



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:45 AM UTC

PDB ID : 2EXY / pdb_00002exy
Title : Crystal structure of the E148Q Mutant of EcClC, Fab complexed in absence of bound ions
Authors : Lobet, S.; Dutzler, R.
Deposited on : 2005-11-09
Resolution : 3.10 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
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

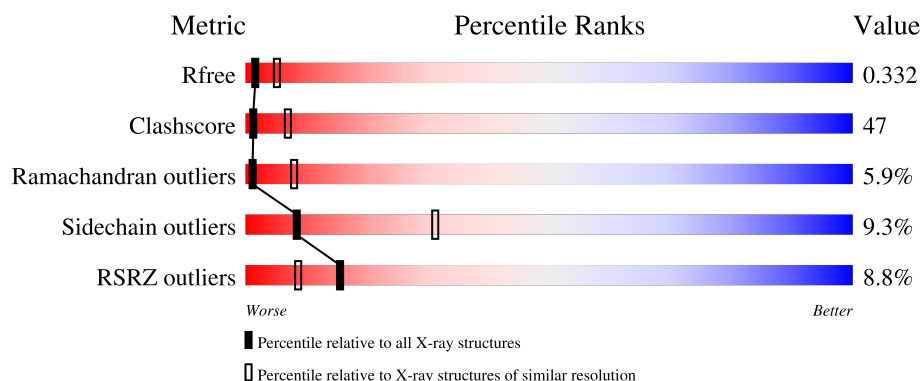
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

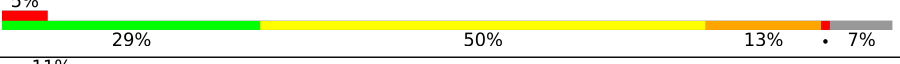
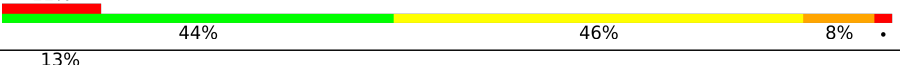
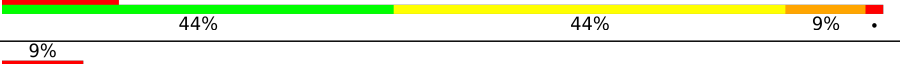
The reported resolution of this entry is 3.10 Å.

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))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	473	
1	B	473	
2	C	222	
2	E	222	
3	D	211	

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Mol	Chain	Length	Quality of chain
3	F	211	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (10%), green (40%), yellow (51%), and orange (9%). The percentages are labeled below the bar.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13223 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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	561	562	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	554	556	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLN	GLU	engineered mutation	UNP P37019
B	148	GLN	GLU	engineered mutation	UNP P37019

- Molecule 2 is a protein called Fab Fragment (Heavy Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			
2	E	221	Total	C	N	O	S	0	0	0
			1672	1077	274	315	6			

