



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:27 PM UTC

PDB ID : 1NFD / pdb_00001nfd
Title : AN ALPHA-BETA T CELL RECEPTOR (TCR) HETERODIMER IN COM-
PLEX WITH AN ANTI-TCR FAB FRAGMENT DERIVED FROM A MI-
TOGENIC ANTIBODY
Authors : Wang, J.-H.; Lim, K.; Smolyar, A.; Teng, M.-K.; Sacchittini, J.; Reinherz,
E.L.
Deposited on : 1997-08-04
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

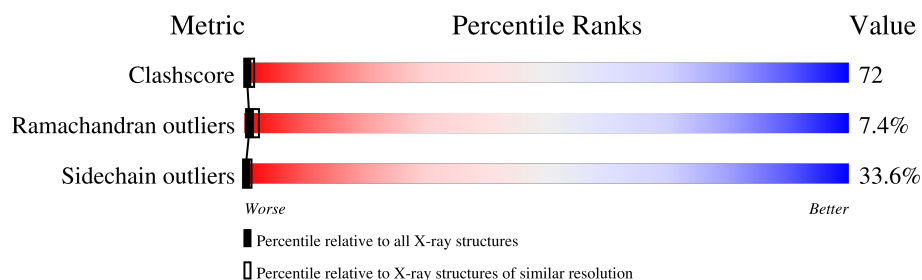
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	203	24% 48% 28%
1	C	203	25% 49% 25% .
2	B	239	24% 52% 22% .
2	D	239	25% 52% 23%
3	E	212	20% 54% 25% .
3	G	212	17% 47% 33% .
4	F	222	16% 56% 27% .
4	H	222	22% 53% 23% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	248	X	-	-	-
5	NAG	C	214	X	-	-	-
5	NAG	C	215	X	-	-	-
5	NAG	C	216	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13884 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called N15 ALPHA-BETA T-CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1589	1002	259	320	8			
1	C	203	Total	C	N	O	S	0	0	0
			1589	1002	259	320	8			

- Molecule 2 is a protein called N15 ALPHA-BETA T-CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1926	1218	338	362	8			
2	D	239	Total	C	N	O	S	0	0	0
			1926	1218	338	362	8			

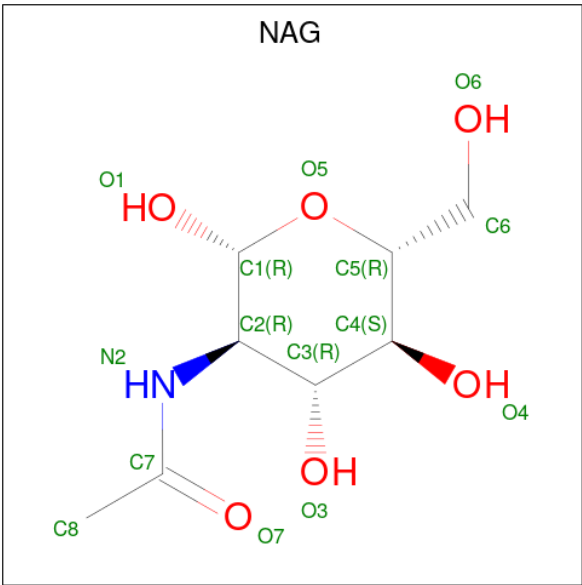
- Molecule 3 is a protein called H57 FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	212	Total	C	N	O	S	0	0	0
			1618	1012	269	330	7			
3	G	212	Total	C	N	O	S	0	0	0
			1618	1012	269	330	7			

- Molecule 4 is a protein called H57 FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	222	Total	C	N	O	S	0	0	0
			1711	1081	289	333	8			
4	H	222	Total	C	N	O	S	0	0	0
			1711	1081	289	333	8			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



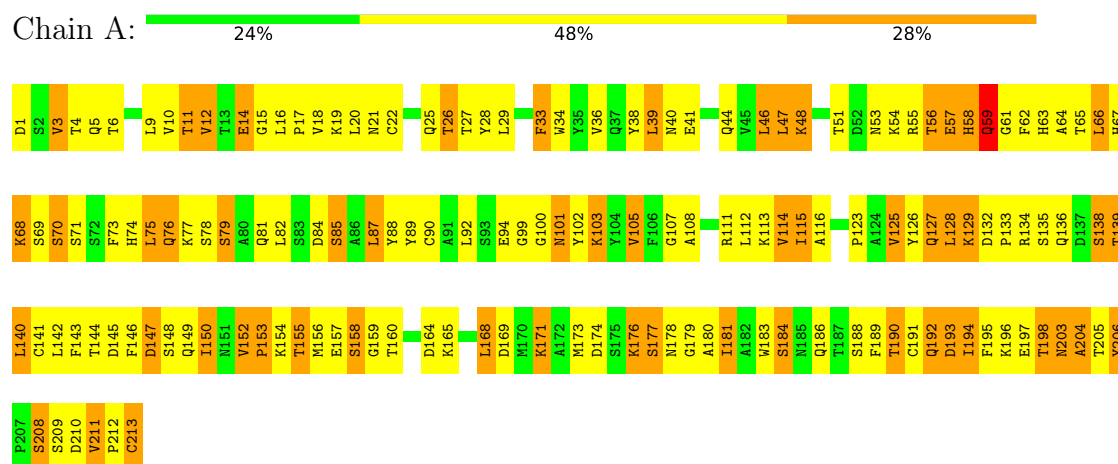
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots [i](#)

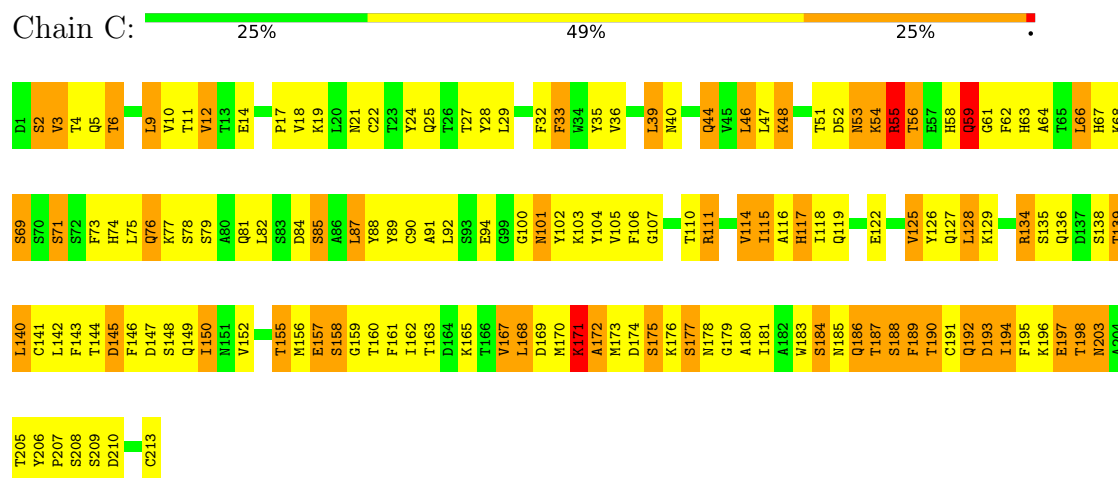
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

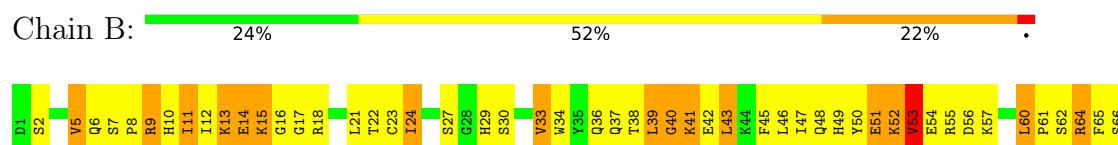
• Molecule 1: N15 ALPHA-BETA T-CELL RECEPTOR

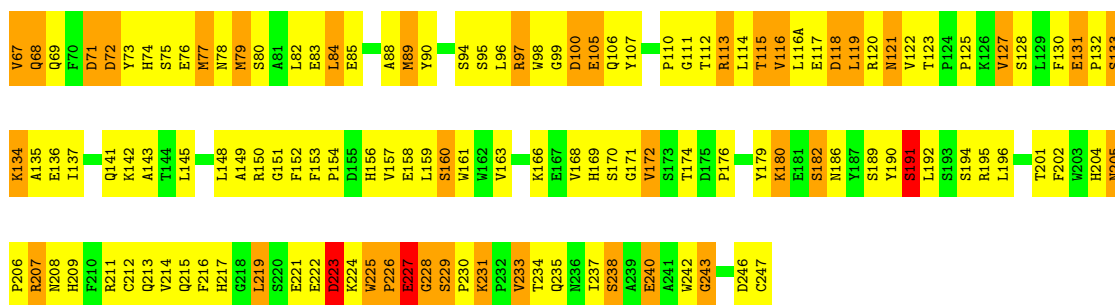


• Molecule 1: N15 ALPHA-BETA T-CELL RECEPTOR



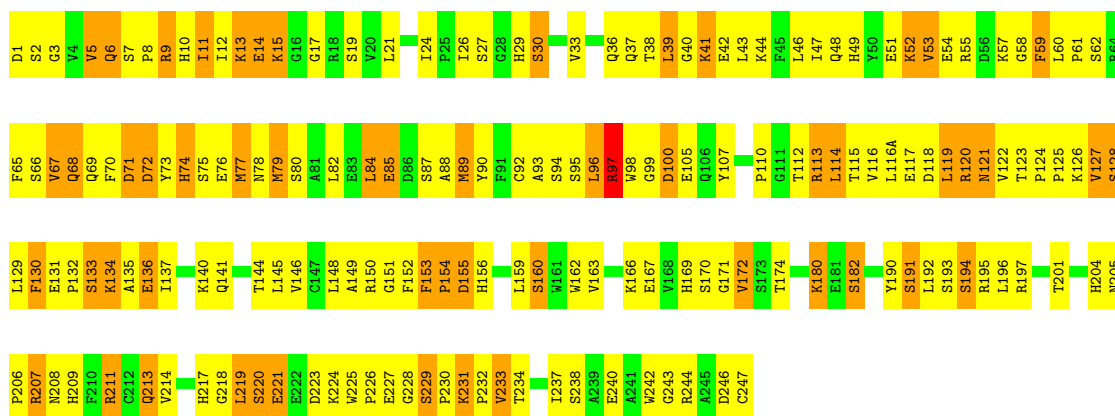
• Molecule 2: N15 ALPHA-BETA T-CELL RECEPTOR





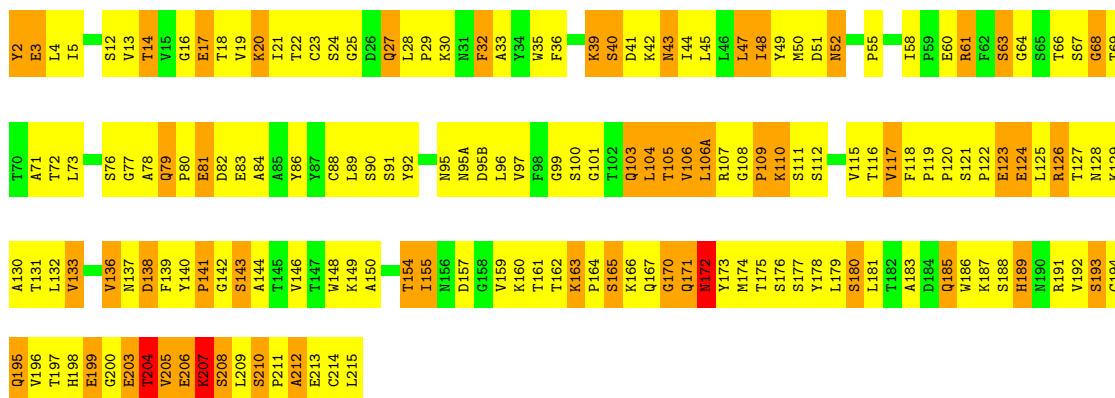
• Molecule 2: N15 ALPHA-BETA T-CELL RECEPTOR

Chain D: 25% 52% 23%



• Molecule 3: H57 FAB

Chain E: 20% 54% 25%



• Molecule 3: H57 FAB

Chain G: 17% 47% 33%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.74Å 122.30Å 115.84Å 90.00° 107.95° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	73.5 (15.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.243 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13884	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.45	0/1625	0.94	8/2208 (0.4%)
1	C	0.46	1/1625 (0.1%)	0.95	6/2208 (0.3%)
2	B	0.59	1/1981 (0.1%)	0.92	12/2683 (0.4%)
2	D	0.59	1/1981 (0.1%)	0.94	3/2683 (0.1%)
3	E	0.38	0/1653	0.87	4/2249 (0.2%)
3	G	0.34	0/1653	0.92	4/2249 (0.2%)
4	F	0.38	0/1759	0.89	2/2404 (0.1%)
4	H	0.35	0/1759	0.91	5/2404 (0.2%)
All	All	0.46	3/14036 (0.0%)	0.92	44/19088 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	191	SER	CB-OG	19.88	1.81	1.42
2	B	191	SER	CB-OG	18.87	1.79	1.42
1	C	203	ASN	CA-C	-5.89	1.44	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	ASN	OD1-CG-ND2	-10.40	112.20	122.60
1	A	211	VAL	N-CA-C	9.90	117.14	108.63
1	C	203	ASN	CB-CG-ND2	8.92	129.78	116.40
1	A	203	ASN	N-CA-C	8.10	121.50	109.59
4	H	134	THR	N-CA-C	-7.51	103.43	112.59
2	D	54	GLU	N-CA-C	-6.88	98.48	109.76
1	A	56	THR	N-CA-C	6.66	119.58	108.13
1	C	46	LEU	N-CA-C	-6.63	105.72	113.88
2	B	99	GLY	N-CA-C	-6.59	104.35	111.93
2	B	57	LYS	N-CA-C	6.58	120.61	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	50	MET	N-CA-C	-6.50	102.43	111.39
2	D	55	ARG	N-CA-C	6.42	118.94	109.24
4	H	30	SER	N-CA-C	6.38	117.93	110.97
2	B	16	GLY	N-CA-C	-6.34	107.37	115.42
4	H	212	HIS	CA-C-N	6.04	127.39	119.84
4	H	212	HIS	C-N-CA	6.04	127.39	119.84
2	B	205	ASN	CA-C-N	5.85	125.56	119.82
2	B	205	ASN	C-N-CA	5.85	125.56	119.82
1	C	197	GLU	CA-C-N	-5.72	114.92	122.99
1	C	197	GLU	C-N-CA	-5.72	114.92	122.99
3	G	185	GLN	N-CA-C	-5.68	106.39	113.55
3	E	185	GLN	N-CA-C	-5.68	105.09	111.28
2	B	60	LEU	CA-C-N	5.67	125.96	119.83
2	B	60	LEU	C-N-CA	5.67	125.96	119.83
2	D	99	GLY	N-CA-C	5.57	122.44	114.64
3	E	99	GLY	N-CA-C	-5.48	102.18	112.64
2	B	131	GLU	CA-C-N	5.46	126.67	119.84
2	B	131	GLU	C-N-CA	5.46	126.67	119.84
2	B	225	TRP	N-CA-C	5.44	116.80	109.24
4	H	33	TRP	N-CA-C	-5.41	100.88	109.96
1	A	46	LEU	N-CA-C	-5.38	106.85	113.41
1	A	16	LEU	CA-C-N	5.36	125.57	120.31
1	A	16	LEU	C-N-CA	5.36	125.57	120.31
3	G	137	ASN	N-CA-C	5.34	117.38	109.69
4	F	199	TRP	N-CA-C	5.29	119.36	112.17
4	F	54	ASN	N-CA-C	5.26	118.84	111.74
3	E	112	SER	CA-C-N	5.24	125.24	120.21
3	E	112	SER	C-N-CA	5.24	125.24	120.21
1	A	59	GLN	N-CA-C	-5.17	99.78	110.80
1	C	2	SER	N-CA-C	5.16	116.68	108.79
1	A	105	VAL	N-CA-C	5.06	116.11	109.58
3	G	125	LEU	N-CA-C	-5.06	105.95	111.82
2	B	127	VAL	N-CA-C	5.04	115.57	108.36
2	B	246	ASP	N-CA-C	5.02	117.08	108.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1589	0	1526	247	1
1	C	1589	0	1525	166	0
2	B	1926	0	1835	258	2
2	D	1926	0	1836	266	1
3	E	1618	0	1576	276	0
3	G	1618	0	1576	265	0
4	F	1711	0	1647	302	0
4	H	1711	0	1647	293	2
5	A	42	0	39	4	0
5	B	56	0	52	7	0
5	C	42	0	37	8	0
5	D	56	0	52	4	0
All	All	13884	0	13348	1949	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 72.

