



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 05:30 AM UTC

PDB ID : 1D9K / pdb_00001d9k
Title : CRYSTAL STRUCTURE OF COMPLEX BETWEEN D10 TCR AND PMHC I-AK/CA
Authors : Reinherz, E.L.; Tan, K.; Tang, L.; Kern, P.; Liu, J.-H.; Xiong, Y.; Hussey, R.E.; Smolyar, A.; Hare, B.; Zhang, R.; Joachimiak, A.; Chang, H.-C.; Wagner, G.; Wang, J.-H.
Deposited on : 1999-10-28
Resolution : 3.20 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

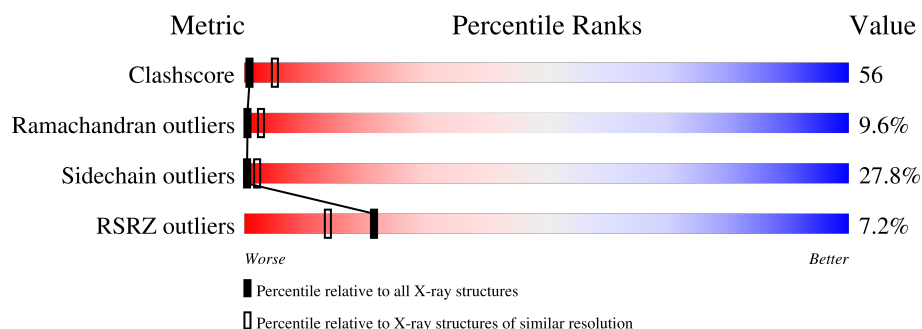
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	110	3% 22% 45% 30% .
1	E	110	3% 29% 47% 17% 6%
2	B	112	3% 27% 42% 21% 10%
2	F	112	6% 25% 50% 19% 6%
3	C	183	2% 32% 53% 14% .
3	G	183	13% 21% 56% 19% .

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Mol	Chain	Length	Quality of chain
4	D	188	
4	H	188	
5	P	16	
5	Q	16	
6	I	2	
6	J	2	
6	K	2	
6	L	2	

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
6	NAG	I	1	X	-	-	-
6	NAG	J	1	X	-	-	-
6	NAG	K	1	X	-	-	-
7	NAG	C	201	X	-	-	-
7	NAG	G	201	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9962 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 T-CELL RECEPTOR D10 (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	0	0
			877	563	145	167	2			
1	E	110	Total	C	N	O	S	0	0	0
			877	563	145	167	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	CYS	engineered mutation	GB 5724764
E	115	SER	CYS	engineered mutation	GB 5724764

- Molecule 2 is a protein called T-CELL RECEPTOR D10 (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	112	Total	C	N	O	S	0	0	0
			854	528	155	168	3			
2	F	112	Total	C	N	O	S	0	0	0
			854	528	155	168	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	116B	GLY	GLU	SEE REMARK 999	GB 1791255
B	116C	SER	ASP	SEE REMARK 999	GB 1791255
F	116B	GLY	GLU	SEE REMARK 999	GB 1791255
F	116C	SER	ASP	SEE REMARK 999	GB 1791255

- Molecule 3 is a protein called MHC I-AK A CHAIN (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	183	Total	C	N	O	S	0	0	0
			1485	959	237	286	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	183	Total	C	N	O	S	0	0	0
			1485	959	237	286	3			

- Molecule 4 is a protein called MHC I-AK B CHAIN (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	188	Total	C	N	O	S	0	0	0
			1575	991	287	291	6			
4	H	188	Total	C	N	O	S	0	0	0
			1575	991	287	291	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	GLY	ASN	conflict	UNP P06343
H	2	GLY	ASN	conflict	UNP P06343

- Molecule 5 is a protein called CONALBUMIN PEPTIDE.

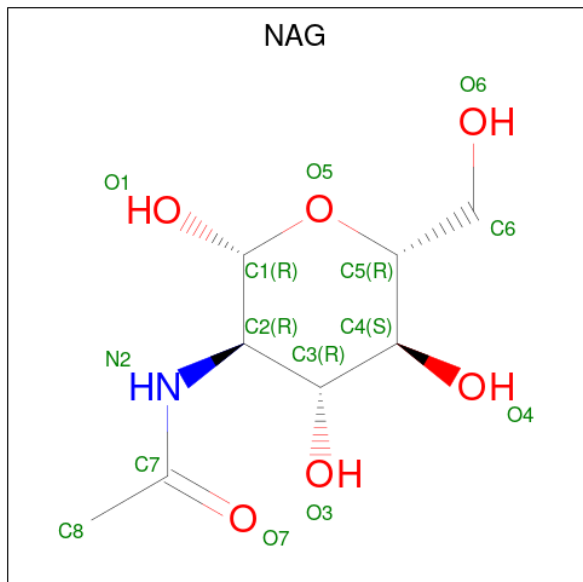
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	16	Total	C	N	O	0	0	0
			120	71	23	26			
5	Q	16	Total	C	N	O	0	0	0
			120	71	23	26			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

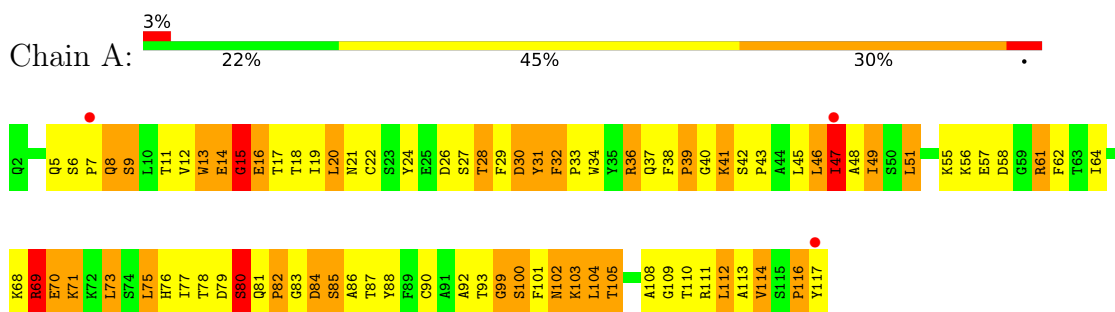


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		

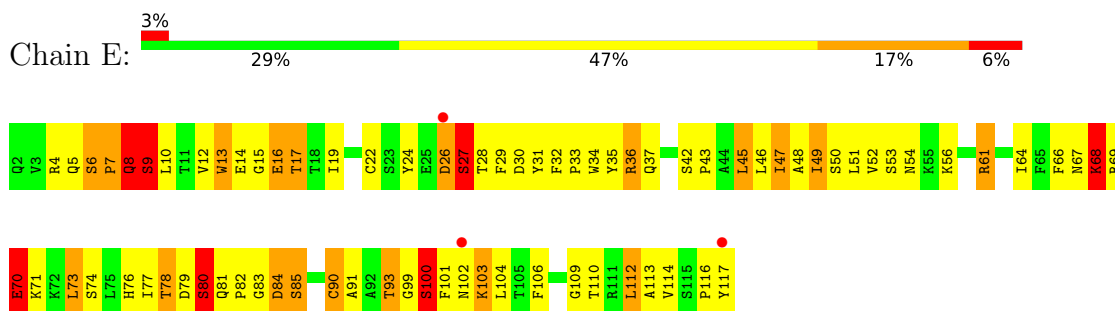
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

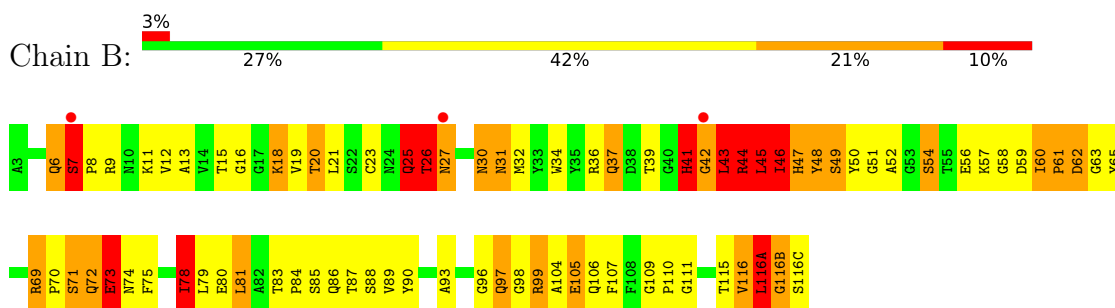
- Molecule 1: T-CELL RECEPTOR D10 (ALPHA CHAIN)



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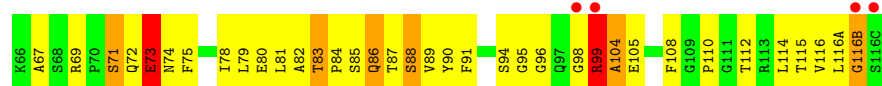


- Molecule 2: T-CELL RECEPTOR D10 (BETA CHAIN)

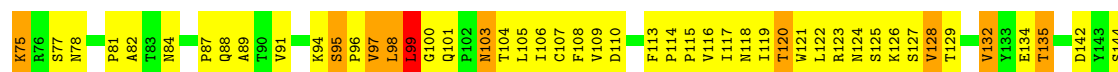


- Molecule 2: T-CELL RECEPTOR D10 (BETA CHAIN)

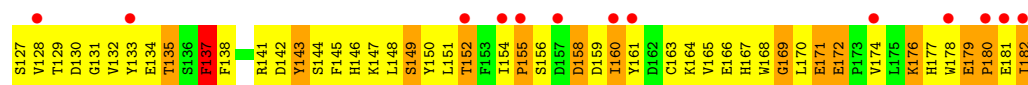
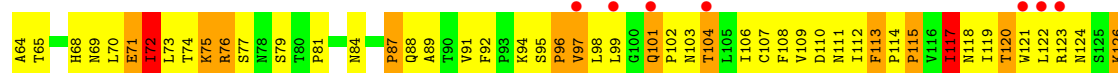




- Molecule 3: MHC I-AK A CHAIN (ALPHA CHAIN)



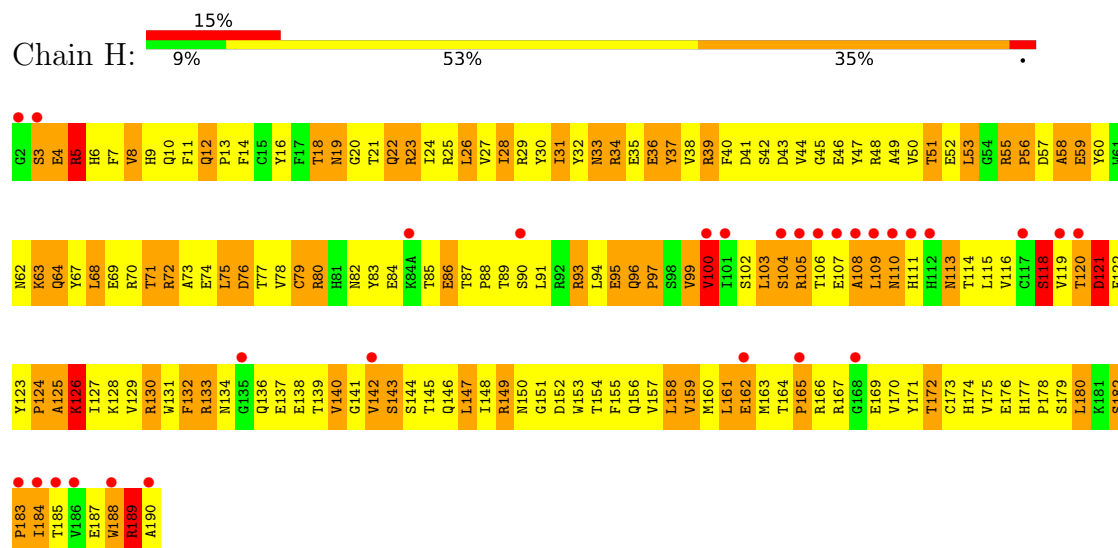
- Molecule 3: MHC I-AK A CHAIN (ALPHA CHAIN)



- Molecule 4: MHC I-AK B CHAIN (BETA CHAIN)



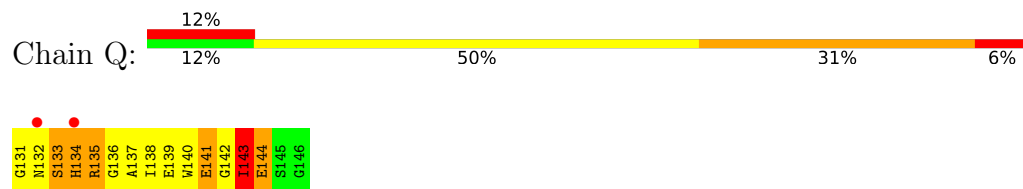
- Molecule 4: MHC I-AK B CHAIN (BETA CHAIN)



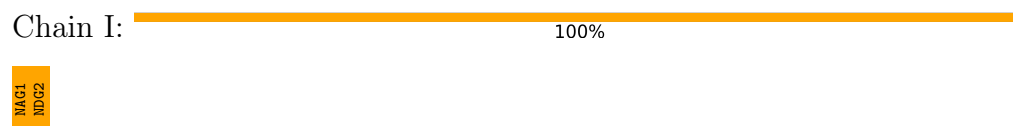
- Molecule 5: CONALBUMIN PEPTIDE



- Molecule 5: CONALBUMIN PEPTIDE



- Molecule 6: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

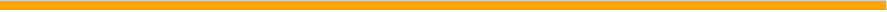


- Molecule 6: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

MDG1
MDG2

- Molecule 6: 2-acetamido-2-deoxy- α -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain L:  100%

MDG1
MDG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.60Å 345.30Å 97.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (15.00-3.20) 90.4 (15.00-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.19Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.247 , 0.293 0.266 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.840	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9962	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: NDG, 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	0.74	4/901 (0.4%)	1.23	12/1220 (1.0%)
1	E	0.74	3/901 (0.3%)	1.19	11/1220 (0.9%)
2	B	0.75	5/873 (0.6%)	1.20	13/1181 (1.1%)
2	F	0.56	1/873 (0.1%)	1.08	11/1181 (0.9%)
3	C	0.32	0/1530	0.87	4/2087 (0.2%)
3	G	0.32	0/1530	0.91	5/2087 (0.2%)
4	D	0.35	0/1615	0.88	5/2191 (0.2%)
4	H	0.35	0/1615	0.83	5/2191 (0.2%)
5	P	0.41	0/122	1.02	1/161 (0.6%)
5	Q	0.43	0/122	1.20	1/161 (0.6%)
All	All	0.50	13/10082 (0.1%)	1.00	68/13680 (0.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	41	HIS	C-N	-8.07	1.24	1.33
1	E	69	ARG	C-N	-7.31	1.23	1.33
2	B	47	HIS	C-N	-7.01	1.23	1.33
2	B	43	LEU	C-N	-6.47	1.24	1.33
2	B	42	GLY	C-N	-6.42	1.24	1.33
1	E	112	LEU	C-N	-6.18	1.25	1.33
1	A	16	GLU	C-N	-5.90	1.25	1.33
2	F	53	GLY	CA-C	5.70	1.59	1.51
1	A	15	GLY	C-N	-5.64	1.26	1.33
1	A	17	THR	N-CA	-5.32	1.39	1.46
1	E	68	LYS	C-N	-5.31	1.26	1.33
2	B	48	TYR	N-CA	-5.29	1.39	1.46
1	A	13	TRP	NE1-CE2	-5.17	1.31	1.37

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	GLU	N-CA-C	-13.95	92.45	111.28
1	E	84	ASP	N-CA-C	-11.84	98.86	113.18
2	F	52	ALA	O-C-N	-10.51	108.62	122.59
2	B	46	ILE	CB-CA-C	-10.15	99.83	111.09
2	B	43	LEU	O-C-N	-9.04	110.56	122.59
2	F	45	LEU	N-CA-C	8.36	122.56	110.10
1	A	47	ILE	O-C-N	8.26	132.90	122.57
5	Q	133	SER	N-CA-C	8.16	122.36	110.28
1	A	84	ASP	N-CA-C	-8.02	103.50	113.28
2	B	47	HIS	CB-CA-C	-7.41	95.67	110.42
2	F	29	HIS	N-CA-C	-7.41	97.05	108.76
1	E	83	GLY	N-CA-C	-7.20	104.56	114.64
3	C	181	GLU	N-CA-C	-7.05	104.68	112.72
3	G	48	PHE	N-CA-C	-6.84	103.88	111.82
4	D	120	THR	N-CA-C	6.81	120.22	109.81
2	B	46	ILE	O-C-N	6.76	129.27	122.71
1	A	16	GLU	N-CA-CB	-6.68	101.22	110.38
1	A	105	THR	N-CA-C	-6.57	98.03	108.73
1	E	71	LYS	O-C-N	6.53	130.65	122.55
1	A	69	ARG	N-CA-C	-6.40	102.54	110.41
2	F	43	LEU	CB-CA-C	-6.33	109.26	116.54
2	B	78	ILE	N-CA-C	6.20	117.94	108.71
1	E	70	GLU	N-CA-C	-6.19	97.62	110.80
2	B	63	GLY	N-CA-C	-6.16	106.01	114.64
1	A	83	GLY	N-CA-C	-6.11	106.09	114.64
1	E	70	GLU	CB-CA-C	6.08	122.51	110.42
3	G	117	ILE	N-CA-C	5.86	116.08	107.75
4	H	31	ILE	N-CA-C	5.84	117.84	108.85
4	D	46	GLU	N-CA-C	5.80	117.35	108.42
3	G	45	LEU	CA-C-N	5.79	127.07	119.84
3	G	45	LEU	C-N-CA	5.79	127.07	119.84
1	E	27	SER	N-CA-C	-5.78	106.27	113.38
2	B	26	THR	N-CA-C	-5.76	101.75	110.28
2	F	7	SER	CA-C-N	-5.73	113.65	120.13
2	F	7	SER	C-N-CA	-5.73	113.65	120.13
1	A	82	PRO	N-CA-C	-5.65	102.40	111.38
2	B	45	LEU	N-CA-C	5.65	119.30	110.32
2	F	30	ASN	N-CA-C	5.63	117.49	111.36
4	H	12	GLN	CA-C-N	5.63	126.87	119.84
4	H	12	GLN	C-N-CA	5.63	126.87	119.84
1	A	103	LYS	N-CA-C	-5.61	98.86	110.80
2	F	99	ARG	N-CA-C	-5.52	99.05	110.80
3	C	9	TYR	N-CA-C	5.51	117.69	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	GLU	N-CA-C	5.48	117.15	110.41
3	C	45	LEU	CA-C-N	5.37	126.55	119.84
3	C	45	LEU	C-N-CA	5.37	126.55	119.84
2	F	108	PHE	N-CA-C	5.35	118.71	110.42
3	G	169	GLY	N-CA-C	-5.34	107.24	115.73
4	H	182	SER	CA-C-N	5.33	126.50	119.84
4	H	182	SER	C-N-CA	5.33	126.50	119.84
2	F	25	GLN	N-CA-C	5.32	117.06	108.34
4	D	84(A)	LYS	N-CA-C	5.27	119.71	113.28
1	E	16	GLU	N-CA-C	5.27	122.02	110.80
1	E	100	SER	N-CA-C	5.21	121.42	113.19
2	B	25	GLN	N-CA-C	5.15	117.37	107.44
2	B	59	ASP	N-CA-C	-5.14	107.13	113.41
2	B	44	ARG	NE-CZ-NH2	5.13	123.81	119.20
2	B	60	ILE	CA-C-N	-5.12	113.44	119.84
2	B	60	ILE	C-N-CA	-5.12	113.44	119.84
5	P	137	ALA	N-CA-C	-5.10	102.97	110.52
2	F	49	SER	N-CA-C	5.10	116.27	108.52
4	D	112	HIS	N-CA-C	5.08	117.68	109.40
1	A	16	GLU	CA-C-N	-5.06	114.18	121.42
1	A	16	GLU	C-N-CA	-5.06	114.18	121.42
4	D	102	SER	N-CA-C	5.04	121.53	110.80
1	E	68	LYS	CA-C-N	-5.03	114.12	122.32
1	E	68	LYS	C-N-CA	-5.03	114.12	122.32
1	E	69	ARG	N-CA-C	5.01	117.70	108.58

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	877	0	848	99	0
1	E	877	0	848	102	0
2	B	854	0	813	109	0
2	F	854	0	813	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1485	0	1413	125	0
3	G	1485	0	1413	209	0
4	D	1575	0	1518	159	0
4	H	1575	0	1517	271	0
5	P	120	0	102	16	0
5	Q	120	0	102	39	0
6	I	28	0	24	3	0
6	J	28	0	24	0	0
6	K	28	0	24	0	0
6	L	28	0	24	4	0
7	C	14	0	13	0	0
7	G	14	0	13	0	0
All	All	9962	0	9509	1092	0

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 56.