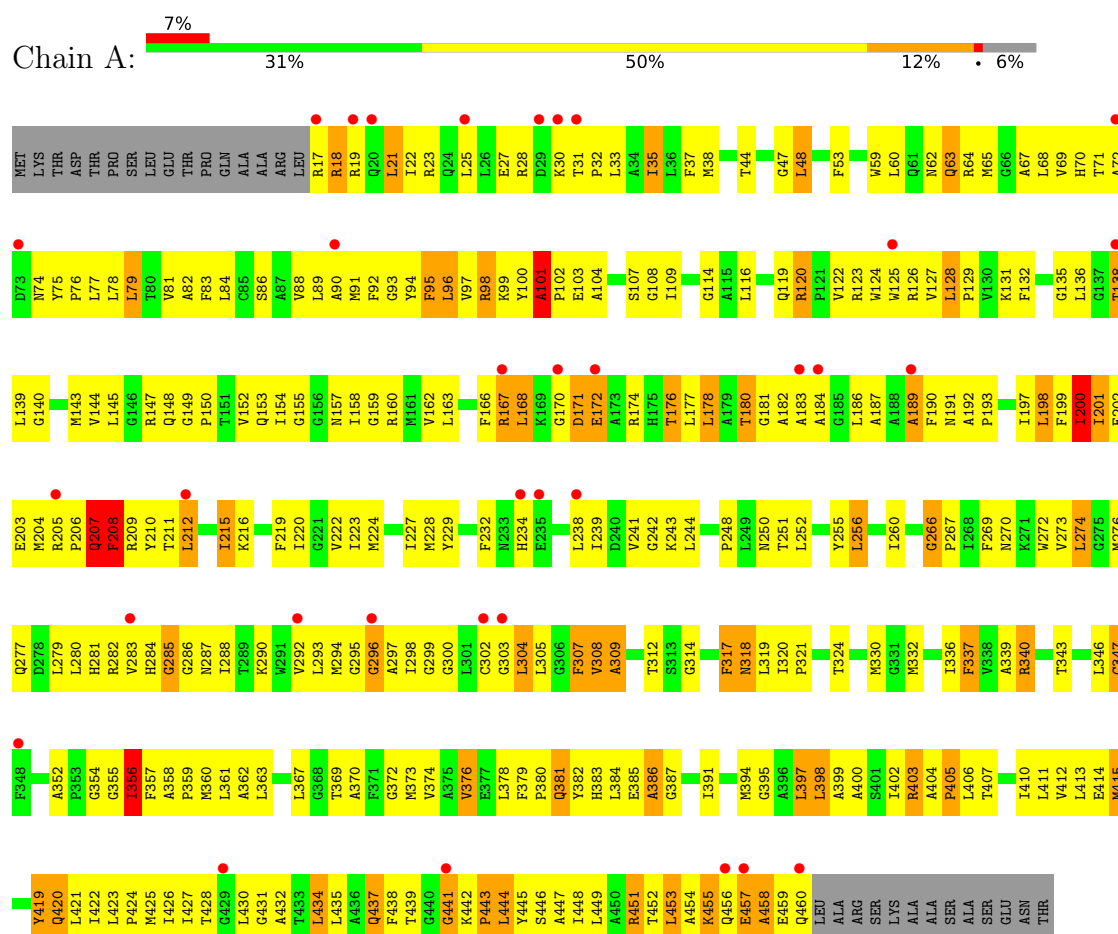
- Molecule 3 is a protein called Fab Fragment (Light Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			
3	F	211	Total	C	N	O	S	0	0	0
			1621	1008	271	334	8			

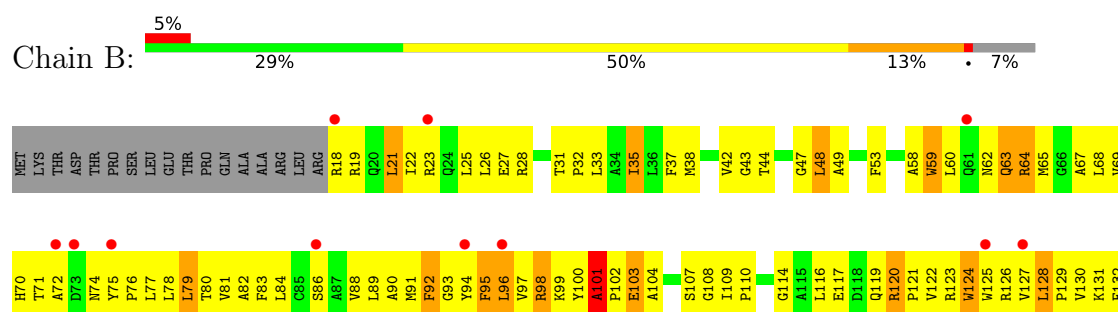
3 Residue-property plots [i](#)