All (1949) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:117:VAL:HG22	3:E:209:LEU:CD2	1.55	1.35
1:A:34:TRP:HD1	1:A:73:PHE:CE1	1.44	1.34
1:C:203:ASN:ND2	5:C:216:NAG:O7	1.65	1.30
3:E:165:SER:HB2	3:E:173:TYR:CD1	1.66	1.30
1:A:34:TRP:CD1	1:A:73:PHE:HE1	1.49	1.29
1:A:34:TRP:CD1	1:A:73:PHE:CE1	2.21	1.29
2:B:191:SER:CB	2:B:191:SER:OG	1.79	1.28
2:D:191:SER:CB	2:D:191:SER:OG	1.81	1.26
2:B:113:ARG:HD2	2:B:156:HIS:CE1	1.73	1.23
1:C:203:ASN:ND2	5:C:216:NAG:C7	1.98	1.22
3:E:209:LEU:O	3:E:211:PRO:HD3	1.40	1.20
3:E:115:VAL:HG12	3:E:209:LEU:HD22	1.21	1.18
1:C:48:LYS:NZ	2:D:100:ASP:OD1	1.78	1.17
3:G:41:ASP:HB3	3:G:43:ASN:HD21	1.04	1.16
1:A:55:ARG:CZ	2:D:97:ARG:HH22	1.60	1.13
2:D:5:VAL:HG23	2:D:24:ILE:HB	1.29	1.13
3:G:79:GLN:HG3	3:G:80:PRO:HD2	1.17	1.11
4:H:195:SER:O	4:H:199:TRP:CZ3	2.04	1.11
1:A:58:HIS:C	1:A:61:GLY:H	1.47	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:115:VAL:HG21	3:E:207:LYS:HB3	1.27	1.11
2:B:217:HIS:HA	2:B:234:THR:HG22	1.26	1.10
4:H:40:ALA:HB3	4:H:43:LYS:HB2	1.29	1.10
3:G:132:LEU:HD22	3:G:192:VAL:HG11	1.32	1.09
3:E:149:LYS:HG3	3:E:195:GLN:HE21	1.10	1.09
4:H:174:PHE:O	4:H:187:LEU:HD11	1.51	1.09
3:G:83:GLU:HB2	3:G:106:VAL:HG23	1.31	1.09
3:E:79:GLN:HG3	3:E:80:PRO:HD2	1.34	1.08
3:G:146:VAL:CG1	3:G:196:VAL:HG22	1.83	1.08
2:B:96:LEU:O	2:B:97:ARG:HG2	1.52	1.08
3:G:132:LEU:CD2	3:G:192:VAL:HG11	1.83	1.08
1:C:59:GLN:OE1	1:C:59:GLN:HA	1.41	1.07
4:H:212:HIS:CE1	4:H:214:ALA:HB3	1.89	1.07
2:B:97:ARG:HH22	1:C:56:THR:HG23	1.18	1.07
2:B:36:GLN:HG3	2:B:90:TYR:CE1	1.90	1.07
2:B:227:GLU:OE2	4:F:50:ARG:NH1	1.87	1.06
1:A:75:LEU:HD12	1:A:76:GLN:N	1.70	1.05
1:A:155:THR:HG21	1:A:160:THR:O	1.56	1.05
2:D:217:HIS:HA	2:D:234:THR:HG22	1.39	1.04
3:E:41:ASP:HB3	3:E:43:ASN:HD21	1.16	1.04
2:B:60:LEU:HD12	2:B:61:PRO:HD2	1.07	1.04
3:E:117:VAL:CG2	3:E:209:LEU:HD21	1.88	1.04
1:A:47:LEU:HB2	1:A:55:ARG:HD2	1.38	1.03
1:A:123:PRO:HB2	1:A:204:ALA:HB3	1.40	1.03
4:H:205:ILE:HG22	4:H:205:ILE:O	1.59	1.02
3:E:41:ASP:HB3	3:E:43:ASN:ND2	1.74	1.02
1:A:55:ARG:CZ	2:D:97:ARG:NH2	2.22	1.02
1:A:171:LYS:HB2	2:B:170:SER:OG	1.59	1.02
2:D:153:PHE:HB3	2:D:154:PRO:CD	1.88	1.02
3:E:89:LEU:HD12	3:E:90:SER:H	1.22	1.02
4:F:40:ALA:HB3	4:F:43:LYS:HB2	1.38	1.02
1:A:125:VAL:HG22	1:A:205:THR:HG23	1.41	1.01
4:H:153:THR:HG23	4:H:211:ALA:HB3	1.39	1.01
2:D:174:THR:HA	2:D:194:SER:HB2	1.42	1.01
2:D:223:ASP:CB	2:D:231:LYS:HE3	1.90	1.01
4:H:67:PHE:CE1	4:H:82:MET:HB3	1.96	1.01
3:E:117:VAL:HG22	3:E:209:LEU:CG	1.90	1.01
4:F:212:HIS:CD2	4:F:214:ALA:H	1.79	1.00
3:E:115:VAL:CG1	3:E:209:LEU:HD22	1.91	1.00
3:E:193:SER:HA	3:E:211:PRO:HD2	1.43	0.99
2:D:125:PRO:HD2	2:D:237:ILE:HD12	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:52(B):ILE:CG2	4:H:52(C):PRO:HD3	1.93	0.99
3:E:117:VAL:HG22	3:E:209:LEU:HD21	1.01	0.98
3:E:198:HIS:HB3	3:E:205:VAL:HG21	1.40	0.98
2:D:223:ASP:HB2	2:D:231:LYS:HE3	1.41	0.98
3:G:41:ASP:HB3	3:G:43:ASN:ND2	1.77	0.98
4:H:199:TRP:CD2	4:H:200:PRO:HD3	1.98	0.98
1:A:55:ARG:HE	2:D:97:ARG:NH1	1.61	0.98
3:G:198:HIS:HB3	3:G:205:VAL:HG21	1.43	0.97
1:A:171:LYS:HD2	2:B:170:SER:HB2	1.46	0.97
3:E:165:SER:HB2	3:E:173:TYR:HD1	1.20	0.97
3:G:43:ASN:ND2	3:G:43:ASN:H	1.58	0.97
4:F:212:HIS:HB3	4:F:217:THR:OG1	1.63	0.97
4:H:134:THR:O	4:H:136:ASP:N	1.95	0.97
1:A:168:LEU:C	1:A:168:LEU:HD12	1.89	0.96
2:B:50:TYR:HD1	2:B:51:GLU:N	1.62	0.96
2:B:97:ARG:NH2	1:C:56:THR:HG23	1.81	0.96
4:F:144:VAL:HG23	4:F:187:LEU:O	1.66	0.96
1:A:82:LEU:HD23	1:A:114:VAL:HG22	1.46	0.96
1:A:58:HIS:C	1:A:61:GLY:N	2.13	0.95
1:A:61:GLY:HA3	1:A:77:LYS:HE3	1.47	0.95
4:F:11:LEU:HG	4:F:11:LEU:O	1.62	0.95
2:B:60:LEU:HD12	2:B:61:PRO:CD	1.95	0.95
1:A:48:LYS:HZ2	2:B:100:ASP:HB2	1.31	0.95
3:G:52:ASN:O	3:G:52:ASN:OD1	1.85	0.94
4:F:134:THR:O	4:F:136:ASP:N	1.98	0.94
4:H:140:LEU:HD11	4:H:205:ILE:HG21	1.49	0.94
2:B:52:LYS:HD3	2:B:53:VAL:HG23	1.45	0.94
2:D:40:GLY:O	2:D:41:LYS:HG3	1.66	0.94
2:B:96:LEU:C	2:B:97:ARG:HG2	1.92	0.94
2:D:52:LYS:HG2	2:D:53:VAL:H	1.32	0.94
2:B:18:ARG:HH21	5:B:248:NAG:H61	1.31	0.94
4:H:199:TRP:CE2	4:H:200:PRO:HD3	2.03	0.93
3:E:25:GLY:HA3	3:E:28:LEU:HG	1.49	0.93
3:E:192:VAL:O	3:E:211:PRO:HD2	1.68	0.93
2:B:118:ASP:CG	5:B:249:NAG:H82	1.94	0.93
2:D:70:PHE:CZ	2:D:74:HIS:HE1	1.86	0.93
2:B:209:HIS:HB2	2:B:242:TRP:CZ3	2.02	0.92
2:D:49:HIS:CE1	2:D:53:VAL:HG13	2.03	0.92
1:A:55:ARG:NH2	2:D:97:ARG:HH22	1.65	0.92
4:H:52(B):ILE:HG22	4:H:52(C):PRO:HD3	1.48	0.92
2:D:153:PHE:HB3	2:D:154:PRO:HD2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:ASP:HB2	2:D:231:LYS:CE	1.98	0.92
2:D:5:VAL:CG2	2:D:24:ILE:HB	2.00	0.92
3:G:43:ASN:H	3:G:43:ASN:HD22	1.08	0.91
2:D:49:HIS:HE1	2:D:53:VAL:CG1	1.83	0.91
3:E:143:SER:HB3	3:E:163:LYS:HG2	1.52	0.91
4:F:87:THR:HG23	4:F:110:THR:HA	1.51	0.91
3:E:144:ALA:HB1	3:E:196:VAL:HG12	1.51	0.91
3:E:61:ARG:NH1	3:E:82:ASP:OD2	2.04	0.90
3:E:132:LEU:HD22	3:E:192:VAL:HG11	1.50	0.90
3:E:138:ASP:HA	3:E:172:ASN:HD22	1.36	0.90
4:F:36:TRP:NE1	4:F:78:ILE:HD12	1.86	0.90
1:A:58:HIS:O	1:A:61:GLY:N	2.03	0.90
4:H:94:ARG:HH21	4:H:101:ASP:CG	1.80	0.90
4:H:87:THR:HG23	4:H:110:THR:HA	1.52	0.90
4:F:219:VAL:CG1	4:F:221:LYS:HE2	2.01	0.90
1:A:55:ARG:HD3	1:A:56:THR:N	1.86	0.89
1:A:75:LEU:HD12	1:A:76:GLN:H	1.31	0.89
1:A:55:ARG:NE	2:D:97:ARG:CZ	2.36	0.89
3:G:79:GLN:CG	3:G:80:PRO:HD2	2.03	0.89
2:B:18:ARG:NH2	5:B:248:NAG:H61	1.87	0.89
3:E:89:LEU:HD12	3:E:90:SER:N	1.87	0.89
3:E:165:SER:HB2	3:E:173:TYR:CE1	2.08	0.89
4:F:52(B):ILE:HG23	4:F:55:TYR:CZ	2.06	0.89
1:A:102:TYR:HB3	2:B:98:TRP:NE1	1.87	0.88
3:G:145:THR:HG23	3:G:197:THR:OG1	1.73	0.88
2:B:132:PRO:HD3	2:B:145:LEU:CD2	2.04	0.88
3:E:148:TRP:CD2	3:E:179:LEU:HD13	2.08	0.88
3:E:149:LYS:HG3	3:E:195:GLN:NE2	1.88	0.88
4:H:117:THR:HG22	4:H:146:GLY:O	1.74	0.88
3:E:149:LYS:HE2	3:E:154:THR:OG1	1.74	0.88
1:A:47:LEU:HB3	1:A:55:ARG:HH11	1.38	0.88
1:A:48:LYS:NZ	2:B:100:ASP:HB2	1.88	0.88
1:A:174:ASP:OD1	1:A:176:LYS:HD2	1.74	0.87
3:E:115:VAL:HG21	3:E:207:LYS:CB	2.03	0.87
1:A:34:TRP:CD1	1:A:73:PHE:CD1	2.61	0.87
1:C:59:GLN:OE1	1:C:59:GLN:CA	2.19	0.87
3:G:193:SER:HA	3:G:211:PRO:HD2	1.56	0.87
1:A:125:VAL:CG2	1:A:205:THR:HG23	2.04	0.87
2:B:134:LYS:H	2:B:134:LYS:HE2	1.38	0.87
2:D:30:SER:HB3	2:D:51:GLU:OE1	1.73	0.87
3:G:146:VAL:HG13	3:G:196:VAL:HG22	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:207:LYS:O	3:E:209:LEU:N	2.07	0.87
2:D:60:LEU:HD11	2:D:65:PHE:HB2	1.55	0.86
3:E:162:THR:O	3:E:175:THR:HG23	1.75	0.86
4:H:20:VAL:HG11	4:H:107:THR:HG21	1.54	0.86
1:A:102:TYR:HB3	2:B:98:TRP:HE1	1.37	0.86
1:C:205:THR:O	1:C:207:PRO:HD3	1.76	0.86
3:G:143:SER:HB3	3:G:163:LYS:HG2	1.55	0.86
1:A:53:ASN:O	1:A:65:THR:HG23	1.75	0.86
4:H:119:PRO:HB3	4:H:147:TYR:HB3	1.55	0.86
1:C:54:LYS:O	1:C:56:THR:N	2.07	0.86
3:G:83:GLU:HG3	3:G:105:THR:HA	1.58	0.86
3:E:140:TYR:CD1	3:E:173:TYR:HE2	1.94	0.86
3:E:66:THR:HA	3:E:71:ALA:HA	1.58	0.85
3:E:136:VAL:HG22	3:E:139:PHE:CE1	2.11	0.85
3:E:163:LYS:HZ2	3:E:175:THR:HG21	1.40	0.85
3:G:51:ASP:O	3:G:52:ASN:HB3	1.75	0.85
4:H:138:VAL:HG21	4:H:199:TRP:CH2	2.12	0.85
4:H:34:MET:HE3	4:H:93:THR:O	1.76	0.85
2:B:50:TYR:CD1	2:B:51:GLU:N	2.44	0.85
2:D:49:HIS:CE1	2:D:53:VAL:CG1	2.57	0.85
3:E:161:THR:HG22	3:E:177:SER:OG	1.77	0.85
1:C:205:THR:C	1:C:207:PRO:HD3	2.02	0.85
3:G:192:VAL:HB	3:G:212:ALA:HB2	1.57	0.84
1:A:55:ARG:HH12	1:A:57:GLU:CG	1.89	0.84
2:D:40:GLY:C	2:D:41:LYS:CG	2.48	0.84
2:B:223:ASP:HB2	2:B:231:LYS:CE	2.07	0.84
4:F:108:MET:HB3	4:F:150:GLU:OE2	1.78	0.83
2:D:40:GLY:O	2:D:41:LYS:CG	2.26	0.83
4:H:131:THR:O	4:H:132:THR:HG23	1.78	0.83
4:H:199:TRP:CD2	4:H:200:PRO:CD	2.61	0.83
4:F:40:ALA:HB3	4:F:43:LYS:HD3	1.60	0.83
2:D:65:PHE:HA	2:D:78:ASN:O	1.79	0.83
4:H:117:THR:O	4:H:146:GLY:O	1.96	0.83
3:G:146:VAL:HG12	3:G:196:VAL:HG22	1.59	0.83
1:A:34:TRP:HE1	1:A:73:PHE:HD1	1.23	0.83
2:D:48:GLN:NE2	2:D:98:TRP:HH2	1.75	0.83
3:E:115:VAL:CG2	3:E:207:LYS:HB3	2.07	0.83
4:H:148:PHE:H	4:H:149:PRO:CD	1.92	0.83
3:E:43:ASN:ND2	3:E:43:ASN:H	1.77	0.82
1:A:144:THR:HG22	1:A:145:ASP:OD1	1.78	0.82
1:C:82:LEU:HD23	1:C:114:VAL:HG22	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:140:TYR:HD1	3:E:141:PRO:HA	1.44	0.82
1:A:34:TRP:NE1	1:A:73:PHE:HD1	1.78	0.82
4:F:82:MET:HE1	4:F:109:VAL:HG21	1.61	0.82
4:F:212:HIS:NE2	4:F:214:ALA:HB2	1.95	0.82
1:A:33:PHE:HD2	1:A:48:LYS:HB2	1.44	0.82
3:E:140:TYR:CD1	3:E:141:PRO:HA	2.15	0.82
3:G:61:ARG:NH1	3:G:79:GLN:HB2	1.93	0.82
3:E:39:LYS:HG3	3:E:84:ALA:HB2	1.61	0.82
1:C:145:ASP:HB2	2:D:140:LYS:NZ	1.94	0.81
1:A:55:ARG:NE	2:D:97:ARG:NH2	2.27	0.81
2:B:228:GLY:HA3	4:F:96:GLY:O	1.79	0.81
1:C:144:THR:HG22	1:C:145:ASP:H	1.45	0.81
4:F:40:ALA:CB	4:F:43:LYS:HD3	2.10	0.81
1:C:75:LEU:HD12	1:C:76:GLN:N	1.95	0.81
4:F:121:VAL:CG2	4:F:219:VAL:HG11	2.09	0.81
2:B:113:ARG:CD	2:B:156:HIS:CE1	2.61	0.81
2:D:48:GLN:NE2	2:D:98:TRP:CH2	2.48	0.81
4:F:208:CYS:O	4:F:208:CYS:SG	2.39	0.81
3:G:128:ASN:C	3:G:183:ALA:HB2	2.06	0.81
2:B:113:ARG:HD2	2:B:156:HIS:HE1	1.40	0.81
4:F:199:TRP:O	4:F:200:PRO:C	2.21	0.81
4:F:122:TYR:O	4:F:124:LEU:HD23	1.81	0.81
2:D:72:ASP:O	2:D:73:TYR:HB2	1.79	0.81
3:E:19:VAL:HG22	3:E:20:LYS:H	1.45	0.81
3:G:16:GLY:O	3:G:77:GLY:HA2	1.81	0.81
3:G:89:LEU:HD12	3:G:90:SER:H	1.46	0.81
1:A:34:TRP:NE1	1:A:73:PHE:CD1	2.49	0.80
4:F:68:THR:O	4:F:80:LEU:HD12	1.79	0.80
4:H:51:ILE:HD13	4:H:71:ARG:HB2	1.62	0.80
3:G:61:ARG:NH1	3:G:82:ASP:OD2	2.14	0.80
1:A:140:LEU:HD13	1:A:141:CYS:N	1.96	0.80
3:E:203:GLU:C	3:E:205:VAL:H	1.88	0.80
4:F:139:THR:HG23	4:F:192:THR:OG1	1.79	0.80
2:B:67:VAL:HG12	2:B:77:MET:HA	1.62	0.80
1:C:147:ASP:N	1:C:150:ILE:HD11	1.96	0.80
4:H:141:GLY:HA3	4:H:189:SER:O	1.80	0.80
2:B:96:LEU:O	2:B:97:ARG:CG	2.28	0.80
2:B:132:PRO:HD3	2:B:145:LEU:HD23	1.61	0.80
3:G:6:GLN:NE2	3:G:88:CYS:H	1.80	0.80
3:G:113:PRO:HB2	3:G:207:LYS:HG2	1.62	0.80
3:E:117:VAL:CG2	3:E:209:LEU:CG	2.60	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLU:O	1:A:59:GLN:N	2.14	0.80
3:E:117:VAL:HG21	3:E:211:PRO:HG3	1.63	0.80
3:E:140:TYR:HD1	3:E:173:TYR:HE2	1.28	0.80
2:B:84:LEU:HA	2:B:116:VAL:HB	1.63	0.80
4:H:35:TYR:CD2	4:H:50:ARG:HB2	2.16	0.80
1:A:171:LYS:CD	2:B:170:SER:HB2	2.12	0.80
4:F:210:VAL:CG2	4:F:219:VAL:HB	2.11	0.80
4:F:52(B):ILE:O	4:F:54:ASN:N	2.15	0.79
3:G:122:PRO:HA	3:G:125:LEU:HD12	1.63	0.79
3:G:133:VAL:HG21	4:H:124:LEU:CD2	2.12	0.79
4:H:133:SER:OG	4:H:135:THR:HG23	1.82	0.79
4:H:199:TRP:CG	4:H:200:PRO:HD3	2.17	0.79
3:E:123:GLU:O	3:E:126:ARG:HB2	1.81	0.79
2:B:50:TYR:OH	2:B:97:ARG:HD2	1.83	0.79
2:B:11:ILE:HD11	2:B:112:THR:HG21	1.64	0.79
1:C:203:ASN:CG	5:C:216:NAG:C7	2.54	0.79
4:F:140:LEU:CD1	4:F:225:ILE:HD13	2.13	0.79
4:H:198:THR:O	4:H:203:GLN:HB3	1.83	0.79
4:H:169:GLY:O	4:H:191:VAL:HA	1.82	0.78
1:A:22:CYS:H	1:A:74:HIS:CD2	2.02	0.78
3:E:206:GLU:O	3:E:208:SER:N	2.14	0.78
4:F:147:TYR:CD1	4:F:185:TYR:O	2.37	0.78
4:H:217:THR:O	4:H:217:THR:HG22	1.84	0.78
2:D:14:GLU:HG3	2:D:119:LEU:HD13	1.64	0.78
2:D:230:PRO:HD3	4:H:33:TRP:HZ2	1.47	0.78
3:G:6:GLN:HE22	3:G:88:CYS:H	1.29	0.78
3:G:182:THR:HG23	3:G:185:GLN:OE1	1.82	0.78
2:B:100:ASP:O	2:B:105:GLU:OE2	2.01	0.78
4:F:2:VAL:HG13	4:F:27:PHE:CD1	2.19	0.78
4:F:133:SER:C	4:F:135:THR:H	1.91	0.78
3:G:142:GLY:HA3	3:G:199:GLU:CB	2.14	0.78
2:D:70:PHE:CZ	2:D:74:HIS:CE1	2.71	0.78
1:A:39:LEU:HD22	1:A:40:ASN:N	1.99	0.78
1:A:55:ARG:HH12	1:A:57:GLU:HG2	1.47	0.78
3:G:183:ALA:HB1	3:G:187:LYS:NZ	1.98	0.78
2:B:36:GLN:OE1	2:B:38:THR:HG23	1.84	0.77
2:B:38:THR:HG22	2:B:88:ALA:HB2	1.63	0.77
4:F:140:LEU:HD13	4:F:225:ILE:HG21	1.65	0.77
3:G:47:LEU:HA	3:G:58:ILE:HD12	1.66	0.77
2:D:60:LEU:HD12	2:D:61:PRO:HD2	1.66	0.77
4:H:195:SER:C	4:H:199:TRP:CZ3	2.62	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:72:ASP:OD2	2:D:74:HIS:HB3	1.83	0.77
3:G:41:ASP:CB	3:G:43:ASN:HD21	1.91	0.77
3:G:203:GLU:C	3:G:205:VAL:H	1.92	0.77
2:D:134:LYS:CE	2:D:134:LYS:H	1.98	0.77
4:H:32:PHE:CE1	4:H:96:GLY:HA3	2.19	0.77
3:E:203:GLU:HB2	3:E:205:VAL:CG2	2.15	0.77
4:F:99:ASP:HB3	4:F:101:ASP:OD2	1.84	0.77
2:D:230:PRO:HD3	4:H:33:TRP:CZ2	2.20	0.77
3:G:133:VAL:HG21	4:H:124:LEU:HD21	1.65	0.77
1:C:92:LEU:C	1:C:92:LEU:HD12	2.10	0.77
1:A:92:LEU:HD12	1:A:92:LEU:C	2.10	0.77
2:D:74:HIS:NE2	2:D:76:GLU:OE2	2.18	0.77
2:D:217:HIS:CA	2:D:234:THR:HG22	2.15	0.76
3:G:58:ILE:HG23	3:G:59:PRO:HD2	1.66	0.76
4:H:13:GLN:O	4:H:16:SER:HB2	1.85	0.76
1:A:55:ARG:NH1	1:A:57:GLU:HG2	2.01	0.76
1:A:125:VAL:CG2	1:A:125:VAL:O	2.33	0.76
3:E:28:LEU:N	3:E:29:PRO:HD2	2.01	0.76
3:E:83:GLU:HG3	3:E:105:THR:HA	1.65	0.76
1:A:144:THR:HG22	1:A:145:ASP:N	2.00	0.76
4:H:210:VAL:HB	4:H:219:VAL:CG1	2.15	0.76
2:B:230:PRO:HB3	4:F:53:ASN:HD21	1.48	0.76
3:E:108:GLY:N	3:E:109:PRO:HD2	1.99	0.76
3:E:165:SER:CB	3:E:173:TYR:CD1	2.60	0.76
3:G:142:GLY:HA3	3:G:199:GLU:HB3	1.68	0.76
1:C:6:THR:HA	5:C:214:NAG:H83	1.67	0.76
3:G:203:GLU:HB2	3:G:205:VAL:HG23	1.66	0.76
2:B:209:HIS:NE2	2:B:240:GLU:OE1	2.16	0.76
1:A:14:GLU:CD	1:A:176:LYS:HE2	2.11	0.75
3:G:83:GLU:HB2	3:G:106:VAL:CG2	2.14	0.75
4:H:205:ILE:O	4:H:205:ILE:CG2	2.33	0.75
2:B:65:PHE:HA	2:B:78:ASN:O	1.87	0.75
4:F:199:TRP:CE3	4:F:200:PRO:HD3	2.21	0.75
4:F:68:THR:CG2	4:F:69:ILE:N	2.49	0.75
3:E:104:LEU:HD23	3:E:104:LEU:O	1.86	0.75
1:C:168:LEU:C	1:C:168:LEU:HD12	2.11	0.75
3:E:41:ASP:CB	3:E:43:ASN:HD21	1.96	0.75
4:H:55:TYR:OH	4:H:73:ASP:OD2	2.05	0.75
1:A:55:ARG:NE	2:D:97:ARG:NH1	2.33	0.75
3:G:121:SER:O	3:G:125:LEU:HG	1.85	0.75
2:B:50:TYR:CZ	2:B:97:ARG:HB3	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:197:THR:HA	3:E:205:VAL:O	1.86	0.74
2:D:125:PRO:HB3	2:D:152:PHE:CD2	2.21	0.74
4:F:176:SER:O	4:F:177:VAL:HG13	1.87	0.74
4:F:116:THR:HG23	4:F:214:ALA:HB1	1.69	0.74
4:H:52(A):ASN:ND2	4:H:52(A):ASN:H	1.85	0.74
1:C:58:HIS:O	1:C:61:GLY:N	2.20	0.74
4:F:68:THR:HG22	4:F:69:ILE:N	2.02	0.74
4:F:174:PHE:O	4:F:187:LEU:HD11	1.87	0.74
3:E:193:SER:HA	3:E:211:PRO:CD	2.17	0.74
1:A:144:THR:HG22	1:A:145:ASP:H	1.53	0.74
4:H:29:PHE:HB3	4:H:76:ASN:OD1	1.88	0.74
4:H:94:ARG:NH2	4:H:101:ASP:OD2	2.21	0.74
3:E:41:ASP:HB3	3:E:43:ASN:CG	2.12	0.74
1:A:125:VAL:O	1:A:125:VAL:HG23	1.88	0.74
4:F:52(B):ILE:HG23	4:F:55:TYR:OH	1.87	0.74
4:F:210:VAL:HG23	4:F:219:VAL:HB	1.68	0.74
3:E:198:HIS:H	3:E:205:VAL:HB	1.52	0.73
4:H:199:TRP:CG	4:H:200:PRO:CD	2.70	0.73
1:A:5:GLN:NE2	1:A:107:GLY:HA3	2.03	0.73
3:E:117:VAL:CG2	3:E:209:LEU:HG	2.18	0.73
2:B:223:ASP:HB2	2:B:231:LYS:HE3	1.68	0.73
2:B:223:ASP:HB2	2:B:231:LYS:NZ	2.02	0.73
4:F:119:PRO:HD2	4:F:217:THR:HG21	1.69	0.73
4:F:126:PRO:O	4:F:128:CYS:N	2.20	0.73
3:G:181:LEU:HD23	3:G:185:GLN:HB3	1.70	0.73
1:C:144:THR:HG22	1:C:145:ASP:N	2.02	0.73
4:F:36:TRP:HE1	4:F:78:ILE:HD12	1.52	0.73
3:G:79:GLN:HG3	3:G:80:PRO:CD	2.09	0.73
4:H:117:THR:O	4:H:147:TYR:HA	1.89	0.73
1:C:145:ASP:HB2	2:D:140:LYS:HZ1	1.51	0.73
1:A:203:ASN:O	1:A:204:ALA:HB3	1.87	0.73
2:D:153:PHE:CB	2:D:154:PRO:CD	2.64	0.73
3:G:33:ALA:HB3	3:G:51:ASP:HB3	1.71	0.73
3:G:141:PRO:HD2	3:G:199:GLU:HG2	1.71	0.73
2:B:158:GLU:OE2	2:B:217:HIS:HE1	1.70	0.72
2:B:221:GLU:C	2:B:223:ASP:H	1.96	0.72
3:G:108:GLY:N	3:G:109:PRO:HD2	2.04	0.72
1:A:3:VAL:HG12	1:A:105:VAL:HG12	1.70	0.72
2:D:49:HIS:HE1	2:D:53:VAL:HG12	1.53	0.72
4:H:148:PHE:O	4:H:185:TYR:CE2	2.42	0.72
3:G:192:VAL:O	3:G:211:PRO:HD2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:HD12	1:C:76:GLN:H	1.54	0.72
1:A:54:LYS:HE3	1:A:63:HIS:HB2	1.70	0.72
2:D:89:MET:HE3	2:D:113:ARG:HB2	1.72	0.72
4:F:126:PRO:C	4:F:128:CYS:H	1.97	0.72
3:G:193:SER:HB3	3:G:195:GLN:HE21	1.55	0.72
1:A:190:THR:CG2	1:A:192:GLN:H	2.03	0.72
3:G:164:PRO:HG3	4:H:175:PRO:CD	2.20	0.72
4:H:212:HIS:HB3	4:H:217:THR:OG1	1.89	0.72
1:A:54:LYS:HB2	1:A:65:THR:OG1	1.88	0.72
4:F:133:SER:OG	4:F:135:THR:HG23	1.90	0.72
2:B:134:LYS:H	2:B:134:LYS:CE	2.03	0.72
3:E:165:SER:CB	3:E:173:TYR:CE1	2.72	0.72
3:G:123:GLU:O	3:G:126:ARG:HB2	1.90	0.72
1:A:47:LEU:CB	1:A:55:ARG:HH11	2.03	0.71
2:B:154:PRO:HG2	2:B:156:HIS:HD2	1.54	0.71
2:D:229:SER:OG	2:D:230:PRO:HD2	1.90	0.71
4:F:118:ALA:HB1	4:F:217:THR:HG21	1.72	0.71
1:C:139:THR:O	1:C:183:TRP:HA	1.90	0.71
3:G:117:VAL:HG21	3:G:211:PRO:HG3	1.71	0.71
1:A:55:ARG:HE	2:D:97:ARG:CZ	2.02	0.71
3:E:136:VAL:HG13	3:E:175:THR:HB	1.72	0.71
3:G:182:THR:OG1	3:G:185:GLN:HB2	1.90	0.71
1:A:47:LEU:HB3	1:A:55:ARG:NH1	2.05	0.71
2:D:8:PRO:HG2	2:D:11:ILE:HG12	1.72	0.71
3:E:132:LEU:CD2	3:E:192:VAL:HG11	2.21	0.71
3:E:136:VAL:CG1	3:E:175:THR:HB	2.21	0.71
3:G:113:PRO:HG2	3:G:205:VAL:HG11	1.73	0.71
3:G:167:GLN:O	3:G:170:GLY:C	2.33	0.71
4:F:57:THR:HG21	4:F:59:TYR:OH	1.91	0.71
4:F:212:HIS:HD2	4:F:214:ALA:H	1.39	0.71
3:E:140:TYR:CE1	3:E:141:PRO:HB3	2.25	0.71
3:G:89:LEU:HD12	3:G:90:SER:N	2.06	0.71
1:C:33:PHE:HD2	1:C:48:LYS:HB2	1.55	0.71
3:G:28:LEU:N	3:G:29:PRO:HD2	2.05	0.71
4:H:40:ALA:HB3	4:H:43:LYS:CB	2.15	0.71
4:F:39:GLN:HG3	4:F:44:GLY:O	1.91	0.70
4:H:52(B):ILE:HG23	4:H:52(C):PRO:HD3	1.73	0.70
4:H:195:SER:C	4:H:199:TRP:HZ3	1.98	0.70
3:E:148:TRP:CG	3:E:179:LEU:HD13	2.26	0.70
2:B:8:PRO:O	2:B:112:THR:HG23	1.91	0.70
1:C:197:GLU:OE1	1:C:197:GLU:HA	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:138:ASP:HA	3:E:172:ASN:ND2	2.06	0.70
3:E:159:VAL:HG23	3:E:178:TYR:O	1.92	0.70
3:G:192:VAL:HB	3:G:212:ALA:CB	2.21	0.70
2:B:127:VAL:HG12	2:B:237:ILE:HG22	1.73	0.70
4:F:199:TRP:O	4:F:202:LYS:N	2.24	0.70
4:H:63:VAL:HB	4:H:67:PHE:HB2	1.73	0.70
4:H:203:GLN:CD	4:H:204:PRO:HD2	2.16	0.70
1:A:82:LEU:HD23	1:A:114:VAL:CG2	2.21	0.70
2:B:83:GLU:O	2:B:116:VAL:HG21	1.92	0.70
2:B:159:LEU:HD23	2:B:160:SER:N	2.07	0.70
4:H:199:TRP:CD1	4:H:200:PRO:HD3	2.27	0.70
4:F:17:SER:HA	4:F:82(A):ASN:HA	1.73	0.70
4:F:79:TYR:N	4:F:79:TYR:CD1	2.59	0.70
4:H:210:VAL:HB	4:H:219:VAL:HG13	1.74	0.70
2:B:100:ASP:O	2:B:105:GLU:CD	2.35	0.70
3:E:47:LEU:O	3:E:55:PRO:HD2	1.90	0.70
3:E:148:TRP:CZ3	3:E:179:LEU:HB2	2.27	0.70
4:F:209:ASN:N	4:F:209:ASN:OD1	2.25	0.70
3:E:79:GLN:CG	3:E:80:PRO:HD2	2.20	0.69
4:F:166:LEU:HD11	4:F:205:ILE:HD12	1.74	0.69
3:G:113:PRO:HD2	3:G:207:LYS:NZ	2.07	0.69
2:D:52:LYS:HG2	2:D:53:VAL:N	2.03	0.69
2:D:209:HIS:HB2	2:D:242:TRP:CZ3	2.28	0.69
3:G:136:VAL:CG1	3:G:175:THR:HB	2.22	0.69
1:A:139:THR:O	1:A:183:TRP:HA	1.91	0.69
1:C:47:LEU:HD13	1:C:56:THR:CG2	2.22	0.69
2:D:154:PRO:O	2:D:156:HIS:N	2.23	0.69
1:A:53:ASN:CG	1:A:54:LYS:H	1.98	0.69
2:B:100:ASP:O	2:B:105:GLU:CG	2.41	0.69
4:F:20:VAL:HG11	4:F:107:THR:HG21	1.74	0.69
4:H:144:VAL:HG23	4:H:187:LEU:O	1.92	0.69
1:A:14:GLU:OE1	1:A:176:LYS:HE2	1.92	0.69
3:E:61:ARG:HB2	3:E:76:SER:O	1.92	0.69
4:F:219:VAL:HG12	4:F:221:LYS:HE2	1.73	0.69
1:A:146:PHE:HB2	1:A:150:ILE:HD11	1.74	0.69
3:E:106(A):LEU:HA	3:E:140:TYR:OH	1.93	0.69
4:F:157:TRP:CZ3	4:F:208:CYS:HB3	2.27	0.69
4:F:124:LEU:HD21	4:F:142:CYS:C	2.17	0.69
1:C:52:ASP:HA	1:C:66:LEU:HD23	1.75	0.69
1:A:39:LEU:HD13	1:A:40:ASN:HB2	1.74	0.69
1:C:82:LEU:HD23	1:C:114:VAL:CG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:11:LEU:O	4:H:11:LEU:HG	1.91	0.69
1:A:168:LEU:HD12	1:A:169:ASP:N	2.08	0.68
2:B:49:HIS:CE1	2:B:55:ARG:NH2	2.61	0.68
2:B:49:HIS:HE1	2:B:55:ARG:NH2	1.91	0.68
3:G:48:ILE:HD13	3:G:64:GLY:HA3	1.75	0.68
4:H:195:SER:O	4:H:199:TRP:CH2	2.46	0.68
1:A:190:THR:HG22	1:A:192:GLN:H	1.59	0.68
2:B:105:GLU:HB3	2:B:107:TYR:CZ	2.29	0.68
1:C:168:LEU:HD12	1:C:169:ASP:N	2.08	0.68
1:C:205:THR:O	1:C:207:PRO:CD	2.41	0.68
2:D:125:PRO:HD2	2:D:237:ILE:CD1	2.22	0.68
2:D:204:HIS:O	2:D:206:PRO:HD3	1.94	0.68
4:F:125:ALA:HB1	4:F:126:PRO:HD2	1.76	0.68
4:H:126:PRO:O	4:H:127:ALA:HB3	1.92	0.68
3:G:43:ASN:ND2	3:G:43:ASN:N	2.33	0.68
1:C:186:GLN:C	1:C:188:SER:H	2.02	0.68
2:B:9:ARG:CZ	2:B:110:PRO:HB3	2.24	0.68
2:B:221:GLU:O	2:B:223:ASP:N	2.23	0.68
4:H:51:ILE:HG23	4:H:51:ILE:O	1.93	0.68
2:D:52:LYS:CG	2:D:53:VAL:H	2.05	0.68
3:E:163:LYS:NZ	3:E:175:THR:CG2	2.57	0.68
3:E:203:GLU:HB2	3:E:205:VAL:HG23	1.74	0.68
4:H:137:THR:HB	4:H:192:THR:HG22	1.76	0.68
2:B:38:THR:O	2:B:39:LEU:C	2.37	0.68
2:B:50:TYR:OH	2:B:97:ARG:CB	2.41	0.68
2:B:50:TYR:CE2	2:B:97:ARG:CB	2.77	0.68
2:B:118:ASP:OD2	5:B:249:NAG:H82	1.92	0.68
3:E:136:VAL:HG22	3:E:139:PHE:HE1	1.57	0.68
2:D:226:PRO:HG3	3:G:50:MET:HE3	1.76	0.68
3:E:48:ILE:HD13	3:E:64:GLY:HA3	1.76	0.68
3:E:148:TRP:CE3	3:E:179:LEU:HD22	2.29	0.68
3:G:144:ALA:HA	3:G:197:THR:O	1.94	0.68
1:C:3:VAL:HG12	1:C:105:VAL:HG12	1.76	0.67
1:C:56:THR:O	1:C:56:THR:HG22	1.94	0.67
4:F:116:THR:CG2	4:F:214:ALA:HB1	2.24	0.67
3:E:139:PHE:CD2	3:E:173:TYR:HB2	2.30	0.67
3:G:214:CYS:HB2	3:G:215:LEU:HD23	1.74	0.67
3:G:14:THR:HG23	3:G:106(A):LEU:HB2	1.77	0.67
1:C:3:VAL:O	1:C:3:VAL:HG22	1.94	0.67
3:E:133:VAL:HG13	3:E:178:TYR:CE1	2.30	0.67
1:A:128:LEU:HD12	1:A:140:LEU:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ARG:HH22	1:C:56:THR:CG2	2.02	0.67
3:G:198:HIS:H	3:G:205:VAL:HB	1.58	0.67
4:H:138:VAL:HG21	4:H:199:TRP:CZ2	2.29	0.67
2:B:51:GLU:OE1	2:B:51:GLU:HA	1.88	0.67
2:D:124:PRO:HD3	2:D:232:PRO:HB3	1.77	0.67
1:C:140:LEU:HD13	1:C:141:CYS:N	2.09	0.67
3:E:51:ASP:O	3:E:52:ASN:HB3	1.93	0.67
3:E:163:LYS:HZ2	3:E:175:THR:CG2	2.08	0.67
3:G:66:THR:HG23	3:G:66:THR:O	1.94	0.67
3:G:89:LEU:HD12	3:G:97:VAL:O	1.95	0.67
1:A:102:TYR:CB	2:B:98:TRP:HE1	2.08	0.67
2:B:217:HIS:CA	2:B:234:THR:HG22	2.16	0.67
1:C:203:ASN:OD1	5:C:216:NAG:N2	2.27	0.67
3:G:206:GLU:C	3:G:208:SER:H	2.03	0.67
1:C:140:LEU:HD13	1:C:141:CYS:H	1.60	0.66