All (1092) 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)
1:E:67:ASN:OD1	1:E:70:GLU:HB2	1.25	1.36
1:A:7:PRO:HB2	1:A:110:THR:HG21	1.20	1.17
3:C:179:GLU:H	3:C:180:PRO:CD	1.59	1.16
1:E:102:ASN:HA	2:F:104:ALA:HA	1.24	1.15
1:E:26:ASP:HB3	1:E:29:PHE:CD1	1.84	1.13
3:C:179:GLU:H	3:C:180:PRO:HD2	0.92	1.07
4:H:56:PRO:HB2	5:Q:143:ILE:HG21	1.36	1.06
3:G:118:ASN:HB2	3:G:166:GLU:HB2	1.30	1.06
1:A:47:ILE:HD11	1:A:58:ASP:HB3	1.36	1.04
2:F:69:ARG:HH11	2:F:72:GLN:HA	1.21	1.03
3:G:81:PRO:HB3	4:H:5:ARG:HG2	1.36	1.03
2:B:7:SER:HB3	2:B:8:PRO:HD3	1.39	1.03
2:F:7:SER:HB3	2:F:8:PRO:HD3	1.38	1.03
4:D:34:ARG:HH11	4:D:34:ARG:HG2	1.20	1.01
2:F:87:THR:HG23	2:F:115:THR:HA	1.37	1.01
4:H:134:ASN:HA	4:H:170:VAL:HB	1.38	1.00
3:C:179:GLU:N	3:C:180:PRO:HD2	1.75	0.99
4:H:176:GLU:HG3	4:H:183:PRO:HG3	1.42	0.99
2:F:69:ARG:NH1	2:F:72:GLN:HA	1.79	0.97
1:A:85:SER:HB3	1:A:113:ALA:HA	1.45	0.96
1:A:13:TRP:O	1:A:15:GLY:N	1.97	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:174:HIS:HA	4:H:185:THR:HG22	1.48	0.95
4:D:108:ALA:HB1	4:D:111:HIS:HB2	1.43	0.95
4:H:113:ASN:HB2	4:H:165:PRO:HD3	1.49	0.94
1:A:45:LEU:HD12	1:A:46:LEU:H	1.30	0.94
4:H:108:ALA:HB1	4:H:111:HIS:HB2	1.49	0.94
4:H:33:ASN:O	4:H:34:ARG:HG2	1.65	0.93
2:F:6:GLN:HG3	2:F:110:PRO:HD2	1.48	0.93
1:A:30:ASP:HA	1:A:51:LEU:HD21	1.50	0.93
1:E:26:ASP:CB	1:E:29:PHE:CE1	2.53	0.91
3:G:119:ILE:HG12	3:G:165:VAL:HG22	1.49	0.91
2:F:15:THR:OG1	2:F:116(B):GLY:HA3	1.70	0.90
3:G:181:GLU:HG3	3:G:182:ILE:H	1.36	0.90
3:C:103:ASN:HD22	3:C:104:THR:H	1.17	0.90
4:H:172:THR:HG23	4:H:187:GLU:HG3	1.53	0.89
2:B:32:MET:HG3	2:B:69:ARG:HH21	1.38	0.89
1:E:26:ASP:HB3	1:E:29:PHE:HD1	1.36	0.89
3:C:171:GLU:CD	3:C:171:GLU:H	1.80	0.88
3:C:118:ASN:HB2	3:C:166:GLU:HB3	1.54	0.88
3:C:160:ILE:HA	3:C:179:GLU:HB3	1.55	0.88
3:C:180:PRO:HB2	3:C:182:ILE:HG13	1.55	0.88
4:D:99:VAL:HG13	4:D:119:VAL:HG13	1.55	0.88
3:G:120:THR:HG23	3:G:164:LYS:HB3	1.54	0.87
4:D:128:LYS:HE2	4:D:130:ARG:HD2	1.54	0.87
4:D:87:THR:HA	4:D:91:LEU:HD12	1.56	0.86
4:H:104:SER:HB2	4:H:114:THR:HB	1.57	0.86
1:A:7:PRO:HB2	1:A:110:THR:CG2	2.05	0.86
2:B:6:GLN:HG3	2:B:110:PRO:HD2	1.57	0.86
3:G:144:SER:HB3	4:H:34:ARG:HH12	1.40	0.86
4:H:134:ASN:CA	4:H:170:VAL:HB	2.06	0.86
2:F:65:TYR:CE2	2:F:79:LEU:HD21	2.11	0.85
4:D:34:ARG:HG2	4:D:34:ARG:NH1	1.87	0.85
4:D:116:VAL:HG22	4:D:160:MET:HG2	1.59	0.85
3:G:1:ILE:HG22	3:G:2:GLU:H	1.42	0.85
4:H:76:ASP:HA	4:H:80:ARG:HB3	1.59	0.85
4:H:37:TYR:HA	4:H:51:THR:HG23	1.57	0.85
1:A:47:ILE:HD12	1:A:62:PHE:CB	2.06	0.84
1:E:8:GLN:O	1:E:8:GLN:HG3	1.78	0.84
1:E:5:GLN:HE22	1:E:90:CYS:H	1.25	0.83
3:G:45:LEU:O	3:G:48:PHE:HB2	1.78	0.83
1:E:102:ASN:HA	2:F:104:ALA:CA	2.08	0.83
2:B:44:ARG:HG2	2:B:60:ILE:HD11	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ASN:O	1:E:68:LYS:O	1.97	0.83
1:A:30:ASP:HA	1:A:51:LEU:CD2	2.09	0.82
1:E:26:ASP:HB3	1:E:29:PHE:CE1	2.13	0.82
3:C:53:ARG:O	5:P:134:HIS:HB2	1.80	0.82
2:B:87:THR:HG23	2:B:115:THR:HA	1.63	0.81
2:F:36:ARG:HH21	2:F:86:GLN:HA	1.43	0.81
5:Q:143:ILE:HD12	5:Q:144:GLU:H	1.46	0.81
1:A:16:GLU:O	1:A:80:SER:OG	1.99	0.81
1:A:61:ARG:HB3	1:A:78:THR:HB	1.62	0.81
2:F:31:ASN:HB3	2:F:50:TYR:HA	1.63	0.81
3:G:71:GLU:HB3	3:G:75:LYS:HZ1	1.44	0.80
4:D:131:TRP:CD1	4:D:161:LEU:HB2	2.16	0.80
3:G:45:LEU:HD12	3:G:45:LEU:H	1.47	0.80
3:G:135:THR:HG21	3:G:148:LEU:HB2	1.62	0.80
3:C:71:GLU:HG2	3:C:75:LYS:HE3	1.63	0.80
2:F:16:GLY:HA2	2:F:81:LEU:HA	1.62	0.80
3:G:3:ALA:HA	4:H:18:THR:HG23	1.64	0.80
2:F:7:SER:HB3	2:F:8:PRO:CD	2.12	0.79
1:E:51:LEU:HD23	1:E:66:PHE:CE2	2.16	0.79
2:F:98:GLY:O	4:H:67:TYR:CE1	2.36	0.79
1:E:36:ARG:HG2	1:E:46:LEU:HD13	1.64	0.78
4:H:41:ASP:HB3	4:H:44:VAL:HG23	1.63	0.78
4:H:68:LEU:HG	4:H:69:GLU:N	1.98	0.78
1:A:47:ILE:HD12	1:A:62:PHE:HB3	1.65	0.78
3:G:71:GLU:HB3	3:G:75:LYS:NZ	1.99	0.78
4:H:109:LEU:O	4:H:110:ASN:HB2	1.82	0.78
2:B:57:LYS:HB3	2:B:61:PRO:HG3	1.65	0.78
4:D:36:GLU:HG2	4:D:50:VAL:HG21	1.66	0.78
1:E:26:ASP:CB	1:E:29:PHE:CD1	2.67	0.78
2:B:26:THR:O	2:B:27:ASN:HB2	1.83	0.77
4:H:74:GLU:HA	4:H:77:THR:OG1	1.84	0.77
4:H:93:ARG:HG3	4:H:93:ARG:HH11	1.50	0.77
2:B:7:SER:HB3	2:B:8:PRO:CD	2.15	0.77
1:E:81:GLN:O	1:E:84:ASP:HB2	1.85	0.77
1:A:14:GLU:HG2	1:A:14:GLU:O	1.85	0.76
3:G:14:GLN:HB3	3:G:19:ILE:HB	1.66	0.76
3:G:134:GLU:HG2	3:G:135:THR:H	1.48	0.76
2:F:43:LEU:O	2:F:44:ARG:HG2	1.85	0.76
4:D:99:VAL:HG11	4:D:175:VAL:HG21	1.68	0.75
2:B:25:GLN:NE2	2:B:32:MET:HE2	2.02	0.75
2:F:60:ILE:N	2:F:61:PRO:HD3	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:THR:HG21	1:A:112:LEU:HD22	1.68	0.75
3:G:60:LEU:HD12	3:G:60:LEU:H	1.51	0.75
3:G:10:ILE:HG13	4:H:13:PRO:HD2	1.68	0.75
3:G:53:ARG:HH21	5:Q:131:GLY:HA3	1.52	0.75
1:A:47:ILE:CD1	1:A:58:ASP:HB3	2.16	0.75
1:E:67:ASN:OD1	1:E:70:GLU:CB	2.21	0.75
5:Q:143:ILE:CG1	5:Q:144:GLU:H	1.97	0.75
1:A:102:ASN:HA	2:B:104:ALA:HA	1.67	0.74
4:H:22:GLN:HE22	6:L:1:NAG:H2	1.52	0.74
1:E:5:GLN:NE2	1:E:90:CYS:H	1.84	0.74
5:Q:143:ILE:CD1	5:Q:144:GLU:H	2.00	0.74
2:B:49:SER:HB2	2:B:54:SER:O	1.88	0.74
1:A:47:ILE:HD12	1:A:62:PHE:HB2	1.70	0.74
3:G:8:SER:HB3	3:G:10:ILE:HD11	1.68	0.74
3:G:113:PHE:CZ	4:H:33:ASN:O	2.40	0.74
2:B:41:HIS:HB2	2:B:44:ARG:HD2	1.68	0.73
4:D:172:THR:HA	4:D:187:GLU:HA	1.71	0.73
2:B:15:THR:OG1	2:B:116(B):GLY:HA3	1.87	0.73
1:E:82:PRO:HA	1:E:114:VAL:HB	1.69	0.73
3:G:65:THR:HG23	5:Q:140:TRP:O	1.89	0.73
4:H:103:LEU:HD21	4:H:188:TRP:CZ2	2.24	0.73
2:B:46:ILE:HG23	2:B:60:ILE:O	1.87	0.73
4:D:129:VAL:HG11	4:D:159:VAL:HG21	1.70	0.73
2:F:3:ALA:HB3	2:F:26:THR:HB	1.70	0.72
1:E:37:GLN:HB2	1:E:43:PRO:HB3	1.70	0.72
3:G:128:VAL:HG11	3:G:151:LEU:HD11	1.70	0.72
3:C:81:PRO:HB3	4:D:5:ARG:HG2	1.72	0.72
2:B:15:THR:HG23	2:B:84:PRO:HD3	1.71	0.72
4:D:85:THR:O	4:D:88:PRO:HD2	1.90	0.72
4:D:160:MET:H	4:D:160:MET:CE	2.01	0.72
3:C:179:GLU:N	3:C:180:PRO:CD	2.36	0.72
3:G:135:THR:O	3:G:147:LYS:HD3	1.89	0.72
3:C:135:THR:O	3:C:147:LYS:HE2	1.90	0.72
3:G:147:LYS:C	3:G:148:LEU:HD12	2.15	0.72
1:A:82:PRO:HG3	1:A:116:PRO:HB3	1.72	0.72
4:D:85:THR:C	4:D:88:PRO:HD2	2.15	0.72
3:G:123:ARG:HG2	3:G:124:ASN:HD22	1.55	0.71
1:E:93:THR:HG22	1:E:99:GLY:H	1.55	0.71
1:E:101:PHE:H	4:H:70:ARG:HH22	1.38	0.71
3:G:65:THR:HG21	5:Q:139:GLU:HB3	1.72	0.71
4:H:56:PRO:HB2	5:Q:143:ILE:CG2	2.18	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:HA	1:A:111:ARG:HA	1.73	0.71
4:D:103:LEU:HD23	4:D:114:THR:O	1.91	0.71
2:B:69:ARG:HG2	2:B:75:PHE:CD1	2.26	0.71
3:G:142:ASP:HB2	4:H:34:ARG:HH22	1.54	0.71
3:C:68:HIS:NE2	3:C:72:ILE:HD11	2.06	0.70
2:B:6:GLN:CG	2:B:110:PRO:HD2	2.21	0.70
2:F:25:GLN:O	2:F:25:GLN:HG2	1.90	0.70
4:H:71:THR:O	4:H:74:GLU:HG3	1.92	0.70
1:E:51:LEU:HD23	1:E:66:PHE:HE2	1.57	0.70
2:B:47:HIS:O	2:B:48:TYR:HB3	1.90	0.70
4:H:75:LEU:O	4:H:79:CYS:HB2	1.92	0.70
4:H:108:ALA:CB	4:H:111:HIS:HB2	2.22	0.70
4:H:93:ARG:HG3	4:H:93:ARG:NH1	2.04	0.69
3:G:43:TRP:HH2	5:Q:134:HIS:HE1	1.39	0.69
3:G:117:ILE:HG21	3:G:119:ILE:HD12	1.74	0.69
3:C:52:ARG:HD3	4:D:89:THR:HG21	1.74	0.69
1:E:61:ARG:HG3	1:E:78:THR:O	1.92	0.69
3:G:118:ASN:CB	3:G:166:GLU:HB2	2.18	0.69
3:C:103:ASN:ND2	3:C:104:THR:H	1.90	0.69
1:A:8:GLN:O	1:A:8:GLN:HG3	1.91	0.69
1:E:22:CYS:HB3	1:E:73:LEU:HD23	1.75	0.69
1:A:6:SER:N	1:A:7:PRO:HD2	2.07	0.69
4:D:114:THR:HA	4:D:162:GLU:HA	1.74	0.69
3:G:1:ILE:HG22	3:G:2:GLU:N	2.07	0.69
3:G:8:SER:HA	4:H:13:PRO:O	1.93	0.69
4:H:118:SER:HA	4:H:158:LEU:HB3	1.74	0.69
3:C:120:THR:HG23	3:C:164:LYS:HB3	1.73	0.69
1:E:102:ASN:CA	2:F:104:ALA:HA	2.14	0.69
2:F:72:GLN:O	2:F:74:ASN:N	2.26	0.69
2:B:52:ALA:O	2:B:69:ARG:HB3	1.93	0.69
1:A:5:GLN:NE2	1:A:109:GLY:H	1.91	0.68
4:H:49:ALA:HB2	4:H:58:ALA:HB2	1.74	0.68
2:F:87:THR:HG22	2:F:87:THR:O	1.92	0.68
3:G:144:SER:HB3	4:H:34:ARG:NH1	2.07	0.68
2:F:36:ARG:NH2	2:F:86:GLN:HA	2.06	0.68
3:G:181:GLU:CG	3:G:182:ILE:H	2.06	0.68
3:C:57:GLN:HA	3:C:57:GLN:HE21	1.59	0.68
1:A:29:PHE:HD2	1:A:92:ALA:HB1	1.58	0.68
2:B:32:MET:HG3	2:B:69:ARG:NH2	2.08	0.68
4:H:188:TRP:O	4:H:189:ARG:HB2	1.94	0.68
1:A:45:LEU:CD1	1:A:46:LEU:H	2.04	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:GLU:HG2	1:E:82:PRO:HD3	1.76	0.68
2:B:32:MET:HE3	2:B:69:ARG:HE	1.58	0.67
4:D:131:TRP:HB3	4:D:161:LEU:HD13	1.75	0.67
4:H:134:ASN:HA	4:H:170:VAL:CB	2.22	0.67
3:C:56:PRO:O	3:C:60:LEU:HD12	1.95	0.67
4:D:164:THR:O	4:D:166:ARG:HG3	1.94	0.67
3:G:148:LEU:HB3	3:G:150:TYR:HE2	1.60	0.67
4:H:56:PRO:CB	5:Q:143:ILE:HG21	2.19	0.67
1:A:22:CYS:HB3	1:A:73:LEU:HD23	1.77	0.67
4:H:12:GLN:HB2	4:H:29:ARG:HB2	1.76	0.67
3:C:135:THR:HG23	3:C:148:LEU:O	1.93	0.67
2:B:44:ARG:CG	2:B:60:ILE:HD11	2.25	0.67
3:G:142:ASP:HB2	4:H:34:ARG:NH2	2.10	0.67
4:H:115:LEU:O	4:H:160:MET:HA	1.95	0.67
4:H:138:GLU:O	4:H:142:VAL:HG21	1.95	0.67
1:E:26:ASP:CB	1:E:29:PHE:HE1	2.06	0.66
2:F:28:ASN:HB2	2:F:72:GLN:OE1	1.95	0.66
1:A:26:ASP:HB3	1:A:29:PHE:CD1	2.29	0.66
2:F:32:MET:HE3	2:F:69:ARG:CZ	2.26	0.66
3:G:43:TRP:HH2	5:Q:134:HIS:CE1	2.14	0.66
4:H:133:ARG:HB2	4:H:138:GLU:HG3	1.77	0.66
4:H:133:ARG:HH11	4:H:133:ARG:HB3	1.61	0.66
3:G:156:SER:HB3	3:G:159:ASP:OD2	1.95	0.66
1:E:26:ASP:HB2	1:E:29:PHE:CE1	2.31	0.66
4:H:111:HIS:O	4:H:165:PRO:HD2	1.95	0.66
2:B:25:GLN:HE21	2:B:32:MET:HE2	1.61	0.66
6:I:1:NAG:H61	6:I:2:NDG:C8	2.25	0.66
2:F:98:GLY:O	4:H:67:TYR:HE1	1.78	0.66
3:G:49:ALA:O	3:G:51:LEU:N	2.28	0.66
3:G:123:ARG:HA	3:G:161:TYR:HD2	1.61	0.66
5:Q:143:ILE:O	5:Q:144:GLU:HB2	1.95	0.65
3:C:162:ASP:HB3	3:C:175:LEU:HD22	1.78	0.65
2:F:38:ASP:C	2:F:40:GLY:H	2.05	0.65
4:D:130:ARG:HB3	4:D:132:PHE:HE1	1.62	0.65
5:Q:134:HIS:N	5:Q:134:HIS:CD2	2.65	0.65
1:A:43:PRO:HG2	2:B:43:LEU:HD21	1.79	0.65
4:H:47:TYR:HB2	4:H:62:ASN:OD1	1.97	0.65
1:A:11:THR:HB	1:E:9:SER:HB2	1.79	0.64
2:B:7:SER:CB	2:B:8:PRO:HD3	2.23	0.64
2:F:49:SER:HB2	2:F:54:SER:O	1.96	0.64
3:G:137:PHE:HB3	3:G:145:PHE:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:16:TYR:O	4:H:24:ILE:HA	1.97	0.64
2:F:71:SER:O	2:F:72:GLN:C	2.40	0.64
4:H:29:ARG:HA	4:H:39:ARG:HB2	1.79	0.64
1:E:34:TRP:HE1	1:E:73:LEU:HD21	1.61	0.64
3:G:147:LYS:O	3:G:148:LEU:HD12	1.97	0.64
4:H:163:MET:HE3	4:H:188:TRP:HZ3	1.63	0.64
3:G:137:PHE:H	3:G:137:PHE:HD2	1.43	0.64
4:H:134:ASN:HD21	4:H:169:GLU:HG3	1.62	0.64
2:B:72:GLN:O	2:B:74:ASN:N	2.31	0.64
2:B:52:ALA:O	2:B:69:ARG:O	2.15	0.64
2:F:44:ARG:HG3	2:F:60:ILE:CD1	2.27	0.64
3:G:107:CYS:HB2	3:G:121:TRP:CZ2	2.33	0.64
4:H:86:GLU:OE1	4:H:86:GLU:HA	1.98	0.64
4:H:175:VAL:HB	4:H:184:ILE:O	1.97	0.64
5:Q:143:ILE:CG1	5:Q:144:GLU:N	2.56	0.64
6:I:1:NAG:H61	6:I:2:NDG:C7	2.28	0.63
2:F:8:PRO:O	2:F:112:THR:HG23	1.98	0.63
1:E:116:PRO:O	1:E:117:TYR:HB2	1.97	0.63
4:H:50:VAL:HG23	4:H:51:THR:H	1.63	0.63
4:H:132:PHE:HB2	4:H:172:THR:HB	1.80	0.63
2:B:49:SER:OG	2:B:69:ARG:HG3	1.98	0.63
4:H:119:VAL:HG21	4:H:129:VAL:HG21	1.80	0.63
2:F:31:ASN:HA	2:F:69:ARG:NH2	2.12	0.63
2:F:46:ILE:O	2:F:58:GLY:HA3	1.98	0.63
4:H:114:THR:HA	4:H:161:LEU:O	1.99	0.63
2:F:32:MET:HG3	2:F:69:ARG:NH2	2.14	0.63
2:B:32:MET:HE3	2:B:69:ARG:NE	2.12	0.63
1:E:34:TRP:CZ2	1:E:90:CYS:HB2	2.34	0.63
2:F:44:ARG:HG3	2:F:60:ILE:HD11	1.81	0.63
3:G:110:ASP:OD1	3:G:111:ASN:N	2.28	0.63
1:A:47:ILE:CD1	1:A:62:PHE:HB2	2.29	0.63
1:A:36:ARG:O	1:A:36:ARG:HG3	1.99	0.62
1:E:68:LYS:O	1:E:70:GLU:N	2.32	0.62
4:D:11:PHE:CD1	5:P:139:GLU:HG3	2.34	0.62
4:D:163:MET:SD	4:D:163:MET:N	2.71	0.62
1:E:100:SER:O	1:E:101:PHE:HB3	1.98	0.62
2:F:32:MET:HE3	2:F:69:ARG:NH1	2.14	0.62
6:I:1:NAG:H61	6:I:2:NDG:H8C3	1.82	0.62
4:D:149:ARG:HG3	4:D:155:PHE:CE2	2.34	0.62
4:H:144:SER:HB2	4:H:159:VAL:HG13	1.82	0.62
2:F:6:GLN:CG	2:F:110:PRO:HD2	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:122:PHE:CE2	4:D:155:PHE:HB2	2.35	0.62
3:G:181:GLU:HG3	3:G:182:ILE:N	2.09	0.62
4:H:148:ILE:HB	4:H:156:GLN:O	2.00	0.62