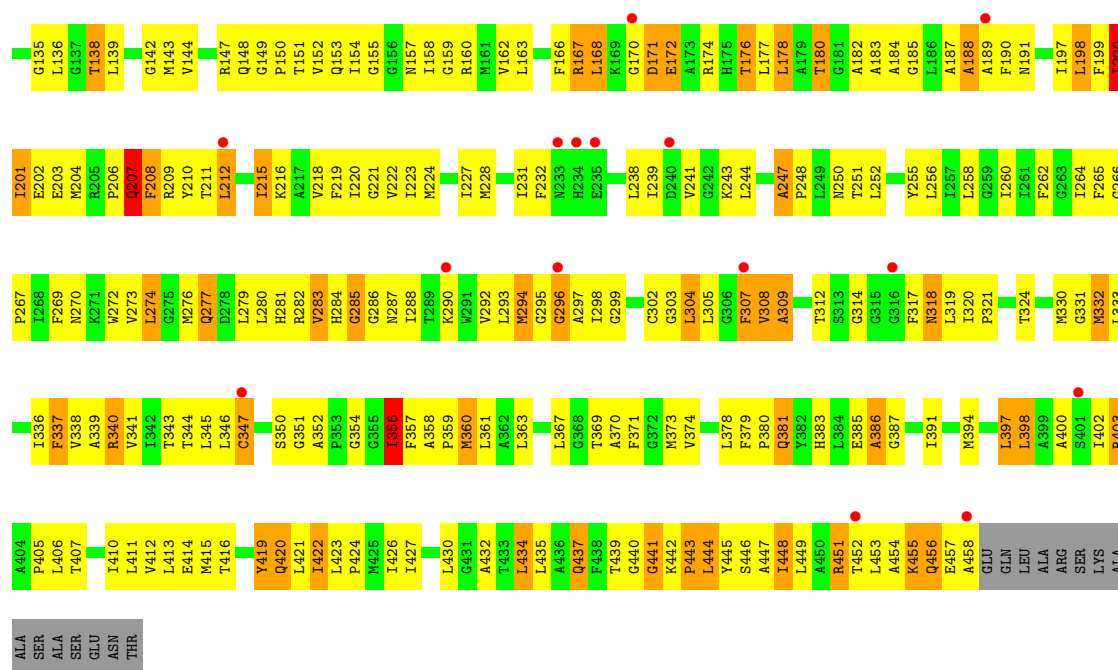
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: H(+)/Cl(-) exchange transporter clcA