4:H:52(B):ILE:CG2	4:H:52(C):PRO:CD	2.72	0.66
2:D:52:LYS:C	2:D:69:GLN:HE21	2.04	0.66
2:D:68:GLN:HE21	2:D:68:GLN:H	1.43	0.66
2:D:113:ARG:HD2	2:D:156:HIS:HE2	1.58	0.66
2:D:159:LEU:HD23	2:D:160:SER:N	2.11	0.66
2:D:223:ASP:HB2	2:D:231:LYS:CD	2.26	0.66
3:E:192:VAL:O	3:E:211:PRO:CD	2.43	0.66
4:H:195:SER:HA	4:H:199:TRP:CZ3	2.30	0.66
2:D:204:HIS:HA	2:D:244:ARG:HB2	1.77	0.66
3:E:198:HIS:N	3:E:205:VAL:HB	2.10	0.66
4:F:141:GLY:HA2	4:F:157:TRP:CZ2	2.30	0.66
4:H:148:PHE:H	4:H:149:PRO:HD2	1.58	0.66
2:B:17:GLY:O	2:B:82:LEU:HG	1.95	0.66
2:B:120:ARG:HD2	3:E:50:MET:SD	2.36	0.66
1:A:55:ARG:NH2	1:A:57:GLU:HG2	2.10	0.66
2:D:70:PHE:CE1	2:D:74:HIS:CE1	2.83	0.66
3:E:140:TYR:CD1	3:E:141:PRO:CA	2.78	0.66
3:E:207:LYS:HD2	3:E:207:LYS:N	2.09	0.66
4:H:2:VAL:HB	4:H:102:TYR:CE2	2.30	0.66
4:H:124:LEU:O	4:H:140:LEU:HB2	1.96	0.66
4:H:153:THR:CG2	4:H:211:ALA:HB3	2.21	0.66
2:D:115:THR:CG2	2:D:116(A):LEU:HD21	2.25	0.66
3:E:136:VAL:HG13	3:E:175:THR:O	1.95	0.66
2:D:49:HIS:CE1	2:D:53:VAL:HG12	2.30	0.66
3:E:183:ALA:O	3:E:187:LYS:HG3	1.95	0.66
3:G:6:GLN:NE2	3:G:88:CYS:SG	2.66	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:157:TRP:CZ3	4:H:208:CYS:HB3	2.30	0.66
1:A:125:VAL:HA	1:A:142:LEU:O	1.95	0.66
2:B:174:THR:HG23	2:B:194:SER:HB2	1.78	0.66
1:C:171:LYS:HA	2:D:170:SER:OG	1.96	0.66
3:E:115:VAL:CG2	3:E:207:LYS:CB	2.72	0.66
4:F:174:PHE:HB3	4:F:175:PRO:CD	2.26	0.66
4:F:212:HIS:CE1	4:F:214:ALA:HB2	2.31	0.66
2:D:74:HIS:CE1	2:D:76:GLU:OE2	2.49	0.66
3:E:61:ARG:NH1	3:E:79:GLN:HB2	2.11	0.66
4:F:142:CYS:O	4:F:188:SER:HA	1.96	0.66
1:A:39:LEU:HD22	1:A:40:ASN:H	1.60	0.65
2:B:227:GLU:OE1	2:B:227:GLU:HA	1.95	0.65
3:E:66:THR:HG23	3:E:66:THR:O	1.95	0.65
3:E:117:VAL:HG11	3:E:211:PRO:CG	2.26	0.65
1:C:159:GLY:O	1:C:184:SER:HA	1.96	0.65
2:D:96:LEU:O	2:D:97:ARG:O	2.12	0.65
4:F:36:TRP:O	4:F:37:VAL:CG2	2.45	0.65
4:F:199:TRP:HE3	4:F:200:PRO:HD3	1.60	0.65
2:B:5:VAL:HG23	2:B:24:ILE:HB	1.76	0.65
2:D:12:ILE:C	2:D:13:LYS:HG2	2.20	0.65
4:F:203:GLN:OE1	4:F:204:PRO:HD2	1.96	0.65
4:H:105:GLN:OE1	4:H:105:GLN:HA	1.97	0.65
2:B:65:PHE:CD1	2:B:79:MET:HA	2.31	0.65
2:D:93:ALA:HA	2:D:107:TYR:O	1.95	0.65
4:F:17:SER:OG	4:F:82(A):ASN:HB3	1.96	0.65
3:G:146:VAL:HG21	3:G:177:SER:HB2	1.78	0.65
1:A:108:ALA:HA	2:B:42:GLU:OE2	1.97	0.65
1:A:123:PRO:HB2	1:A:204:ALA:CB	2.23	0.65
1:A:160:THR:OG1	1:A:184:SER:HB2	1.95	0.65
4:H:37:VAL:HG13	4:H:47:TRP:HA	1.77	0.65
1:A:57:GLU:C	1:A:59:GLN:H	2.05	0.65
2:D:37:GLN:CG	2:D:41:LYS:HA	2.27	0.65
4:F:36:TRP:NE1	4:F:78:ILE:CD1	2.59	0.65
4:F:121:VAL:HG21	4:F:219:VAL:HG11	1.79	0.65
4:H:52(B):ILE:HG23	4:H:52(C):PRO:CD	2.27	0.65
1:C:17:PRO:HA	1:C:78:SER:O	1.97	0.65
3:E:163:LYS:HZ3	3:E:175:THR:HG23	1.61	0.65
3:E:167:GLN:O	3:E:170:GLY:C	2.40	0.65
3:G:113:PRO:HG3	3:G:198:HIS:HB2	1.77	0.65
3:G:149:LYS:HG2	3:G:154:THR:HA	1.79	0.65
4:H:212:HIS:HB3	4:H:217:THR:CB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ARG:HH22	1:A:57:GLU:HG2	1.60	0.65
2:D:127:VAL:HG23	2:D:237:ILE:HG22	1.78	0.65
2:D:160:SER:HB2	2:D:162:TRP:HE1	1.62	0.65
2:B:233:VAL:O	2:B:235:GLN:HG2	1.98	0.65
3:G:80:PRO:C	3:G:82:ASP:H	2.02	0.65
4:H:141:GLY:HA2	4:H:157:TRP:CZ2	2.32	0.64
4:H:217:THR:HG22	4:H:219:VAL:HG12	1.78	0.64
1:C:68:LYS:O	1:C:69:SER:C	2.39	0.64
2:D:70:PHE:CG	2:D:74:HIS:ND1	2.63	0.64
4:H:19:LYS:HA	4:H:80:LEU:O	1.97	0.64
1:A:14:GLU:HG2	1:A:116:ALA:HA	1.80	0.64
1:C:155:THR:HG21	1:C:160:THR:O	1.98	0.64
2:D:74:HIS:NE2	2:D:76:GLU:CG	2.61	0.64
3:E:144:ALA:CB	3:E:196:VAL:HG12	2.24	0.64
4:H:199:TRP:HB2	4:H:205:ILE:HG13	1.80	0.64
1:A:87:LEU:HD12	2:B:41:LYS:HD3	1.80	0.64
2:D:78:ASN:ND2	5:D:248:NAG:O7	2.30	0.64
4:F:83:ARG:C	4:F:111:VAL:HG11	2.22	0.64
1:A:33:PHE:CD2	1:A:48:LYS:HB2	2.31	0.64
1:C:47:LEU:HB2	1:C:56:THR:CG2	2.27	0.64
2:D:128:SER:HB3	2:D:130:PHE:CE1	2.32	0.64
3:E:139:PHE:CE2	3:E:173:TYR:HB3	2.33	0.64
3:G:47:LEU:HA	3:G:58:ILE:CD1	2.27	0.64
1:A:14:GLU:OE2	1:A:176:LYS:HE2	1.98	0.64
2:B:132:PRO:HD3	2:B:145:LEU:HD21	1.76	0.64
2:D:37:GLN:NE2	2:D:41:LYS:HB3	2.13	0.64
4:F:52(A):ASN:HA	4:F:71:ARG:NH2	2.13	0.64
4:H:35:TYR:N	4:H:35:TYR:CD1	2.63	0.64
4:H:149:PRO:O	4:H:150:GLU:O	2.15	0.64
1:A:77:LYS:NZ	1:A:84:ASP:OD2	2.31	0.64
1:A:146:PHE:HB2	1:A:150:ILE:CD1	2.27	0.64
1:C:159:GLY:HA3	1:C:185:ASN:OD1	1.98	0.64
2:D:60:LEU:HD11	2:D:65:PHE:CB	2.27	0.64
4:F:125:ALA:C	4:F:127:ALA:H	2.05	0.64
4:F:148:PHE:H	4:F:149:PRO:HD2	1.62	0.64
3:E:167:GLN:HB3	3:E:172:ASN:OD1	1.98	0.64
4:F:29:PHE:HB3	4:F:76:ASN:OD1	1.98	0.64
4:F:36:TRP:O	4:F:37:VAL:HG22	1.97	0.64
2:B:68:GLN:HE21	2:B:68:GLN:H	1.46	0.63
1:C:122:GLU:HB3	2:D:140:LYS:CE	2.28	0.63
3:E:143:SER:HB3	3:E:163:LYS:CG	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:146:VAL:HG12	3:G:196:VAL:CG2	2.25	0.63
4:H:139:THR:HA	4:H:191:VAL:O	1.98	0.63
4:H:99:ASP:HB3	4:H:101:ASP:OD2	1.98	0.63
4:F:131:THR:O	4:F:132:THR:HG23	1.97	0.63
3:G:192:VAL:H	3:G:212:ALA:HB3	1.62	0.63
4:H:18:LEU:HD13	4:H:109:VAL:HG22	1.81	0.63
2:B:100:ASP:O	2:B:105:GLU:HG2	1.98	0.63
2:B:221:GLU:C	2:B:223:ASP:N	2.57	0.63
2:B:150:ARG:HG2	2:B:191:SER:OG	1.99	0.63
1:C:33:PHE:CD2	1:C:48:LYS:HB2	2.33	0.63
4:F:6:GLU:HB2	4:F:106:GLY:O	1.98	0.63
1:A:168:LEU:C	1:A:168:LEU:CD1	2.64	0.63
2:D:154:PRO:C	2:D:156:HIS:H	2.06	0.63
3:E:107:ARG:CB	3:E:109:PRO:HD2	2.29	0.63
3:G:47:LEU:O	3:G:55:PRO:HD2	1.99	0.63
3:G:125:LEU:O	3:G:128:ASN:N	2.31	0.63
2:B:71:ASP:C	2:B:73:TYR:H	2.06	0.63
2:B:133:SER:O	2:B:137:ILE:HD13	1.99	0.63
2:B:223:ASP:CG	2:B:223:ASP:O	2.42	0.63
2:D:60:LEU:CD1	2:D:65:PHE:HB2	2.28	0.63
4:H:171:VAL:O	4:H:172:HIS:ND1	2.31	0.63
1:A:193:ASP:OD1	1:A:193:ASP:N	2.28	0.62
2:B:105:GLU:CD	2:D:96:LEU:HD23	2.24	0.62
4:F:140:LEU:HD11	4:F:225:ILE:HD13	1.80	0.62
3:G:41:ASP:O	3:G:42:LYS:HB2	1.98	0.62
1:C:117:HIS:O	1:C:117:HIS:CG	2.52	0.62
1:A:171:LYS:HD2	2:B:170:SER:CB	2.25	0.62
1:C:62:PHE:HB3	1:C:75:LEU:HD11	1.79	0.62
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.80	0.62
3:E:163:LYS:NZ	3:E:175:THR:HG21	2.15	0.62
4:H:195:SER:CA	4:H:199:TRP:HZ3	2.12	0.62
1:A:126:TYR:CE2	2:B:136:GLU:HG3	2.34	0.62
2:B:118:ASP:O	2:B:121:ASN:HB2	1.99	0.62
2:D:70:PHE:CE2	2:D:74:HIS:CE1	2.87	0.62
2:B:50:TYR:CZ	2:B:97:ARG:CB	2.82	0.62
1:A:205:THR:C	1:A:206:TYR:HD1	2.08	0.62
3:E:119:PRO:HG2	4:F:127:ALA:HB3	1.81	0.62
3:E:203:GLU:HB2	3:E:205:VAL:HG22	1.81	0.62
3:G:86:TYR:HE2	3:G:104:LEU:HD22	1.64	0.62
2:B:72:ASP:O	2:B:73:TYR:HB2	1.99	0.62
2:D:26:ILE:HB	2:D:29:HIS:ND1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:GLY:C	2:D:41:LYS:HG3	2.21	0.62
5:D:249:NAG:O7	5:D:249:NAG:H3	1.99	0.62
3:E:52:ASN:C	3:E:52:ASN:OD1	2.42	0.62
3:E:79:GLN:HG3	3:E:80:PRO:CD	2.23	0.62
4:F:124:LEU:HG	4:F:141:GLY:C	2.24	0.62
4:F:140:LEU:O	4:F:190:SER:HA	1.99	0.62
4:F:193:VAL:HB	4:F:198:THR:HG21	1.82	0.62
3:G:162:THR:HB	3:G:164:PRO:HD3	1.82	0.62
2:B:52:LYS:HD3	2:B:53:VAL:CG2	2.25	0.61
3:E:118:PHE:CE1	4:F:124:LEU:O	2.52	0.61
1:A:129:LYS:CE	1:A:210:ASP:OD2	2.48	0.61
4:H:164:GLY:O	4:H:165:ALA:C	2.43	0.61
2:D:2:SER:HA	2:D:26:ILE:HG23	1.81	0.61
3:E:91:SER:HA	3:E:95(B):ASP:O	2.00	0.61
3:G:192:VAL:HG23	3:G:212:ALA:CB	2.30	0.61
2:D:52:LYS:O	2:D:69:GLN:NE2	2.33	0.61
4:F:150:GLU:HB3	4:F:151:PRO:HD2	1.81	0.61
4:H:52(A):ASN:HD22	4:H:52(A):ASN:N	1.96	0.61
4:H:178:LEU:HD23	4:H:185:TYR:CE1	2.36	0.61
2:D:40:GLY:O	2:D:41:LYS:CB	2.48	0.61
4:H:52(A):ASN:HA	4:H:71:ARG:NH2	2.15	0.61
4:F:124:LEU:HG	4:F:141:GLY:O	2.00	0.61
2:D:11:ILE:HD11	2:D:112:THR:HG21	1.82	0.61
2:D:84:LEU:CD2	2:D:117:GLU:HG2	2.31	0.61
4:F:29:PHE:CZ	4:F:71:ARG:HD2	2.35	0.61
4:F:68:THR:CG2	4:F:69:ILE:H	2.12	0.61
3:G:183:ALA:HB1	3:G:187:LYS:HZ1	1.66	0.61
3:E:162:THR:HB	3:E:164:PRO:HD3	1.83	0.61
4:F:36:TRP:C	4:F:37:VAL:HG23	2.26	0.61
4:F:72:ASP:OD1	4:F:74:SER:OG	2.17	0.61
2:D:40:GLY:C	2:D:41:LYS:HG2	2.23	0.61
2:D:153:PHE:HB3	2:D:154:PRO:HD3	1.80	0.61
3:G:132:LEU:O	3:G:148:TRP:HH2	1.84	0.61
4:F:47:TRP:CE3	4:F:60:ALA:HB2	2.35	0.61
4:F:141:GLY:HA2	4:F:157:TRP:CH2	2.36	0.61
1:C:168:LEU:HD21	2:D:197:ARG:HB2	1.83	0.60
4:F:119:PRO:HB3	4:F:147:TYR:HB3	1.82	0.60
3:G:132:LEU:O	3:G:148:TRP:CH2	2.53	0.60
3:G:193:SER:HB3	3:G:195:GLN:NE2	2.14	0.60
1:C:193:ASP:OD1	1:C:193:ASP:N	2.32	0.60
4:H:33:TRP:CH2	4:H:52:LYS:HE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ALA:HB2	1:C:167:VAL:HG11	1.82	0.60
1:C:170:MET:HA	2:D:171:GLY:HA2	1.84	0.60
3:E:19:VAL:HG22	3:E:20:LYS:N	2.15	0.60
3:E:140:TYR:HD1	3:E:173:TYR:CE2	2.14	0.60
3:G:96:LEU:HD12	4:H:47:TRP:NE1	2.17	0.60
2:B:131:GLU:HA	2:B:145:LEU:HD23	1.84	0.60
1:C:52:ASP:O	1:C:53:ASN:HB2	2.01	0.60
1:A:140:LEU:HD13	1:A:141:CYS:H	1.67	0.60
2:B:95:SER:HB3	2:B:106:GLN:HG2	1.84	0.60
1:C:89:TYR:OH	2:D:37:GLN:NE2	2.35	0.60
3:E:118:PHE:CZ	4:F:140:LEU:HA	2.36	0.60
4:F:3:TYR:N	4:F:25:SER:O	2.35	0.60
4:H:153:THR:HG23	4:H:211:ALA:CB	2.22	0.60
1:A:171:LYS:N	2:B:170:SER:OG	2.35	0.60
2:B:125:PRO:HD2	2:B:237:ILE:HD12	1.84	0.60
2:B:169:HIS:O	2:B:172:VAL:HG22	2.02	0.60
4:F:57:THR:HG21	4:F:59:TYR:CZ	2.35	0.60
1:C:19:LYS:HA	1:C:75:LEU:O	2.02	0.60
2:D:51:GLU:OE2	2:D:73:TYR:OH	2.18	0.60
4:F:138:VAL:O	4:F:192:THR:HA	2.02	0.60
1:A:77:LYS:HE2	1:A:79:SER:O	2.01	0.60
1:A:155:THR:HG23	1:A:160:THR:HG22	1.83	0.60
2:B:131:GLU:HA	2:B:145:LEU:CD2	2.31	0.60
4:H:33:TRP:CZ2	4:H:53:ASN:ND2	2.69	0.60
1:A:15:GLY:O	1:A:79:SER:HA	2.02	0.60
1:C:170:MET:HA	2:D:171:GLY:CA	2.32	0.60
4:H:52(A):ASN:ND2	4:H:52(A):ASN:N	2.48	0.60
4:H:141:GLY:O	4:H:225:ILE:HD11	2.02	0.60
4:H:174:PHE:HD1	4:H:174:PHE:H	1.49	0.60
3:G:21:ILE:O	3:G:72:THR:HG23	2.02	0.59
2:D:128:SER:HB3	2:D:130:PHE:HE1	1.67	0.59
3:E:166:LYS:CG	3:E:167:GLN:H	2.14	0.59
4:F:10:ASP:CG	4:F:11:LEU:N	2.59	0.59
4:H:174:PHE:N	4:H:174:PHE:CD1	2.70	0.59
3:E:148:TRP:CE3	3:E:179:LEU:HD13	2.36	0.59
4:F:109:VAL:O	4:F:109:VAL:HG12	2.02	0.59
3:G:80:PRO:O	3:G:82:ASP:N	2.35	0.59
1:C:47:LEU:HD13	1:C:56:THR:HG21	1.84	0.59
4:F:29:PHE:CE1	4:F:71:ARG:NH1	2.66	0.59
1:A:203:ASN:O	1:A:204:ALA:CB	2.50	0.59
2:B:226:PRO:HG3	3:E:50:MET:SD	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:ASP:OD1	2:D:120:ARG:HD3	2.03	0.59
4:F:150:GLU:HB3	4:F:151:PRO:CD	2.32	0.59
3:E:25:GLY:CA	3:E:28:LEU:HG	2.28	0.59
4:H:148:PHE:O	4:H:185:TYR:CD2	2.55	0.59
1:A:155:THR:CG2	1:A:160:THR:O	2.42	0.59
1:C:77:LYS:NZ	1:C:84:ASP:OD2	2.35	0.59
4:F:191:VAL:HG13	4:F:191:VAL:O	2.02	0.59
3:G:122:PRO:HG3	4:H:228:ARG:CZ	2.32	0.59
3:G:206:GLU:O	3:G:208:SER:N	2.36	0.59
1:A:55:ARG:CZ	1:A:57:GLU:HG2	2.32	0.59
2:B:60:LEU:HD11	2:B:65:PHE:HB2	1.84	0.59
4:F:174:PHE:O	4:F:187:LEU:CD1	2.50	0.59
2:D:74:HIS:NE2	2:D:76:GLU:HG2	2.17	0.59
2:D:167:GLU:HG2	2:D:169:HIS:HE1	1.67	0.59
2:D:172:VAL:HG12	2:D:196:LEU:HD13	1.84	0.59
4:F:138:VAL:N	4:F:193:VAL:O	2.34	0.59
1:A:102:TYR:CB	2:B:98:TRP:NE1	2.64	0.59
3:E:150:ALA:HA	3:E:191:ARG:O	2.03	0.59
4:F:93:THR:HG21	4:F:100(A):PHE:HD1	1.68	0.59
4:F:199:TRP:C	4:F:202:LYS:N	2.60	0.59
3:G:63:SER:OG	3:G:74:THR:HB	2.03	0.59
3:G:148:TRP:HZ2	3:G:177:SER:O	1.86	0.59
4:H:34:MET:C	4:H:35:TYR:CD1	2.81	0.59
1:A:68:LYS:O	1:A:71:SER:N	2.28	0.58
3:G:182:THR:HG23	3:G:185:GLN:CD	2.27	0.58
4:H:68:THR:O	4:H:80:LEU:HD12	2.03	0.58
1:A:48:LYS:HZ1	2:B:100:ASP:CG	2.11	0.58
1:A:55:ARG:HD3	1:A:55:ARG:C	2.28	0.58
2:D:119:LEU:O	2:D:121:ASN:N	2.35	0.58
3:E:41:ASP:HB3	3:E:43:ASN:OD1	2.03	0.58
4:F:36:TRP:C	4:F:37:VAL:CG2	2.76	0.58
4:F:40:ALA:HB3	4:F:43:LYS:CD	2.33	0.58
4:H:121:VAL:HG11	4:H:210:VAL:HG21	1.83	0.58
4:H:128:CYS:O	4:H:130:SER:N	2.35	0.58
2:B:29:HIS:HB3	2:B:95:SER:O	2.04	0.58
4:F:40:ALA:HB3	4:F:43:LYS:CB	2.23	0.58
3:G:43:ASN:HD22	3:G:43:ASN:N	1.89	0.58
3:G:121:SER:OG	3:G:123:GLU:HG2	2.03	0.58
4:H:107:THR:HG23	4:H:107:THR:O	2.02	0.58
4:H:137:THR:HG22	4:H:193:VAL:C	2.29	0.58
4:H:210:VAL:HB	4:H:219:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:HB3	2:D:131:GLU:O	2.04	0.58
2:D:79:MET:HE1	2:D:114:LEU:HD22	1.85	0.58
1:A:47:LEU:CB	1:A:55:ARG:HD2	2.25	0.58
3:E:108:GLY:N	3:E:109:PRO:CD	2.65	0.58
4:F:115:THR:CG2	4:F:116:THR:N	2.67	0.58
3:G:19:VAL:HG22	3:G:20:LYS:H	1.68	0.58
3:E:139:PHE:CE2	3:E:173:TYR:CB	2.87	0.58
2:D:51:GLU:O	2:D:52:LYS:HB3	2.03	0.58
2:D:206:PRO:HA	2:D:243:GLY:HA3	1.85	0.58
3:E:128:ASN:O	3:E:129:LYS:HD3	2.03	0.58
4:F:157:TRP:HZ3	4:F:225:ILE:CD1	2.17	0.58
4:H:84:VAL:C	4:H:86:ASP:H	2.12	0.58
4:F:108:MET:CB	4:F:150:GLU:CD	2.77	0.58
3:E:28:LEU:HD12	3:E:69:THR:O	2.04	0.58
3:G:192:VAL:HG23	3:G:212:ALA:HB1	1.85	0.58
3:G:192:VAL:N	3:G:212:ALA:HB3	2.18	0.58
2:B:9:ARG:HD2	2:B:110:PRO:HB2	1.86	0.57
1:C:58:HIS:O	1:C:59:GLN:C	2.47	0.57
2:D:118:ASP:OD2	2:D:120:ARG:HB2	2.03	0.57
1:A:5:GLN:HE21	1:A:107:GLY:HA3	1.67	0.57
3:E:148:TRP:CH2	3:E:179:LEU:HB2	2.39	0.57
3:E:163:LYS:NZ	3:E:175:THR:HG23	2.18	0.57
3:E:205:VAL:CG1	3:E:207:LYS:HD3	2.34	0.57
4:F:133:SER:O	4:F:135:THR:N	2.35	0.57
3:G:25:GLY:HA3	3:G:28:LEU:HG	1.86	0.57
4:H:195:SER:HA	4:H:199:TRP:HZ3	1.68	0.57
1:C:47:LEU:HD13	1:C:56:THR:HG22	1.86	0.57
3:G:198:HIS:N	3:G:205:VAL:HB	2.20	0.57
1:A:87:LEU:HD13	1:A:89:TYR:CE2	2.39	0.57
1:A:101:ASN:C	1:A:103:LYS:N	2.60	0.57
2:B:34:TRP:O	2:B:46:LEU:HB2	2.04	0.57
2:B:50:TYR:CE2	2:B:97:ARG:HB3	2.38	0.57
2:B:214:VAL:O	2:B:214:VAL:HG12	2.03	0.57
3:E:164:PRO:HG3	4:F:175:PRO:CG	2.35	0.57
4:F:147:TYR:CE1	4:F:185:TYR:O	2.58	0.57
3:G:166:LYS:O	3:G:167:GLN:C	2.47	0.57
4:H:17:SER:HA	4:H:82:MET:O	2.04	0.57
1:A:38:TYR:O	1:A:41:GLU:HB2	2.05	0.57
2:B:202:PHE:CE1	2:B:208:ASN:ND2	2.72	0.57
2:D:180:LYS:HG2	2:D:190:TYR:CZ	2.39	0.57
2:D:229:SER:HA	4:H:33:TRP:CZ2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:52:ASN:O	3:G:52:ASN:CG	2.48	0.57
1:C:21:ASN:HB2	5:C:214:NAG:HN2	1.69	0.57
1:C:144:THR:HG22	1:C:145:ASP:OD1	2.05	0.57
2:D:13:LYS:HD2	2:D:19:SER:HB2	1.87	0.57
2:D:225:TRP:CD2	2:D:226:PRO:HD2	2.39	0.57
4:F:108:MET:HB3	4:F:150:GLU:CD	2.30	0.57
3:G:123:GLU:HA	3:G:126:ARG:HB2	1.87	0.57
3:G:192:VAL:CB	3:G:212:ALA:CB	2.82	0.57
4:H:19:LYS:HE3	4:H:81:GLN:HG2	1.85	0.57
4:H:141:GLY:CA	4:H:189:SER:O	2.53	0.57
2:B:209:HIS:HE2	2:B:240:GLU:CD	2.12	0.57
2:D:8:PRO:O	2:D:112:THR:OG1	2.19	0.57
2:D:89:MET:HE3	2:D:113:ARG:CB	2.33	0.57
3:E:211:PRO:O	3:E:212:ALA:O	2.22	0.57
4:H:126:PRO:O	4:H:127:ALA:CB	2.53	0.57
1:A:159:GLY:O	1:A:184:SER:HA	2.05	0.57
1:C:186:GLN:O	1:C:188:SER:N	2.36	0.57
2:D:60:LEU:HD12	2:D:61:PRO:CD	2.34	0.57
4:F:9:GLY:HA3	4:F:108:MET:O	2.04	0.57
3:G:2:TYR:CD1	3:G:2:TYR:N	2.72	0.57
3:G:214:CYS:C	3:G:215:LEU:HD23	2.29	0.57
2:B:114:LEU:HG	2:B:115:THR:N	2.20	0.57
1:C:125:VAL:CG2	1:C:125:VAL:O	2.52	0.57
2:D:180:LYS:HG2	2:D:190:TYR:CE2	2.40	0.57
2:D:205:ASN:HB3	2:D:208:ASN:ND2	2.20	0.57
3:G:34:TYR:HB2	3:G:89:LEU:HB3	1.87	0.57
3:G:115:VAL:HB	3:G:209:LEU:HD13	1.86	0.57
4:H:52(A):ASN:H	4:H:52(A):ASN:HD22	1.50	0.57
4:H:59:TYR:O	4:H:64:ARG:NH2	2.38	0.57
4:H:63:VAL:HG12	4:H:66:ARG:CZ	2.35	0.57
4:H:215:SER:O	4:H:216:SER:C	2.46	0.57
1:A:47:LEU:CB	1:A:55:ARG:NH1	2.66	0.57
2:D:38:THR:O	2:D:39:LEU:C	2.48	0.57
2:D:134:LYS:H	2:D:134:LYS:HE2	1.69	0.57
4:F:22:CYS:HB3	4:F:78:ILE:HG13	1.87	0.57
4:H:52(A):ASN:HA	4:H:71:ARG:HH21	1.68	0.57
2:B:71:ASP:C	2:B:73:TYR:N	2.63	0.56
2:D:127:VAL:HG23	2:D:237:ILE:CG2	2.35	0.56
2:D:153:PHE:CD2	2:D:154:PRO:HD3	2.40	0.56
4:F:39:GLN:O	4:F:88:ALA:HB1	2.04	0.56
4:F:78:ILE:C	4:F:79:TYR:CD1	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:84:VAL:HA	4:H:111:VAL:O	2.05	0.56
1:C:66:LEU:HG	1:C:67:HIS:N	2.20	0.56
1:C:144:THR:CG2	1:C:145:ASP:H	2.16	0.56
2:D:1:ASP:O	2:D:26:ILE:HA	2.05	0.56
2:D:10:HIS:HD2	2:D:156:HIS:HD2	1.53	0.56
2:D:134:LYS:H	2:D:134:LYS:CD	2.17	0.56
3:E:17:GLU:O	3:E:78:ALA:N	2.37	0.56
4:F:52(A):ASN:ND2	4:F:52(A):ASN:H	2.02	0.56
4:H:38:ARG:HB3	4:H:90:TYR:CE2	2.40	0.56
1:A:77:LYS:HZ2	1:A:84:ASP:CG	2.13	0.56
2:B:15:LYS:C	2:B:17:GLY:H	2.11	0.56
1:C:189:PHE:HB3	1:C:194:ILE:HD12	1.86	0.56
1:C:195:PHE:O	1:C:198:THR:HG23	2.06	0.56
2:D:1:ASP:C	2:D:3:GLY:H	2.13	0.56
3:E:198:HIS:O	3:E:203:GLU:O	2.22	0.56
3:G:108:GLY:N	3:G:109:PRO:CD	2.68	0.56
3:G:186:TRP:HA	3:G:189:HIS:HB2	1.87	0.56
3:G:191:ARG:HG3	3:G:213:GLU:OE2	2.05	0.56
3:G:214:CYS:O	3:G:215:LEU:C	2.48	0.56
4:H:140:LEU:O	4:H:190:SER:HA	2.06	0.56
1:A:12:VAL:O	1:A:115:ILE:HG13	2.05	0.56
4:F:141:GLY:HA3	4:F:189:SER:O	2.06	0.56
4:F:205:ILE:O	4:F:225:ILE:HD12	2.05	0.56
3:G:116:THR:O	3:G:116:THR:HG22	2.03	0.56
3:G:124:GLU:CD	3:G:131:THR:HG1	2.13	0.56
3:G:214:CYS:HB2	3:G:215:LEU:CD2	2.35	0.56
4:H:138:VAL:CG2	4:H:199:TRP:CH2	2.88	0.56
4:H:143:LEU:C	4:H:143:LEU:HD12	2.30	0.56
1:A:92:LEU:C	1:A:92:LEU:CD1	2.77	0.56
1:A:144:THR:CG2	1:A:145:ASP:H	2.18	0.56
4:H:199:TRP:NE1	4:H:200:PRO:HD3	2.19	0.56
2:D:68:GLN:H	2:D:68:GLN:NE2	2.03	0.56
3:E:179:LEU:O	3:E:180:SER:C	2.48	0.56
4:F:148:PHE:O	4:F:149:PRO:O	2.22	0.56
1:A:68:LYS:O	1:A:69:SER:C	2.49	0.56
1:A:129:LYS:HE3	1:A:210:ASP:OD2	2.05	0.56
3:E:13:VAL:HB	3:E:19:VAL:HB	1.88	0.56
3:G:151:ASN:CG	3:G:151:ASN:O	2.48	0.56
1:A:143:PHE:O	1:A:146:PHE:HE2	1.89	0.56
2:D:84:LEU:HD21	2:D:117:GLU:HG2	1.86	0.56
1:A:48:LYS:NZ	2:B:100:ASP:CB	2.67	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:11:LEU:HA	4:F:110:THR:O	2.06	0.56
4:F:71:ARG:HD3	4:F:78:ILE:HG22	1.88	0.56
4:F:198:THR:HG22	4:F:199:TRP:N	2.19	0.56
3:G:114:LYS:HD3	3:G:138:ASP:HB2	1.88	0.56
4:H:75:ARG:O	4:H:76:ASN:HB2	2.06	0.56
4:H:147:TYR:O	4:H:185:TYR:N	2.38	0.56
4:H:152:VAL:HB	4:H:211:ALA:O	2.06	0.56
1:C:126:TYR:CE1	2:D:136:GLU:HG3	2.39	0.55
4:F:77:SER:C	4:F:78:ILE:HG23	2.30	0.55
4:F:157:TRP:CZ3	4:F:225:ILE:HD11	2.41	0.55
4:F:210:VAL:N	4:F:219:VAL:O	2.39	0.55
1:A:89:TYR:OH	2:B:37:GLN:NE2	2.38	0.55
1:A:127:GLN:OE1	1:A:208:SER:HB3	2.06	0.55
2:B:105:GLU:OE2	2:D:96:LEU:HD23	2.06	0.55
2:D:219:LEU:HD12	2:D:219:LEU:N	2.20	0.55
3:G:17:GLU:O	3:G:78:ALA:N	2.39	0.55
3:G:95:ASN:O	3:G:95(A):ASN:C	2.49	0.55
4:H:18:LEU:CD1	4:H:109:VAL:HG22	2.35	0.55
1:A:57:GLU:C	1:A:59:GLN:N	2.62	0.55
1:A:82:LEU:CD2	1:A:114:VAL:HG22	2.30	0.55
1:A:203:ASN:ND2	5:A:216:NAG:O7	2.40	0.55
1:C:104:TYR:HE1	1:C:106:PHE:CZ	2.23	0.55
3:G:164:PRO:HB3	4:H:175:PRO:CG	2.36	0.55
1:A:46:LEU:CD1	1:A:59:GLN:OE1	2.55	0.55
1:A:46:LEU:O	1:A:47:LEU:HB3	2.06	0.55
2:B:172:VAL:HG12	2:B:196:LEU:HD13	1.88	0.55
2:D:159:LEU:HD13	2:D:194:SER:HB3	1.88	0.55
4:F:57:THR:HG22	4:F:58:GLU:N	2.21	0.55
4:F:82:MET:SD	4:F:82(C):LEU:HD21	2.47	0.55
3:G:91:SER:HA	3:G:95(B):ASP:O	2.06	0.55
3:G:115:VAL:HG12	3:G:116:THR:N	2.20	0.55
3:G:171:GLN:HG2	3:G:171:GLN:O	2.05	0.55
4:H:174:PHE:HB3	4:H:175:PRO:CD	2.36	0.55
1:A:140:LEU:HD21	1:A:181:ILE:HD12	1.89	0.55
1:A:171:LYS:CE	2:B:170:SER:HB2	2.36	0.55
4:H:38:ARG:HD2	4:H:90:TYR:CE2	2.42	0.55
2:B:113:ARG:HD2	2:B:156:HIS:ND1	2.15	0.55
3:E:66:THR:CA	3:E:71:ALA:HA	2.35	0.55
4:F:52(A):ASN:HD22	4:F:52(A):ASN:N	2.05	0.55
3:G:113:PRO:HD2	3:G:207:LYS:HZ2	1.71	0.55
1:C:36:VAL:HG13	1:C:36:VAL:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:ILE:HD12	1:C:162:ILE:N	2.21	0.55
3:E:48:ILE:CG2	3:E:49:TYR:N	2.70	0.55
4:F:84:VAL:C	4:F:86:ASP:H	2.15	0.55
3:G:175:THR:CG2	3:G:176:SER:N	2.70	0.55
2:B:6:GLN:OE1	2:B:111:GLY:HA2	2.06	0.55
2:B:50:TYR:CE2	2:B:97:ARG:HB2	2.41	0.55
2:B:127:VAL:HG11	2:B:238:SER:HA	1.89	0.55
3:E:181:LEU:HD11	3:E:185:GLN:HB3	1.89	0.55
3:G:141:PRO:CG	3:G:142:GLY:H	2.20	0.55
4:F:16:SER:OG	4:F:17:SER:N	2.39	0.55
4:F:37:VAL:HG13	4:F:47:TRP:HA	1.87	0.55
4:F:40:ALA:HB1	4:F:43:LYS:HD3	1.88	0.55
3:G:181:LEU:HD21	3:G:189:HIS:HD1	1.71	0.55
3:G:192:VAL:CG2	3:G:212:ALA:CB	2.84	0.55
4:H:78:ILE:O	4:H:78:ILE:HG13	2.04	0.55
1:A:144:THR:CG2	1:A:145:ASP:N	2.69	0.54
1:A:171:LYS:HB2	2:B:170:SER:CB	2.36	0.54
2:B:227:GLU:O	4:F:95:ALA:HB1	2.07	0.54
4:F:147:TYR:HB2	4:F:212:HIS:CE1	2.42	0.54
3:G:144:ALA:HB2	3:G:198:HIS:HA	1.90	0.54
4:H:29:PHE:CE2	4:H:71:ARG:HD2	2.41	0.54
1:A:190:THR:HG22	1:A:192:GLN:N	2.21	0.54
4:F:157:TRP:CH2	4:F:208:CYS:HB3	2.42	0.54
4:F:157:TRP:HZ2	4:F:189:SER:O	1.91	0.54
3:G:181:LEU:HD21	3:G:189:HIS:ND1	2.22	0.54
4:H:38:ARG:HB3	4:H:90:TYR:CD2	2.42	0.54
1:A:101:ASN:C	1:A:103:LYS:H	2.15	0.54
1:C:39:LEU:HD13	1:C:40:ASN:HB2	1.88	0.54
4:F:154:VAL:HG22	4:F:210:VAL:HG13	1.90	0.54
1:A:102:TYR:HB3	2:B:98:TRP:CD1	2.43	0.54
3:G:11:ALA:O	3:G:104:LEU:HA	2.07	0.54
4:H:32:PHE:CD1	4:H:96:GLY:CA	2.90	0.54
1:A:123:PRO:HB2	1:A:203:ASN:O	2.08	0.54
1:C:55:ARG:HH21	1:C:63:HIS:CD2	2.24	0.54
1:C:92:LEU:C	1:C:92:LEU:CD1	2.81	0.54
3:E:35:TRP:CH2	3:E:88:CYS:HB3	2.42	0.54
4:F:68:THR:HG23	4:F:69:ILE:H	1.71	0.54
4:F:148:PHE:H	4:F:149:PRO:CD	2.20	0.54
2:B:10:HIS:HD2	2:B:156:HIS:ND1	2.06	0.54
2:D:129:LEU:HD11	2:D:145:LEU:HD22	1.89	0.54
3:E:43:ASN:ND2	3:E:43:ASN:N	2.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:117:VAL:HG11	3:E:211:PRO:HG2	1.89	0.54
3:E:170:GLY:O	3:E:171:GLN:CB	2.55	0.54
4:F:19:LYS:HE3	4:F:81:GLN:HE21	1.72	0.54
3:G:58:ILE:CG2	3:G:59:PRO:HD2	2.37	0.54
3:G:146:VAL:CG1	3:G:196:VAL:CG2	2.71	0.54
1:C:147:ASP:O	1:C:150:ILE:HG12	2.07	0.54
3:E:149:LYS:HA	3:E:154:THR:HA	1.90	0.54
3:E:163:LYS:N	3:E:164:PRO:CD	2.71	0.54
4:F:68:THR:O	4:F:69:ILE:HG13	2.08	0.54
3:G:132:LEU:HD22	3:G:192:VAL:CG1	2.21	0.54
3:G:193:SER:CB	3:G:195:GLN:NE2	2.70	0.54
2:B:105:GLU:HG3	2:B:107:TYR:OH	2.07	0.54
1:C:91:ALA:HB1	1:C:105:VAL:O	2.08	0.54
3:G:55:PRO:HG2	3:G:58:ILE:HG13	1.90	0.54