2:B:87:THR:CG2	2:B:115:THR:HA	2.27	0.62
4:D:166:ARG:O	4:D:169:GLU:HG3	1.99	0.62
1:A:26:ASP:OD1	1:A:28:THR:HB	1.99	0.62
3:C:52:ARG:CD	4:D:89:THR:HG21	2.27	0.62
2:F:16:GLY:HA2	2:F:81:LEU:CA	2.29	0.62
3:G:108:PHE:CZ	3:G:110:ASP:HB2	2.35	0.62
3:G:129:THR:HG22	3:G:129:THR:O	1.98	0.62
4:D:40:PHE:HB2	4:D:47:TYR:CD1	2.34	0.62
4:H:116:VAL:HG13	4:H:160:MET:HG3	1.80	0.62
4:H:147:LEU:HD11	4:H:155:PHE:HB3	1.79	0.62
4:D:25:ARG:HD2	4:D:43:ASP:OD2	2.00	0.62
2:F:37:GLN:HE21	2:F:43:LEU:H	1.46	0.62
2:B:83:THR:HG22	2:B:85:SER:H	1.65	0.61
3:G:135:THR:HG23	3:G:148:LEU:O	2.00	0.61
4:D:127:ILE:HG13	4:D:176:GLU:O	2.00	0.61
3:G:107:CYS:HB2	3:G:121:TRP:CH2	2.35	0.61
4:H:164:THR:O	4:H:166:ARG:HG3	2.00	0.61
1:E:61:ARG:HH22	1:E:81:GLN:HB2	1.65	0.61
3:C:171:GLU:CD	3:C:171:GLU:N	2.54	0.61
4:D:152:ASP:O	4:D:153:TRP:HB2	2.00	0.61
4:H:129:VAL:HA	4:H:174:HIS:O	2.01	0.61
1:A:104:LEU:HD21	2:B:104:ALA:O	2.00	0.61
1:A:8:GLN:HE21	1:E:12:VAL:HA	1.65	0.61
4:D:36:GLU:O	4:D:50:VAL:HB	2.01	0.61
4:D:160:MET:H	4:D:160:MET:HE2	1.65	0.61
1:E:30:ASP:OD1	4:H:70:ARG:HD2	2.01	0.61
3:G:48:PHE:CZ	4:H:89:THR:HB	2.36	0.61
4:H:97:PRO:HB3	4:H:122:PHE:HB3	1.81	0.61
1:E:30:ASP:HB3	4:H:77:THR:HG21	1.82	0.61
2:F:83:THR:O	2:F:86:GLN:HG3	2.00	0.60
4:H:147:LEU:HD12	4:H:148:ILE:N	2.16	0.60
1:E:19:ILE:HG23	1:E:76:HIS:HE1	1.65	0.60
4:H:103:LEU:HD22	4:H:115:LEU:HD23	1.83	0.60
4:D:32:TYR:O	4:D:33:ASN:HB2	2.00	0.60
1:E:14:GLU:CG	1:E:82:PRO:HD3	2.31	0.60
1:E:34:TRP:N	1:E:47:ILE:O	2.35	0.60
4:H:87:THR:HB	4:H:88:PRO:HD3	1.83	0.60
2:B:71:SER:O	2:B:72:GLN:C	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:TYR:CD2	5:P:143:ILE:HG12	2.37	0.60
4:D:108:ALA:O	4:D:165:PRO:HG2	2.01	0.60
4:H:21:THR:HG21	4:H:84:GLU:OE2	2.02	0.60
4:H:21:THR:HG21	4:H:84:GLU:CG	2.31	0.60
2:B:65:TYR:CE2	2:B:79:LEU:HD21	2.36	0.60
1:E:102:ASN:HD21	2:F:95:GLY:HA3	1.67	0.60
2:F:47:HIS:O	2:F:48:TYR:HB3	2.01	0.60
4:H:149:ARG:NH1	4:H:149:ARG:HG3	2.17	0.60
2:B:84:PRO:HA	2:B:116:VAL:HB	1.83	0.59
4:H:72:ARG:O	4:H:75:LEU:HB2	2.01	0.59
4:H:130:ARG:HD3	4:H:174:HIS:HB3	1.84	0.59
4:H:134:ASN:N	4:H:170:VAL:HB	2.16	0.59
3:C:3:ALA:HA	4:D:18:THR:HG23	1.85	0.59
3:C:61:GLN:O	3:C:64:ALA:HB3	2.03	0.59
4:D:25:ARG:HH11	4:D:43:ASP:HB2	1.66	0.59
4:D:99:VAL:HG11	4:D:175:VAL:CG2	2.32	0.59
2:F:60:ILE:N	2:F:61:PRO:CD	2.64	0.59
4:H:19:ASN:ND2	6:L:1:NAG:C6	2.64	0.59
4:H:113:ASN:HB2	4:H:165:PRO:CD	2.29	0.59
1:A:93:THR:HG23	1:A:99:GLY:N	2.18	0.59
3:C:45:LEU:O	3:C:48:PHE:HB2	2.03	0.59
4:D:76:ASP:OD1	4:D:80:ARG:HD2	2.02	0.59
4:H:57:ASP:OD1	5:Q:142:GLY:HA3	2.02	0.59
3:C:32:PHE:HB2	3:C:42:VAL:O	2.02	0.59
4:D:132:PHE:CZ	4:D:137:GLU:HB2	2.38	0.59
4:H:149:ARG:HG3	4:H:149:ARG:HH11	1.66	0.59
3:G:134:GLU:HG2	3:G:135:THR:N	2.17	0.59
1:A:45:LEU:HD12	1:A:46:LEU:N	2.10	0.59
3:C:108:PHE:HE2	3:C:110:ASP:HB2	1.68	0.59
4:D:134:ASN:HD21	4:D:169:GLU:HB3	1.68	0.59
4:D:144:SER:HB2	4:D:159:VAL:HG12	1.85	0.59
4:H:33:ASN:O	4:H:34:ARG:CG	2.46	0.59
4:H:144:SER:CB	4:H:159:VAL:HG13	2.33	0.59
2:B:37:GLN:O	2:B:88:SER:HB2	2.02	0.59
3:G:14:GLN:HE21	4:H:6:HIS:HB3	1.67	0.59
4:H:41:ASP:HB3	4:H:44:VAL:CG2	2.30	0.59
1:A:101:PHE:HB2	5:P:138:ILE:HG21	1.84	0.59
2:B:87:THR:HG23	2:B:116:VAL:H	1.68	0.59
1:E:28:THR:HG23	5:Q:135:ARG:HB3	1.83	0.59
4:H:184:ILE:O	4:H:184:ILE:HG22	2.02	0.59
2:B:32:MET:HE3	2:B:69:ARG:HH21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:16:TYR:HB2	4:D:25:ARG:HB3	1.85	0.58
4:D:108:ALA:HB1	4:D:111:HIS:CB	2.25	0.58
3:G:159:ASP:O	3:G:180:PRO:HD3	2.03	0.58
1:A:104:LEU:HD11	2:B:106:GLN:HG3	1.84	0.58
3:C:180:PRO:CB	3:C:182:ILE:HG13	2.31	0.58
2:F:84:PRO:HA	2:F:116:VAL:HB	1.85	0.58
3:G:76:ARG:HH22	4:H:57:ASP:CG	2.11	0.58
3:G:124:ASN:OD1	3:G:159:ASP:HA	2.02	0.58
3:G:171:GLU:C	3:G:172:GLU:HG3	2.28	0.58
2:B:20:THR:HG23	2:B:78:ILE:HG23	1.84	0.58
3:C:113:PHE:HA	3:C:114:PRO:C	2.27	0.58
2:B:31:ASN:HB3	2:B:50:TYR:HA	1.85	0.58
3:G:117:ILE:HD12	3:G:167:HIS:ND1	2.19	0.58
4:H:38:VAL:HA	4:H:49:ALA:HA	1.85	0.58
3:G:12:VAL:O	3:G:20:GLY:HA2	2.02	0.58
5:Q:143:ILE:HG13	5:Q:144:GLU:N	2.18	0.58
1:A:24:TYR:CZ	1:A:71:LYS:HG2	2.39	0.58
2:B:31:ASN:HB2	2:B:49:SER:O	2.03	0.58
1:E:85:SER:HB3	1:E:113:ALA:HA	1.84	0.58
4:D:71:THR:HA	4:D:74:GLU:HG3	1.86	0.58
1:E:116:PRO:O	1:E:117:TYR:CB	2.52	0.58
4:H:113:ASN:CB	4:H:165:PRO:HD3	2.29	0.58
3:C:57:GLN:HE21	3:C:57:GLN:CA	2.15	0.58
1:E:7:PRO:HB2	1:E:110:THR:HG21	1.85	0.58
1:E:101:PHE:N	4:H:70:ARG:HH22	2.01	0.58
3:C:99:LEU:HA	3:C:155:PRO:HB2	1.86	0.57
1:E:31:TYR:HB2	4:H:70:ARG:HD3	1.83	0.57
3:G:6:VAL:HG22	4:H:16:TYR:CE1	2.38	0.57
4:H:152:ASP:O	4:H:153:TRP:HB2	2.03	0.57
3:C:73:LEU:O	3:C:77:SER:HB3	2.04	0.57
2:B:98:GLY:C	2:B:104:ALA:H	2.12	0.57
2:F:7:SER:CB	2:F:8:PRO:HD3	2.23	0.57
4:H:133:ARG:HA	4:H:170:VAL:O	2.04	0.57
4:H:163:MET:HE1	4:H:165:PRO:HA	1.87	0.57
2:B:43:LEU:O	2:B:44:ARG:C	2.44	0.57
4:D:102:SER:O	4:D:115:LEU:HD22	2.02	0.57
3:G:32:PHE:HB2	3:G:42:VAL:O	2.04	0.57
4:H:115:LEU:HD21	4:H:188:TRP:CD2	2.40	0.57
4:H:129:VAL:HG22	4:H:175:VAL:HA	1.87	0.57
2:B:32:MET:HE3	2:B:69:ARG:NH2	2.18	0.57
2:F:83:THR:HG22	2:F:85:SER:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:18:THR:O	4:H:19:ASN:HB3	2.04	0.57
2:B:62:ASP:OD1	2:B:62:ASP:O	2.22	0.57
2:F:29:HIS:HB3	2:F:95:GLY:O	2.05	0.57
3:G:84:ASN:HD21	3:G:168:TRP:HB3	1.69	0.57
4:H:68:LEU:O	4:H:71:THR:HB	2.05	0.57
3:G:45:LEU:HD12	3:G:45:LEU:N	2.18	0.57
3:G:52:ARG:HA	5:Q:132:ASN:HB3	1.86	0.57
4:H:21:THR:HA	4:H:24:ILE:HD11	1.86	0.57
4:H:111:HIS:O	4:H:164:THR:HA	2.03	0.57
1:A:61:ARG:HD2	1:A:78:THR:O	2.05	0.56
2:B:32:MET:CE	2:B:69:ARG:HH21	2.18	0.56
2:F:57:LYS:HD3	2:F:61:PRO:HB3	1.87	0.56
3:G:24:PHE:O	3:G:31:LEU:HB2	2.05	0.56
3:G:124:ASN:HA	3:G:160:ILE:O	2.05	0.56
4:D:39:ARG:HG2	4:D:40:PHE:N	2.19	0.56
4:D:56:PRO:O	5:P:143:ILE:HD11	2.05	0.56
4:D:103:LEU:HD23	4:D:114:THR:C	2.30	0.56
1:A:32:PHE:CD1	1:A:32:PHE:N	2.73	0.56
3:C:32:PHE:HD1	3:C:33:TYR:N	2.04	0.56
4:D:34:ARG:HH11	4:D:34:ARG:CG	2.04	0.56
2:F:71:SER:O	2:F:73:GLU:HG2	2.04	0.56
3:G:121:TRP:CG	3:G:151:LEU:HD22	2.40	0.56
4:H:30:TYR:HH	5:Q:140:TRP:CD1	2.24	0.56
1:E:17:THR:HA	1:E:77:ILE:O	2.05	0.56
3:G:135:THR:CG2	3:G:148:LEU:HB2	2.33	0.56
3:C:95:SER:H	3:C:103:ASN:HD21	1.53	0.56
4:D:25:ARG:NH1	4:D:43:ASP:HB2	2.20	0.56
2:F:41:HIS:N	2:F:41:HIS:CD2	2.73	0.56
2:F:50:TYR:CE2	3:G:61:GLN:HG2	2.40	0.56
4:H:127:ILE:HG13	4:H:176:GLU:O	2.05	0.56
3:G:72:ILE:HG22	3:G:73:LEU:HD22	1.88	0.56
1:A:37:GLN:O	1:A:86:ALA:HB1	2.06	0.56
1:A:81:GLN:O	1:A:114:VAL:HG21	2.06	0.56
3:C:89:ALA:HB3	3:C:176:LYS:HG3	1.87	0.56
2:F:24:ASN:HA	2:F:73:GLU:O	2.06	0.56
3:C:122:LEU:HA	3:C:126:LYS:O	2.06	0.56
1:E:26:ASP:CG	1:E:29:PHE:HE1	2.12	0.56
2:F:36:ARG:O	2:F:36:ARG:HG2	2.06	0.56
1:A:79:ASP:O	1:A:80:SER:C	2.48	0.56
3:G:13:TYR:HA	3:G:19:ILE:O	2.06	0.56
3:G:84:ASN:ND2	3:G:168:TRP:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:93:ARG:HH11	4:H:93:ARG:CG	2.17	0.56
4:H:114:THR:HG23	4:H:161:LEU:C	2.31	0.56
1:E:24:TYR:HE1	1:E:26:ASP:O	1.89	0.55
4:H:96:GLN:HA	4:H:179:SER:OG	2.06	0.55
3:G:10:ILE:N	3:G:10:ILE:HD12	2.21	0.55
1:E:19:ILE:HG23	1:E:76:HIS:CE1	2.41	0.55
4:D:93:ARG:O	4:D:94:LEU:HD23	2.05	0.55
1:A:101:PHE:HB2	5:P:138:ILE:CG2	2.36	0.55
2:F:6:GLN:HG3	2:F:110:PRO:CD	2.28	0.55
4:D:114:THR:OG1	4:D:162:GLU:HB2	2.07	0.55
3:G:65:THR:CG2	5:Q:139:GLU:HB3	2.37	0.55
3:G:91:VAL:HA	3:G:106:ILE:O	2.07	0.55
4:H:78:VAL:O	4:H:82:ASN:HB2	2.06	0.55
4:H:116:VAL:HA	4:H:159:VAL:O	2.07	0.55
1:E:33:PRO:HA	1:E:48:ALA:HA	1.88	0.54
3:G:112:ILE:O	3:G:113:PHE:HB2	2.07	0.54
3:G:170:LEU:HD13	3:G:174:VAL:HG23	1.88	0.54
4:H:36:GLU:HG2	4:H:50:VAL:HG21	1.90	0.54
2:B:42:GLY:O	2:B:44:ARG:N	2.41	0.54
4:D:55:ARG:HB3	4:D:56:PRO:HD3	1.88	0.54
4:H:21:THR:CA	4:H:24:ILE:HD11	2.37	0.54
2:B:97:GLN:C	2:B:98:GLY:O	2.48	0.54
4:D:160:MET:H	4:D:160:MET:HE3	1.73	0.54
2:F:18:LYS:HA	2:F:79:LEU:O	2.07	0.54
3:G:72:ILE:HD12	5:Q:142:GLY:O	2.06	0.54
2:F:16:GLY:CA	2:F:81:LEU:HA	2.34	0.54
4:D:129:VAL:CG1	4:D:159:VAL:HG21	2.36	0.54
3:G:91:VAL:HG13	3:G:106:ILE:O	2.07	0.54
3:C:105:LEU:HD11	3:C:178:TRP:CE3	2.43	0.54
4:D:116:VAL:HG13	4:D:160:MET:HG3	1.89	0.54
4:H:113:ASN:HB3	4:H:163:MET:SD	2.47	0.54
1:A:8:GLN:N	1:A:110:THR:HG23	2.23	0.54
3:C:24:PHE:O	3:C:31:LEU:HB2	2.08	0.54
3:C:110:ASP:OD1	3:C:146:HIS:HB3	2.08	0.54
3:C:109:VAL:HG21	3:C:119:ILE:HG12	1.90	0.54
3:G:81:PRO:CB	4:H:5:ARG:HG2	2.25	0.54
2:B:16:GLY:HA2	2:B:81:LEU:HD12	1.89	0.54
1:E:17:THR:HG23	1:E:78:THR:HG23	1.90	0.54
2:F:41:HIS:CD2	2:F:41:HIS:H	2.26	0.54
1:A:7:PRO:HG3	1:A:21:ASN:H	1.74	0.53
4:H:21:THR:HB	4:H:24:ILE:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:113:PHE:HZ	4:H:33:ASN:O	1.91	0.53
4:H:178:PRO:C	4:H:180:LEU:H	2.15	0.53
2:B:51:GLY:C	2:B:69:ARG:HH11	2.17	0.53
2:B:70:PRO:O	2:B:71:SER:HB3	2.08	0.53
3:C:123:ARG:H	3:C:128:VAL:HG22	1.73	0.53
1:A:11:THR:HA	1:A:113:ALA:O	2.09	0.53
4:D:22:GLN:HG3	4:D:23:ARG:N	2.23	0.53
1:A:26:ASP:HB3	1:A:29:PHE:CE1	2.44	0.53
3:G:6:VAL:HG13	4:H:16:TYR:HE1	1.73	0.53
3:G:160:ILE:O	3:G:160:ILE:HD12	2.09	0.53
1:A:47:ILE:O	1:A:64:ILE:HD11	2.09	0.53
1:E:51:LEU:HD23	1:E:66:PHE:CZ	2.42	0.53
1:A:61:ARG:HB2	1:A:78:THR:H	1.74	0.53
3:G:65:THR:HG22	5:Q:139:GLU:OE2	2.08	0.53
3:G:137:PHE:CD2	3:G:137:PHE:N	2.76	0.53
4:H:116:VAL:HG22	4:H:160:MET:HG2	1.89	0.53
4:H:134:ASN:H	4:H:170:VAL:HB	1.73	0.53
1:A:31:TYR:HB2	4:D:70:ARG:HD3	1.91	0.53
2:F:38:ASP:OD1	2:F:88:SER:HB2	2.08	0.53
4:H:95:GLU:HA	4:H:95:GLU:OE1	2.09	0.53
3:C:68:HIS:CE1	3:C:72:ILE:HD11	2.43	0.53
1:A:69:ARG:O	1:A:70:GLU:HB3	2.09	0.52
1:A:100:SER:O	1:A:101:PHE:HB3	2.09	0.52
4:D:129:VAL:HG11	4:D:159:VAL:CG2	2.39	0.52
4:D:148:ILE:HB	4:D:156:GLN:HG2	1.89	0.52
2:F:116(A):LEU:O	2:F:116(B):GLY:C	2.52	0.52
4:H:11:PHE:O	4:H:13:PRO:HD3	2.08	0.52
4:D:132:PHE:CE2	4:D:137:GLU:HB2	2.45	0.52
3:G:123:ARG:HG2	3:G:124:ASN:ND2	2.24	0.52
1:A:18:THR:HB	1:A:77:ILE:HB	1.92	0.52
3:C:106:ILE:HG12	3:C:150:TYR:CD1	2.43	0.52
2:F:98:GLY:O	2:F:99:ARG:HG3	2.10	0.52
3:G:10:ILE:HG13	4:H:13:PRO:CD	2.37	0.52
3:G:28:GLY:HA3	4:H:149:ARG:NH2	2.25	0.52
4:H:12:GLN:HG3	4:H:31:ILE:CD1	2.40	0.52
4:H:57:ASP:O	4:H:60:TYR:HB3	2.10	0.52
1:E:28:THR:HG23	5:Q:135:ARG:CB	2.40	0.52
3:G:117:ILE:HG23	3:G:119:ILE:H	1.74	0.52
2:B:116(A):LEU:O	2:B:116(B):GLY:C	2.52	0.52
3:C:65:THR:O	3:C:68:HIS:HB3	2.09	0.52
3:C:154:ILE:O	3:C:156:SER:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:60:ILE:O	2:F:60:ILE:HG22	2.09	0.52
4:H:32:TYR:CD1	4:H:32:TYR:C	2.86	0.52
4:H:73:ALA:O	4:H:77:THR:HG23	2.10	0.52
2:B:20:THR:CG2	2:B:78:ILE:HD13	2.39	0.52
4:D:18:THR:HG21	4:D:23:ARG:HH11	1.75	0.52
1:E:67:ASN:O	1:E:68:LYS:C	2.53	0.52
2:F:6:GLN:NE2	2:F:34:TRP:CH2	2.76	0.52
3:C:148:LEU:N	3:C:148:LEU:HD12	2.24	0.52
4:D:31:ILE:HG23	4:D:35:GLU:C	2.34	0.52
4:D:37:TYR:HA	4:D:51:THR:HG23	1.92	0.52
4:H:82:ASN:HD21	5:Q:134:HIS:HB2	1.74	0.52
4:D:164:THR:HG21	4:D:166:ARG:NH2	2.24	0.52
4:H:78:VAL:HG13	5:Q:135:ARG:O	2.10	0.52
4:H:166:ARG:O	4:H:190:ALA:HB1	2.10	0.52
1:A:19:ILE:HG12	1:A:76:HIS:CE1	2.45	0.52
2:B:49:SER:CB	2:B:69:ARG:HG3	2.39	0.52
3:C:43:TRP:CH2	3:C:52:ARG:HG3	2.44	0.52
2:B:60:ILE:O	2:B:60:ILE:HG22	2.09	0.51
3:C:11:THR:HB	4:D:11:PHE:HB3	1.92	0.51
3:G:84:ASN:HD22	3:G:168:TRP:C	2.17	0.51
4:H:25:ARG:HD2	4:H:43:ASP:OD1	2.10	0.51
3:C:32:PHE:CD1	3:C:32:PHE:C	2.87	0.51
3:C:117:ILE:HG12	3:C:118:ASN:H	1.74	0.51
2:F:36:ARG:NH2	2:F:85:SER:O	2.44	0.51
3:G:1:ILE:CG2	3:G:2:GLU:H	2.19	0.51
3:C:15:SER:OG	3:C:16:PRO:HA	2.09	0.51
3:C:146:HIS:NE2	4:D:149:ARG:NH2	2.59	0.51
3:C:167:HIS:ND1	3:C:168:TRP:N	2.57	0.51
3:C:178:TRP:C	3:C:179:GLU:HG3	2.35	0.51
4:D:188:TRP:CG	4:D:189:ARG:N	2.78	0.51