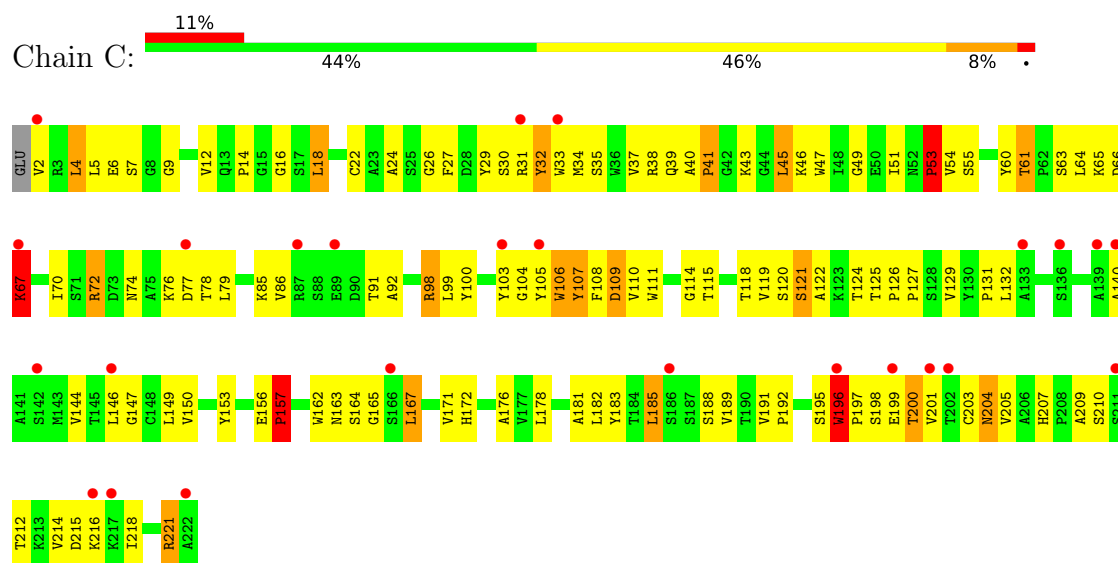


- Molecule 1: H(+)/Cl(-) exchange transporter clcA

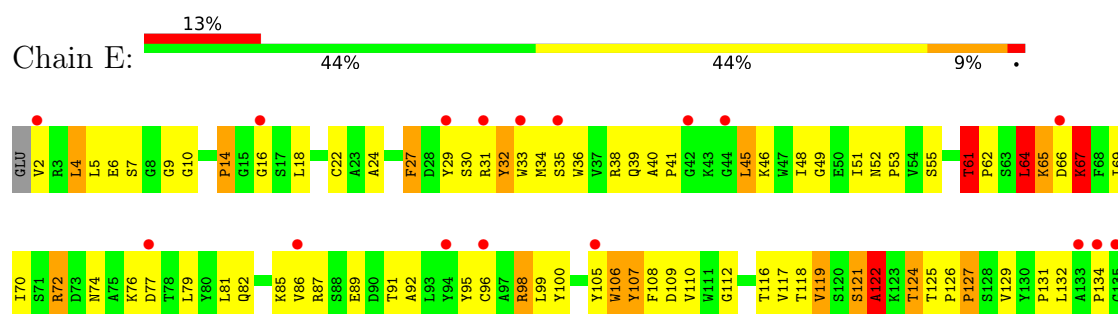


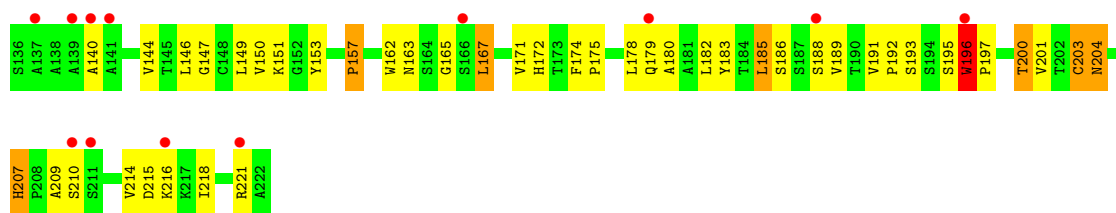


• Molecule 2: Fab Fragment (Heavy Chain)

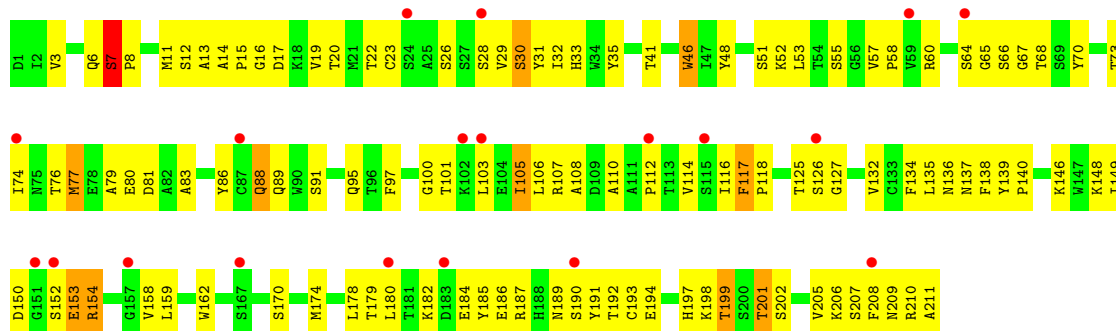


• Molecule 2: Fab Fragment (Heavy Chain)

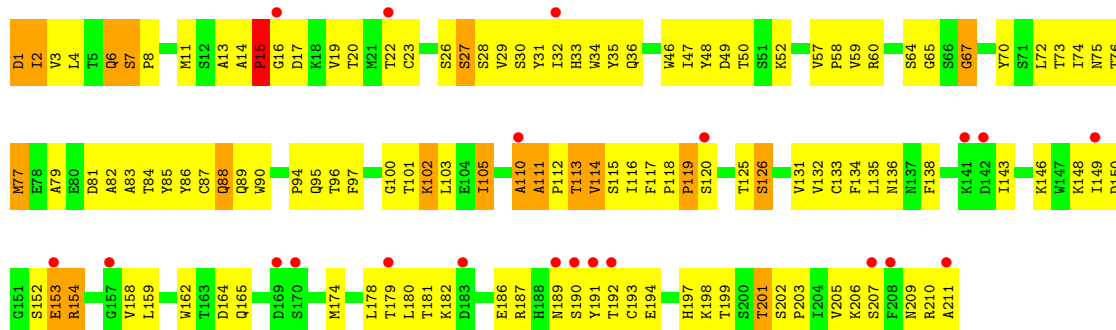




● Molecule 3: Fab Fragment (Light Chain)



● Molecule 3: Fab Fragment (Light Chain)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.64Å 119.79Å 151.30Å 90.00° 128.09° 90.00°	Depositor
Resolution (Å)	19.97 – 3.10 19.97 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.97-3.10) 95.3 (19.97-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.328 , 0.352 0.309 , 0.332	Depositor DCC
R_{free} test set	2595 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	82.6	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