3:G:117:VAL:HG23	3:G:209:LEU:HD22	1.90	0.54
4:H:128:CYS:O	4:H:129:ASP:C	2.50	0.54
4:H:142:CYS:O	4:H:188:SER:HA	2.07	0.54
2:D:229:SER:CB	2:D:230:PRO:HD2	2.38	0.54
3:G:163:LYS:N	3:G:164:PRO:CD	2.70	0.54
4:H:171:VAL:CG1	4:H:172:HIS:N	2.71	0.54
4:H:212:HIS:N	4:H:217:THR:HB	2.23	0.54
4:F:83:ARG:O	4:F:86:ASP:HB2	2.08	0.54
4:F:157:TRP:HZ3	4:F:225:ILE:HD11	1.73	0.54
4:H:52:LYS:HD2	4:H:56:ALA:HB3	1.90	0.54
4:H:195:SER:CA	4:H:199:TRP:CZ3	2.91	0.54
1:A:48:LYS:O	2:D:97:ARG:NE	2.41	0.53
2:B:50:TYR:OH	2:B:97:ARG:HB2	2.07	0.53
2:B:120:ARG:HA	2:B:225:TRP:CH2	2.43	0.53
3:E:107:ARG:C	3:E:109:PRO:HD2	2.32	0.53
3:E:170:GLY:O	3:E:171:GLN:HB3	2.07	0.53
4:H:121:VAL:HG12	4:H:144:VAL:HG13	1.89	0.53
1:A:19:LYS:C	1:A:20:LEU:HD23	2.33	0.53
1:C:24:TYR:CD2	1:C:32:PHE:HE2	2.26	0.53
4:F:213:PRO:O	4:F:214:ALA:O	2.26	0.53
2:B:15:LYS:CD	2:B:84:LEU:HD21	2.38	0.53
1:C:128:LEU:HD12	1:C:140:LEU:HD12	1.89	0.53
2:D:96:LEU:O	2:D:97:ARG:C	2.51	0.53
3:E:193:SER:OG	3:E:210:SER:HA	2.07	0.53
4:F:119:PRO:HB2	4:F:144:VAL:HG12	1.90	0.53
4:F:126:PRO:C	4:F:128:CYS:N	2.62	0.53
4:F:133:SER:CB	4:F:135:THR:HG23	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:192:VAL:CB	3:G:212:ALA:HB2	2.32	0.53
4:H:18:LEU:HB3	4:H:82:MET:HE3	1.89	0.53
1:A:1:ASP:HB3	1:A:25:GLN:O	2.08	0.53
1:A:143:PHE:HB2	1:A:195:PHE:CE2	2.44	0.53
2:D:167:GLU:HG2	2:D:169:HIS:CE1	2.43	0.53
2:D:219:LEU:O	2:D:233:VAL:HG12	2.08	0.53
3:E:121:SER:OG	3:E:123:GLU:HG2	2.07	0.53
3:E:148:TRP:HA	3:E:193:SER:O	2.07	0.53
3:E:166:LYS:O	3:E:167:GLN:C	2.50	0.53
4:H:17:SER:OG	4:H:82(A):ASN:ND2	2.40	0.53
1:A:92:LEU:HD12	1:A:92:LEU:O	2.07	0.53
2:D:219:LEU:N	2:D:219:LEU:CD1	2.72	0.53
3:E:117:VAL:HG23	3:E:209:LEU:HD11	1.90	0.53
3:G:46:LEU:O	3:G:58:ILE:HD11	2.07	0.53
3:G:164:PRO:HB3	4:H:175:PRO:HG3	1.91	0.53
4:H:2:VAL:HG11	4:H:102:TYR:CG	2.43	0.53
4:H:29:PHE:CZ	4:H:71:ARG:HD2	2.43	0.53
1:A:158:SER:C	1:A:160:THR:H	2.16	0.53
1:C:190:THR:HG22	1:C:193:ASP:OD1	2.09	0.53
3:E:117:VAL:N	3:E:209:LEU:HD21	2.23	0.53
3:G:192:VAL:O	3:G:211:PRO:CD	2.55	0.53
3:E:96:LEU:HB2	4:F:47:TRP:CD2	2.43	0.53
4:F:3:TYR:HB2	4:F:25:SER:OG	2.09	0.53
3:G:206:GLU:C	3:G:208:SER:N	2.67	0.53
4:H:82(A):ASN:O	4:H:82(B):ARG:C	2.52	0.53
4:H:148:PHE:N	4:H:149:PRO:CD	2.62	0.53
1:A:58:HIS:O	1:A:59:GLN:C	2.51	0.53
3:E:104:LEU:HD23	3:E:104:LEU:C	2.33	0.53
4:F:51:ILE:HG23	4:F:51:ILE:O	2.09	0.53
4:F:169:GLY:O	4:F:191:VAL:HA	2.08	0.53
2:B:36:GLN:OE1	2:B:38:THR:CG2	2.57	0.53
1:C:125:VAL:O	1:C:125:VAL:HG23	2.09	0.53
3:E:80:PRO:C	3:E:82:ASP:H	2.16	0.53
3:E:140:TYR:CD1	3:E:141:PRO:HB3	2.43	0.53
3:G:121:SER:CB	3:G:124:GLU:HB2	2.39	0.53
4:H:140:LEU:HD11	4:H:205:ILE:CG2	2.32	0.53
1:C:128:LEU:HD11	2:D:146:VAL:HG21	1.90	0.52
3:E:35:TRP:O	3:E:47:LEU:N	2.39	0.52
3:E:103:GLN:OE1	3:E:103:GLN:HA	2.08	0.52
4:F:6:GLU:OE2	4:F:104:GLY:HA3	2.09	0.52
3:G:2:TYR:N	3:G:2:TYR:HD1	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:71:ARG:HD3	4:H:78:ILE:HG22	1.91	0.52
4:H:108:MET:HB3	4:H:150:GLU:CD	2.34	0.52
1:A:55:ARG:NH1	1:A:57:GLU:CG	2.62	0.52
1:A:64:ALA:HB2	1:A:75:LEU:HA	1.91	0.52
2:B:11:ILE:HD11	2:B:112:THR:CG2	2.36	0.52
2:B:226:PRO:O	2:B:227:GLU:C	2.53	0.52
3:E:89:LEU:HD12	3:E:97:VAL:O	2.10	0.52
3:E:139:PHE:HZ	3:E:175:THR:HG1	1.58	0.52
3:G:61:ARG:HH12	3:G:79:GLN:HB2	1.70	0.52
4:H:29:PHE:CB	4:H:76:ASN:OD1	2.56	0.52
4:H:133:SER:OG	4:H:135:THR:CG2	2.56	0.52
4:H:144:VAL:HG13	4:H:210:VAL:HG11	1.92	0.52
4:H:154:VAL:O	4:H:154:VAL:HG12	2.08	0.52
1:C:12:VAL:O	1:C:115:ILE:N	2.33	0.52
2:D:225:TRP:CE3	2:D:226:PRO:HD2	2.45	0.52
3:E:136:VAL:CG1	3:E:175:THR:O	2.57	0.52
1:A:12:VAL:O	1:A:115:ILE:N	2.39	0.52
1:A:146:PHE:O	1:A:147:ASP:C	2.52	0.52
2:D:36:GLN:HG3	2:D:90:TYR:CE1	2.44	0.52
3:E:16:GLY:O	3:E:77:GLY:HA2	2.10	0.52
4:F:35:TYR:CE2	4:F:50:ARG:HD3	2.44	0.52
4:F:125:ALA:O	4:F:127:ALA:N	2.37	0.52
4:F:203:GLN:CD	4:F:204:PRO:HD2	2.35	0.52
4:H:52:LYS:HD3	4:H:53:ASN:HB3	1.92	0.52
1:A:21:ASN:HD22	5:A:214:NAG:C7	2.23	0.52
3:E:77:GLY:O	3:E:78:ALA:C	2.52	0.52
4:H:29:PHE:CE2	4:H:71:ARG:NH1	2.70	0.52
1:A:171:LYS:CB	2:B:170:SER:OG	2.44	0.52
1:A:206:TYR:HD1	1:A:206:TYR:N	2.08	0.52
2:D:127:VAL:CG2	2:D:237:ILE:HG22	2.39	0.52
3:E:44:ILE:HD13	3:E:44:ILE:N	2.24	0.52
4:F:8:GLY:CA	4:F:20:VAL:HG13	2.40	0.52
4:F:10:ASP:OD1	4:F:12:VAL:HG22	2.09	0.52
4:F:40:ALA:O	4:F:41:PRO:C	2.51	0.52
4:F:212:HIS:CD2	4:F:214:ALA:HB2	2.44	0.52
4:F:215:SER:O	4:F:216:SER:C	2.53	0.52
4:H:199:TRP:CD2	4:H:200:PRO:HD2	2.43	0.52
1:A:38:TYR:O	1:A:39:LEU:C	2.53	0.52
2:B:137:ILE:O	2:B:141:GLN:HA	2.09	0.52
1:C:145:ASP:HB2	2:D:140:LYS:HZ3	1.71	0.52
2:D:15:LYS:C	2:D:17:GLY:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:37:GLN:HB2	3:G:47:LEU:HD11	1.92	0.52
3:G:123:GLU:C	3:G:126:ARG:HB2	2.35	0.52
4:H:199:TRP:C	4:H:202:LYS:N	2.66	0.52
1:C:77:LYS:NZ	1:C:84:ASP:OD1	2.43	0.52
3:E:115:VAL:HG12	3:E:116:THR:N	2.25	0.52
3:E:138:ASP:CA	3:E:172:ASN:HD22	2.17	0.52
4:F:63:VAL:HB	4:F:67:PHE:CD1	2.45	0.52
4:H:121:VAL:HG23	4:H:121:VAL:O	2.10	0.52
1:A:6:THR:HG21	5:A:214:NAG:H81	1.91	0.52
1:A:155:THR:HG21	1:A:160:THR:C	2.31	0.52
1:A:171:LYS:HE3	2:B:170:SER:HB2	1.90	0.52
2:B:113:ARG:CD	2:B:156:HIS:HE1	2.14	0.52
1:C:12:VAL:O	1:C:114:VAL:HA	2.09	0.52
4:F:210:VAL:HB	4:F:219:VAL:CG2	2.40	0.52
4:H:83:ARG:O	4:H:86:ASP:HB2	2.10	0.52
2:D:6:GLN:HB2	2:D:110:PRO:HD2	1.91	0.52
3:E:2:TYR:N	3:E:2:TYR:CD1	2.77	0.52
4:F:178:LEU:HD23	4:F:185:TYR:CE1	2.44	0.52
3:G:159:VAL:O	3:G:160:LYS:HG2	2.10	0.52
4:H:59:TYR:HE1	4:H:69:ILE:HG13	1.75	0.52
4:H:148:PHE:O	4:H:185:TYR:HE2	1.88	0.52
1:A:17:PRO:HA	1:A:77:LYS:O	2.10	0.51
1:A:55:ARG:HE	2:D:97:ARG:HH12	1.50	0.51
1:A:75:LEU:HD12	1:A:75:LEU:C	2.31	0.51
2:D:9:ARG:CZ	2:D:110:PRO:HB3	2.40	0.51
3:E:117:VAL:HG11	3:E:211:PRO:HG3	1.92	0.51
3:E:141:PRO:HD2	3:E:199:GLU:HG2	1.92	0.51
4:F:97:ARG:HB3	4:F:98:PHE:CD1	2.44	0.51
4:F:124:LEU:HD21	4:F:142:CYS:CA	2.40	0.51
3:G:207:LYS:O	3:G:209:LEU:N	2.43	0.51
4:H:28:THR:C	4:H:30:SER:N	2.66	0.51
1:A:77:LYS:HG2	1:A:79:SER:O	2.10	0.51
3:E:107:ARG:HB2	3:E:109:PRO:HD2	1.92	0.51
4:F:55:TYR:OH	4:F:73:ASP:OD2	2.20	0.51
4:F:140:LEU:O	4:F:191:VAL:HG12	2.10	0.51
1:A:206:TYR:N	1:A:206:TYR:CD1	2.75	0.51
2:B:45:PHE:HZ	2:B:48:GLN:CB	2.23	0.51
2:D:6:GLN:OE1	2:D:92:CYS:N	2.44	0.51
2:D:229:SER:HA	4:H:33:TRP:CH2	2.45	0.51
3:G:80:PRO:C	3:G:82:ASP:N	2.68	0.51
4:H:215:SER:O	4:H:217:THR:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:C	1:A:65:THR:HG23	2.35	0.51
2:D:67:VAL:HG12	2:D:77:MET:HA	1.92	0.51
4:F:133:SER:C	4:F:135:THR:N	2.59	0.51
3:G:146:VAL:CG2	3:G:177:SER:HB2	2.40	0.51
4:H:156:SER:OG	4:H:157:TRP:N	2.42	0.51
1:C:125:VAL:HA	1:C:142:LEU:O	2.10	0.51
3:E:2:TYR:N	3:E:2:TYR:HD1	2.09	0.51
3:E:107:ARG:HB2	3:E:140:TYR:HE2	1.75	0.51
4:F:38:ARG:HD2	4:F:90:TYR:CZ	2.46	0.51
4:F:121:VAL:HG23	4:F:221:LYS:HE3	1.93	0.51
3:G:204:THR:O	3:G:205:VAL:O	2.29	0.51
1:A:19:LYS:HA	1:A:75:LEU:O	2.11	0.51
1:A:55:ARG:HH21	2:D:97:ARG:HH12	1.58	0.51
2:B:36:GLN:HG3	2:B:90:TYR:HE1	1.64	0.51
2:D:65:PHE:N	2:D:65:PHE:CD1	2.77	0.51
1:A:164:ASP:N	2:B:179:TYR:OH	2.41	0.51
1:C:157:GLU:OE2	1:C:189:PHE:CE2	2.64	0.51
2:D:119:LEU:C	2:D:121:ASN:N	2.68	0.51
3:G:204:THR:O	3:G:205:VAL:C	2.53	0.51
1:A:22:CYS:H	1:A:74:HIS:HD2	1.56	0.51
2:B:22:THR:CG2	2:B:23:CYS:N	2.74	0.51
4:F:38:ARG:HD2	4:F:90:TYR:CE2	2.46	0.51
3:G:203:GLU:HB2	3:G:205:VAL:CG2	2.37	0.51
4:H:199:TRP:CB	4:H:205:ILE:HG13	2.40	0.51
2:D:153:PHE:O	2:D:154:PRO:C	2.54	0.51
3:E:43:ASN:H	3:E:43:ASN:HD22	1.56	0.51
4:H:35:TYR:N	4:H:35:TYR:HD1	2.09	0.51
4:H:82:MET:HE1	4:H:109:VAL:HG21	1.92	0.51
4:H:212:HIS:HB3	4:H:217:THR:HB	1.92	0.51
2:B:158:GLU:OE2	2:B:217:HIS:CE1	2.59	0.51
2:D:9:ARG:HD2	2:D:110:PRO:HB2	1.92	0.51
3:E:21:ILE:O	3:E:72:THR:HG23	2.11	0.51
3:G:19:VAL:HG22	3:G:20:LYS:N	2.26	0.51
3:G:203:GLU:C	3:G:205:VAL:N	2.62	0.51
4:H:32:PHE:CE1	4:H:96:GLY:CA	2.92	0.51
1:A:144:THR:CG2	1:A:145:ASP:OD1	2.56	0.50
1:C:77:LYS:NZ	1:C:84:ASP:CG	2.69	0.50
3:E:108:GLY:O	3:E:110:LYS:N	2.44	0.50
4:H:137:THR:HG22	4:H:193:VAL:O	2.11	0.50
4:H:172:HIS:O	4:H:174:PHE:CE1	2.64	0.50
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PRO:C	1:A:154:LYS:HG2	2.37	0.50
2:B:12:ILE:C	2:B:13:LYS:HG2	2.36	0.50
2:B:45:PHE:HZ	2:B:48:GLN:HB3	1.76	0.50
1:C:52:ASP:OD1	1:C:67:HIS:HA	2.11	0.50
2:D:113:ARG:HD2	2:D:156:HIS:NE2	2.26	0.50
3:E:142:GLY:HA3	3:E:199:GLU:HB3	1.93	0.50
4:F:174:PHE:C	4:F:187:LEU:HD11	2.37	0.50
4:F:210:VAL:HB	4:F:219:VAL:HG23	1.92	0.50
2:B:15:LYS:HD2	2:B:84:LEU:HD21	1.93	0.50
2:B:118:ASP:OD2	5:B:249:NAG:C8	2.60	0.50
1:C:170:MET:O	1:C:171:LYS:C	2.53	0.50
3:E:28:LEU:N	3:E:29:PRO:CD	2.73	0.50
4:F:63:VAL:HG12	4:F:66:ARG:NH2	2.27	0.50
4:F:139:THR:CG2	4:F:192:THR:OG1	2.55	0.50
4:H:115:THR:CG2	4:H:116:THR:N	2.75	0.50
4:H:138:VAL:O	4:H:192:THR:HA	2.12	0.50
1:A:17:PRO:HA	1:A:78:SER:O	2.11	0.50
1:A:165:LYS:HA	1:A:179:GLY:O	2.11	0.50
2:D:70:PHE:CD1	2:D:74:HIS:ND1	2.78	0.50
3:G:193:SER:HA	3:G:211:PRO:CD	2.36	0.50
4:H:101:ASP:OD1	4:H:102:TYR:HD1	1.94	0.50
4:H:121:VAL:O	4:H:121:VAL:CG2	2.58	0.50
4:F:77:SER:O	4:F:78:ILE:CG2	2.59	0.50
3:G:120:PRO:HB2	3:G:125:LEU:HD21	1.93	0.50
2:B:226:PRO:O	2:B:228:GLY:N	2.44	0.50
3:E:141:PRO:CG	3:E:142:GLY:H	2.25	0.50
4:H:52(A):ASN:CA	4:H:71:ARG:HH21	2.25	0.50
1:A:22:CYS:O	1:A:74:HIS:CD2	2.65	0.50
2:B:205:ASN:OD1	2:B:207:ARG:N	2.44	0.50
2:D:52:LYS:H	2:D:69:GLN:HE22	1.58	0.50
2:D:119:LEU:C	2:D:121:ASN:H	2.19	0.50
3:E:148:TRP:CE3	3:E:179:LEU:HB2	2.47	0.50
3:G:28:LEU:HD12	3:G:69:THR:C	2.37	0.50
3:G:86:TYR:CE2	3:G:104:LEU:HD22	2.46	0.50
3:G:142:GLY:CA	3:G:199:GLU:HB3	2.39	0.50
1:C:157:GLU:OE2	1:C:186:GLN:NE2	2.45	0.50
3:E:115:VAL:HG11	3:E:209:LEU:HB2	1.94	0.50
3:E:198:HIS:HB3	3:E:205:VAL:CG2	2.27	0.50
4:F:147:TYR:O	4:F:185:TYR:N	2.45	0.50
2:B:9:ARG:CZ	2:B:110:PRO:CB	2.90	0.50
2:B:225:TRP:HD1	2:B:229:SER:O	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:8:GLY:HA3	4:F:20:VAL:HG13	1.94	0.50
4:F:84:VAL:O	4:F:86:ASP:N	2.45	0.50
3:G:167:GLN:HB3	3:G:172:ASN:HB3	1.93	0.50
4:H:38:ARG:HD2	4:H:90:TYR:CZ	2.46	0.50
4:H:219:VAL:CG2	4:H:220:ASP:N	2.74	0.50
2:D:47:ILE:CG2	2:D:60:LEU:HD22	2.42	0.49
2:D:229:SER:OG	2:D:230:PRO:CD	2.57	0.49
3:E:136:VAL:HB	3:E:196:VAL:HG21	1.92	0.49
4:F:38:ARG:HB3	4:F:90:TYR:CE2	2.47	0.49
4:F:68:THR:C	4:F:69:ILE:HG13	2.37	0.49
4:F:121:VAL:HA	4:F:143:LEU:O	2.11	0.49
3:G:209:LEU:O	3:G:210:SER:C	2.54	0.49
4:H:2:VAL:CG1	4:H:102:TYR:CG	2.95	0.49
2:B:159:LEU:HD13	2:B:194:SER:HB3	1.93	0.49
1:C:87:LEU:HD13	1:C:89:TYR:CE2	2.48	0.49
2:D:48:GLN:NE2	2:D:98:TRP:CZ2	2.80	0.49
3:E:136:VAL:HG22	3:E:136:VAL:O	2.12	0.49
3:E:162:THR:C	3:E:164:PRO:HD2	2.37	0.49
4:F:18:LEU:CD1	4:F:109:VAL:HG22	2.41	0.49
4:H:134:THR:C	4:H:136:ASP:N	2.68	0.49
1:A:138:SER:HB2	2:B:130:PHE:HE2	1.76	0.49
3:E:162:THR:O	3:E:175:THR:CG2	2.53	0.49
3:G:48:ILE:CD1	3:G:63:SER:C	2.85	0.49
3:G:61:ARG:HH12	3:G:79:GLN:CB	2.25	0.49
4:H:55:TYR:O	4:H:56:ALA:C	2.56	0.49
1:A:168:LEU:HD13	2:B:171:GLY:HA2	1.93	0.49
2:B:219:LEU:CD1	2:B:219:LEU:N	2.75	0.49
1:C:161:PHE:C	1:C:162:ILE:HD12	2.37	0.49
2:D:226:PRO:HG3	3:G:50:MET:CE	2.42	0.49
4:F:18:LEU:HB3	4:F:82:MET:HE3	1.93	0.49
4:F:66:ARG:HB3	4:F:82(B):ARG:HD3	1.94	0.49
4:H:150:GLU:HB3	4:H:151:PRO:HD2	1.95	0.49
4:H:199:TRP:O	4:H:200:PRO:C	2.55	0.49
1:A:147:ASP:O	1:A:150:ILE:HG12	2.12	0.49
2:B:79:MET:HE3	2:B:82:LEU:CD2	2.42	0.49
2:B:202:PHE:CD1	2:B:208:ASN:ND2	2.80	0.49
2:D:44:LYS:HG3	2:D:59:PHE:HD2	1.77	0.49
4:F:57:THR:HG22	4:F:58:GLU:H	1.77	0.49
4:F:79:TYR:N	4:F:79:TYR:HD1	2.08	0.49
4:F:149:PRO:O	4:F:150:GLU:O	2.31	0.49
2:B:125:PRO:HG2	2:B:237:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:228:ARG:HG2	4:F:228:ARG:O	2.12	0.49
3:G:143:SER:HB3	3:G:163:LYS:CG	2.36	0.49
4:H:35:TYR:OH	4:H:95:ALA:HB3	2.12	0.49
4:H:141:GLY:HA2	4:H:157:TRP:CH2	2.48	0.49
1:C:186:GLN:C	1:C:188:SER:N	2.69	0.49
2:D:119:LEU:O	2:D:122:VAL:HG23	2.13	0.49
3:E:83:GLU:HB2	3:E:106:VAL:HG23	1.94	0.49
4:F:222:LYS:HE2	4:F:226:GLU:HG2	1.94	0.49
4:H:172:HIS:HB2	4:H:190:SER:HB3	1.94	0.49
1:A:203:ASN:ND2	5:A:216:NAG:C7	2.76	0.49
2:D:133:SER:O	2:D:137:ILE:HD13	2.12	0.49
3:G:83:GLU:CB	3:G:106:VAL:HG23	2.23	0.49
4:H:68:THR:HG23	4:H:69:ILE:N	2.27	0.49
2:D:53:VAL:HG22	2:D:69:GLN:H	1.77	0.49
4:F:11:LEU:HB2	4:F:110:THR:HB	1.94	0.49
3:G:181:LEU:CD2	3:G:185:GLN:HB3	2.41	0.49
1:A:28:TYR:HB2	1:A:94:GLU:HG3	1.94	0.49
1:A:190:THR:HG22	1:A:192:GLN:HB3	1.94	0.49
2:D:131:GLU:HA	2:D:145:LEU:HD23	1.94	0.49
3:E:25:GLY:O	3:E:69:THR:HB	2.13	0.49
3:E:48:ILE:CD1	3:E:64:GLY:HA3	2.42	0.49
3:E:148:TRP:CZ3	3:E:179:LEU:CB	2.96	0.49
4:F:52(A):ASN:ND2	4:F:52(A):ASN:N	2.58	0.49
4:F:84:VAL:HA	4:F:111:VAL:O	2.13	0.49
4:F:115:THR:HG23	4:F:116:THR:N	2.28	0.49
3:G:207:LYS:O	3:G:208:SER:C	2.55	0.49
2:B:224:LYS:O	3:E:32:PHE:CE2	2.66	0.48
2:D:51:GLU:O	2:D:52:LYS:CB	2.60	0.48
3:E:203:GLU:O	3:E:205:VAL:N	2.46	0.48
3:G:106(A):LEU:HA	3:G:140:TYR:OH	2.13	0.48
3:G:136:VAL:HG13	3:G:175:THR:HB	1.93	0.48
2:D:159:LEU:HD23	2:D:159:LEU:C	2.37	0.48
3:E:146:VAL:HG11	3:E:177:SER:CB	2.43	0.48
4:H:2:VAL:HG12	4:H:102:TYR:CD2	2.48	0.48
2:B:83:GLU:C	2:B:116:VAL:HG21	2.37	0.48
1:C:146:PHE:HB2	1:C:150:ILE:CD1	2.44	0.48
2:D:220:SER:O	2:D:221:GLU:C	2.57	0.48
3:E:67:SER:O	3:E:68:GLY:C	2.56	0.48
4:F:174:PHE:HB3	4:F:175:PRO:HD2	1.93	0.48
3:G:140:TYR:CD1	3:G:141:PRO:HA	2.48	0.48
1:A:11:THR:HG22	1:A:115:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:VAL:HG12	1:C:143:PHE:CD1	2.49	0.48
1:C:165:LYS:HA	1:C:179:GLY:O	2.13	0.48
3:E:39:LYS:C	3:E:41:ASP:N	2.70	0.48
4:F:35:TYR:HE1	4:F:95:ALA:HB3	1.76	0.48
3:G:126:ARG:C	3:G:128:ASN:H	2.22	0.48
3:G:193:SER:OG	3:G:195:GLN:NE2	2.46	0.48
1:C:189:PHE:HB3	1:C:194:ILE:CD1	2.43	0.48
3:G:2:TYR:CE2	3:G:26:ASP:HB3	2.49	0.48
1:A:46:LEU:O	1:A:57:GLU:HB2	2.13	0.48
1:A:155:THR:CG2	1:A:160:THR:C	2.86	0.48
1:A:177:SER:O	2:B:195:ARG:NH2	2.41	0.48
1:A:194:ILE:HG22	1:A:195:PHE:N	2.27	0.48
2:B:174:THR:HA	2:B:194:SER:HB2	1.96	0.48
2:D:121:ASN:HA	4:H:97:ARG:HH21	1.77	0.48
4:H:219:VAL:HG22	4:H:220:ASP:N	2.28	0.48
1:A:129:LYS:HE2	1:A:210:ASP:OD2	2.13	0.48
1:C:39:LEU:HD22	1:C:40:ASN:N	2.28	0.48
2:D:125:PRO:HB3	2:D:152:PHE:HB3	1.96	0.48
3:E:33:ALA:N	3:E:51:ASP:OD1	2.47	0.48
3:E:117:VAL:CG2	3:E:209:LEU:HD11	2.43	0.48
4:H:26:GLY:O	4:H:27:PHE:HB3	2.13	0.48
4:H:52(A):ASN:CA	4:H:71:ARG:NH2	2.77	0.48
1:A:146:PHE:C	1:A:150:ILE:HD11	2.39	0.48
2:D:44:LYS:HG3	2:D:59:PHE:CD2	2.48	0.48
3:E:144:ALA:HB2	3:E:198:HIS:HA	1.95	0.48
1:A:190:THR:HG23	1:A:191:CYS:N	2.28	0.48
2:B:135:ALA:O	2:B:136:GLU:C	2.57	0.48
2:D:149:ALA:HB2	2:D:214:VAL:HG21	1.95	0.48
3:E:120:PRO:HB3	3:E:130:ALA:HA	1.96	0.48
3:G:141:PRO:HG2	3:G:142:GLY:H	1.79	0.48
4:H:117:THR:CB	4:H:184:LEU:HD21	2.44	0.48
2:B:97:ARG:NH2	1:C:56:THR:CG2	2.64	0.48
2:D:169:HIS:O	2:D:172:VAL:HG22	2.14	0.48
3:E:35:TRP:C	3:E:47:LEU:HD12	2.39	0.48
3:E:86:TYR:O	3:E:101:GLY:HA2	2.14	0.48
3:E:132:LEU:HB2	3:E:179:LEU:HB3	1.96	0.48
4:F:20:VAL:HG23	4:F:82:MET:HE2	1.96	0.48
4:F:82(A):ASN:C	4:F:82(B):ARG:HG3	2.39	0.48
2:B:9:ARG:CD	2:B:110:PRO:HB2	2.44	0.47
1:C:128:LEU:CD1	2:D:146:VAL:HG21	2.44	0.47
1:C:158:SER:C	1:C:160:THR:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:PHE:CE1	2:D:74:HIS:HE1	2.22	0.47
2:D:137:ILE:O	2:D:141:GLN:HA	2.14	0.47
3:E:89:LEU:CD1	3:E:90:SER:N	2.69	0.47
4:F:84:VAL:C	4:F:86:ASP:N	2.72	0.47
4:F:184:LEU:HD23	4:F:184:LEU:HA	1.73	0.47
3:G:138:ASP:HA	3:G:172:ASN:ND2	2.29	0.47
4:H:40:ALA:CB	4:H:43:LYS:HD3	2.44	0.47
4:H:84:VAL:C	4:H:86:ASP:N	2.72	0.47
2:B:46:LEU:CD1	2:B:77:MET:HE1	2.44	0.47
2:B:79:MET:CE	2:B:114:LEU:HD22	2.44	0.47
2:B:225:TRP:CD1	2:B:229:SER:O	2.67	0.47
1:C:144:THR:CG2	1:C:145:ASP:N	2.72	0.47
2:D:78:ASN:ND2	5:D:248:NAG:C7	2.77	0.47
3:E:166:LYS:HG2	3:E:167:GLN:H	1.79	0.47
3:G:15:VAL:HG23	3:G:106(A):LEU:O	2.13	0.47
3:G:48:ILE:HD13	3:G:64:GLY:CA	2.44	0.47
4:H:51:ILE:O	4:H:51:ILE:CG2	2.60	0.47
4:H:212:HIS:HD1	4:H:215:SER:H	1.61	0.47
2:B:67:VAL:CG1	2:B:77:MET:HA	2.40	0.47
2:B:226:PRO:HB2	4:F:100:HIS:CE1	2.48	0.47
5:B:251:NAG:O7	5:B:251:NAG:O3	2.28	0.47
2:D:74:HIS:CE1	2:D:76:GLU:CG	2.97	0.47
3:E:136:VAL:CG2	3:E:139:PHE:CE1	2.90	0.47
3:E:203:GLU:C	3:E:205:VAL:N	2.57	0.47
4:F:35:TYR:CE1	4:F:95:ALA:HB3	2.49	0.47
4:F:162:ASN:HB3	4:F:165:ALA:HB3	1.97	0.47
3:G:37:GLN:NE2	3:G:45:LEU:HD23	2.29	0.47
3:G:48:ILE:CG2	3:G:49:TYR:N	2.77	0.47
4:H:131:THR:O	4:H:132:THR:CG2	2.58	0.47
1:A:3:VAL:HG12	1:A:105:VAL:CG1	2.44	0.47
2:B:122:VAL:HA	2:B:153:PHE:O	2.14	0.47
1:C:6:THR:CA	5:C:214:NAG:H83	2.42	0.47
1:C:54:LYS:C	1:C:56:THR:N	2.72	0.47
1:C:126:TYR:CE2	1:C:207:PRO:HG2	2.49	0.47
1:C:168:LEU:HD13	2:D:171:GLY:HA2	1.97	0.47
3:E:213:GLU:HG3	3:E:213:GLU:O	2.14	0.47
4:F:54:ASN:CG	4:F:54:ASN:O	2.56	0.47
4:F:63:VAL:HB	4:F:67:PHE:CG	2.50	0.47
3:G:215:LEU:HD23	3:G:215:LEU:N	2.29	0.47
4:H:6:GLU:OE2	4:H:91:TYR:HA	2.14	0.47
4:H:52(A):ASN:HB3	4:H:71:ARG:NH2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:148:PHE:HA	4:H:185:TYR:CD2	2.49	0.47
1:A:47:LEU:C	1:A:47:LEU:HD12	2.38	0.47
1:A:190:THR:HG23	1:A:192:GLN:H	1.78	0.47
2:B:182:SER:HB3	2:B:189:SER:HB3	1.96	0.47
2:D:21:LEU:HG	2:D:112:THR:HG21	1.97	0.47
2:D:130:PHE:N	2:D:130:PHE:CD1	2.83	0.47
4:F:22:CYS:HB3	4:F:78:ILE:CG1	2.44	0.47
4:F:35:TYR:CD2	4:F:50:ARG:HB2	2.50	0.47
3:G:14:THR:O	3:G:15:VAL:C	2.57	0.47
4:H:40:ALA:HB3	4:H:43:LYS:HD3	1.96	0.47
4:H:52(A):ASN:HB3	4:H:71:ARG:HH22	1.80	0.47
2:B:125:PRO:CD	2:B:237:ILE:HD12	2.44	0.47
1:C:160:THR:HG22	1:C:161:PHE:N	2.30	0.47
3:E:39:LYS:O	3:E:41:ASP:N	2.47	0.47
3:E:146:VAL:HG13	3:E:194:CYS:SG	2.55	0.47
4:F:2:VAL:HG13	4:F:27:PHE:CE1	2.50	0.47
4:F:22:CYS:O	4:F:77:SER:HB2	2.14	0.47
4:F:77:SER:C	4:F:78:ILE:CG2	2.88	0.47
3:G:175:THR:HG23	3:G:176:SER:N	2.30	0.47
1:A:47:LEU:HA	2:D:97:ARG:HH21	1.80	0.47
1:A:61:GLY:CA	1:A:77:LYS:HE3	2.34	0.47
1:A:123:PRO:O	1:A:204:ALA:HB1	2.14	0.47
2:B:49:HIS:HE1	2:B:55:ARG:HH21	1.60	0.47
2:B:130:PHE:CD1	2:B:130:PHE:N	2.81	0.47
1:C:171:LYS:O	1:C:172:ALA:C	2.57	0.47
2:D:148:LEU:HG	2:D:150:ARG:HG3	1.96	0.47
3:E:36:PHE:C	3:E:47:LEU:CD1	2.88	0.47
3:E:118:PHE:HZ	4:F:140:LEU:HA	1.80	0.47
3:E:200:GLY:C	3:E:203:GLU:HG2	2.37	0.47
4:F:6:GLU:CD	4:F:104:GLY:HA3	2.39	0.47
4:F:148:PHE:HD1	4:F:149:PRO:HD3	1.80	0.47
3:G:28:LEU:N	3:G:29:PRO:CD	2.76	0.47
3:G:39:LYS:C	3:G:41:ASP:N	2.72	0.47
3:G:142:GLY:HA3	3:G:199:GLU:CG	2.44	0.47
4:H:2:VAL:CG1	4:H:102:TYR:CD2	2.98	0.47
4:H:6:GLU:HB2	4:H:106:GLY:O	2.15	0.47
4:H:19:LYS:HB2	4:H:81:GLN:NE2	2.30	0.47
4:H:40:ALA:O	4:H:41:PRO:C	2.58	0.47
4:H:68:THR:CG2	4:H:69:ILE:N	2.71	0.47
4:H:199:TRP:O	4:H:202:LYS:N	2.47	0.47
1:A:3:VAL:HG22	1:A:3:VAL:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLN:HE21	1:C:44:GLN:HB2	1.56	0.47
1:C:205:THR:HG22	1:C:207:PRO:HD3	1.96	0.47
2:D:160:SER:N	2:D:213:GLN:O	2.42	0.47
4:F:140:LEU:HD12	4:F:225:ILE:HD13	1.93	0.47
3:G:50:MET:O	3:G:52:ASN:N	2.47	0.47
4:H:139:THR:HG23	4:H:192:THR:OG1	2.14	0.47
2:B:8:PRO:HG2	2:B:11:ILE:HG12	1.97	0.47
2:B:29:HIS:CG	2:B:95:SER:C	2.93	0.47
2:B:207:ARG:HD3	2:B:207:ARG:HA	1.51	0.47
1:C:46:LEU:HD22	1:C:88:TYR:HE2	1.80	0.47
3:E:83:GLU:HA	3:E:104:LEU:CD2	2.45	0.47
3:E:142:GLY:HA3	3:E:199:GLU:CB	2.45	0.47
3:E:209:LEU:O	3:E:211:PRO:CD	2.35	0.47
4:F:87:THR:HA	4:F:109:VAL:O	2.14	0.47
3:G:153:ALA:O	3:G:154:THR:C	2.58	0.47
1:A:63:HIS:ND1	1:A:63:HIS:C	2.73	0.47
1:A:212:PRO:O	1:A:213:CYS:C	2.58	0.47
2:B:39:LEU:O	2:B:41:LYS:N	2.47	0.47
2:D:29:HIS:HB3	2:D:95:SER:O	2.15	0.47
2:D:118:ASP:CG	2:D:120:ARG:HD3	2.39	0.47
2:B:219:LEU:N	2:B:219:LEU:HD12	2.31	0.46
1:C:3:VAL:HA	1:C:24:TYR:HA	1.97	0.46
1:C:90:CYS:O	1:C:107:GLY:N	2.47	0.46
2:D:233:VAL:O	2:D:234:THR:C	2.57	0.46
4:F:148:PHE:CD1	4:F:149:PRO:N	2.83	0.46
4:H:226:GLU:HG3	4:H:227:PRO:HD2	1.97	0.46
1:A:62:PHE:HB3	1:A:75:LEU:HD11	1.96	0.46
3:E:206:GLU:C	3:E:208:SER:N	2.71	0.46
4:H:11:LEU:HA	4:H:110:THR:O	2.15	0.46
4:H:33:TRP:CZ3	4:H:52:LYS:HE2	2.50	0.46
4:H:52(B):ILE:N	4:H:52(C):PRO:CD	2.79	0.46
2:B:161:TRP:NE1	2:B:194:SER:OG	2.44	0.46
1:C:17:PRO:CA	1:C:78:SER:O	2.63	0.46
2:D:156:HIS:HB3	2:D:217:HIS:HB2	1.98	0.46
2:D:207:ARG:HD3	2:D:207:ARG:HA	1.53	0.46
2:D:214:VAL:O	2:D:214:VAL:HG12	2.16	0.46
2:D:219:LEU:O	2:D:233:VAL:CG1	2.63	0.46
3:E:186:TRP:O	3:E:189:HIS:HB2	2.15	0.46
4:F:52(B):ILE:HG23	4:F:55:TYR:CE2	2.49	0.46
2:B:50:TYR:OH	2:B:97:ARG:HB3	2.08	0.46
2:B:68:GLN:HE21	2:B:68:GLN:N	2.10	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:MET:HE1	2:B:114:LEU:HD22	1.97	0.46
2:B:84:LEU:H	2:B:84:LEU:HG	1.48	0.46
1:C:64:ALA:HB1	1:C:74:HIS:O	2.15	0.46
2:D:29:HIS:HA	2:D:96:LEU:HD13	1.97	0.46
2:D:155:ASP:OD1	2:D:155:ASP:N	2.49	0.46
3:E:154:THR:CG2	3:E:155:ILE:N	2.78	0.46
4:F:52:LYS:O	4:F:55:TYR:HA	2.16	0.46
1:A:36:VAL:HG11	1:A:46:LEU:HD13	1.98	0.46
2:D:15:LYS:HD3	2:D:117:GLU:HA	1.97	0.46
3:E:36:PHE:HA	3:E:45:LEU:O	2.15	0.46
4:F:172:HIS:O	4:F:174:PHE:CE1	2.68	0.46
1:A:115:ILE:HG13	1:A:115:ILE:H	1.50	0.46
2:D:218:GLY:H	2:D:234:THR:CG2	2.28	0.46
4:F:69:ILE:HA	4:F:79:TYR:O	2.16	0.46
3:G:107:ARG:CB	3:G:109:PRO:HD2	2.45	0.46
4:H:119:PRO:CB	4:H:147:TYR:HB3	2.36	0.46
4:H:150:GLU:HB3	4:H:151:PRO:CD	2.45	0.46