4:H:188:TRP:CG	4:H:189:ARG:N	2.76	0.51
4:D:114:THR:HG22	4:D:115:LEU:N	2.25	0.51
5:Q:134:HIS:N	5:Q:134:HIS:HD2	2.09	0.51
4:D:26:LEU:HB2	4:D:75:LEU:HD13	1.92	0.51
1:E:112:LEU:HG	1:E:113:ALA:N	2.24	0.51
1:E:112:LEU:HD21	1:E:114:VAL:HG22	1.92	0.51
5:Q:143:ILE:O	5:Q:144:GLU:CB	2.57	0.51
2:F:88:SER:OG	2:F:89:VAL:N	2.40	0.51
3:G:95:SER:O	3:G:103:ASN:ND2	2.44	0.51
3:G:179:GLU:CD	3:G:179:GLU:H	2.19	0.51
4:H:32:TYR:C	4:H:32:TYR:HD1	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:35:GLU:HG2	4:H:51:THR:HG21	1.92	0.51
4:D:74:GLU:OE2	5:P:135:ARG:NH2	2.44	0.51
2:F:38:ASP:C	2:F:40:GLY:N	2.68	0.51
3:G:71:GLU:O	3:G:72:ILE:C	2.54	0.51
4:H:93:ARG:HD3	4:H:123:TYR:CD1	2.46	0.51
4:H:104:SER:CB	4:H:114:THR:HB	2.35	0.51
1:A:101:PHE:H	4:D:70:ARG:HH22	1.58	0.51
3:C:48:PHE:HZ	4:D:90:SER:HA	1.76	0.51
4:D:103:LEU:CD2	4:D:114:THR:HB	2.41	0.51
1:E:15:GLY:HA2	1:E:79:ASP:HA	1.92	0.51
3:G:121:TRP:CZ3	3:G:163:CYS:HB2	2.46	0.51
1:A:29:PHE:HA	1:A:93:THR:O	2.11	0.51
2:B:32:MET:HE3	2:B:69:ARG:CZ	2.41	0.51
2:B:43:LEU:O	2:B:44:ARG:O	2.29	0.51
3:C:103:ASN:HD22	3:C:104:THR:N	1.96	0.51
2:F:26:THR:O	2:F:27:ASN:HB2	2.10	0.51
3:G:98:LEU:O	3:G:155:PRO:HG2	2.10	0.50
4:H:97:PRO:HD2	4:H:180:LEU:HD21	1.93	0.50
2:B:57:LYS:HD3	2:B:61:PRO:HB2	1.92	0.50
4:D:72:ARG:O	4:D:75:LEU:HB2	2.10	0.50
3:G:120:THR:CG2	3:G:164:LYS:HB3	2.34	0.50
3:G:158:ASP:N	3:G:158:ASP:OD1	2.42	0.50
1:A:28:THR:HG23	5:P:135:ARG:CD	2.41	0.50
3:C:35:ASP:CG	3:C:38:LYS:HB2	2.37	0.50
1:E:93:THR:HG21	1:E:103:LYS:O	2.10	0.50
3:G:92:PHE:CZ	3:G:106:ILE:HG21	2.46	0.50
3:G:123:ARG:HA	3:G:161:TYR:CD2	2.44	0.50
1:A:7:PRO:HG3	1:A:20:LEU:HA	1.94	0.50
1:A:61:ARG:CB	1:A:78:THR:HB	2.36	0.50
3:C:154:ILE:O	3:C:155:PRO:C	2.55	0.50
3:G:9(A):GLY:N	3:G:24:PHE:CD1	2.80	0.50
1:E:47:ILE:HG21	1:E:64:ILE:HG13	1.92	0.50
4:D:104:SER:C	4:D:106:THR:H	2.20	0.50
2:F:16:GLY:HA2	2:F:81:LEU:C	2.36	0.50
3:G:74:THR:HA	4:H:32:TYR:OH	2.12	0.50
4:H:32:TYR:C	4:H:34:ARG:H	2.20	0.50
3:C:142:ASP:OD1	3:C:144:SER:HB3	2.11	0.50
2:F:43:LEU:O	2:F:44:ARG:CG	2.59	0.50
2:B:36:ARG:HB3	2:B:46:ILE:HD11	1.93	0.50
3:G:45:LEU:HD21	4:H:153:TRP:CD2	2.46	0.50
1:E:24:TYR:CE1	1:E:26:ASP:O	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:TRP:CD1	1:E:64:ILE:HD11	2.46	0.49
2:B:16:GLY:CA	2:B:81:LEU:HD12	2.42	0.49
2:F:44:ARG:CG	2:F:60:ILE:HD11	2.42	0.49
3:G:91:VAL:HG12	3:G:92:PHE:N	2.26	0.49
4:H:133:ARG:O	4:H:134:ASN:HB2	2.11	0.49
3:C:47:GLU:O	3:C:50:GLN:HG3	2.12	0.49
1:E:12:VAL:HG12	1:E:13:TRP:H	1.76	0.49
3:G:14:GLN:HB2	4:H:8:VAL:HG13	1.94	0.49
2:B:58:GLY:C	2:B:61:PRO:HD3	2.37	0.49
4:D:99:VAL:HA	4:D:118:SER:O	2.12	0.49
2:F:37:GLN:HG3	2:F:91:PHE:CE1	2.47	0.49
3:G:14:GLN:CG	4:H:8:VAL:HG13	2.42	0.49
3:G:52:ARG:HD3	4:H:89:THR:HG21	1.94	0.49
3:G:57:GLN:HE21	3:G:57:GLN:HA	1.77	0.49
2:B:37:GLN:HG2	2:B:43:LEU:CD1	2.42	0.49
2:B:45:LEU:HG	2:B:46:ILE:N	2.27	0.49
2:B:48:TYR:HH	3:C:57:GLN:CD	2.21	0.49
3:C:32:PHE:CD1	3:C:33:TYR:N	2.80	0.49
5:Q:140:TRP:O	5:Q:141:GLU:HB3	2.12	0.49
2:B:6:GLN:HG3	2:B:110:PRO:CD	2.36	0.49
3:C:1:ILE:HG21	4:D:16:TYR:CZ	2.48	0.49
3:G:26:PHE:O	3:G:27:ASP:HB2	2.12	0.49
3:G:130:ASP:OD1	3:G:131:GLY:N	2.44	0.49
4:H:83:TYR:HA	4:H:86:GLU:HB2	1.95	0.49
1:A:13:TRP:O	1:A:14:GLU:C	2.53	0.49
3:C:9(A):GLY:O	3:C:10:ILE:C	2.55	0.49
4:D:61:TRP:NE1	5:P:141:GLU:O	2.41	0.49
4:H:148:ILE:HB	4:H:156:GLN:HG2	1.94	0.49
4:H:171:TYR:HD2	4:H:190:ALA:HB2	1.78	0.49
1:A:46:LEU:HD23	1:A:46:LEU:O	2.13	0.49
1:E:93:THR:HG22	1:E:100:SER:OG	2.12	0.49
3:G:14:GLN:HG3	4:H:7:PHE:O	2.11	0.49
4:H:173:CYS:O	4:H:185:THR:HA	2.13	0.49
1:A:33:PRO:HB3	1:A:48:ALA:HB2	1.95	0.49
2:F:57:LYS:HB3	2:F:61:PRO:CG	2.43	0.49
2:B:36:ARG:HH21	2:B:88:SER:HB3	1.77	0.48
2:B:61:PRO:O	2:B:62:ASP:OD1	2.31	0.48
2:B:83:THR:O	2:B:116:VAL:HG21	2.12	0.48
2:F:99:ARG:O	2:F:104:ALA:HB3	2.13	0.48
3:G:6:VAL:HG13	4:H:16:TYR:CE1	2.48	0.48
3:G:70:LEU:HD12	4:H:9:HIS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:MET:O	2:B:48:TYR:HB2	2.12	0.48
4:H:118:SER:OG	4:H:158:LEU:HD23	2.13	0.48
1:A:5:GLN:NE2	1:A:90:CYS:H	2.11	0.48
1:A:75:LEU:HD12	1:A:76:HIS:N	2.29	0.48
4:D:74:GLU:HA	4:D:78:VAL:HG23	1.94	0.48
1:A:34:TRP:CH2	1:A:90:CYS:HB2	2.48	0.48
2:B:37:GLN:HB2	2:B:89:VAL:HB	1.95	0.48
3:C:87:PRO:HD3	3:C:167:HIS:CD2	2.48	0.48
4:D:87:THR:HB	4:D:88:PRO:HD3	1.95	0.48
4:H:163:MET:HE3	4:H:188:TRP:CZ3	2.48	0.48
4:D:134:ASN:OD1	4:D:169:GLU:HA	2.14	0.48
4:D:148:ILE:HD12	4:D:148:ILE:N	2.28	0.48
4:H:62:ASN:O	4:H:68:LEU:HB3	2.13	0.48
1:A:42:SER:HB3	2:B:109:GLY:O	2.13	0.48
1:E:34:TRP:CH2	1:E:90:CYS:HB2	2.48	0.48
1:E:47:ILE:HG22	1:E:64:ILE:CD1	2.44	0.48
3:G:104:THR:HG23	3:G:152:THR:HA	1.95	0.48
4:H:122:PHE:O	4:H:155:PHE:HB2	2.14	0.48
3:C:15:SER:HA	3:C:16:PRO:C	2.38	0.48
3:G:89:ALA:HA	3:G:109:VAL:HG22	1.95	0.48
3:C:129:THR:HA	3:C:132:VAL:HG21	1.94	0.48
4:D:25:ARG:HD2	4:D:43:ASP:CG	2.39	0.48
1:E:32:PHE:CD1	1:E:32:PHE:N	2.81	0.48
3:G:10:ILE:HG23	4:H:11:PHE:O	2.14	0.48
3:G:142:ASP:O	3:G:143:TYR:HB2	2.14	0.48
4:H:113:ASN:O	4:H:162:GLU:HA	2.13	0.48
3:C:91:VAL:HA	3:C:106:ILE:O	2.14	0.48
3:C:169:GLY:C	3:C:170:LEU:HG	2.39	0.48
1:E:93:THR:OG1	1:E:104:LEU:HA	2.14	0.48
1:E:61:ARG:HH21	1:E:84:ASP:CG	2.22	0.47
2:F:114:LEU:HD12	2:F:115:THR:N	2.28	0.47
4:D:97:PRO:HB2	4:D:119:VAL:HG12	1.96	0.47
4:H:126:LYS:NZ	4:H:178:PRO:HG3	2.29	0.47
3:C:87:PRO:HD3	3:C:167:HIS:HD2	1.79	0.47
3:G:73:LEU:HB3	4:H:32:TYR:CD2	2.49	0.47
4:H:52:GLU:O	4:H:55:ARG:HB3	2.15	0.47
4:H:131:TRP:CD1	4:H:161:LEU:HB2	2.49	0.47
3:C:84:ASN:HD21	3:C:168:TRP:HB3	1.79	0.47
4:D:114:THR:O	4:D:115:LEU:HD23	2.14	0.47
4:D:133:ARG:N	4:D:136:GLN:O	2.36	0.47
4:H:128:LYS:HE2	4:H:130:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:164:THR:O	4:H:166:ARG:N	2.47	0.47
2:B:36:ARG:O	2:B:36:ARG:HG3	2.14	0.47
4:D:29:ARG:HD3	4:D:36:GLU:OE2	2.14	0.47
4:H:123:TYR:CG	4:H:124:PRO:HA	2.49	0.47
1:A:13:TRP:CH2	1:E:8:GLN:HB2	2.50	0.47
3:C:98:LEU:O	3:C:99:LEU:C	2.57	0.47
3:C:115:PRO:HB3	3:C:145:PHE:CD1	2.50	0.47
4:D:31:ILE:HG23	4:D:36:GLU:N	2.30	0.47
1:E:35:TYR:CE2	1:E:45:LEU:HD12	2.50	0.47
1:E:47:ILE:HG22	1:E:64:ILE:HD11	1.95	0.47
2:F:28:ASN:C	2:F:28:ASN:OD1	2.57	0.47
3:G:28:GLY:HA3	4:H:149:ARG:HH22	1.78	0.47
3:G:29:ASP:HB3	4:H:153:TRP:NE1	2.30	0.47
3:G:60:LEU:HD12	3:G:60:LEU:N	2.26	0.47
2:B:26:THR:O	2:B:27:ASN:CB	2.58	0.47
4:D:47:TYR:HB2	4:D:62:ASN:OD1	2.15	0.47
2:F:32:MET:H	2:F:69:ARG:HH21	1.61	0.47
3:G:14:GLN:HB3	3:G:19:ILE:CB	2.39	0.47
3:G:15:SER:OG	3:G:16:PRO:HA	2.15	0.47
3:G:62:ASN:CG	5:Q:139:GLU:H	2.23	0.47
3:G:63:ILE:HG22	3:G:64:ALA:N	2.30	0.47
3:G:123:ARG:H	3:G:128:VAL:HG23	1.80	0.47
4:H:157:VAL:O	4:H:157:VAL:HG13	2.15	0.47
1:A:13:TRP:C	1:A:15:GLY:N	2.68	0.47
2:B:74:ASN:OD1	2:B:74:ASN:C	2.58	0.47
3:C:97:VAL:HG12	3:C:155:PRO:HB3	1.97	0.47
1:E:36:ARG:O	1:E:36:ARG:HG3	2.14	0.47
3:G:164:LYS:HE2	3:G:166:GLU:CG	2.45	0.47
4:H:46:GLU:HG3	4:H:47:TYR:O	2.14	0.47
4:H:150:ASN:HB2	4:H:154:THR:OG1	2.15	0.47
4:H:177:HIS:CE1	4:H:179:SER:HB3	2.50	0.47
4:D:15:CYS:HB3	4:D:17:PHE:CZ	2.50	0.47
1:E:12:VAL:HG12	1:E:13:TRP:N	2.30	0.47
3:G:46:PRO:C	3:G:48:PHE:H	2.23	0.47
1:A:11:THR:HB	1:E:9:SER:CB	2.43	0.46
1:E:49:ILE:HG23	1:E:50:SER:N	2.30	0.46
1:A:38:PHE:O	1:A:39:PRO:C	2.58	0.46
3:C:41:THR:HG21	3:C:54:PHE:O	2.15	0.46
3:C:125:SER:H	3:C:160:ILE:HD11	1.80	0.46
3:C:160:ILE:C	3:C:160:ILE:HD12	2.41	0.46
3:G:50:GLN:H	3:G:50:GLN:HG2	1.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:31:ILE:HG22	4:H:32:TYR:N	2.30	0.46
4:D:188:TRP:CG	4:D:189:ARG:H	2.33	0.46
3:G:65:THR:O	3:G:68:HIS:HB3	2.15	0.46
3:G:76:ARG:HE	5:Q:143:ILE:HD13	1.81	0.46
3:G:138:PHE:HB2	3:G:146:HIS:NE2	2.29	0.46
4:H:130:ARG:O	4:H:174:HIS:N	2.46	0.46
1:E:102:ASN:ND2	2:F:95:GLY:HA3	2.30	0.46
3:G:73:LEU:HD12	4:H:32:TYR:HD2	1.80	0.46
2:B:83:THR:C	2:B:85:SER:N	2.74	0.46
3:C:9:TYR:HB3	3:C:24:PHE:CZ	2.50	0.46
3:G:9:TYR:OH	4:H:86:GLU:HG2	2.15	0.46
3:G:60:LEU:HA	3:G:63:ILE:HB	1.98	0.46
4:H:19:ASN:ND2	4:H:22:GLN:NE2	2.63	0.46
2:B:83:THR:C	2:B:85:SER:H	2.22	0.46
1:E:106:PHE:CG	2:F:43:LEU:HD12	2.51	0.46
3:G:56:PRO:O	3:G:57:GLN:C	2.57	0.46
3:G:150:TYR:HE1	4:H:152:ASP:HB3	1.81	0.46
4:H:63:LYS:HE2	4:H:63:LYS:O	2.15	0.46
4:H:151:GLY:C	4:H:153:TRP:H	2.23	0.46
3:C:34:VAL:O	3:C:36:LEU:HD23	2.16	0.46
1:E:51:LEU:HD22	1:E:68:LYS:HD2	1.96	0.46
2:F:114:LEU:HD12	2:F:115:THR:H	1.81	0.46
1:A:49:ILE:HD11	1:A:55:LYS:C	2.41	0.46
2:B:105:GLU:OE1	2:B:107:PHE:CZ	2.69	0.46
3:C:52:ARG:NH1	4:D:89:THR:OG1	2.48	0.46
4:H:14:PHE:N	4:H:27:VAL:O	2.38	0.46
4:H:140:VAL:C	4:H:142:VAL:H	2.24	0.46
3:C:82:ALA:HB1	3:C:113:PHE:HE2	1.79	0.46
4:D:38:VAL:CA	4:D:50:VAL:HG23	2.46	0.46
2:F:32:MET:HE1	2:F:72:GLN:O	2.16	0.46
1:A:112:LEU:HD12	1:A:113:ALA:H	1.80	0.46
3:C:98:LEU:HD23	3:C:98:LEU:HA	1.82	0.46
4:D:130:ARG:HB3	4:D:132:PHE:CE1	2.47	0.46
1:E:15:GLY:O	1:E:17:THR:N	2.46	0.46
3:G:43:TRP:CH2	5:Q:134:HIS:HE1	2.27	0.46
3:G:123:ARG:HG3	3:G:161:TYR:HE2	1.80	0.46
4:H:25:ARG:HD2	4:H:43:ASP:CG	2.41	0.46
4:H:114:THR:HG23	4:H:162:GLU:N	2.30	0.46
4:H:133:ARG:CB	4:H:138:GLU:HG3	2.45	0.46
4:H:145:THR:HG21	4:H:158:LEU:HD12	1.98	0.46
1:A:101:PHE:HD2	1:A:101:PHE:O	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:THR:HG21	4:D:23:ARG:NH1	2.30	0.45
4:D:25:ARG:HH11	4:D:43:ASP:CB	2.28	0.45
4:D:131:TRP:HB2	4:D:142:VAL:HG22	1.99	0.45
4:D:163:MET:HG2	4:D:171:TYR:CE1	2.51	0.45
4:D:21:THR:HG21	4:D:84:GLU:CD	2.42	0.45
4:D:49:ALA:HB2	4:D:55:ARG:HA	1.98	0.45
4:D:100:VAL:O	4:D:117:CYS:O	2.35	0.45
3:G:45:LEU:HA	3:G:46:PRO:HD2	1.82	0.45
1:A:7:PRO:HG3	1:A:21:ASN:N	2.31	0.45
3:C:162:ASP:OD1	3:C:177:HIS:ND1	2.50	0.45
4:D:100:VAL:O	4:D:100:VAL:HG23	2.17	0.45
3:G:137:PHE:HB3	3:G:145:PHE:CB	2.45	0.45
3:G:176:LYS:HA	3:G:176:LYS:HD3	1.54	0.45
4:H:125:ALA:O	4:H:126:LYS:C	2.60	0.45
1:A:101:PHE:CZ	5:P:141:GLU:HG2	2.51	0.45
3:C:51:LEU:HD12	4:D:89:THR:HG22	1.98	0.45
4:D:52:GLU:OE1	4:D:55:ARG:NH1	2.50	0.45
3:G:76:ARG:NH2	4:H:57:ASP:CG	2.74	0.45
2:B:23:CYS:O	2:B:74:ASN:HA	2.16	0.45
3:C:135:THR:O	3:C:147:LYS:HG3	2.16	0.45
3:G:123:ARG:NH1	3:G:161:TYR:HE2	2.14	0.45
3:C:35:ASP:OD1	3:C:38:LYS:HB2	2.16	0.45
3:G:106:ILE:N	3:G:106:ILE:HD12	2.32	0.45
4:H:63:LYS:O	4:H:64:GLN:CG	2.65	0.45
2:B:18:LYS:HE3	2:B:80:GLU:HG2	1.98	0.45
4:D:146:GLN:O	4:D:148:ILE:HD12	2.17	0.45
3:G:26:PHE:C	3:G:28:GLY:H	2.24	0.45
3:G:76:ARG:HH21	5:Q:143:ILE:CG2	2.30	0.45
3:G:81:PRO:HA	4:H:7:PHE:CD1	2.52	0.45
4:H:19:ASN:ND2	6:L:1:NAG:H62	2.32	0.45
4:H:97:PRO:CB	4:H:122:PHE:HB3	2.45	0.45
4:H:131:TRP:HD1	4:H:142:VAL:HG13	1.82	0.45
1:A:16:GLU:H	1:A:16:GLU:HG3	1.24	0.45
4:D:62:ASN:O	4:D:68:LEU:HB2	2.15	0.45
3:G:95:SER:HB2	3:G:101:GLN:HE22	1.82	0.45
4:H:128:LYS:HE2	4:H:130:ARG:NH1	2.31	0.45
3:C:47:GLU:HG2	3:C:48:PHE:H	1.82	0.45
4:D:166:ARG:NH1	4:D:166:ARG:HG2	2.31	0.45
3:G:9:TYR:HD1	3:G:24:PHE:CD2	2.34	0.45
3:G:46:PRO:O	3:G:48:PHE:N	2.50	0.45
4:H:52:GLU:HG3	4:H:55:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:109:LEU:O	4:H:110:ASN:CB	2.59	0.45
4:H:145:THR:HG21	4:H:158:LEU:CD1	2.47	0.45
4:H:167:ARG:HA	4:H:190:ALA:O	2.16	0.45
1:E:54:ASN:HB2	1:E:66:PHE:O	2.17	0.44
4:H:87:THR:CB	4:H:88:PRO:HD3	2.46	0.44
2:B:43:LEU:HA	2:B:43:LEU:HD12	1.40	0.44
2:B:44:ARG:HB3	2:B:60:ILE:HD11	1.99	0.44
2:B:72:GLN:O	2:B:73:GLU:C	2.61	0.44
2:F:58:GLY:N	2:F:61:PRO:HG3	2.32	0.44
3:G:87:PRO:HB2	3:G:109:VAL:CG1	2.48	0.44
4:H:26:LEU:HB3	4:H:75:LEU:HD13	1.98	0.44
1:A:33:PRO:HA	1:A:48:ALA:HA	1.99	0.44
3:C:3:ALA:HB1	4:D:17:PHE:O	2.17	0.44
3:C:101:GLN:O	3:C:155:PRO:HD2	2.16	0.44
4:D:56:PRO:C	5:P:143:ILE:HD11	2.41	0.44
4:D:130:ARG:CB	4:D:132:PHE:HE1	2.29	0.44
4:D:142:VAL:O	4:D:142:VAL:HG12	2.15	0.44