5.1 Standard geometry

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	0.61	0/3405	1.06	21/4621 (0.5%)
1	B	0.62	0/3376	1.04	23/4583 (0.5%)
2	C	0.95	4/1721 (0.2%)	1.19	7/2355 (0.3%)
2	E	0.95	6/1721 (0.3%)	1.19	10/2355 (0.4%)
3	D	0.75	0/1660	1.07	5/2257 (0.2%)
3	F	0.85	2/1660 (0.1%)	1.13	5/2257 (0.2%)
All	All	0.76	12/13543 (0.1%)	1.10	71/18428 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	E	0	1
3	F	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	121	SER	C-N	-10.15	1.19	1.33
2	E	121	SER	CA-C	9.20	1.66	1.52
2	E	121	SER	C-O	7.35	1.33	1.24
2	C	61	THR	CB-CG2	-7.13	1.29	1.52
2	E	122	ALA	CA-CB	-6.09	1.43	1.53
2	C	121	SER	CA-C	5.88	1.60	1.52
2	E	124	THR	CA-CB	5.77	1.60	1.53
2	C	121	SER	C-N	-5.76	1.25	1.33
2	C	63	SER	C-N	5.49	1.40	1.33
3	F	110	ALA	CA-CB	-5.24	1.48	1.53
3	F	201	THR	CB-CG2	-5.21	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	61	THR	CB-CG2	-5.10	1.35	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	121	SER	N-CA-C	-11.06	99.29	113.12
1	A	356	ILE	N-CA-C	-10.76	102.53	112.43
2	C	61	THR	OG1-CB-CG2	-10.18	88.94	109.30
1	A	207	GLN	N-CA-C	8.90	121.94	111.71
1	B	356	ILE	N-CA-C	-8.63	103.97	112.17
1	A	398	LEU	N-CA-C	-8.00	103.54	113.38
1	B	398	LEU	N-CA-C	-7.64	103.55	113.17
2	E	67	LYS	N-CA-C	-7.59	102.00	111.11
1	B	207	GLN	N-CA-C	7.48	121.50	112.38
1	B	296	GLY	N-CA-C	-7.16	106.79	114.67
3	D	136	ASN	N-CA-C	7.13	121.30	109.46
2	E	121	SER	N-CA-C	-7.04	104.26	112.92
2	C	61	THR	N-CA-C	-6.88	102.22	110.13
3	F	111	ALA	CA-C-N	6.63	128.13	119.84
3	F	111	ALA	C-N-CA	6.63	128.13	119.84
2	C	67	LYS	N-CA-C	-6.60	103.34	111.33
1	A	437	GLN	N-CA-C	-6.59	102.67	111.96
3	F	114	VAL	N-CA-C	6.38	117.42	110.21
1	A	238	LEU	N-CA-C	-6.37	105.15	113.12
3	F	136	ASN	N-CA-C	6.23	120.42	109.96
3	D	91	SER	N-CA-C	-6.20	105.72	113.28
1	A	308	VAL	N-CA-C	-6.12	107.32	113.20
1	B	437	GLN	N-CA-C	-6.09	103.37	111.96
1	A	403	ARG	N-CA-C	6.08	119.74	111.17
1	A	296	GLY	N-CA-C	-6.05	107.68	114.40
2	E	32	TYR	N-CA-C	6.03	118.72	108.90
2	E	121	SER	O-C-N	6.02	129.57	122.34
2	E	196	TRP	N-CA-C	6.02	123.12	109.81
2	C	32	TYR	N-CA-C	5.98	118.70	109.07
1	B	308	VAL	N-CA-C	-5.98	107.46	113.20
1	A	458	ALA	N-CA-C	-5.96	105.28	113.56
1	A	168	LEU	N-CA-C	-5.92	101.65	110.23
1	B	256	LEU	N-CA-C	-5.92	104.18	111.40
3	D	201	THR	OG1-CB-CG2	-5.91	97.48	109.30
3	D	7	SER	CA-C-N	-5.90	113.13	119.98
3	D	7	SER	C-N-CA	-5.90	113.13	119.98
1	A	256	LEU	N-CA-C	-5.88	104.23	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455	LYS	N-CA-C	-5.86	105.80	113.12
2	E	207	HIS	CA-C-N	5.78	127.07	119.84
2	E	207	HIS	C-N-CA	5.78	127.07	119.84
1	A	397	LEU	N-CA-C	-5.78	105.99	113.16
2	E	7	SER	CB-CA-C	-5.78	107.18	114.40
2	C	196	TRP	N-CA-C	5.67	122.34	109.81
1	A	455	LYS	N-CA-C	-5.67	106.50	113.41
2	E	64	LEU	N-CA-C	5.65	122.83	110.80
1	B	456	GLN	N-CA-C	-5.58	104.22	111.02
1	A	456	GLN	N-CA-C	-5.52	104.28	111.02
1	B	101	ALA	CA-C-N	5.49	126.71	119.84
1	B	101	ALA	C-N-CA	5.49	126.71	119.84
1	B	403	ARG	N-CA-C	5.45	118.85	111.17
1	B	397	LEU	N-CA-C	-5.44	106.41	113.16
2	E	61	THR	CB-CA-C	-5.38	99.25	111.89
3	F	27	SER	CA-C-O	5.36	121.71	118.33
1	A	266	GLY	CA-C-N	5.36	124.69	118.85
1	A	266	GLY	C-N-CA	5.36	124.69	118.85
1	B	168	LEU	N-CA-C	-5.34	102.49	110.23
1	B	294	MET	N-CA-C	-5.34	106.84	113.19
1	A	101	ALA	CA-C-N	5.29	126.45	119.84
1	A	101	ALA	C-N-CA	5.29	126.45	119.84
1	B	247	ALA	CA-C-N	5.27	125.18	119.85
1	B	247	ALA	C-N-CA	5.27	125.18	119.85
1	B	238	LEU	N-CA-C	-5.26	106.55	113.12
1	A	457	GLU	N-CA-C	-5.25	102.23	110.17
1	B	277	GLN	N-CA-C	-5.23	106.95	113.38
1	A	453	LEU	N-CA-C	-5.22	107.46	113.88
1	B	371	PHE	N-CA-C	-5.21	105.60	111.28
1	B	448	ILE	N-CA-C	-5.19	106.62	111.45
1	B	124	TRP	N-CA-C	5.19	116.94	111.28
1	B	360	MET	N-CA-C	-5.10	105.91	111.82
1	A	208	PHE	N-CA-C	5.04	118.51	111.30
2	C	7	SER	CB-CA-C	-5.01	108.14	114.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	419	TYR	Sidechain
2	E	95	TYR	Sidechain
3	F	31	TYR	Sidechain