4:H:195:SER:HA	4:H:199:TRP:CH2	2.50	0.46
2:B:12:ILE:HG12	2:B:154:PRO:HG3	1.98	0.46
2:B:64:ARG:H	2:B:64:ARG:HG2	1.34	0.46
2:B:67:VAL:HB	2:B:76:GLU:O	2.15	0.46
2:B:156:HIS:CB	2:B:217:HIS:HB2	2.46	0.46
1:C:28:TYR:HB2	1:C:94:GLU:HG3	1.97	0.46
1:C:101:ASN:O	1:C:102:TYR:HB2	2.16	0.46
2:D:223:ASP:CG	2:D:223:ASP:O	2.58	0.46
3:E:51:ASP:HB3	3:E:66:THR:HG21	1.98	0.46
3:E:148:TRP:O	3:E:154:THR:HG23	2.15	0.46
4:F:212:HIS:CD2	4:F:214:ALA:CB	2.99	0.46
3:G:198:HIS:HB3	3:G:205:VAL:CG2	2.31	0.46
1:A:144:THR:HA	1:A:178:ASN:O	2.16	0.46
2:B:79:MET:HB3	2:B:82:LEU:HD21	1.97	0.46
2:B:217:HIS:HA	2:B:234:THR:CG2	2.19	0.46
1:C:5:GLN:HA	1:C:21:ASN:O	2.16	0.46
3:E:124:GLU:O	3:E:127:THR:OG1	2.27	0.46
4:F:57:THR:CG2	4:F:59:TYR:CZ	2.98	0.46
3:G:113:PRO:HD2	3:G:207:LYS:HZ3	1.79	0.46
4:H:36:TRP:C	4:H:37:VAL:CG2	2.89	0.46
1:A:61:GLY:O	1:A:77:LYS:HG3	2.16	0.46
1:A:138:SER:HB2	2:B:130:PHE:CE2	2.51	0.46
1:A:153:PRO:HD3	1:A:198:THR:HG23	1.96	0.46
1:C:144:THR:HG23	2:D:195:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:221:GLU:O	2:D:223:ASP:N	2.45	0.46
3:E:133:VAL:HG21	4:F:143:LEU:HD22	1.97	0.46
4:F:36:TRP:CD1	4:F:78:ILE:HD12	2.51	0.46
1:A:87:LEU:CD1	2:B:41:LYS:HD3	2.45	0.46
2:B:6:GLN:HB2	2:B:110:PRO:HG2	1.98	0.46
2:B:125:PRO:HA	2:B:152:PHE:HB3	1.97	0.46
2:B:172:VAL:HG12	2:B:196:LEU:CD1	2.46	0.46
1:C:87:LEU:HD13	1:C:89:TYR:CZ	2.50	0.46
1:C:155:THR:HG21	1:C:160:THR:C	2.40	0.46
2:D:12:ILE:O	2:D:13:LYS:HG2	2.16	0.46
2:D:96:LEU:C	2:D:97:ARG:O	2.59	0.46
3:E:2:TYR:N	3:E:92:TYR:CE2	2.84	0.46
4:F:107:THR:O	4:F:107:THR:HG23	2.15	0.46
3:G:13:VAL:HG11	3:G:78:ALA:CB	2.46	0.46
3:E:148:TRP:C	3:E:155:ILE:HD12	2.40	0.45
4:F:29:PHE:HZ	4:F:77:SER:O	2.00	0.45
4:F:212:HIS:CD2	4:F:214:ALA:N	2.64	0.45
3:G:153:ALA:O	3:G:154:THR:O	2.34	0.45
2:B:38:THR:HG22	2:B:88:ALA:CB	2.40	0.45
1:C:2:SER:O	1:C:25:GLN:N	2.48	0.45
1:C:32:PHE:N	1:C:32:PHE:CD1	2.84	0.45
1:C:144:THR:HA	1:C:178:ASN:O	2.17	0.45
2:D:11:ILE:HD11	2:D:112:THR:CG2	2.44	0.45
3:E:27:GLN:C	3:E:29:PRO:HD2	2.40	0.45
3:G:123:GLU:CA	3:G:126:ARG:HB2	2.46	0.45
3:G:167:GLN:O	3:G:170:GLY:O	2.33	0.45
4:H:63:VAL:HG11	4:H:67:PHE:CD2	2.51	0.45
2:D:59:PHE:CD1	2:D:59:PHE:N	2.83	0.45
3:E:121:SER:O	3:E:125:LEU:HG	2.16	0.45
3:G:183:ALA:HB1	3:G:187:LYS:HZ3	1.77	0.45
3:G:192:VAL:H	3:G:212:ALA:CB	2.29	0.45
4:H:28:THR:O	4:H:30:SER:N	2.49	0.45
1:A:66:LEU:HG	1:A:67:HIS:N	2.32	0.45
2:B:105:GLU:HB3	2:B:107:TYR:CE2	2.51	0.45
1:C:155:THR:OG1	1:C:161:PHE:HA	2.17	0.45
2:D:70:PHE:CD2	2:D:74:HIS:ND1	2.84	0.45
2:D:125:PRO:CA	2:D:152:PHE:HB3	2.47	0.45
1:A:128:LEU:HB3	2:B:131:GLU:O	2.16	0.45
1:C:122:GLU:O	2:D:140:LYS:NZ	2.48	0.45
1:C:197:GLU:OE1	1:C:197:GLU:CA	2.63	0.45
2:D:220:SER:HB3	2:D:221:GLU:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:115:VAL:HG11	3:E:209:LEU:CB	2.46	0.45
4:F:4:LEU:O	4:F:104:GLY:HA2	2.15	0.45
3:G:154:THR:HG22	3:G:155:ILE:N	2.31	0.45
4:H:2:VAL:HB	4:H:102:TYR:CZ	2.51	0.45
1:A:5:GLN:HE21	1:A:107:GLY:CA	2.28	0.45
2:D:223:ASP:HB3	2:D:231:LYS:HE3	1.93	0.45
3:E:144:ALA:CB	3:E:196:VAL:CG1	2.94	0.45
3:E:149:LYS:C	3:E:155:ILE:HD11	2.42	0.45
4:F:19:LYS:HG3	4:F:81:GLN:HG2	1.98	0.45
4:F:147:TYR:HB2	4:F:212:HIS:HE1	1.80	0.45
4:F:164:GLY:O	4:F:165:ALA:C	2.60	0.45
4:H:81:GLN:OE1	4:H:81:GLN:HA	2.17	0.45
4:H:190:SER:C	4:H:191:VAL:HG23	2.41	0.45
1:A:36:VAL:HG23	1:A:88:TYR:CE2	2.51	0.45
2:B:47:ILE:CD1	2:B:55:ARG:NH1	2.80	0.45
2:B:225:TRP:HA	2:B:225:TRP:CE3	2.52	0.45
1:C:145:ASP:CB	2:D:140:LYS:NZ	2.75	0.45
2:D:153:PHE:O	2:D:155:ASP:N	2.50	0.45
3:E:36:PHE:C	3:E:47:LEU:HD11	2.41	0.45
3:G:39:LYS:O	3:G:40:SER:C	2.60	0.45
3:G:164:PRO:HG3	4:H:175:PRO:CG	2.46	0.45
4:H:199:TRP:O	4:H:203:GLN:O	2.34	0.45
2:B:5:VAL:CG2	2:B:24:ILE:HB	2.43	0.45
3:E:48:ILE:HG23	3:E:49:TYR:N	2.31	0.45
4:F:32:PHE:HD1	4:F:95:ALA:C	2.24	0.45
4:F:125:ALA:C	4:F:127:ALA:N	2.73	0.45
4:H:20:VAL:HG23	4:H:82:MET:HE2	1.99	0.45
4:H:119:PRO:HG3	4:H:212:HIS:HB2	1.99	0.45
1:A:22:CYS:N	1:A:74:HIS:CD2	2.80	0.45
1:A:55:ARG:NH2	2:D:97:ARG:NH2	2.47	0.45
3:E:115:VAL:HG23	3:E:207:LYS:CG	2.47	0.45
3:E:137:ASN:ND2	3:E:138:ASP:H	2.15	0.45
3:G:29:PRO:HD3	3:G:69:THR:HA	1.98	0.45
3:G:125:LEU:CD2	3:G:186:TRP:HE1	2.30	0.45
3:G:139:PHE:CE1	3:G:173:TYR:C	2.95	0.45
4:H:93:THR:OG1	4:H:94:ARG:N	2.50	0.45
4:H:149:PRO:C	4:H:150:GLU:O	2.59	0.45
1:A:63:HIS:CE1	1:A:76:GLN:HG3	2.52	0.45
2:D:52:LYS:C	2:D:69:GLN:NE2	2.71	0.45
3:E:119:PRO:CG	4:F:127:ALA:HB3	2.47	0.45
4:F:18:LEU:HD13	4:F:109:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:93:THR:HG21	4:F:100(A):PHE:CD1	2.52	0.45
2:B:14:GLU:OE2	2:B:118:ASP:HA	2.17	0.44
1:C:5:GLN:O	1:C:6:THR:C	2.60	0.44
2:D:223:ASP:CG	2:D:231:LYS:HE3	2.39	0.44
4:F:89:ILE:CD1	4:F:108:MET:SD	3.05	0.44
4:H:121:VAL:CG1	4:H:210:VAL:HG21	2.46	0.44
1:A:85:SER:HA	1:A:112:LEU:O	2.17	0.44
2:B:182:SER:OG	2:B:186:ASN:N	2.48	0.44
1:C:168:LEU:C	1:C:168:LEU:CD1	2.80	0.44
2:D:84:LEU:H	2:D:84:LEU:HG	1.34	0.44
2:D:162:TRP:HB2	2:D:211:ARG:HB3	1.99	0.44
3:E:92:TYR:CE1	3:E:95(B):ASP:HB2	2.52	0.44
3:G:66:THR:HA	3:G:71:ALA:HA	1.98	0.44
3:G:132:LEU:HD12	3:G:132:LEU:N	2.32	0.44
4:H:28:THR:C	4:H:30:SER:H	2.24	0.44
4:H:199:TRP:C	4:H:202:LYS:H	2.25	0.44
1:A:99:GLY:O	1:A:101:ASN:N	2.50	0.44
1:A:193:ASP:O	1:A:194:ILE:C	2.59	0.44
1:C:146:PHE:HB2	1:C:150:ILE:HD11	1.99	0.44
1:C:168:LEU:CD1	2:D:171:GLY:HA2	2.48	0.44
4:F:52(B):ILE:H	4:F:52(B):ILE:HG13	1.41	0.44
4:F:162:ASN:C	4:F:163:SER:OG	2.61	0.44
3:G:31:ASN:HD21	3:G:95(A):ASN:ND2	2.16	0.44
3:G:34:TYR:O	3:G:89:LEU:N	2.46	0.44
4:H:83:ARG:NH2	4:H:85:ASP:OD2	2.50	0.44
4:H:107:THR:O	4:H:107:THR:CG2	2.65	0.44
1:C:3:VAL:HG12	1:C:105:VAL:CG1	2.45	0.44
3:E:149:LYS:HB2	3:E:193:SER:HB3	1.99	0.44
4:F:52(B):ILE:O	4:F:52(C):PRO:C	2.60	0.44
3:G:94:ASP:OD1	3:G:94:ASP:N	2.51	0.44
1:A:51:THR:O	1:A:66:LEU:HD23	2.17	0.44
1:A:55:ARG:HH12	1:A:57:GLU:CB	2.28	0.44
3:E:13:VAL:O	3:E:106:VAL:HA	2.17	0.44
3:E:117:VAL:CG2	3:E:209:LEU:CD1	2.96	0.44
4:F:33:TRP:N	4:F:95:ALA:O	2.49	0.44
4:F:52(A):ASN:HA	4:F:71:ARG:HH21	1.83	0.44
4:F:141:GLY:CA	4:F:189:SER:O	2.66	0.44
4:F:178:LEU:HD23	4:F:185:TYR:CD1	2.53	0.44
3:G:31:ASN:HD21	3:G:95(A):ASN:HD22	1.64	0.44
3:G:96:LEU:HB2	4:H:47:TRP:CD2	2.52	0.44
3:G:150:ALA:O	3:G:151:ASN:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:34:MET:CE	4:H:93:THR:O	2.57	0.44
4:H:86:ASP:HB2	4:H:111:VAL:HG21	1.98	0.44
1:A:147:ASP:N	1:A:150:ILE:HD11	2.33	0.44
1:A:179:GLY:HA3	2:B:195:ARG:CZ	2.47	0.44
2:D:71:ASP:OD1	2:D:71:ASP:N	2.49	0.44
2:D:136:GLU:CD	2:D:144:THR:HG1	2.24	0.44
3:E:136:VAL:HG11	3:E:175:THR:HB	1.95	0.44
4:F:139:THR:HA	4:F:191:VAL:O	2.18	0.44
4:H:101:ASP:OD1	4:H:102:TYR:N	2.46	0.44
3:E:39:LYS:O	3:E:42:LYS:N	2.46	0.44
3:E:115:VAL:CG1	3:E:209:LEU:CD2	2.80	0.44
3:E:141:PRO:HG2	3:E:142:GLY:H	1.83	0.44
4:F:83:ARG:O	4:F:84:VAL:C	2.60	0.44
3:G:154:THR:CG2	3:G:155:ILE:N	2.81	0.44
1:A:194:ILE:HG22	1:A:195:PHE:CD1	2.53	0.44
2:B:18:ARG:HH21	5:B:248:NAG:C6	2.14	0.44
2:B:120:ARG:NH1	4:F:100:HIS:NE2	2.66	0.44
2:B:228:GLY:CA	4:F:96:GLY:O	2.59	0.44
1:C:3:VAL:HG23	1:C:22:CYS:SG	2.57	0.44
2:D:46:LEU:O	2:D:58:GLY:HA3	2.18	0.44
3:E:121:SER:HB3	3:E:124:GLU:HB2	2.00	0.44
3:E:166:LYS:HG2	3:E:167:GLN:N	2.33	0.44
4:F:67:PHE:N	4:F:67:PHE:HD1	2.16	0.44
1:A:190:THR:CG2	1:A:192:GLN:HB3	2.48	0.44
2:B:168:VAL:HG22	2:B:169:HIS:N	2.33	0.44
2:D:74:HIS:NE2	2:D:76:GLU:CD	2.76	0.44
2:D:242:TRP:HB3	2:D:243:GLY:H	1.64	0.44
3:G:35:TRP:CH2	3:G:88:CYS:HB3	2.53	0.44
4:H:70:SER:O	4:H:78:ILE:HA	2.17	0.44
4:H:70:SER:O	4:H:79:TYR:N	2.45	0.44
1:A:87:LEU:HD12	2:B:41:LYS:CD	2.47	0.43
2:B:209:HIS:CB	2:B:242:TRP:CZ3	2.90	0.43
1:C:122:GLU:HB3	2:D:140:LYS:HE2	2.00	0.43
2:D:228:GLY:HA2	4:H:95:ALA:HB1	2.00	0.43
4:F:13:GLN:NE2	4:F:113:SER:HA	2.33	0.43
4:F:212:HIS:CD2	4:F:212:HIS:C	2.95	0.43
3:G:22:THR:HG22	3:G:70:THR:CG2	2.48	0.43
3:G:37:GLN:N	3:G:45:LEU:O	2.45	0.43
3:G:133:VAL:HG21	4:H:124:LEU:HD22	1.94	0.43
4:H:144:VAL:CG1	4:H:210:VAL:HG11	2.48	0.43
1:A:53:ASN:OD1	1:A:54:LYS:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:14:THR:O	3:E:17:GLU:HB2	2.18	0.43
4:F:67:PHE:CD1	4:F:67:PHE:N	2.86	0.43
4:F:93:THR:CG2	4:F:100(A):PHE:HD1	2.29	0.43
3:G:25:GLY:CA	3:G:28:LEU:HG	2.47	0.43
3:G:99:GLY:C	3:G:101:GLY:H	2.25	0.43
4:H:33:TRP:HZ2	4:H:53:ASN:HD21	1.66	0.43
4:H:84:VAL:O	4:H:86:ASP:N	2.51	0.43
2:B:22:THR:HG22	2:B:23:CYS:N	2.32	0.43
2:B:127:VAL:HG11	2:B:238:SER:CA	2.48	0.43
1:C:17:PRO:HB3	1:C:78:SER:HA	2.00	0.43
1:C:104:TYR:CE1	1:C:106:PHE:CZ	3.05	0.43
3:E:14:THR:HG23	3:E:106(A):LEU:HB2	1.99	0.43
4:F:33:TRP:O	4:F:35:TYR:CE1	2.71	0.43
4:F:47:TRP:CZ3	4:F:60:ALA:HB2	2.53	0.43
3:G:183:ALA:O	3:G:187:LYS:HD2	2.18	0.43
1:C:92:LEU:HD12	1:C:92:LEU:O	2.16	0.43
2:D:79:MET:HE2	2:D:114:LEU:HD13	1.99	0.43
4:F:51:ILE:HD13	4:F:71:ARG:HB2	2.00	0.43
4:H:139:THR:HG23	4:H:192:THR:HG23	2.00	0.43
1:A:189:PHE:N	1:A:189:PHE:CD1	2.86	0.43
2:B:60:LEU:HA	2:B:61:PRO:HD3	1.88	0.43
2:B:105:GLU:CD	2:D:96:LEU:CD2	2.92	0.43
2:B:157:VAL:HA	2:B:215:GLN:O	2.18	0.43
1:C:177:SER:O	2:D:195:ARG:NH2	2.51	0.43
1:C:203:ASN:OD1	5:C:216:NAG:C5	2.67	0.43
2:D:68:GLN:HE21	2:D:68:GLN:N	2.13	0.43
2:D:174:THR:CA	2:D:194:SER:HB2	2.30	0.43
3:E:164:PRO:HG3	4:F:175:PRO:HG2	1.99	0.43
4:F:2:VAL:HA	4:F:25:SER:O	2.19	0.43
1:A:5:GLN:HE22	1:A:90:CYS:H	1.66	0.43
1:A:53:ASN:CG	1:A:54:LYS:N	2.67	0.43
2:B:133:SER:O	2:B:134:LYS:C	2.62	0.43
2:B:149:ALA:HB2	2:B:214:VAL:HG21	1.99	0.43
2:D:227:GLU:O	2:D:227:GLU:HG3	2.19	0.43
4:F:35:TYR:CD1	4:F:35:TYR:N	2.86	0.43
3:G:182:THR:O	3:G:185:GLN:N	2.45	0.43
4:H:94:ARG:NE	4:H:101:ASP:OD1	2.46	0.43
4:H:125:ALA:HA	4:H:126:PRO:HD3	1.82	0.43
1:C:144:THR:CG2	1:C:177:SER:OG	2.66	0.43
2:D:37:GLN:HG3	2:D:41:LYS:HA	2.00	0.43
2:D:140:LYS:O	2:D:141:GLN:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:140:TYR:CD1	3:E:141:PRO:CB	3.01	0.43
3:E:204:THR:O	3:E:205:VAL:C	2.61	0.43
4:F:150:GLU:CB	4:F:151:PRO:CD	2.93	0.43
3:G:104:LEU:O	3:G:104:LEU:HD23	2.17	0.43
4:H:1:GLU:O	4:H:1:GLU:HG2	2.18	0.43
4:H:63:VAL:HB	4:H:67:PHE:CB	2.47	0.43
4:H:80:LEU:HG	4:H:82:MET:HG2	1.99	0.43
4:H:141:GLY:HA2	4:H:157:TRP:HZ2	1.79	0.43
4:H:148:PHE:CD1	4:H:148:PHE:C	2.93	0.43
4:H:150:GLU:CB	4:H:151:PRO:CD	2.96	0.43
4:H:193:VAL:HB	4:H:194:PRO:CD	2.48	0.43
1:A:67:HIS:O	1:A:68:LYS:C	2.61	0.43
2:B:40:GLY:O	2:B:41:LYS:C	2.61	0.43
2:B:180:LYS:HG2	2:B:190:TYR:CE2	2.54	0.43
2:B:205:ASN:HA	2:B:206:PRO:HD3	1.88	0.43
1:C:5:GLN:HE22	1:C:90:CYS:H	1.66	0.43
4:F:205:ILE:HG22	4:F:225:ILE:CD1	2.48	0.43
3:G:49:TYR:O	3:G:50:MET:C	2.61	0.43
3:G:66:THR:O	3:G:66:THR:CG2	2.65	0.43
4:H:148:PHE:H	4:H:149:PRO:HD3	1.76	0.43
2:B:15:LYS:C	2:B:17:GLY:N	2.77	0.43
2:B:119:LEU:HA	2:B:119:LEU:HD12	1.78	0.43
1:C:160:THR:OG1	1:C:184:SER:HB2	2.18	0.43
2:D:70:PHE:CD1	2:D:70:PHE:N	2.85	0.43
4:F:35:TYR:CE1	4:F:95:ALA:CB	3.02	0.43
4:F:94:ARG:HH21	4:F:101:ASP:CG	2.26	0.43
1:A:54:LYS:CB	1:A:65:THR:OG1	2.63	0.43
3:E:2:TYR:CG	3:E:3:GLU:N	2.87	0.43
4:F:32:PHE:HA	4:F:95:ALA:O	2.19	0.43
4:F:205:ILE:HG22	4:F:225:ILE:HD12	2.01	0.43
4:H:33:TRP:HZ2	4:H:53:ASN:ND2	2.15	0.43
4:H:124:LEU:HD12	4:H:142:CYS:N	2.34	0.43
1:A:46:LEU:O	1:A:55:ARG:NH1	2.52	0.42
2:B:79:MET:HE3	2:B:82:LEU:HD22	2.00	0.42
3:E:117:VAL:HG21	3:E:209:LEU:HG	1.96	0.42
3:G:139:PHE:HE1	3:G:174:MET:HA	1.83	0.42
3:G:148:TRP:CH2	3:G:179:LEU:HB3	2.53	0.42
3:G:148:TRP:CD2	3:G:179:LEU:HD13	2.54	0.42
4:H:117:THR:HB	4:H:184:LEU:HD21	2.01	0.42
1:A:48:LYS:HZ1	2:B:100:ASP:CB	2.33	0.42
1:A:87:LEU:CD1	2:B:41:LYS:CD	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:148:PHE:N	4:F:149:PRO:CD	2.82	0.42
3:G:125:LEU:HD22	3:G:186:TRP:HE1	1.84	0.42
4:H:33:TRP:CD2	4:H:52:LYS:HG2	2.54	0.42
2:B:50:TYR:CZ	2:B:97:ARG:HB2	2.54	0.42
2:B:89:MET:HE2	2:B:89:MET:HB3	1.70	0.42
3:E:95:ASN:O	3:E:95(A):ASN:C	2.63	0.42
3:E:183:ALA:O	3:E:187:LYS:CG	2.66	0.42
3:E:203:GLU:O	3:E:205:VAL:HG23	2.20	0.42
4:F:38:ARG:HB3	4:F:90:TYR:CD2	2.55	0.42
4:H:39:GLN:HG3	4:H:44:GLY:O	2.18	0.42
4:H:171:VAL:HG13	4:H:172:HIS:N	2.34	0.42
3:E:115:VAL:CG2	3:E:207:LYS:CG	2.97	0.42
3:E:119:PRO:HA	3:E:120:PRO:HD3	1.90	0.42
3:E:140:TYR:CD1	3:E:173:TYR:CE2	2.87	0.42
4:F:67:PHE:CD2	4:F:82:MET:HB3	2.55	0.42
4:H:174:PHE:HB3	4:H:175:PRO:HD2	2.00	0.42
1:A:55:ARG:NH1	1:A:57:GLU:CB	2.82	0.42
1:C:35:TYR:HB2	1:C:89:TYR:HB2	2.01	0.42
1:C:47:LEU:CD1	1:C:56:THR:HG21	2.49	0.42
1:C:174:ASP:HB3	1:C:175:SER:H	1.57	0.42
2:D:125:PRO:HB3	2:D:152:PHE:HD2	1.80	0.42
2:D:180:LYS:HD2	2:D:182:SER:O	2.19	0.42
3:E:61:ARG:NH1	3:E:82:ASP:CG	2.76	0.42
4:H:84:VAL:HA	4:H:111:VAL:HB	2.01	0.42
4:H:117:THR:HG21	4:H:184:LEU:HD11	2.01	0.42
1:A:158:SER:C	1:A:160:THR:N	2.78	0.42
2:B:71:ASP:OD1	2:B:71:ASP:N	2.50	0.42
2:B:179:TYR:O	2:B:190:TYR:HA	2.19	0.42
1:C:9:LEU:HD13	1:C:111:ARG:HB3	2.01	0.42
1:C:119:GLN:OE1	1:C:119:GLN:HA	2.19	0.42
2:D:231:LYS:HG2	2:D:233:VAL:HG22	2.02	0.42
3:G:46:LEU:C	3:G:46:LEU:HD12	2.44	0.42
3:G:120:PRO:HD3	3:G:132:LEU:HG	2.00	0.42
3:G:121:SER:HG	4:H:122:TYR:HD1	1.63	0.42
3:G:137:ASN:OD1	4:H:172:HIS:CD2	2.73	0.42
1:A:26:THR:HB	1:A:94:GLU:OE1	2.20	0.42
1:A:164:ASP:HB2	2:B:179:TYR:OH	2.20	0.42
2:B:71:ASP:O	2:B:73:TYR:N	2.52	0.42
2:B:154:PRO:HG2	2:B:156:HIS:CD2	2.44	0.42
2:B:29:HIS:CD2	2:B:96:LEU:HB2	2.54	0.42
3:E:122:PRO:HA	3:E:125:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:138:ASP:CA	3:E:172:ASN:ND2	2.79	0.42
3:E:139:PHE:CE2	3:E:173:TYR:HB2	2.52	0.42
4:F:2:VAL:HG13	4:F:27:PHE:HD1	1.77	0.42
4:F:116:THR:HG23	4:F:214:ALA:CB	2.44	0.42
4:F:212:HIS:HD2	4:F:213:PRO:N	2.18	0.42
4:H:69:ILE:HG22	4:H:70:SER:N	2.34	0.42
1:A:47:LEU:HA	2:D:97:ARG:NH2	2.35	0.42
2:B:148:LEU:HG	2:B:150:ARG:HG3	2.02	0.42
2:B:156:HIS:HB3	2:B:217:HIS:HB2	2.02	0.42
2:B:228:GLY:O	4:F:96:GLY:HA2	2.20	0.42
2:D:115:THR:HG22	2:D:116(A):LEU:HD21	2.02	0.42
3:E:4:LEU:HA	3:E:4:LEU:HD23	1.86	0.42
3:E:35:TRP:CZ3	3:E:88:CYS:HB3	2.54	0.42
4:F:89:ILE:HD11	4:F:108:MET:SD	2.60	0.42
3:G:44:ILE:HG21	4:H:103:TRP:CE2	2.55	0.42
3:G:163:LYS:HD3	3:G:175:THR:OG1	2.20	0.42
1:A:5:GLN:O	1:A:6:THR:C	2.63	0.42
1:A:36:VAL:HG23	1:A:88:TYR:CZ	2.55	0.42
2:B:21:LEU:HD12	2:B:21:LEU:N	2.34	0.42
2:B:141:GLN:O	2:B:142:LYS:HG3	2.19	0.42
2:D:52:LYS:N	2:D:69:GLN:HE22	2.17	0.42
2:D:85:GLU:H	2:D:85:GLU:HG2	1.67	0.42
3:E:123:GLU:O	3:E:126:ARG:CB	2.61	0.42
4:F:108:MET:HG2	4:F:150:GLU:CG	2.50	0.42
3:G:141:PRO:O	3:G:142:GLY:C	2.62	0.42
4:H:18:LEU:O	4:H:82:MET:HG3	2.18	0.42
4:H:51:ILE:HD13	4:H:71:ARG:CB	2.41	0.42
4:H:83:ARG:O	4:H:84:VAL:C	2.63	0.42
4:H:89:ILE:HD13	4:H:108:MET:SD	2.59	0.42
4:H:126:PRO:HB2	4:H:127:ALA:H	1.66	0.42
4:H:157:TRP:CH2	4:H:208:CYS:HB3	2.55	0.42
4:H:178:LEU:HD23	4:H:185:TYR:CD1	2.55	0.42
3:E:28:LEU:C	3:E:30:LYS:N	2.78	0.41
4:F:32:PHE:CD1	4:F:94:ARG:HG3	2.55	0.41
4:F:52(B):ILE:CB	4:F:52(C):PRO:HD3	2.50	0.41
4:H:171:VAL:HG22	4:H:191:VAL:HG22	2.01	0.41
4:H:210:VAL:HG12	4:H:211:ALA:N	2.35	0.41
1:A:58:HIS:O	1:A:58:HIS:ND1	2.53	0.41
1:A:69:SER:OG	1:A:70:SER:N	2.51	0.41
1:A:144:THR:CG2	1:A:177:SER:OG	2.67	0.41
2:B:132:PRO:CG	2:B:143:ALA:HB1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLU:HB3	2:D:140:LYS:HE3	1.99	0.41
1:C:190:THR:CG2	1:C:192:GLN:H	2.33	0.41
3:G:36:PHE:HZ	4:H:100(A):PHE:CB	2.33	0.41
1:A:132:ASP:HA	1:A:133:PRO:HD2	1.95	0.41
2:B:204:HIS:O	2:B:206:PRO:HD3	2.20	0.41
2:D:74:HIS:CE1	2:D:76:GLU:HG3	2.54	0.41
3:E:109:PRO:O	3:E:110:LYS:C	2.61	0.41
3:E:148:TRP:O	3:E:154:THR:HA	2.20	0.41
4:F:52(B):ILE:N	4:F:52(C):PRO:HD2	2.36	0.41
4:F:61:ASP:OD1	4:F:64:ARG:NH1	2.46	0.41
3:G:9:SER:O	3:G:11:ALA:HB2	2.19	0.41
3:G:112:SER:HB2	3:G:207:LYS:HZ3	1.84	0.41
3:G:176:SER:O	3:G:178:TYR:HD1	2.04	0.41
4:H:32:PHE:CD1	4:H:94:ARG:HG3	2.54	0.41
4:H:116:THR:HG23	4:H:149:PRO:HG2	2.02	0.41
4:H:190:SER:O	4:H:191:VAL:CG2	2.68	0.41
2:B:15:LYS:HD3	2:B:84:LEU:HD21	2.02	0.41
2:B:219:LEU:O	2:B:233:VAL:HG12	2.21	0.41
1:C:143:PHE:HB2	1:C:195:PHE:CE2	2.55	0.41
2:D:97:ARG:H	2:D:97:ARG:HG2	1.55	0.41
3:E:5:ILE:O	3:E:23:CYS:HA	2.20	0.41
3:E:120:PRO:HG2	3:E:130:ALA:HB1	2.01	0.41
4:F:107:THR:O	4:F:107:THR:CG2	2.68	0.41
4:F:121:VAL:HG21	4:F:210:VAL:HG21	2.01	0.41
3:G:214:CYS:CB	3:G:215:LEU:HD23	2.47	0.41
2:B:17:GLY:O	2:B:82:LEU:CG	2.66	0.41
1:C:134:ARG:HD3	1:C:134:ARG:HA	1.88	0.41
1:C:171:LYS:HA	2:D:170:SER:HG	1.86	0.41
1:C:179:GLY:HA3	2:D:195:ARG:CZ	2.50	0.41
2:D:47:ILE:HG21	2:D:60:LEU:HD22	2.01	0.41
2:D:218:GLY:H	2:D:234:THR:HG23	1.85	0.41
3:E:48:ILE:CD1	3:E:63:SER:C	2.94	0.41
3:E:199:GLU:C	3:E:203:GLU:H	2.28	0.41
4:F:4:LEU:HA	4:F:23:ALA:O	2.21	0.41
4:F:52(B):ILE:HB	4:F:52(C):PRO:HD3	2.02	0.41
4:F:148:PHE:CD1	4:F:148:PHE:C	2.98	0.41
3:G:4:LEU:HD23	3:G:4:LEU:HA	1.88	0.41
3:G:117:VAL:HG11	3:G:211:PRO:CG	2.50	0.41
3:G:182:THR:HG23	3:G:185:GLN:HB2	2.02	0.41
1:A:70:SER:O	1:A:71:SER:C	2.64	0.41
2:B:33:VAL:CG2	2:B:34:TRP:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:LEU:HA	2:B:43:LEU:HD13	1.38	0.41
2:B:115:THR:O	2:B:115:THR:HG22	2.20	0.41
1:C:128:LEU:CD1	2:D:146:VAL:CG2	2.99	0.41
1:C:143:PHE:O	1:C:179:GLY:HA2	2.21	0.41
3:E:129:LYS:HD3	3:E:129:LYS:HA	1.69	0.41
4:F:11:LEU:HA	4:F:110:THR:HB	2.01	0.41
4:F:29:PHE:CE1	4:F:71:ARG:HD2	2.55	0.41
1:A:36:VAL:CG2	1:A:88:TYR:CE2	3.04	0.41
2:B:79:MET:CB	2:B:82:LEU:HD21	2.50	0.41
4:F:52(B):ILE:CB	4:F:52(C):PRO:CD	2.98	0.41
3:G:21:ILE:HG22	3:G:35:TRP:CH2	2.56	0.41
1:A:11:THR:HA	1:A:113:LYS:O	2.21	0.41
1:A:211:VAL:HA	1:A:212:PRO:HD3	1.83	0.41
1:C:171:LYS:CA	2:D:170:SER:OG	2.67	0.41
2:D:1:ASP:C	2:D:3:GLY:N	2.78	0.41
2:D:70:PHE:N	2:D:70:PHE:HD1	2.18	0.41
2:D:88:ALA:HB3	2:D:90:TYR:CE2	2.55	0.41
2:D:154:PRO:C	2:D:156:HIS:N	2.69	0.41
3:E:33:ALA:HA	3:E:89:LEU:O	2.21	0.41
3:E:160:LYS:O	3:E:178:TYR:N	2.54	0.41
3:G:37:GLN:CB	3:G:47:LEU:HD11	2.50	0.41
3:G:140:TYR:HA	3:G:141:PRO:HA	1.86	0.41
4:H:35:TYR:OH	4:H:95:ALA:CB	2.69	0.41
1:A:190:THR:CG2	1:A:191:CYS:N	2.82	0.41
2:B:56:ASP:OD1	2:B:56:ASP:C	2.63	0.41
2:B:125:PRO:HD3	2:B:216:PHE:CG	2.56	0.41
2:B:212:CYS:O	2:B:238:SER:HA	2.21	0.41
1:C:190:THR:HG23	1:C:191:CYS:N	2.34	0.41
2:D:82:LEU:HB3	2:D:116:VAL:HG21	2.03	0.41
2:D:135:ALA:O	2:D:136:GLU:C	2.64	0.41
3:E:107:ARG:HB3	3:E:109:PRO:HD2	2.03	0.41
3:E:120:PRO:CG	3:E:130:ALA:HB1	2.51	0.41
3:E:214:CYS:O	3:E:215:LEU:HB2	2.21	0.41
4:F:144:VAL:HG13	4:F:210:VAL:HG11	2.02	0.41
3:G:46:LEU:HD12	3:G:47:LEU:N	2.36	0.41
4:H:157:TRP:CE2	4:H:191:VAL:CG2	3.03	0.41
4:F:140:LEU:CD1	4:F:225:ILE:HG21	2.43	0.41
4:F:194:PRO:HD2	4:F:198:THR:OG1	2.21	0.41
3:G:79:GLN:O	3:G:82:ASP:HB2	2.21	0.41
2:B:39:LEU:HB3	2:B:40:GLY:H	1.59	0.40
2:B:242:TRP:HB3	2:B:243:GLY:H	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:137:ASN:OD1	4:F:172:HIS:CE1	2.74	0.40
4:F:26:GLY:O	4:F:27:PHE:HB3	2.21	0.40
4:F:166:LEU:HD11	4:F:205:ILE:CD1	2.47	0.40
3:G:124:GLU:OE1	3:G:131:THR:OG1	2.32	0.40
1:A:36:VAL:O	1:A:36:VAL:HG13	2.20	0.40
1:A:140:LEU:HD13	1:A:140:LEU:C	2.46	0.40
2:B:50:TYR:CD1	2:B:50:TYR:C	2.95	0.40
1:C:101:ASN:O	1:C:102:TYR:CB	2.69	0.40
2:D:67:VAL:HB	2:D:76:GLU:O	2.20	0.40
3:G:123:GLU:O	3:G:126:ARG:CB	2.64	0.40
1:A:62:PHE:HD1	1:A:75:LEU:HD11	1.87	0.40
1:A:102:TYR:CG	2:B:98:TRP:NE1	2.89	0.40
1:A:189:PHE:N	1:A:189:PHE:HD1	2.18	0.40
2:B:49:HIS:HA	2:B:54:GLU:O	2.20	0.40
2:B:223:ASP:CB	2:B:231:LYS:HE3	2.44	0.40
1:C:47:LEU:HB2	1:C:56:THR:HG21	2.02	0.40
2:D:118:ASP:CG	5:D:249:NAG:H83	2.46	0.40
3:E:80:PRO:C	3:E:82:ASP:N	2.79	0.40
3:E:161:THR:HA	3:E:177:SER:HA	2.04	0.40
4:F:137:THR:HG22	4:F:193:VAL:C	2.46	0.40
4:F:199:TRP:CZ2	4:F:225:ILE:HG22	2.56	0.40
3:G:118:PHE:CZ	4:H:140:LEU:HA	2.56	0.40
3:G:166:LYS:CG	3:G:167:GLN:H	2.34	0.40
4:H:11:LEU:HB2	4:H:110:THR:HB	2.02	0.40
2:B:137:ILE:N	2:B:137:ILE:HD12	2.37	0.40
2:B:159:LEU:HB3	2:B:174:THR:HG21	2.04	0.40
1:C:32:PHE:HB3	1:C:73:PHE:CD2	2.56	0.40
2:D:44:LYS:HE2	2:D:59:PHE:HB2	2.04	0.40
2:D:68:GLN:NE2	2:D:68:GLN:N	2.67	0.40
2:D:160:SER:HB2	2:D:162:TRP:NE1	2.32	0.40
4:F:2:VAL:HB	4:F:102:TYR:CE2	2.56	0.40
4:F:5:VAL:HB	4:F:23:ALA:HB3	2.04	0.40
3:G:41:ASP:HB3	3:G:43:ASN:CG	2.43	0.40
3:G:181:LEU:HG	3:G:185:GLN:OE1	2.22	0.40
4:H:10:ASP:CG	4:H:11:LEU:N	2.79	0.40
4:H:108:MET:HB3	4:H:150:GLU:OE2	2.20	0.40
2:D:204:HIS:O	2:D:206:PRO:CD	2.68	0.40
4:F:157:TRP:CZ3	4:F:225:ILE:CD1	2.99	0.40
3:G:28:LEU:HD23	3:G:28:LEU:HA	1.63	0.40
3:G:54:ARG:HB3	3:G:54:ARG:CZ	2.52	0.40
3:G:77:GLY:O	3:G:78:ALA:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:182:THR:O	3:G:183:ALA:C	2.65	0.40
3:G:192:VAL:O	3:G:211:PRO:HG2	2.22	0.40
3:G:203:GLU:O	3:G:205:VAL:N	2.54	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:CYS:O	2:D:57:LYS:NZ[2_546]	2.01	0.19
2:B:53:VAL:O	4:H:70:SER:OG[2_656]	2.09	0.11
2:B:55:ARG:NH2	4:H:19:LYS:NZ[2_656]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	201/203 (99%)	156 (78%)	33 (16%)	12 (6%)	1	3
1	C	201/203 (99%)	162 (81%)	23 (11%)	16 (8%)	1	1
2	B	237/239 (99%)	198 (84%)	25 (10%)	14 (6%)	1	3
2	D	237/239 (99%)	195 (82%)	30 (13%)	12 (5%)	1	5
3	E	210/212 (99%)	159 (76%)	35 (17%)	16 (8%)	1	2
3	G	210/212 (99%)	158 (75%)	33 (16%)	19 (9%)	0	1
4	F	220/222 (99%)	160 (73%)	39 (18%)	21 (10%)	0	1
4	H	220/222 (99%)	170 (77%)	32 (14%)	18 (8%)	0	1
All	All	1736/1752 (99%)	1358 (78%)	250 (14%)	128 (7%)	1	2