1:E:26:ASP:OD2	1:E:29:PHE:HE1	2.01	0.44
1:A:116:PRO:O	1:A:117:TYR:HB2	2.15	0.44
3:G:33:TYR:O	3:G:42:VAL:HG23	2.18	0.44
3:G:68:HIS:CD2	3:G:69:ASN:N	2.86	0.44
2:B:81:LEU:HD12	2:B:81:LEU:HA	1.88	0.44
3:C:14:GLN:OE1	3:C:115:PRO:HD2	2.17	0.44
4:D:94:LEU:CD2	4:D:124:PRO:HD3	2.48	0.44
4:H:32:TYR:CE1	4:H:33:ASN:ND2	2.86	0.44
3:C:57:GLN:HA	3:C:57:GLN:NE2	2.28	0.44
3:G:122:LEU:HB3	3:G:126:LYS:H	1.83	0.44
4:H:115:LEU:HD11	4:H:188:TRP:CE3	2.52	0.44
1:A:15:GLY:O	1:A:79:ASP:HA	2.17	0.44
2:B:47:HIS:O	2:B:48:TYR:CB	2.49	0.44
2:B:87:THR:O	2:B:87:THR:HG22	2.18	0.44
3:C:11:THR:HG23	3:C:63:ILE:HD13	2.00	0.44
3:C:117:ILE:HG23	3:C:118:ASN:N	2.33	0.44
3:G:121:TRP:CD2	3:G:151:LEU:HD22	2.53	0.44
3:G:132:VAL:HG12	3:G:133:TYR:H	1.82	0.44
4:H:75:LEU:HD12	4:H:75:LEU:HA	1.88	0.44
1:A:55:LYS:HG2	1:A:56:LYS:N	2.31	0.44
2:F:90:TYR:CD1	2:F:90:TYR:N	2.86	0.44
3:G:149:SER:C	3:G:150:TYR:HD2	2.25	0.44
2:B:34:TRP:CD1	2:B:75:PHE:CE2	3.06	0.43
3:C:108:PHE:C	3:C:108:PHE:CD2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:MET:HE1	2:F:72:GLN:C	2.43	0.43
3:G:39:LYS:HG2	3:G:60:LEU:HD21	2.00	0.43
4:H:4:GLU:O	4:H:5:ARG:HB2	2.18	0.43
4:H:20:GLY:C	4:H:22:GLN:H	2.26	0.43
4:H:74:GLU:HA	4:H:78:VAL:HG23	2.00	0.43
1:A:116:PRO:O	1:A:117:TYR:CB	2.65	0.43
4:D:109:LEU:O	4:D:110:ASN:HB2	2.17	0.43
1:E:8:GLN:O	1:E:9:SER:HB2	2.17	0.43
1:E:91:ALA:HB2	1:E:106:PHE:CD2	2.52	0.43
3:G:35:ASP:OD2	3:G:38:LYS:HB2	2.18	0.43
4:H:120:THR:HA	4:H:156:GLN:HB2	1.99	0.43
1:A:112:LEU:HD12	1:A:113:ALA:N	2.33	0.43
3:C:53:ARG:HH12	5:P:131:GLY:N	2.15	0.43
1:E:78:THR:C	1:E:80:SER:N	2.75	0.43
4:H:83:TYR:CE2	4:H:91:LEU:HD11	2.52	0.43
1:A:81:GLN:O	1:A:84:ASP:HB2	2.18	0.43
3:C:97:VAL:HG21	3:C:178:TRP:CZ2	2.54	0.43
4:D:22:GLN:CG	4:D:23:ARG:N	2.81	0.43
4:D:56:PRO:CB	5:P:143:ILE:HD12	2.48	0.43
4:D:85:THR:HG21	5:P:134:HIS:CE1	2.53	0.43
3:G:71:GLU:O	3:G:74:THR:N	2.51	0.43
3:G:167:HIS:CD2	3:G:169:GLY:H	2.37	0.43
4:H:36:GLU:O	4:H:50:VAL:CG2	2.66	0.43
4:H:79:CYS:O	4:H:80:ARG:C	2.61	0.43
4:H:129:VAL:HG22	4:H:175:VAL:HG22	2.00	0.43
3:C:100:GLY:O	3:C:154:ILE:HG23	2.17	0.43
2:F:54:SER:HB2	2:F:56:GLU:OE2	2.19	0.43
2:F:72:GLN:O	2:F:73:GLU:C	2.60	0.43
4:H:147:LEU:HD12	4:H:147:LEU:C	2.43	0.43
1:A:108:ALA:HA	2:B:42:GLY:H	1.84	0.43
2:B:42:GLY:O	2:B:43:LEU:C	2.61	0.43
4:D:101:ILE:HD11	4:D:173:CYS:HB2	2.00	0.43
2:F:47:HIS:CB	2:F:67:ALA:HB2	2.49	0.43
2:F:67:ALA:HB1	2:F:75:PHE:CE1	2.54	0.43
3:G:99:LEU:HD12	3:G:155:PRO:O	2.19	0.43
4:H:53:LEU:O	4:H:56:PRO:HD2	2.18	0.43
1:A:29:PHE:CD2	1:A:92:ALA:HB1	2.44	0.43
2:B:20:THR:HG21	2:B:78:ILE:HD13	2.01	0.43
2:B:30:ASN:O	2:B:69:ARG:NH2	2.36	0.43
4:D:145:THR:HG22	4:D:158:LEU:O	2.19	0.43
4:D:189:ARG:O	4:D:190:ALA:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:26:PHE:CE1	4:H:86:GLU:HG3	2.53	0.43
4:H:32:TYR:O	4:H:34:ARG:N	2.51	0.43
4:H:82:ASN:ND2	5:Q:134:HIS:CB	2.82	0.43
4:H:141:GLY:O	4:H:161:LEU:HA	2.17	0.43
2:B:80:GLU:O	2:B:81:LEU:CB	2.67	0.43
3:C:66:GLY:O	3:C:67:LYS:C	2.62	0.43
3:C:105:LEU:HD23	3:C:105:LEU:HA	1.76	0.43
3:G:76:ARG:NH2	5:Q:143:ILE:HG12	2.34	0.43
3:G:148:LEU:HD22	4:H:151:GLY:HA3	2.00	0.43
4:H:26:LEU:O	4:H:41:ASP:HA	2.18	0.43
4:H:37:TYR:HA	4:H:51:THR:CG2	2.39	0.43
3:C:124:ASN:HA	3:C:160:ILE:HG13	2.01	0.43
4:D:74:GLU:CA	4:D:78:VAL:HG23	2.49	0.43
1:E:34:TRP:CE2	1:E:90:CYS:HB2	2.53	0.43
1:E:100:SER:O	1:E:101:PHE:CB	2.65	0.43
1:E:102:ASN:HD21	2:F:95:GLY:CA	2.29	0.43
3:G:9(A):GLY:O	4:H:13:PRO:HG3	2.19	0.43
3:G:115:PRO:HG3	3:G:145:PHE:CE1	2.54	0.43
3:G:121:TRP:CD1	3:G:151:LEU:HB2	2.53	0.43
4:H:149:ARG:HH11	4:H:149:ARG:CG	2.31	0.43
3:G:102:PRO:HA	3:G:154:ILE:HG12	2.01	0.43
4:H:56:PRO:O	4:H:57:ASP:C	2.62	0.43
4:H:57:ASP:OD1	5:Q:143:ILE:HG23	2.18	0.43
4:H:134:ASN:ND2	4:H:169:GLU:HG3	2.32	0.43
2:B:98:GLY:C	2:B:104:ALA:N	2.77	0.42
3:C:158:ASP:OD1	3:C:158:ASP:N	2.45	0.42
4:D:40:PHE:HB2	4:D:47:TYR:CE1	2.54	0.42
4:H:26:LEU:HD11	4:H:28:ILE:HG12	2.01	0.42
3:C:125:SER:N	3:C:160:ILE:HD11	2.34	0.42
4:D:74:GLU:O	4:D:78:VAL:HG23	2.19	0.42
4:D:144:SER:HB2	4:D:159:VAL:CG1	2.49	0.42
3:G:1:ILE:HG13	4:H:25:ARG:NH2	2.34	0.42
3:G:60:LEU:H	3:G:60:LEU:CD1	2.26	0.42
3:G:89:ALA:HB3	3:G:176:LYS:HG2	2.01	0.42
3:G:117:ILE:HG13	3:G:166:GLU:O	2.19	0.42
1:A:8:GLN:HE21	1:E:12:VAL:CA	2.32	0.42
3:C:48:PHE:CE1	4:D:89:THR:HB	2.54	0.42
4:D:74:GLU:HB3	4:D:78:VAL:HG21	2.02	0.42
4:D:88:PRO:HA	4:D:92:ARG:NH1	2.34	0.42
4:D:158:LEU:O	4:D:160:MET:HE2	2.19	0.42
3:G:96:PRO:HG3	4:H:100:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:10:GLN:HB2	4:H:31:ILE:HB	2.01	0.42
2:B:20:THR:HG23	2:B:78:ILE:HD13	2.01	0.42
2:B:57:LYS:HD3	2:B:61:PRO:CB	2.50	0.42
2:B:80:GLU:O	2:B:81:LEU:HB2	2.19	0.42
4:D:38:VAL:HA	4:D:50:VAL:HG23	2.02	0.42
4:D:96:GLN:HA	4:D:179:SER:OG	2.19	0.42
4:D:131:TRP:CB	4:D:161:LEU:HD13	2.46	0.42
3:G:124:ASN:OD1	3:G:160:ILE:HG13	2.20	0.42
2:B:97:GLN:O	2:B:98:GLY:O	2.37	0.42
3:C:118:ASN:CB	3:C:166:GLU:HB3	2.36	0.42
4:D:89:THR:OG1	4:D:90:SER:N	2.50	0.42
1:E:5:GLN:HE22	1:E:90:CYS:N	2.04	0.42
4:H:107:GLU:C	4:H:113:ASN:HD21	2.28	0.42
1:A:26:ASP:C	1:A:28:THR:H	2.27	0.42
2:B:47:HIS:N	2:B:47:HIS:CD2	2.86	0.42
4:D:133:ARG:O	4:D:134:ASN:C	2.62	0.42
2:F:15:THR:HG1	2:F:116(B):GLY:HA3	1.78	0.42
2:F:31:ASN:CB	2:F:49:SER:O	2.68	0.42
2:F:59:ASP:C	2:F:60:ILE:HG13	2.44	0.42
4:H:30:TYR:HB2	4:H:38:VAL:O	2.20	0.42
4:H:63:LYS:O	4:H:64:GLN:HG3	2.19	0.42
4:H:105:ARG:CG	4:H:113:ASN:HA	2.50	0.42
4:H:188:TRP:CG	4:H:189:ARG:H	2.38	0.42
2:B:36:ARG:HA	2:B:89:VAL:O	2.19	0.42
4:D:37:TYR:O	4:D:54:GLY:HA3	2.19	0.42
4:D:109:LEU:C	4:D:111:HIS:H	2.26	0.42
2:F:32:MET:N	2:F:69:ARG:HH21	2.17	0.42
3:G:29:ASP:HB3	4:H:153:TRP:CD1	2.54	0.42
1:A:38:PHE:HA	1:A:39:PRO:HD2	1.90	0.42
3:C:104:THR:CG2	3:C:150:TYR:HB3	2.50	0.42
4:D:182:SER:O	4:D:183:PRO:C	2.63	0.42
2:F:43:LEU:HB3	2:F:44:ARG:H	1.50	0.42
4:H:39:ARG:HG2	4:H:40:PHE:N	2.33	0.42
4:H:44:VAL:HG11	4:H:48:ARG:HG3	2.01	0.42
1:A:102:ASN:HD22	2:B:31:ASN:HD21	1.67	0.42
3:C:122:LEU:HD12	3:C:175:LEU:HD21	2.00	0.42
4:D:60:TYR:HB2	5:P:143:ILE:HD11	2.01	0.42
1:E:19:ILE:HG12	1:E:76:HIS:CE1	2.54	0.42
2:F:37:GLN:HG3	2:F:91:PHE:CD1	2.55	0.42
3:G:15:SER:HB2	3:G:70:LEU:CD2	2.49	0.42
3:G:107:CYS:O	3:G:109:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:95:SER:O	3:C:96:PRO:C	2.61	0.42
3:C:172:GLU:H	3:C:172:GLU:HG3	1.63	0.42
3:G:46:PRO:C	3:G:48:PHE:N	2.78	0.42
4:H:50:VAL:HG23	4:H:51:THR:N	2.33	0.42
4:H:142:VAL:HG22	4:H:161:LEU:HD12	2.02	0.42
2:B:18:LYS:HG2	2:B:80:GLU:HA	2.02	0.41
1:E:34:TRP:NE1	1:E:73:LEU:HD21	2.31	0.41
2:F:14:VAL:O	2:F:15:THR:C	2.63	0.41
3:G:135:THR:OG1	3:G:138:PHE:HE1	2.02	0.41
3:G:135:THR:OG1	3:G:147:LYS:HG2	2.20	0.41
1:A:22:CYS:CB	1:A:73:LEU:HD23	2.48	0.41
1:A:101:PHE:HZ	5:P:141:GLU:HG2	1.85	0.41
3:C:71:GLU:O	3:C:72:ILE:C	2.63	0.41
4:D:87:THR:CA	4:D:91:LEU:HD12	2.39	0.41
4:D:149:ARG:HG3	4:D:155:PHE:HE2	1.82	0.41
1:E:47:ILE:CG2	1:E:64:ILE:HG13	2.49	0.41
3:G:6:VAL:O	3:G:26:PHE:HA	2.19	0.41
4:H:38:VAL:HG23	4:H:48:ARG:C	2.44	0.41
4:H:87:THR:HG22	4:H:88:PRO:N	2.35	0.41
4:H:119:VAL:O	4:H:156:GLN:HA	2.20	0.41
4:H:143:SER:O	4:H:160:MET:HE3	2.20	0.41
4:D:34:ARG:NH1	4:D:34:ARG:CG	2.66	0.41
2:F:23:CYS:O	2:F:74:ASN:HA	2.20	0.41
3:C:104:THR:HA	3:C:152:THR:HA	2.01	0.41
3:C:107:CYS:HB2	3:C:121:TRP:CH2	2.56	0.41
4:H:18:THR:OG1	4:H:23:ARG:HD3	2.21	0.41
4:H:45:GLY:O	4:H:46:GLU:HB3	2.21	0.41
6:L:2:NDG:O6	6:L:2:NDG:C1	2.68	0.41
2:B:93:ALA:HA	2:B:107:PHE:O	2.19	0.41
2:B:98:GLY:O	2:B:99:ARG:HB2	2.21	0.41
3:C:82:ALA:HB2	4:D:33:ASN:CG	2.45	0.41
1:E:101:PHE:HA	4:H:70:ARG:NH2	2.35	0.41
3:G:119:ILE:HA	3:G:164:LYS:O	2.21	0.41
4:H:12:GLN:O	4:H:28:ILE:HA	2.20	0.41
4:H:27:VAL:HG22	4:H:41:ASP:OD1	2.21	0.41
4:H:171:TYR:CD2	4:H:190:ALA:HB2	2.56	0.41
2:B:51:GLY:C	2:B:69:ARG:NH1	2.78	0.41
4:D:30:TYR:HB2	4:D:38:VAL:HG12	2.02	0.41
4:D:163:MET:HB2	4:D:164:THR:H	1.66	0.41
3:G:101:GLN:O	3:G:155:PRO:HD2	2.20	0.41
3:G:113:PHE:HA	3:G:114:PRO:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:59:GLU:H	4:H:59:GLU:HG3	1.63	0.41
4:H:87:THR:HA	4:H:91:LEU:HB2	2.03	0.41
1:A:45:LEU:CG	1:A:46:LEU:N	2.83	0.41
2:B:12:VAL:HG12	2:B:13:ALA:N	2.35	0.41
4:D:26:LEU:HD12	4:D:27:VAL:N	2.36	0.41
1:E:26:ASP:OD2	1:E:28:THR:HB	2.20	0.41
2:F:36:ARG:O	2:F:43:LEU:O	2.39	0.41
3:G:48:PHE:CE2	4:H:89:THR:HB	2.55	0.41
3:G:144:SER:CB	4:H:34:ARG:NH1	2.81	0.41
3:G:164:LYS:HE2	3:G:166:GLU:HG3	2.01	0.41
4:H:12:GLN:HB3	4:H:14:PHE:CE2	2.56	0.41
4:H:106:THR:HG22	4:H:107:GLU:HG2	2.01	0.41
4:H:118:SER:HA	4:H:158:LEU:HA	2.03	0.41
2:B:6:GLN:HG3	2:B:111:GLY:H	1.86	0.41
3:C:35:ASP:O	3:C:39:LYS:N	2.54	0.41
3:C:121:TRP:CD1	3:C:132:VAL:HG13	2.56	0.41
4:D:14:PHE:N	4:D:27:VAL:O	2.54	0.41
2:F:18:LYS:HG3	2:F:80:GLU:HA	2.02	0.41
3:G:26:PHE:CZ	4:H:86:GLU:HG3	2.55	0.41
3:G:36:LEU:HD13	3:G:63:ILE:HG13	2.01	0.41
4:H:20:GLY:HA2	4:H:83:TYR:OH	2.21	0.41
4:H:21:THR:HG21	4:H:84:GLU:HG2	2.02	0.41
4:H:21:THR:CB	4:H:24:ILE:HD11	2.49	0.41
4:H:126:LYS:HZ3	4:H:178:PRO:HG3	1.84	0.41
4:H:178:PRO:C	4:H:180:LEU:N	2.79	0.41
1:A:31:TYR:HA	1:A:49:ILE:O	2.21	0.41
2:B:9:ARG:NH2	2:B:110:PRO:HB2	2.35	0.41
2:B:37:GLN:HG2	2:B:43:LEU:HD11	2.02	0.41
2:B:65:TYR:HE2	2:B:90:TYR:CE2	2.39	0.41
3:C:82:ALA:HB2	4:D:33:ASN:OD1	2.20	0.41
3:C:135:THR:CG2	3:C:150:TYR:HE2	2.33	0.41
4:D:81:HIS:O	4:D:82:ASN:C	2.64	0.41
4:D:169:GLU:HG3	4:D:169:GLU:H	1.76	0.41
1:E:27:SER:C	1:E:29:PHE:H	2.29	0.41
2:F:38:ASP:O	2:F:40:GLY:N	2.54	0.41
3:G:52:ARG:HH12	4:H:86:GLU:HA	1.86	0.41
3:G:77:SER:HB3	4:H:32:TYR:CE2	2.56	0.41
3:G:129:THR:O	3:G:129:THR:CG2	2.66	0.41
4:H:99:VAL:HG22	4:H:175:VAL:HG21	2.03	0.41
1:A:101:PHE:CD2	1:A:101:PHE:C	2.99	0.41
4:D:111:HIS:O	4:D:164:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:145:THR:CG2	4:D:158:LEU:O	2.68	0.41
1:E:51:LEU:HD12	4:H:77:THR:CG2	2.51	0.41
3:G:68:HIS:CD2	5:Q:141:GLU:HB2	2.56	0.41
3:G:120:THR:O	3:G:164:LYS:N	2.51	0.41
3:G:137:PHE:CE2	3:G:147:LYS:HE2	2.56	0.41
1:A:34:TRP:O	1:A:45:LEU:HD12	2.21	0.40
3:C:14:GLN:HB3	4:D:6:HIS:NE2	2.36	0.40
3:C:104:THR:OG1	3:C:152:THR:HG22	2.21	0.40
3:C:150:TYR:CD2	3:C:150:TYR:N	2.89	0.40
1:E:6:SER:O	1:E:7:PRO:C	2.64	0.40
1:E:31:TYR:CD1	4:H:70:ARG:HD3	2.56	0.40
2:F:52:ALA:O	2:F:53:GLY:C	2.60	0.40
3:G:95:SER:O	3:G:96:PRO:C	2.64	0.40
3:G:132:VAL:HG12	3:G:133:TYR:N	2.36	0.40
3:C:2:GLU:HG2	3:C:3:ALA:H	1.86	0.40
2:F:18:LYS:CG	2:F:80:GLU:HA	2.52	0.40
3:G:142:ASP:O	3:G:143:TYR:CB	2.69	0.40
4:H:147:LEU:HD11	4:H:155:PHE:CG	2.57	0.40
5:Q:135:ARG:HG2	5:Q:136:GLY:O	2.21	0.40
1:A:30:ASP:CA	1:A:51:LEU:HD21	2.36	0.40
3:C:84:ASN:ND2	3:C:168:TRP:HB3	2.36	0.40
4:D:189:ARG:O	4:D:190:ALA:O	2.39	0.40
3:G:123:ARG:HG3	3:G:161:TYR:CE2	2.56	0.40
3:G:177:HIS:CD2	3:G:178:TRP:N	2.89	0.40
4:H:118:SER:HA	4:H:158:LEU:CB	2.47	0.40
4:H:124:PRO:HB2	4:H:125:ALA:H	1.66	0.40
4:H:134:ASN:HD21	4:H:169:GLU:CG	2.31	0.40
1:A:40:GLY:C	1:A:41:LYS:HG2	2.46	0.40
1:A:45:LEU:CD1	1:A:46:LEU:N	2.80	0.40
3:C:1:ILE:CD1	4:D:25:ARG:HH21	2.35	0.40
3:C:68:HIS:NE2	3:C:72:ILE:CD1	2.81	0.40
2:F:12:VAL:HG13	2:F:116(A):LEU:HG	2.04	0.40
3:G:48:PHE:CZ	4:H:90:SER:N	2.90	0.40
3:G:53:ARG:N	5:Q:134:HIS:NE2	2.69	0.40
3:G:65:THR:CG2	5:Q:140:TRP:O	2.66	0.40
3:G:84:ASN:ND2	3:G:168:TRP:CB	2.83	0.40
4:H:121:ASP:OD1	4:H:121:ASP:N	2.54	0.40
3:C:148:LEU:HD22	4:D:150:ASN:O	2.21	0.40
4:D:99:VAL:CG1	4:D:175:VAL:HG21	2.45	0.40
4:D:114:THR:HG23	4:D:162:GLU:CA	2.52	0.40
1:E:27:SER:C	1:E:29:PHE:N	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:PHE:CD1	1:E:29:PHE:N	2.90	0.40
3:G:69:ASN:O	3:G:70:LEU:C	2.63	0.40
3:G:150:TYR:N	3:G:150:TYR:CD2	2.89	0.40
3:G:156:SER:O	3:G:180:PRO:HG2	2.21	0.40
4:H:149:ARG:HA	4:H:155:PHE:CD2	2.56	0.40