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	3333	0	3486	421	0
1	B	3304	0	3459	408	0
2	C	1672	0	1654	127	0
2	E	1672	0	1654	130	0
3	D	1621	0	1546	103	0
3	F	1621	0	1546	135	0
All	All	13223	0	13345	1249	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 47.

All (1249) 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:D:16:GLY:HA2	3:D:76:THR:HG23	1.28	1.06
1:A:381:GLN:H	1:A:381:GLN:NE2	1.54	1.06
1:B:381:GLN:H	1:B:381:GLN:NE2	1.53	1.05
3:F:192:THR:HA	3:F:207:SER:HB3	1.37	1.05
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.39	1.04
1:A:28:ARG:HD2	1:B:207:GLN:HG2	1.40	1.03
2:C:45:LEU:HD12	2:C:45:LEU:H	1.24	1.03
1:B:381:GLN:HE21	1:B:381:GLN:N	1.57	1.01
1:A:207:GLN:HG2	1:B:28:ARG:HD2	1.43	1.00
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.42	0.99
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.44	0.99
1:A:381:GLN:HE21	1:A:381:GLN:N	1.60	0.98
1:A:98:ARG:HH11	1:A:98:ARG:HB3	1.29	0.98
2:E:45:LEU:HD12	2:E:45:LEU:H	1.26	0.98
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.46	0.97
1:B:287:ASN:ND2	1:B:290:LYS:H	1.62	0.96
1:B:120:ARG:HB3	1:B:120:ARG:HH11	1.28	0.95
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.45	0.94
1:A:252:LEU:HD22	1:A:427:ILE:HD12	1.49	0.94
3:D:192:THR:HA	3:D:207:SER:HB3	1.49	0.94
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HH11	1:B:98:ARG:HB3	1.34	0.92
1:B:154:ILE:O	1:B:158:ILE:HG12	1.69	0.92
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.52	0.91
1:A:287:ASN:ND2	1:A:290:LYS:H	1.69	0.91
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.51	0.90
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.53	0.90
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.55	0.89
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.36	0.88
1:A:274:LEU:HA	1:A:277:GLN:HE21	1.37	0.88
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.38	0.88
1:A:274:LEU:O	1:A:277:GLN:HG2	1.73	0.88
1:A:154:ILE:O	1:A:158:ILE:HG12	1.74	0.88
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.55	0.88
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.55	0.88
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.54	0.88
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.39	0.87
1:B:305:LEU:HA	1:B:308:VAL:HG22	1.58	0.86
1:B:68:LEU:HD21	1:B:82:ALA:HB2	1.58	0.86
3:F:110:ALA:O	3:F:138:PHE:HA	1.76	0.86
1:B:274:LEU:O	1:B:277:GLN:HG2	1.75	0.85
3:F:14:ALA:O	3:F:17:ASP:HB2	1.76	0.85
1:B:109:ILE:HD12	1:B:445:TYR:HE2	1.40	0.85
1:B:287:ASN:HD22	1:B:290:LYS:H	1.17	0.85
1:B:198:LEU:HG	1:B:410:ILE:HD12	1.59	0.84
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.57	0.84
1:A:274:LEU:HA	1:A:277:GLN:NE2	1.93	0.84
1:A:381:GLN:H	1:A:381:GLN:HE21	0.84	0.83
3:F:82:ALA:HB2	3:F:105:ILE:HD11	1.61	0.83
1:A:274:LEU:HD12	1:A:277:GLN:HE22	1.42	0.83
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.61	0.83
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.13	0.83
1:B:37:PHE:HD2	1:B:38:MET:HE2	1.44	0.82
1:A:18:ARG:NH1	1:B:457:GLU:HB3	1.96	0.81
2:C:132:LEU:HB2	2:C:147:GLY:O	1.78	0.81
3:D:95:GLN:OE1	3:D:95:GLN:N	2.14	0.81
2:E:204:ASN:HB3	2:E:215:ASP:OD1	1.80	0.81
1:A:279:LEU:HA	1:A:282:ARG:HH11	1.46	0.81
1:B:65:MET:C	1:B:67:ALA:H	1.89	0.81
1:B:120:ARG:HD3	1:B:453:LEU:CD1	2.11	0.81
1:A:223:ILE:HD11	1:B:426:ILE:CG2	2.09	0.81
1:B:320:ILE:HD13	1:B:394:MET:HE2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.63	0.80
1:B:120:ARG:HB3	1:B:120:ARG:NH1	1.95	0.80
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.16	0.80
1:A:123:ARG:HA	1:A:125:TRP:CH2	2.17	0.80
2:C:172:HIS:HB2	2:C:188:SER:HB3	1.61	0.80