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	134	ARG
1	A	204	ALA
2	B	39	LEU
1	C	53	ASN
1	C	55	ARG
1	C	59	GLN
1	C	134	ARG
1	C	187	THR
2	D	39	LEU
2	D	97	ARG
2	D	105	GLU
2	D	153	PHE
2	D	155	ASP
3	E	52	ASN
3	E	141	PRO
3	E	170	GLY
3	E	207	LYS
3	E	208	SER
3	E	212	ALA
4	F	127	ALA
4	F	135	THR
4	F	149	PRO
4	F	150	GLU
4	F	214	ALA
3	G	51	ASP
3	G	52	ASN
3	G	81	GLU
3	G	141	PRO
3	G	154	THR
3	G	205	VAL
3	G	207	LYS
3	G	208	SER
4	H	129	ASP
4	H	132	THR
4	H	135	THR
4	H	150	GLU
4	H	216	SER
1	A	59	GLN
1	A	100	GLY
1	A	188	SER
2	B	41	LYS
2	B	151	GLY

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Mol	Chain	Res	Type
2	B	227	GLU
1	C	6	THR
1	C	85	SER
1	C	138	SER
1	C	172	ALA
2	D	52	LYS
2	D	120	ARG
2	D	151	GLY
3	E	32	PHE
3	E	172	ASN
4	F	16	SER
4	F	41	PRO
4	F	85	ASP
4	F	176	SER
4	F	191	VAL
3	G	142	GLY
3	G	170	GLY
4	H	41	PRO
4	H	85	ASP
4	H	126	PRO
4	H	131	THR
4	H	148	PHE
4	H	195	SER
4	H	222	LYS
1	A	47	LEU
1	A	138	SER
1	A	147	ASP
1	A	180	ALA
1	A	197	GLU
2	B	40	GLY
2	B	105	GLU
2	B	222	GLU
2	B	223	ASP
2	B	228	GLY
2	B	243	GLY
1	C	145	ASP
1	C	171	LYS
2	D	41	LYS
3	E	171	GLN
3	E	204	THR
3	E	205	VAL
4	F	116	THR