There are no symmetry-related clashes.

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	108/110 (98%)	80 (74%)	12 (11%)	16 (15%)	0	1
1	E	108/110 (98%)	82 (76%)	17 (16%)	9 (8%)	0	4
2	B	110/112 (98%)	77 (70%)	19 (17%)	14 (13%)	0	1
2	F	110/112 (98%)	79 (72%)	15 (14%)	16 (14%)	0	1
3	C	181/183 (99%)	161 (89%)	15 (8%)	5 (3%)	4	25
3	G	181/183 (99%)	133 (74%)	33 (18%)	15 (8%)	0	4
4	D	186/188 (99%)	145 (78%)	30 (16%)	11 (6%)	1	10
4	H	186/188 (99%)	129 (69%)	33 (18%)	24 (13%)	0	1
5	P	14/16 (88%)	12 (86%)	1 (7%)	1 (7%)	1	6
5	Q	14/16 (88%)	9 (64%)	1 (7%)	4 (29%)	0	0
All	All	1198/1218 (98%)	907 (76%)	176 (15%)	115 (10%)	0	3

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	14	GLU

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Mol	Chain	Res	Type
1	A	68	LYS
1	A	71	LYS
1	A	103	LYS
2	B	43	LEU
2	B	73	GLU
3	C	179	GLU
1	E	16	GLU
1	E	68	LYS
2	F	7	SER
2	F	28	ASN
2	F	52	ALA
2	F	71	SER
2	F	73	GLU
2	F	99	ARG
2	F	116(B)	GLY
3	G	49	ALA
3	G	50	GLN
3	G	51	LEU
3	G	180	PRO
4	H	34	ARG
4	H	58	ALA
4	H	79	CYS
4	H	97	PRO
4	H	108	ALA
4	H	110	ASN
4	H	126	LYS
4	H	188	TRP
4	H	189	ARG
5	Q	144	GLU
1	A	31	TYR
1	A	46	LEU
1	A	47	ILE
1	A	88	TYR
1	A	99	GLY
1	A	102	ASN
2	B	27	ASN
2	B	39	THR
2	B	44	ARG
2	B	62	ASP
2	B	71	SER
2	B	116(B)	GLY
3	C	3	ALA

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Mol	Chain	Res	Type
4	D	4	GLU
4	D	102	SER
4	D	103	LEU
1	E	8	GLN
2	F	82	ALA
3	G	46	PRO
3	G	47	GLU
4	H	5	ARG
4	H	64	GLN
4	H	80	ARG
4	H	121	ASP
4	H	165	PRO
1	A	9	SER
1	A	80	SER
2	B	7	SER
2	B	72	GLN
2	B	96	GLY
2	B	116(A)	LEU
3	C	99	LEU
3	C	155	PRO
4	D	64	GLN
4	D	189	ARG
5	P	145	SER
1	E	17	THR
2	F	15	THR
2	F	18	LYS
2	F	104	ALA
3	G	115	PRO
4	H	3	SER
4	H	56	PRO
4	H	104	SER
4	H	118	SER
4	H	183	PRO
5	Q	143	ILE
1	A	116	PRO
2	B	30	ASN
3	C	173	PRO
4	D	5	ARG
1	E	7	PRO
1	E	9	SER
1	E	80	SER
1	E	109	GLY

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Mol	Chain	Res	Type
2	F	39	THR
2	F	44	ARG
2	F	46	ILE
3	G	137	PHE
3	G	143	TYR
4	H	33	ASN
4	H	124	PRO
5	Q	141	GLU
4	D	81	HIS
4	D	134	ASN
4	D	183	PRO
3	G	113	PHE
4	H	19	ASN
4	H	125	ALA
5	Q	137	ALA
1	A	15	GLY
1	A	39	PRO
4	D	118	SER
4	D	163	MET
2	F	10	ASN
2	B	61	PRO
3	G	72	ILE
4	H	100	VAL
1	E	52	VAL
2	F	96	GLY
3	G	96	PRO
3	G	97	VAL
3	G	155	PRO
3	G	87	PRO

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	96/96 (100%)	73 (76%)	23 (24%)	14
1	E	96/96 (100%)	70 (73%)	26 (27%)	02

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	91/91 (100%)	61 (67%)	30 (33%)	0	1
2	F	91/91 (100%)	69 (76%)	22 (24%)	1	4
3	C	166/166 (100%)	131 (79%)	35 (21%)	1	6
3	G	166/166 (100%)	125 (75%)	41 (25%)	1	3
4	D	174/174 (100%)	124 (71%)	50 (29%)	0	1
4	H	174/174 (100%)	113 (65%)	61 (35%)	0	0
5	P	11/11 (100%)	5 (46%)	6 (54%)	0	0
5	Q	11/11 (100%)	6 (54%)	5 (46%)	0	0
All	All	1076/1076 (100%)	777 (72%)	299 (28%)	0	2

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	12	VAL
1	A	20	LEU
1	A	27	SER
1	A	28	THR
1	A	30	ASP
1	A	32	PHE
1	A	36	ARG
1	A	41	LYS
1	A	49	ILE
1	A	51	LEU
1	A	57	GLU
1	A	61	ARG
1	A	69	ARG
1	A	73	LEU
1	A	75	LEU
1	A	80	SER
1	A	85	SER
1	A	100	SER
1	A	104	LEU
1	A	105	THR
1	A	112	LEU
1	A	114	VAL
2	B	6	GLN
2	B	7	SER
2	B	11	LYS

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Mol	Chain	Res	Type
2	B	18	LYS
2	B	19	VAL
2	B	20	THR
2	B	21	LEU
2	B	25	GLN
2	B	26	THR
2	B	31	ASN
2	B	37	GLN
2	B	41	HIS
2	B	43	LEU
2	B	44	ARG
2	B	45	LEU
2	B	46	ILE
2	B	49	SER
2	B	54	SER
2	B	56	GLU
2	B	69	ARG
2	B	73	GLU
2	B	78	ILE
2	B	81	LEU
2	B	86	GLN
2	B	97	GLN
2	B	99	ARG
2	B	105	GLU
2	B	116	VAL
2	B	116(A)	LEU
2	B	116(C)	SER
3	C	21	GLN
3	C	23	THR
3	C	24	PHE
3	C	36	LEU
3	C	39	LYS
3	C	41	THR
3	C	55	GLU
3	C	57	GLN
3	C	62	ASN
3	C	65	THR
3	C	71	GLU
3	C	73	LEU
3	C	74	THR
3	C	75	LYS
3	C	78	ASN

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Mol	Chain	Res	Type
3	C	88	GLN
3	C	94	LYS
3	C	95	SER
3	C	97	VAL
3	C	98	LEU
3	C	99	LEU
3	C	103	ASN
3	C	116	VAL
3	C	120	THR
3	C	127	SER
3	C	128	VAL
3	C	132	VAL
3	C	134	GLU
3	C	135	THR
3	C	147	LYS
3	C	170	LEU
3	C	171	GLU
3	C	172	GLU
3	C	179	GLU
3	C	182	ILE
4	D	4	GLU
4	D	18	THR
4	D	22	GLN
4	D	25	ARG
4	D	28	ILE
4	D	31	ILE
4	D	34	ARG
4	D	50	VAL
4	D	51	THR
4	D	59	GLU
4	D	63	LYS
4	D	64	GLN
4	D	69	GLU
4	D	74	GLU
4	D	75	LEU
4	D	78	VAL
4	D	85	THR
4	D	98	SER
4	D	99	VAL
4	D	104	SER
4	D	105	ARG
4	D	109	LEU