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Mol	Chain	Res	Type
4	F	130	SER
4	F	134	THR
4	F	148	PHE
4	F	195	SER
3	G	172	ASN
3	G	179	LEU
4	H	16	SER
4	H	149	PRO
2	B	226	PRO
1	C	180	ALA
3	E	40	SER
3	E	210	SER
3	G	66	THR
3	G	138	ASP
3	G	167	GLN
3	G	204	THR
2	B	97	ARG
1	C	69	SER
1	C	71	SER
2	D	132	PRO
2	D	221	GLU
3	E	109	PRO
4	F	25	SER
4	F	126	PRO
4	F	133	SER
4	F	177	VAL
3	G	101	GLY
4	H	29	PHE
4	H	127	ALA
4	H	176	SER
1	C	100	GLY
1	C	163	THR
3	E	81	GLU
1	A	153	PRO
2	B	53	VAL
4	F	200	PRO
3	G	210	SER
2	B	176	PRO
3	G	80	PRO
4	H	63	VAL
4	F	123	PRO
2	D	154	PRO

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Mol	Chain	Res	Type
3	E	68	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/181 (100%)	117 (65%)	64 (35%)	0	0
1	C	181/181 (100%)	107 (59%)	74 (41%)	0	0
2	B	212/212 (100%)	145 (68%)	67 (32%)	0	1
2	D	212/212 (100%)	143 (68%)	69 (32%)	0	1
3	E	185/185 (100%)	128 (69%)	57 (31%)	0	1
3	G	185/185 (100%)	110 (60%)	75 (40%)	0	0
4	F	192/192 (100%)	134 (70%)	58 (30%)	0	1
4	H	192/192 (100%)	139 (72%)	53 (28%)	0	1
All	All	1540/1540 (100%)	1023 (66%)	517 (34%)	0	1

All (517) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	4	THR
1	A	9	LEU
1	A	10	VAL
1	A	11	THR
1	A	12	VAL
1	A	14	GLU
1	A	18	VAL
1	A	26	THR
1	A	27	THR
1	A	29	LEU
1	A	33	PHE
1	A	39	LEU
1	A	44	GLN

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Mol	Chain	Res	Type
1	A	48	LYS
1	A	57	GLU
1	A	66	LEU
1	A	68	LYS
1	A	70	SER
1	A	75	LEU
1	A	76	GLN
1	A	79	SER
1	A	81	GLN
1	A	85	SER
1	A	87	LEU
1	A	101	ASN
1	A	103	LYS
1	A	111	ARG
1	A	114	VAL
1	A	115	ILE
1	A	125	VAL
1	A	127	GLN
1	A	128	LEU
1	A	129	LYS
1	A	135	SER
1	A	136	GLN
1	A	139	THR
1	A	140	LEU
1	A	148	SER
1	A	149	GLN
1	A	150	ILE
1	A	152	VAL
1	A	155	THR
1	A	156	MET
1	A	157	GLU
1	A	158	SER
1	A	168	LEU
1	A	171	LYS
1	A	173	MET
1	A	176	LYS
1	A	177	SER
1	A	181	ILE
1	A	184	SER
1	A	186	GLN
1	A	190	THR
1	A	192	GLN

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Mol	Chain	Res	Type
1	A	193	ASP
1	A	194	ILE
1	A	196	LYS
1	A	198	THR
1	A	206	TYR
1	A	208	SER
1	A	209	SER
1	A	213	CYS
2	B	2	SER
2	B	5	VAL
2	B	7	SER
2	B	9	ARG
2	B	11	ILE
2	B	13	LYS
2	B	14	GLU
2	B	15	LYS
2	B	24	ILE
2	B	27	SER
2	B	30	SER
2	B	33	VAL
2	B	43	LEU
2	B	51	GLU
2	B	52	LYS
2	B	53	VAL
2	B	62	SER
2	B	64	ARG
2	B	66	SER
2	B	67	VAL
2	B	68	GLN
2	B	69	GLN
2	B	71	ASP
2	B	72	ASP
2	B	74	HIS
2	B	75	SER
2	B	77	MET
2	B	79	MET
2	B	80	SER
2	B	84	LEU
2	B	85	GLU
2	B	89	MET
2	B	94	SER
2	B	100	ASP

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Mol	Chain	Res	Type
2	B	113	ARG
2	B	115	THR
2	B	116	VAL
2	B	116(A)	LEU
2	B	117	GLU
2	B	118	ASP
2	B	119	LEU
2	B	121	ASN
2	B	123	THR
2	B	128	SER
2	B	133	SER
2	B	134	LYS
2	B	160	SER
2	B	163	VAL
2	B	166	LYS
2	B	172	VAL
2	B	180	LYS
2	B	182	SER
2	B	191	SER
2	B	192	LEU
2	B	201	THR
2	B	207	ARG
2	B	211	ARG
2	B	213	GLN
2	B	219	LEU
2	B	223	ASP
2	B	227	GLU
2	B	229	SER
2	B	231	LYS
2	B	233	VAL
2	B	238	SER
2	B	240	GLU
2	B	247	CYS
1	C	3	VAL
1	C	4	THR
1	C	9	LEU
1	C	10	VAL
1	C	11	THR
1	C	12	VAL
1	C	14	GLU
1	C	18	VAL
1	C	27	THR

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Mol	Chain	Res	Type
1	C	29	LEU
1	C	33	PHE
1	C	39	LEU
1	C	44	GLN
1	C	48	LYS
1	C	51	THR
1	C	54	LYS
1	C	55	ARG
1	C	56	THR
1	C	59	GLN
1	C	66	LEU
1	C	71	SER
1	C	76	GLN
1	C	79	SER
1	C	81	GLN
1	C	85	SER
1	C	87	LEU
1	C	101	ASN
1	C	103	LYS
1	C	110	THR
1	C	111	ARG
1	C	114	VAL
1	C	115	ILE
1	C	117	HIS
1	C	118	ILE
1	C	125	VAL
1	C	127	GLN
1	C	128	LEU
1	C	129	LYS
1	C	135	SER
1	C	136	GLN
1	C	139	THR
1	C	140	LEU
1	C	148	SER
1	C	149	GLN
1	C	150	ILE
1	C	152	VAL
1	C	155	THR
1	C	156	MET
1	C	157	GLU
1	C	158	SER
1	C	167	VAL

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Mol	Chain	Res	Type
1	C	168	LEU
1	C	171	LYS
1	C	173	MET
1	C	175	SER
1	C	176	LYS
1	C	177	SER
1	C	181	ILE
1	C	184	SER
1	C	186	GLN
1	C	187	THR
1	C	188	SER
1	C	189	PHE
1	C	190	THR
1	C	192	GLN
1	C	193	ASP
1	C	194	ILE
1	C	196	LYS
1	C	198	THR
1	C	206	TYR
1	C	208	SER
1	C	209	SER
1	C	210	ASP
1	C	213	CYS
2	D	5	VAL
2	D	6	GLN
2	D	7	SER
2	D	9	ARG
2	D	11	ILE
2	D	13	LYS
2	D	14	GLU
2	D	15	LYS
2	D	27	SER
2	D	30	SER
2	D	33	VAL
2	D	42	GLU
2	D	43	LEU
2	D	53	VAL
2	D	59	PHE
2	D	62	SER
2	D	66	SER
2	D	67	VAL
2	D	68	GLN

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Mol	Chain	Res	Type
2	D	71	ASP
2	D	72	ASP
2	D	74	HIS
2	D	75	SER
2	D	77	MET
2	D	79	MET
2	D	80	SER
2	D	84	LEU
2	D	85	GLU
2	D	87	SER
2	D	89	MET
2	D	94	SER
2	D	96	LEU
2	D	97	ARG
2	D	100	ASP
2	D	113	ARG
2	D	114	LEU
2	D	119	LEU
2	D	121	ASN
2	D	123	THR
2	D	126	LYS
2	D	127	VAL
2	D	128	SER
2	D	130	PHE
2	D	133	SER
2	D	134	LYS
2	D	136	GLU
2	D	160	SER
2	D	163	VAL
2	D	166	LYS
2	D	172	VAL
2	D	180	LYS
2	D	182	SER
2	D	192	LEU
2	D	193	SER
2	D	194	SER
2	D	201	THR
2	D	207	ARG
2	D	211	ARG
2	D	213	GLN
2	D	219	LEU
2	D	220	SER

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Mol	Chain	Res	Type
2	D	224	LYS
2	D	229	SER
2	D	231	LYS
2	D	233	VAL
2	D	238	SER
2	D	240	GLU
2	D	246	ASP
2	D	247	CYS
3	E	2	TYR
3	E	3	GLU
3	E	12	SER
3	E	14	THR
3	E	17	GLU
3	E	18	THR
3	E	20	LYS
3	E	22	THR
3	E	24	SER
3	E	27	GLN
3	E	39	LYS
3	E	40	SER
3	E	43	ASN
3	E	47	LEU
3	E	48	ILE
3	E	58	ILE
3	E	60	GLU
3	E	61	ARG
3	E	63	SER
3	E	73	LEU
3	E	79	GLN
3	E	81	GLU
3	E	100	SER
3	E	103	GLN
3	E	104	LEU
3	E	105	THR
3	E	106	VAL
3	E	106(A)	LEU
3	E	110	LYS
3	E	111	SER
3	E	117	VAL
3	E	123	GLU
3	E	124	GLU
3	E	126	ARG

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Mol	Chain	Res	Type
3	E	131	THR
3	E	133	VAL
3	E	136	VAL
3	E	138	ASP
3	E	143	SER
3	E	154	THR
3	E	155	ILE
3	E	157	ASP
3	E	163	LYS
3	E	165	SER
3	E	172	ASN
3	E	174	MET
3	E	176	SER
3	E	180	SER
3	E	188	SER
3	E	189	HIS
3	E	193	SER
3	E	195	GLN
3	E	199	GLU
3	E	203	GLU
3	E	204	THR
3	E	206	GLU
3	E	207	LYS
4	F	1	GLU
4	F	7	SER
4	F	10	ASP
4	F	11	LEU
4	F	12	VAL
4	F	18	LEU
4	F	20	VAL
4	F	21	SER
4	F	25	SER
4	F	28	THR
4	F	30	SER
4	F	31	ASP
4	F	38	ARG
4	F	43	LYS
4	F	66	ARG
4	F	68	THR
4	F	70	SER
4	F	71	ARG
4	F	75	ARG

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Mol	Chain	Res	Type
4	F	77	SER
4	F	79	TYR
4	F	83	ARG
4	F	89	ILE
4	F	94	ARG
4	F	99	ASP
4	F	101	ASP
4	F	108	MET
4	F	109	VAL
4	F	110	THR
4	F	113	SER
4	F	115	THR
4	F	121	VAL
4	F	124	LEU
4	F	130	SER
4	F	131	THR
4	F	132	THR
4	F	137	THR
4	F	139	THR
4	F	140	LEU
4	F	143	LEU
4	F	144	VAL
4	F	148	PHE
4	F	153	THR
4	F	156	SER
4	F	163	SER
4	F	168	SER
4	F	177	VAL
4	F	178	LEU
4	F	188	SER
4	F	190	SER
4	F	196	SER
4	F	202	LYS
4	F	205	ILE
4	F	209	ASN
4	F	210	VAL
4	F	215	SER
4	F	219	VAL
4	F	226	GLU
3	G	2	TYR
3	G	3	GLU
3	G	6	GLN

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Mol	Chain	Res	Type
3	G	9	SER
3	G	14	THR
3	G	17	GLU
3	G	18	THR
3	G	21	ILE
3	G	22	THR
3	G	24	SER
3	G	27	GLN
3	G	30	LYS
3	G	39	LYS
3	G	43	ASN
3	G	47	LEU
3	G	48	ILE
3	G	52	ASN
3	G	54	ARG
3	G	56	SER
3	G	58	ILE
3	G	60	GLU
3	G	61	ARG
3	G	63	SER
3	G	65	SER
3	G	67	SER
3	G	69	THR
3	G	75	ILE
3	G	76	SER
3	G	79	GLN
3	G	81	GLU
3	G	91	SER
3	G	94	ASP
3	G	100	SER
3	G	104	LEU
3	G	105	THR
3	G	106	VAL
3	G	106(A)	LEU
3	G	111	SER
3	G	114	LYS
3	G	117	VAL
3	G	121	SER
3	G	123	GLU
3	G	124	GLU
3	G	125	LEU
3	G	126	ARG

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Mol	Chain	Res	Type
3	G	131	THR
3	G	133	VAL
3	G	134	CYS
3	G	143	SER
3	G	145	THR
3	G	146	VAL
3	G	162	THR
3	G	163	LYS
3	G	165	SER
3	G	166	LYS
3	G	172	ASN
3	G	174	MET
3	G	175	THR
3	G	176	SER
3	G	181	LEU
3	G	182	THR
3	G	186	TRP
3	G	189	HIS
3	G	190	ASN
3	G	191	ARG
3	G	193	SER
3	G	199	GLU
3	G	203	GLU
3	G	204	THR
3	G	206	GLU
3	G	207	LYS
3	G	209	LEU
3	G	213	GLU
3	G	214	CYS
3	G	215	LEU
4	H	2	VAL
4	H	7	SER
4	H	11	LEU
4	H	12	VAL
4	H	18	LEU
4	H	21	SER
4	H	28	THR
4	H	31	ASP
4	H	35	TYR
4	H	37	VAL
4	H	43	LYS
4	H	50	ARG

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Mol	Chain	Res	Type
4	H	54	ASN
4	H	68	THR
4	H	71	ARG
4	H	74	SER
4	H	75	ARG
4	H	89	ILE
4	H	94	ARG
4	H	97	ARG
4	H	108	MET
4	H	110	THR
4	H	113	SER
4	H	115	THR
4	H	121	VAL
4	H	128	CYS
4	H	130	SER
4	H	131	THR
4	H	132	THR
4	H	137	THR
4	H	138	VAL
4	H	139	THR
4	H	140	LEU
4	H	143	LEU
4	H	144	VAL
4	H	145	LYS
4	H	148	PHE
4	H	153	THR
4	H	156	SER
4	H	163	SER
4	H	168	SER
4	H	171	VAL
4	H	174	PHE
4	H	178	LEU
4	H	180	SER
4	H	192	THR
4	H	195	SER
4	H	196	SER
4	H	198	THR
4	H	202	LYS
4	H	205	ILE
4	H	216	SER
4	H	226	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	37	GLN
1	A	44	GLN
1	A	63	HIS
1	A	74	HIS
1	A	81	GLN
1	A	101	ASN
1	A	117	HIS
1	A	119	GLN
1	A	136	GLN
2	B	10	HIS
2	B	37	GLN
2	B	49	HIS
2	B	68	GLN
2	B	69	GLN
2	B	215	GLN
2	B	217	HIS
1	C	5	GLN
1	C	37	GLN
1	C	44	GLN
1	C	58	HIS
1	C	63	HIS
1	C	67	HIS
1	C	101	ASN
1	C	127	GLN
1	C	186	GLN
2	D	37	GLN
2	D	48	GLN
2	D	49	HIS
2	D	68	GLN
2	D	69	GLN
2	D	156	HIS
2	D	235	GLN
3	E	43	ASN
3	E	95(A)	ASN
3	E	137	ASN
3	E	171	GLN
3	E	195	GLN
4	F	52(A)	ASN
4	F	53	ASN
4	F	172	HIS
4	F	212	HIS

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Mol	Chain	Res	Type
3	G	6	GLN
3	G	31	ASN
3	G	37	GLN
3	G	43	ASN
3	G	95(A)	ASN
3	G	103	GLN
3	G	156	ASN
3	G	172	ASN
3	G	195	GLN
4	H	52(A)	ASN
4	H	54	ASN
4	H	82(A)	ASN
4	H	172	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	D	250	2	14,14,15	0.43	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	D	251	2	14,14,15	0.51	0	17,19,21	0.63	0
5	NAG	C	216	1	14,14,15	4.48	6 (42%)	17,19,21	2.19	6 (35%)
5	NAG	A	214	1	14,14,15	1.08	1 (7%)	17,19,21	1.08	1 (5%)
5	NAG	A	215	1	14,14,15	0.41	0	17,19,21	0.62	1 (5%)
5	NAG	A	216	1	14,14,15	0.53	0	17,19,21	0.78	0
5	NAG	D	249	2	14,14,15	0.53	0	17,19,21	0.67	0
5	NAG	D	248	2	14,14,15	0.38	0	17,19,21	0.55	0
5	NAG	C	215	1	14,14,15	0.43	0	17,19,21	0.67	0
5	NAG	C	214	1	14,14,15	0.45	0	17,19,21	0.62	0
5	NAG	B	251	2	14,14,15	0.52	0	17,19,21	0.64	0
5	NAG	B	250	2	14,14,15	0.40	0	17,19,21	0.86	1 (5%)
5	NAG	B	248	2	14,14,15	0.46	0	17,19,21	0.83	1 (5%)
5	NAG	B	249	2	14,14,15	0.37	0	17,19,21	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	250	2	-	2/6/23/26	0/1/1/1
5	NAG	D	251	2	-	2/6/23/26	0/1/1/1
5	NAG	C	216	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	A	214	1	-	1/6/23/26	0/1/1/1
5	NAG	A	215	1	-	2/6/23/26	0/1/1/1
5	NAG	A	216	1	-	2/6/23/26	0/1/1/1
5	NAG	D	249	2	-	3/6/23/26	0/1/1/1
5	NAG	D	248	2	-	2/6/23/26	0/1/1/1
5	NAG	C	215	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	C	214	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	B	251	2	-	3/6/23/26	0/1/1/1
5	NAG	B	250	2	-	3/6/23/26	0/1/1/1
5	NAG	B	248	2	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	249	2	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	216	NAG	C1-C2	-11.73	1.36	1.52
5	C	216	NAG	O5-C1	7.89	1.56	1.43
5	C	216	NAG	C4-C5	-5.54	1.41	1.53
5	C	216	NAG	C8-C7	4.47	1.59	1.50
5	C	216	NAG	C3-C2	-3.84	1.44	1.52
5	A	214	NAG	O5-C1	2.88	1.48	1.43
5	C	216	NAG	O7-C7	-2.80	1.17	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	216	NAG	O5-C5-C4	4.83	122.58	110.83
5	C	216	NAG	C4-C3-C2	3.92	116.77	111.02
5	C	216	NAG	C1-C2-N2	-3.36	105.14	110.43
5	A	214	NAG	C2-N2-C7	-3.19	118.62	122.90
5	C	216	NAG	C6-C5-C4	2.96	120.28	113.02
5	C	216	NAG	O5-C5-C6	2.94	113.39	107.66
5	C	216	NAG	C1-O5-C5	-2.66	108.63	112.19
5	B	250	NAG	C2-N2-C7	-2.62	119.39	122.90
5	B	248	NAG	C2-N2-C7	-2.38	119.71	122.90
5	A	215	NAG	C2-N2-C7	-2.18	119.98	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	248	NAG	C1
5	C	214	NAG	C1
5	C	215	NAG	C1
5	C	216	NAG	C1

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	216	NAG	C1-C2-N2-C7
5	A	215	NAG	C4-C5-C6-O6
5	C	214	NAG	C4-C5-C6-O6
5	C	216	NAG	O5-C5-C6-O6
5	A	215	NAG	O5-C5-C6-O6
5	C	214	NAG	O5-C5-C6-O6
5	B	250	NAG	C4-C5-C6-O6
5	D	250	NAG	C4-C5-C6-O6
5	B	250	NAG	O5-C5-C6-O6
5	D	250	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	D	248	NAG	O5-C5-C6-O6
5	D	248	NAG	C4-C5-C6-O6
5	C	215	NAG	O5-C5-C6-O6
5	B	251	NAG	O5-C5-C6-O6
5	C	215	NAG	C4-C5-C6-O6
5	D	251	NAG	C4-C5-C6-O6
5	D	251	NAG	O5-C5-C6-O6
5	A	216	NAG	C4-C5-C6-O6
5	A	216	NAG	O5-C5-C6-O6
5	D	249	NAG	C3-C2-N2-C7
5	B	249	NAG	C4-C5-C6-O6
5	C	215	NAG	C1-C2-N2-C7
5	C	216	NAG	C4-C5-C6-O6
5	B	251	NAG	C3-C2-N2-C7
5	C	215	NAG	C3-C2-N2-C7
5	B	249	NAG	O5-C5-C6-O6
5	D	249	NAG	C4-C5-C6-O6
5	B	251	NAG	C4-C5-C6-O6
5	A	214	NAG	C1-C2-N2-C7
5	B	250	NAG	C1-C2-N2-C7
5	D	249	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	216	NAG	5	0
5	A	214	NAG	2	0
5	A	216	NAG	2	0
5	D	249	NAG	2	0
5	D	248	NAG	2	0
5	C	214	NAG	3	0
5	B	251	NAG	1	0
5	B	248	NAG	3	0
5	B	249	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.