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Mol	Chain	Res	Type
4	D	113	ASN
4	D	119	VAL
4	D	120	THR
4	D	121	ASP
4	D	128	LYS
4	D	136	GLN
4	D	138	GLU
4	D	143	SER
4	D	145	THR
4	D	147	LEU
4	D	157	VAL
4	D	158	LEU
4	D	159	VAL
4	D	160	MET
4	D	161	LEU
4	D	162	GLU
4	D	163	MET
4	D	164	THR
4	D	166	ARG
4	D	169	GLU
4	D	171	TYR
4	D	175	VAL
4	D	181	LYS
4	D	182	SER
4	D	184	ILE
4	D	185	THR
4	D	186	VAL
4	D	187	GLU
5	P	133	SER
5	P	134	HIS
5	P	141	GLU
5	P	143	ILE
5	P	144	GLU
5	P	145	SER
1	E	4	ARG
1	E	6	SER
1	E	8	GLN
1	E	9	SER
1	E	10	LEU
1	E	13	TRP
1	E	26	ASP
1	E	27	SER

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Mol	Chain	Res	Type
1	E	36	ARG
1	E	42	SER
1	E	45	LEU
1	E	47	ILE
1	E	49	ILE
1	E	53	SER
1	E	56	LYS
1	E	61	ARG
1	E	70	GLU
1	E	73	LEU
1	E	74	SER
1	E	78	THR
1	E	80	SER
1	E	85	SER
1	E	90	CYS
1	E	93	THR
1	E	100	SER
1	E	103	LYS
2	F	4	VAL
2	F	6	GLN
2	F	7	SER
2	F	9	ARG
2	F	14	VAL
2	F	21	LEU
2	F	25	GLN
2	F	36	ARG
2	F	37	GLN
2	F	39	THR
2	F	41	HIS
2	F	46	ILE
2	F	49	SER
2	F	56	GLU
2	F	59	ASP
2	F	73	GLU
2	F	78	ILE
2	F	83	THR
2	F	86	GLN
2	F	88	SER
2	F	94	SER
2	F	105	GLU
3	G	2	GLU
3	G	8	SER

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Mol	Chain	Res	Type
3	G	11	THR
3	G	15	SER
3	G	18	ASP
3	G	23	THR
3	G	31	LEU
3	G	40	GLU
3	G	42	VAL
3	G	45	LEU
3	G	48	PHE
3	G	50	GLN
3	G	51	LEU
3	G	57	GLN
3	G	63	ILE
3	G	71	GLU
3	G	72	ILE
3	G	75	LYS
3	G	76	ARG
3	G	79	SER
3	G	88	GLN
3	G	94	LYS
3	G	97	VAL
3	G	101	GLN
3	G	104	THR
3	G	117	ILE
3	G	120	THR
3	G	126	LYS
3	G	127	SER
3	G	135	THR
3	G	137	PHE
3	G	141	ARG
3	G	149	SER
3	G	152	THR
3	G	158	ASP
3	G	160	ILE
3	G	171	GLU
3	G	172	GLU
3	G	176	LYS
3	G	179	GLU
3	G	182	ILE
4	H	3	SER
4	H	4	GLU
4	H	5	ARG

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Mol	Chain	Res	Type
4	H	8	VAL
4	H	18	THR
4	H	22	GLN
4	H	23	ARG
4	H	26	LEU
4	H	28	ILE
4	H	36	GLU
4	H	37	TYR
4	H	39	ARG
4	H	42	SER
4	H	51	THR
4	H	53	LEU
4	H	55	ARG
4	H	59	GLU
4	H	63	LYS
4	H	68	LEU
4	H	71	THR
4	H	72	ARG
4	H	75	LEU
4	H	76	ASP
4	H	85	THR
4	H	86	GLU
4	H	93	ARG
4	H	94	LEU
4	H	95	GLU
4	H	96	GLN
4	H	99	VAL
4	H	100	VAL
4	H	102	SER
4	H	103	LEU
4	H	105	ARG
4	H	109	LEU
4	H	113	ASN
4	H	118	SER
4	H	120	THR
4	H	121	ASP
4	H	126	LYS
4	H	130	ARG
4	H	132	PHE
4	H	133	ARG
4	H	136	GLN
4	H	137	GLU

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Mol	Chain	Res	Type
4	H	139	THR
4	H	140	VAL
4	H	142	VAL
4	H	143	SER
4	H	146	GLN
4	H	147	LEU
4	H	149	ARG
4	H	158	LEU
4	H	159	VAL
4	H	161	LEU
4	H	162	GLU
4	H	172	THR
4	H	180	LEU
4	H	182	SER
4	H	184	ILE
4	H	189	ARG
5	Q	133	SER
5	Q	134	HIS
5	Q	135	ARG
5	Q	138	ILE
5	Q	143	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	8	GLN
1	A	21	ASN
1	A	67	ASN
1	A	76	HIS
2	B	31	ASN
2	B	37	GLN
3	C	84	ASN
3	C	103	ASN
4	D	12	GLN
4	D	82	ASN
4	D	156	GLN
1	E	5	GLN
1	E	8	GLN
1	E	76	HIS
1	E	102	ASN
2	F	25	GLN

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Mol	Chain	Res	Type
2	F	29	HIS
2	F	37	GLN
2	F	41	HIS
2	F	74	ASN
3	G	14	GLN
3	G	57	GLN
3	G	84	ASN
4	H	10	GLN
4	H	22	GLN
4	H	82	ASN
4	H	134	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

8 monosaccharides 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	$\# Z > 2$
6	NAG	I	1	3,6	14,14,15	0.61	0	17,19,21	0.66	1 (5%)
6	NDG	I	2	6	14,14,15	0.67	0	17,19,21	0.65	1 (5%)
6	NAG	J	1	4,6	14,14,15	0.70	0	17,19,21	0.74	0
6	NDG	J	2	6	14,14,15	0.74	0	17,19,21	0.70	1 (5%)
6	NAG	K	1	3,6	14,14,15	0.80	0	17,19,21	0.75	1 (5%)
6	NDG	K	2	6	14,14,15	0.70	0	17,19,21	0.81	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	L	1	4,6	14,14,15	0.72	0	17,19,21	1.45	3 (17%)
6	NDG	L	2	6	14,14,15	0.81	0	17,19,21	0.96	2 (11%)

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
6	NAG	I	1	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NDG	I	2	6	-	2/6/23/26	0/1/1/1
6	NAG	J	1	4,6	1/1/5/7	1/6/23/26	0/1/1/1
6	NDG	J	2	6	-	1/6/23/26	0/1/1/1
6	NAG	K	1	3,6	1/1/5/7	2/6/23/26	0/1/1/1
6	NDG	K	2	6	-	2/6/23/26	0/1/1/1
6	NAG	L	1	4,6	-	2/6/23/26	0/1/1/1
6	NDG	L	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1	NAG	C4-C3-C2	3.97	116.83	111.02
6	L	1	NAG	C3-C4-C5	3.20	116.04	110.23
6	L	2	NDG	C2-N2-C7	-2.53	119.50	122.90
6	L	2	NDG	C1-O5-C5	2.30	115.27	112.19
6	J	2	NDG	C2-N2-C7	-2.19	119.96	122.90
6	I	2	NDG	C2-N2-C7	-2.17	119.99	122.90
6	L	1	NAG	C2-N2-C7	-2.14	120.03	122.90
6	K	2	NDG	C1-O5-C5	2.11	115.02	112.19
6	K	1	NAG	C2-N2-C7	-2.06	120.14	122.90
6	I	1	NAG	C2-N2-C7	-2.03	120.17	122.90
6	K	2	NDG	C2-N2-C7	-2.00	120.22	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	I	1	NAG	C1
6	J	1	NAG	C1
6	K	1	NAG	C1

All (10) torsion outliers are listed below:

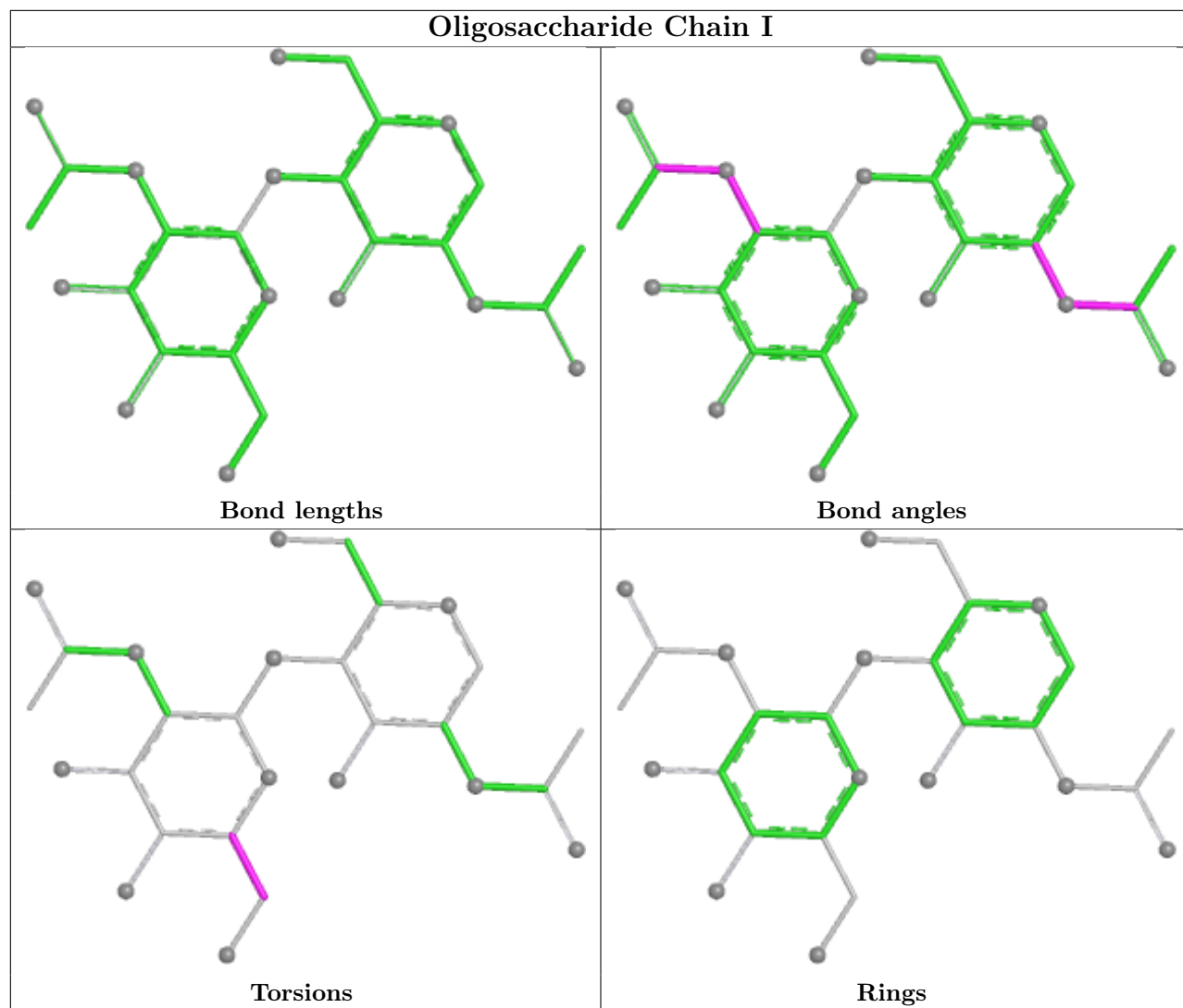
Mol	Chain	Res	Type	Atoms
6	I	2	NDG	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
6	I	2	NDG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
6	J	2	NDG	O5-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
6	K	2	NDG	C1-C2-N2-C7
6	K	2	NDG	C3-C2-N2-C7

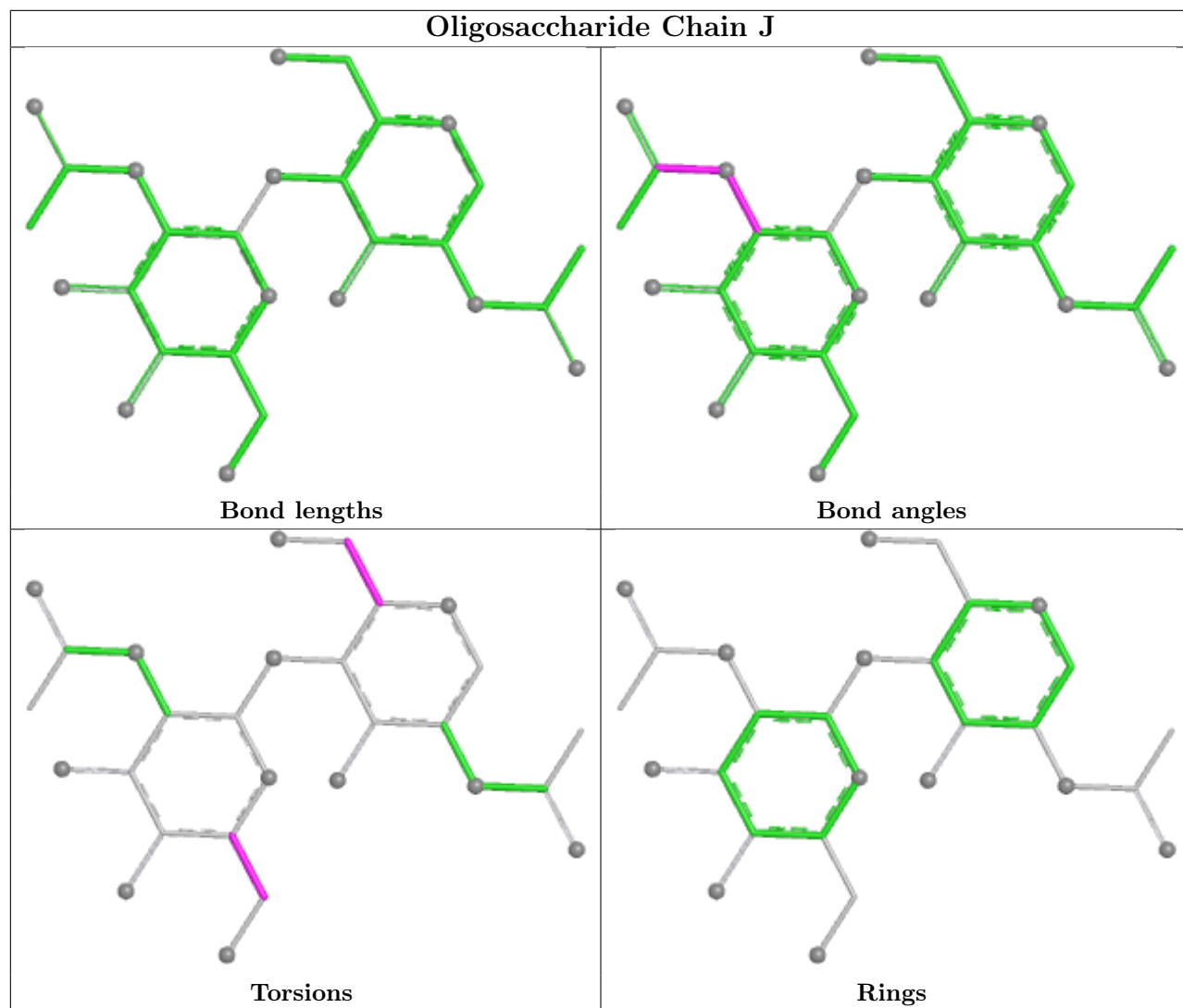
There are no ring outliers.

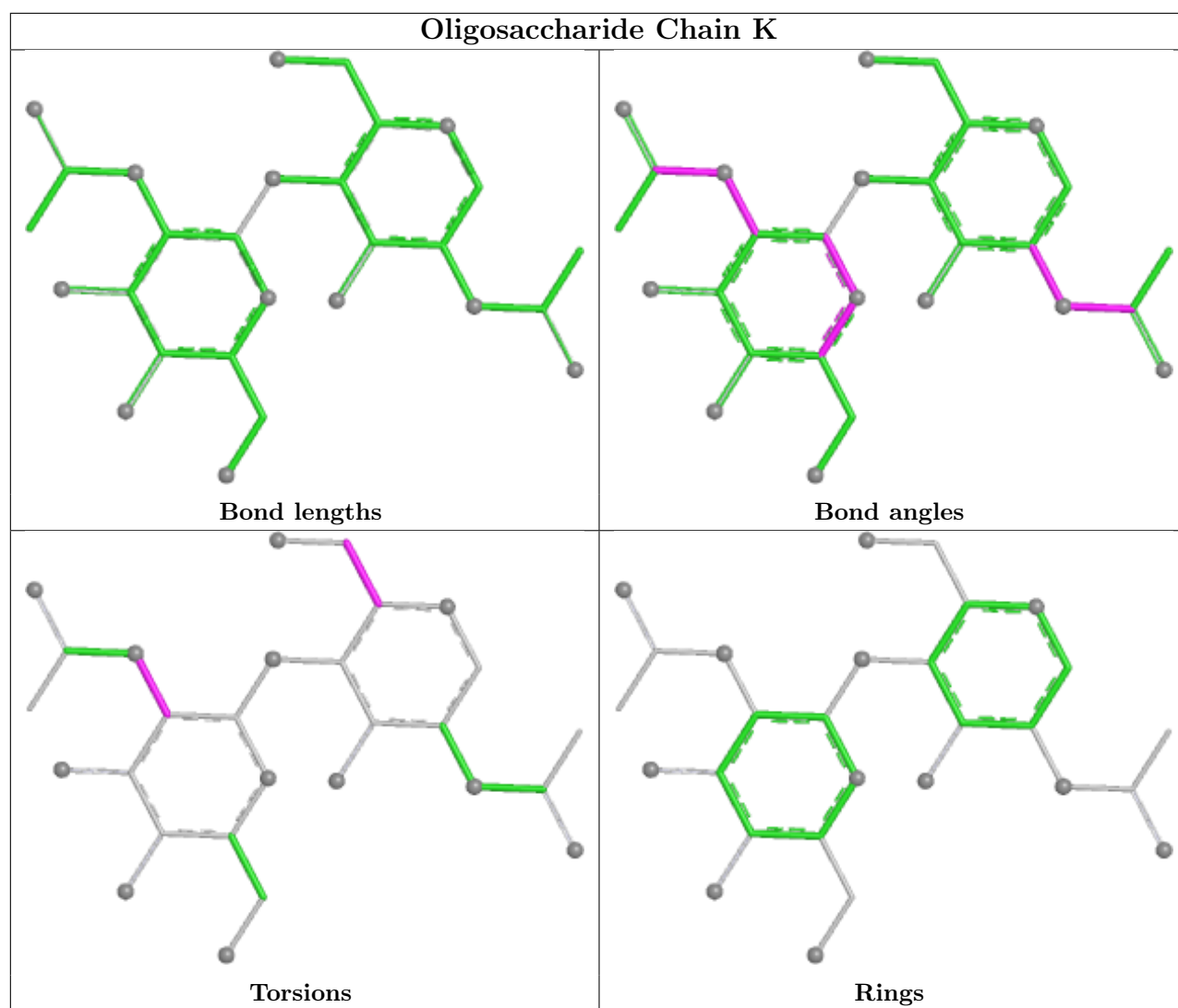
4 monomers are involved in 7 short contacts:

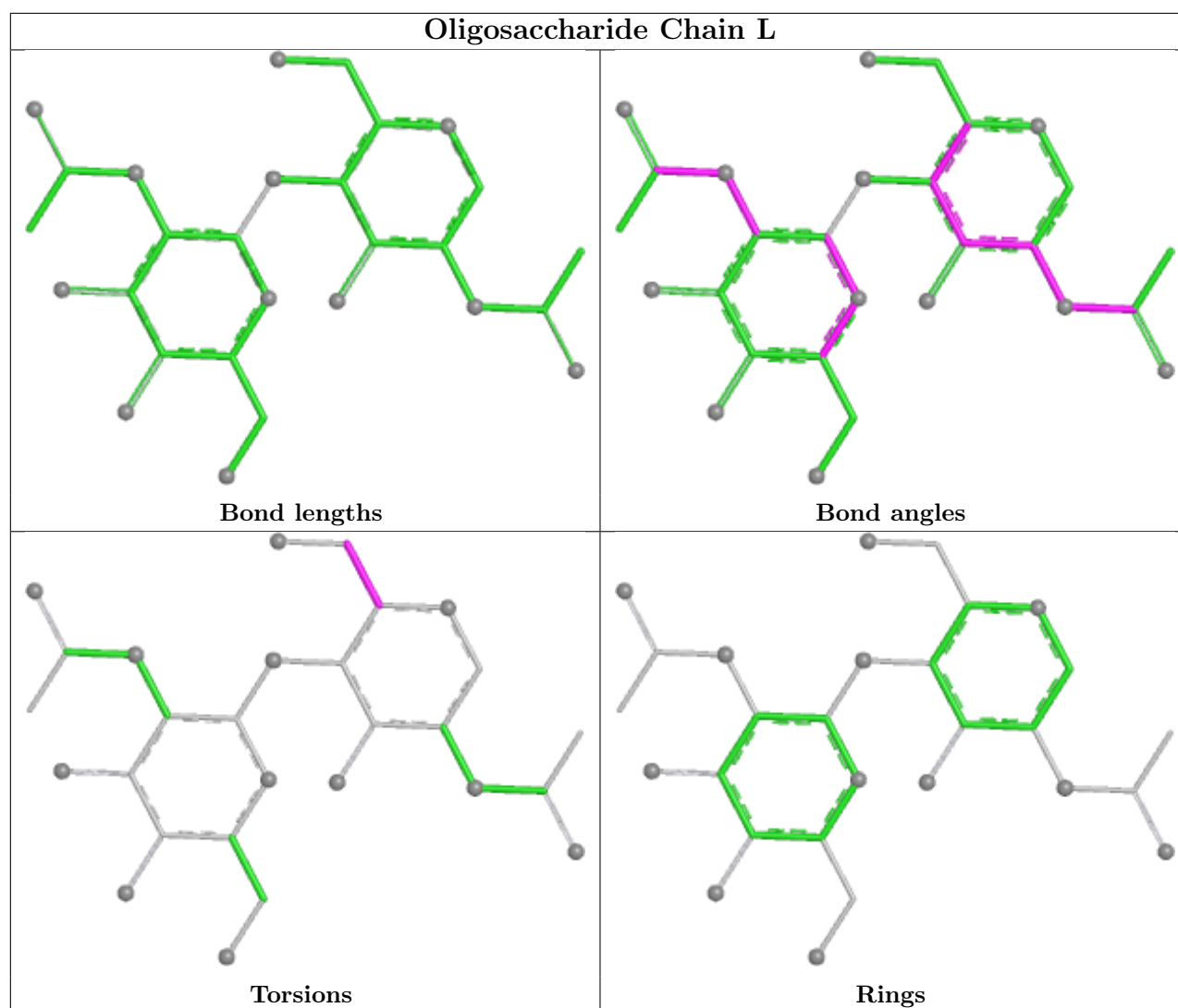
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	2	NDG	1	0
6	I	1	NAG	3	0
6	I	2	NDG	3	0
6	L	1	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
7	NAG	C	201	3	14,14,15	0.66	0	17,19,21	0.81	1 (5%)
7	NAG	G	201	3	14,14,15	0.71	0	17,19,21	0.63	1 (5%)

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
7	NAG	C	201	3	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	G	201	3	1/1/5/7	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	201	NAG	C2-N2-C7	-2.37	119.72	122.90
7	G	201	NAG	C2-N2-C7	-2.17	120.00	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	201	NAG	C1
7	G	201	NAG	C1

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	201	NAG	C4-C5-C6-O6
7	G	201	NAG	O5-C5-C6-O6
7	C	201	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	110/110 (100%)	0.11	3 (2%) 56 36	23, 43, 73, 96	0
1	E	110/110 (100%)	0.18	3 (2%) 56 36	31, 52, 79, 94	0
2	B	112/112 (100%)	0.14	3 (2%) 56 36	29, 48, 69, 91	0
2	F	112/112 (100%)	0.40	7 (6%) 26 17	28, 51, 81, 100	0
3	C	183/183 (100%)	-0.04	4 (2%) 62 42	20, 44, 86, 100	0
3	G	183/183 (100%)	0.86	23 (12%) 8 6	41, 84, 100, 100	0
4	D	188/188 (100%)	0.22	14 (7%) 20 13	18, 48, 100, 100	0
4	H	188/188 (100%)	1.13	29 (15%) 5 4	49, 91, 100, 100	0
5	P	16/16 (100%)	0.52	0 100 100	28, 48, 96, 100	0
5	Q	16/16 (100%)	1.34	2 (12%) 8 6	57, 73, 99, 100	0
All	All	1218/1218 (100%)	0.43	88 (7%) 21 14	18, 58, 100, 100	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	155	PRO	5.7
4	H	109	LEU	5.6
4	H	110	ASN	5.1
4	D	108	ALA	4.8
4	H	168	GLY	4.7
4	D	106	THR	4.7
4	H	107	GLU	4.7
4	H	111	HIS	4.6
4	D	112	HIS	4.5
3	G	160	ILE	4.4
4	D	111	HIS	4.4
3	G	128	VAL	4.3
4	H	105	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
4	H	108	ALA	4.1
4	D	2	GLY	4.1
1	A	117	TYR	3.9
2	F	116(C)	SER	3.8
4	H	2	GLY	3.8
3	G	182	ILE	3.6
2	F	116(B)	GLY	3.6
3	G	180	PRO	3.5
3	G	154	ILE	3.5
4	D	109	LEU	3.5
3	G	2	GLU	3.4
4	H	162	GLU	3.4
4	D	104	SER	3.4
3	G	161	TYR	3.4
4	H	190	ALA	3.4
4	D	110	ASN	3.4
1	E	117	TYR	3.1
1	A	47	ILE	3.1
4	H	106	THR	3.1
3	G	181	GLU	3.0
4	H	165	PRO	2.9
4	H	188	TRP	2.9
4	H	186	VAL	2.9
2	B	27	ASN	2.8
4	H	120	THR	2.8
4	H	3	SER	2.8
2	F	42	GLY	2.8
3	G	174	VAL	2.7
3	G	1	ILE	2.7
3	C	179	GLU	2.7
4	D	105	ARG	2.7
4	H	185	THR	2.7
4	D	161	LEU	2.7
3	G	178	TRP	2.6
2	B	7	SER	2.6
4	H	184	ILE	2.6
4	H	101	ILE	2.6
5	Q	134	HIS	2.5
2	F	17	GLY	2.5
4	H	183	PRO	2.5
2	F	98	GLY	2.5
3	G	99	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	H	112	HIS	2.5
3	G	152	THR	2.4
3	C	180	PRO	2.4
3	G	122	LEU	2.4
4	H	100	VAL	2.3
4	H	117	CYS	2.3
5	Q	132	ASN	2.3
3	G	101	GLN	2.3
3	G	50	GLN	2.2
2	F	41	HIS	2.2
4	H	104	SER	2.2
2	B	42	GLY	2.2
1	E	102	ASN	2.2
4	D	3	SER	2.2
3	G	104	THR	2.1
4	D	170	VAL	2.1
4	H	119	VAL	2.1
3	C	1	ILE	2.1
4	H	135	GLY	2.1
3	G	157	ASP	2.1
4	H	84(A)	LYS	2.1
4	D	188	TRP	2.1
4	H	142	VAL	2.1
4	H	90	SER	2.1
1	A	7	PRO	2.1
2	F	99	ARG	2.1
1	E	26	ASP	2.1
3	G	121	TRP	2.0
4	D	163	MET	2.0
3	G	97	VAL	2.0
3	C	177	HIS	2.0
3	G	133	TYR	2.0
3	G	123	ARG	2.0

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

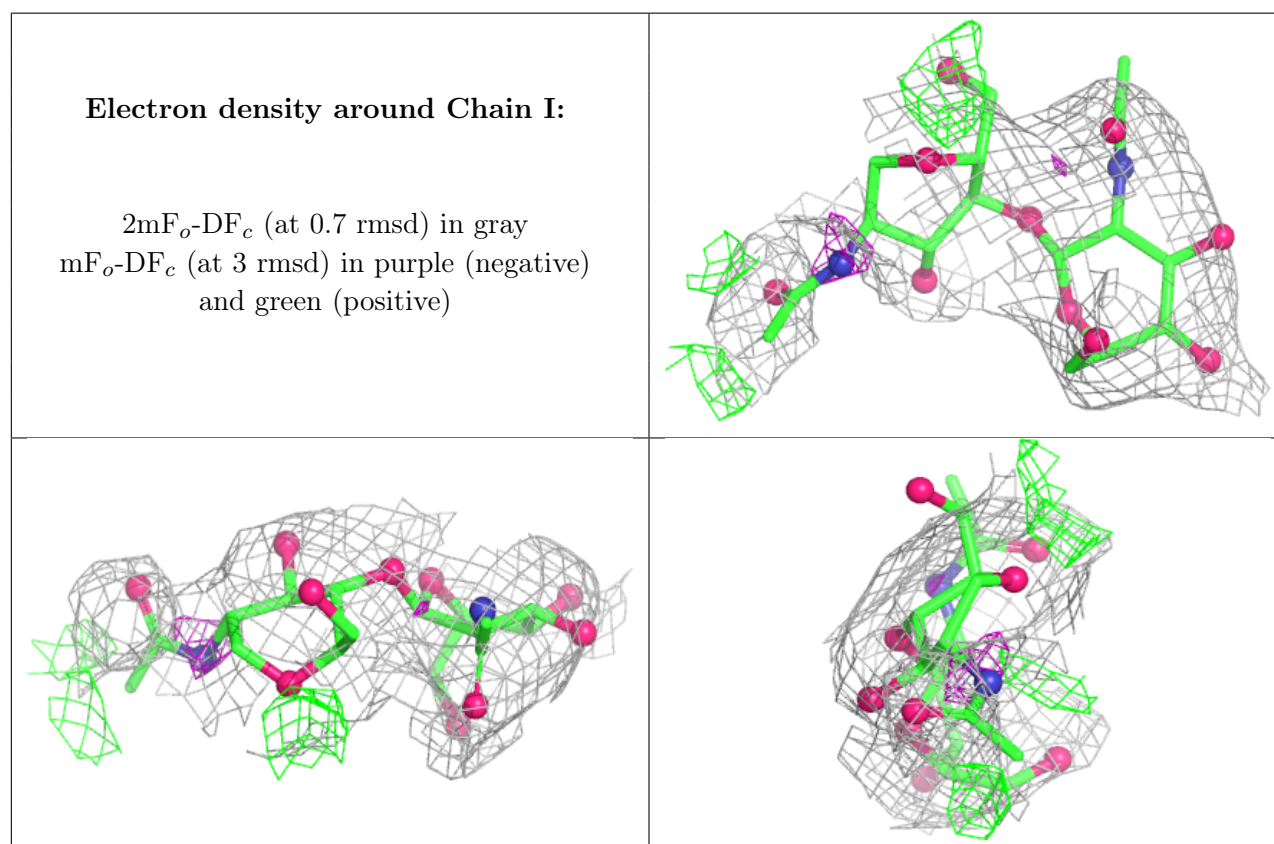
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

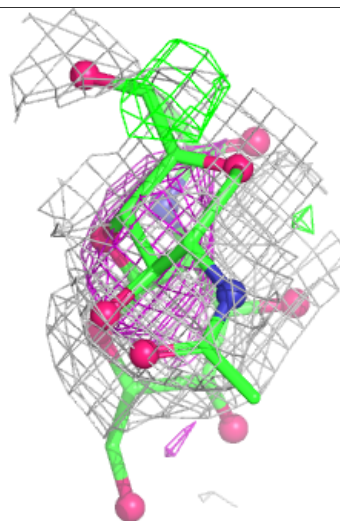
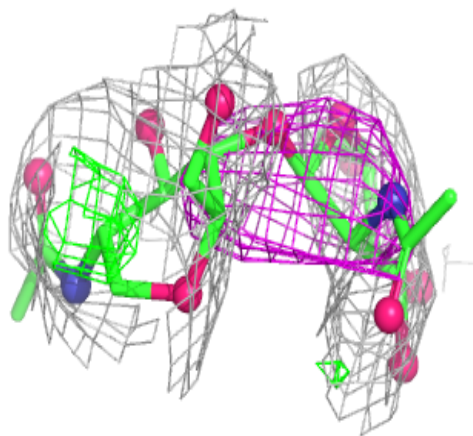
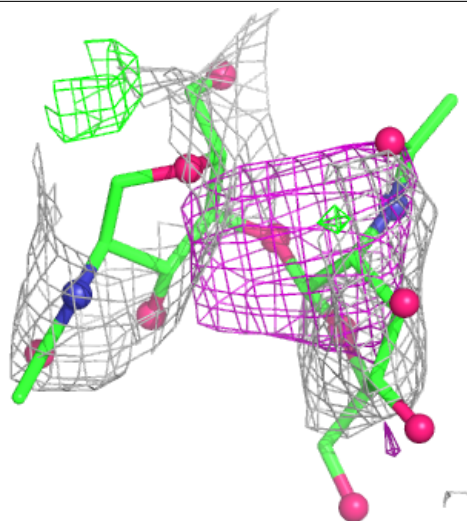
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	I	1	14/15	-	-	80,90,100,100	0
6	NDG	I	2	14/15	-	-	98,100,100,100	0
6	NAG	J	1	14/15	-	-	87,97,100,100	0
6	NDG	J	2	14/15	-	-	98,100,100,100	0
6	NDG	L	2	14/15	0.26	0.24	97,100,100,100	0
6	NAG	L	1	14/15	0.41	0.22	92,100,100,100	0
6	NAG	K	1	14/15	0.66	0.18	93,100,100,100	0
6	NDG	K	2	14/15	0.70	0.15	98,100,100,100	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



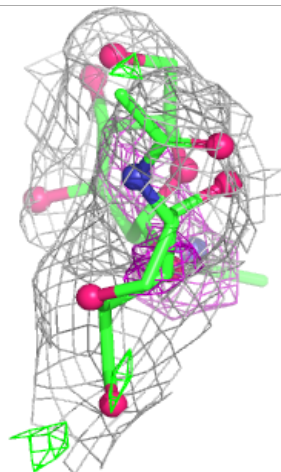
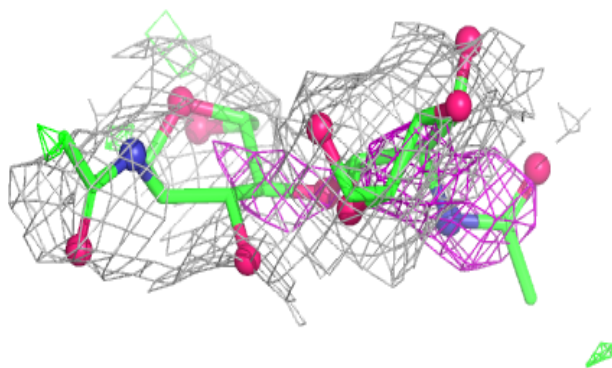
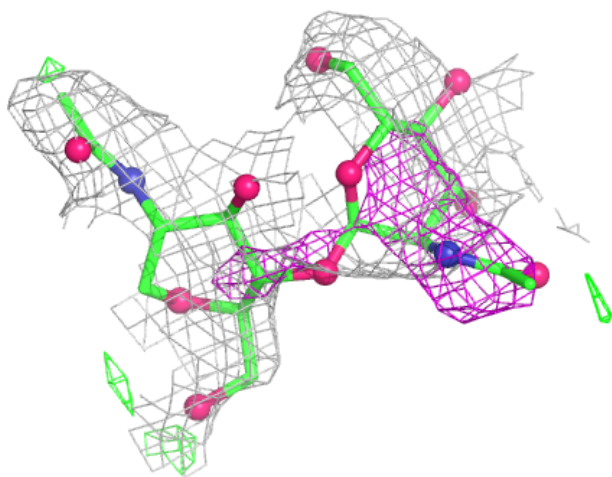
Electron density around Chain J:

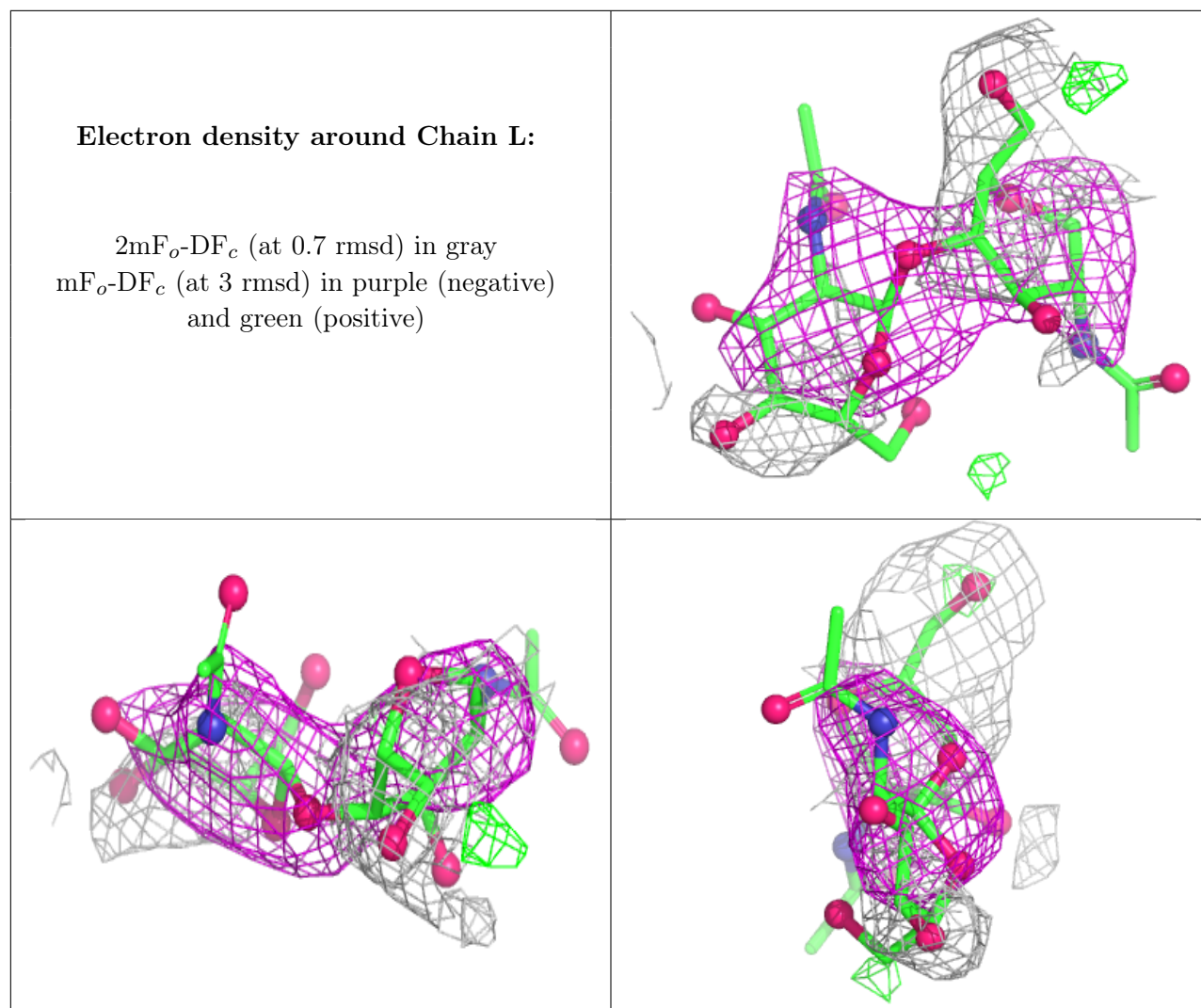
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	G	201	14/15	0.16	0.32	97,100,100,100	0
7	NAG	C	201	14/15	0.76	0.23	95,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.