1:A:65:MET:C	1:A:67:ALA:H	1.90	0.80
3:D:150:ASP:HA	3:D:190:SER:HB3	1.62	0.80
1:A:109:ILE:HD12	1:A:445:TYR:HE2	1.46	0.79
1:B:449:LEU:O	1:B:453:LEU:HB2	1.82	0.79
1:B:241:VAL:HG11	1:B:324:THR:HG21	1.65	0.79
3:D:30:SER:HA	3:D:70:TYR:OH	1.83	0.79
1:B:200:ILE:HG22	1:B:201:ILE:N	1.97	0.79
1:B:201:ILE:HG21	1:B:215:ILE:HD11	1.63	0.78
3:F:111:ALA:N	3:F:199:THR:HG21	1.98	0.78
1:A:120:ARG:HH11	1:A:120:ARG:HB3	1.48	0.78
1:A:44:THR:O	1:A:48:LEU:HD22	1.83	0.78
1:B:120:ARG:HH11	1:B:120:ARG:CB	1.95	0.78
1:A:449:LEU:O	1:A:453:LEU:HB2	1.83	0.78
1:B:451:ARG:HH11	1:B:451:ARG:CB	1.96	0.78
1:A:274:LEU:HD12	1:A:277:GLN:NE2	1.97	0.78
2:E:72:ARG:NH1	2:E:74:ASN:OD1	2.16	0.78
1:A:287:ASN:HD22	1:A:290:LYS:H	1.27	0.78
3:F:95:GLN:N	3:F:95:GLN:OE1	2.16	0.78
1:A:200:ILE:HG22	1:A:201:ILE:N	1.97	0.78
1:A:98:ARG:HB3	1:A:98:ARG:NH1	1.99	0.77
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.64	0.77
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.20	0.77
1:B:279:LEU:HA	1:B:282:ARG:HH11	1.49	0.77
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.64	0.77
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.20	0.77
1:B:44:THR:O	1:B:48:LEU:HD22	1.85	0.76
3:F:192:THR:CA	3:F:207:SER:HB3	2.13	0.76
1:B:421:LEU:O	1:B:424:PRO:HD2	1.84	0.76
1:A:68:LEU:HD21	1:A:82:ALA:HB2	1.66	0.76
1:A:201:ILE:HG21	1:A:215:ILE:HD11	1.66	0.76
3:D:189:ASN:HD21	3:D:211:ALA:H	1.31	0.76
1:B:150:PRO:O	1:B:154:ILE:HG13	1.85	0.76
1:B:374:VAL:HG12	1:B:378:LEU:CD1	2.16	0.76
2:E:45:LEU:HD12	2:E:45:LEU:N	2.00	0.76
1:A:374:VAL:HG12	1:A:378:LEU:CD1	2.16	0.75
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:PRO:HB3	2:C:210:SER:OG	1.86	0.75
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.21	0.75
1:A:119:GLN:HB3	1:A:453:LEU:HD11	1.67	0.75
2:E:221:ARG:HH22	3:F:120:SER:HA	1.51	0.75
3:F:189:ASN:HD21	3:F:211:ALA:H	1.35	0.75
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.70	0.74
1:A:37:PHE:CD2	1:A:38:MET:HE2	2.22	0.74
1:B:274:LEU:HA	1:B:277:GLN:HE21	1.50	0.74
1:B:109:ILE:HD12	1:B:445:TYR:CE2	2.23	0.74
2:C:207:HIS:HE1	2:C:209:ALA:HB3	1.49	0.74
1:B:252:LEU:HD22	1:B:427:ILE:HD12	1.68	0.74
3:D:14:ALA:O	3:D:17:ASP:HB2	1.87	0.74
2:E:45:LEU:HD11	3:F:86:TYR:CD1	2.23	0.74
1:A:150:PRO:O	1:A:154:ILE:HG13	1.88	0.74
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.53	0.73
1:B:123:ARG:HH21	1:B:126:ARG:HH11	1.35	0.73
2:C:18:LEU:HD23	2:C:18:LEU:H	1.53	0.73
3:F:150:ASP:HA	3:F:190:SER:HB3	1.69	0.73
1:A:120:ARG:HD3	1:A:453:LEU:HD13	1.70	0.73
1:A:18:ARG:O	1:A:18:ARG:HG2	1.86	0.73
3:F:148:LYS:HB2	3:F:192:THR:OG1	1.89	0.72
1:A:120:ARG:HD3	1:A:453:LEU:CD1	2.19	0.72
2:C:51:ILE:HD11	2:C:55:SER:HB3	1.70	0.72
2:C:189:VAL:HG13	2:C:189:VAL:O	1.90	0.72
3:F:7:SER:HB3	3:F:8:PRO:CD	2.18	0.72
1:B:287:ASN:HD22	1:B:290:LYS:N	1.87	0.72
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.53	0.72
3:F:1:ASP:HB3	3:F:94:PRO:HD2	1.69	0.72
1:A:17:ARG:HD2	1:A:17:ARG:C	2.14	0.72
1:A:28:ARG:HD2	1:B:207:GLN:CG	2.17	0.72
2:E:41:PRO:HD3	2:E:92:ALA:HA	1.72	0.72
2:E:132:LEU:HD21	3:F:132:VAL:HG21	1.72	0.72
2:C:2:VAL:HA	2:C:26:GLY:HA3	1.71	0.72
2:E:126:PRO:HB3	2:E:210:SER:OG	1.90	0.71
3:F:30:SER:HA	3:F:70:TYR:OH	1.90	0.71
1:B:119:GLN:HB3	1:B:453:LEU:HD11	1.72	0.71
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.73	0.71
1:B:120:ARG:HD3	1:B:453:LEU:HD13	1.70	0.71
1:B:166:PHE:HB2	1:B:168:LEU:HD11	1.73	0.71
1:B:287:ASN:ND2	1:B:290:LYS:N	2.38	0.71
3:D:20:THR:HG23	3:D:73:THR:OG1	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ILE:HG21	1:B:394:MET:CE	2.21	0.71
1:A:18:ARG:NH2	1:B:456:GLN:NE2	2.38	0.71
1:B:168:LEU:HD12	1:B:168:LEU:H	1.56	0.70
2:C:124:THR:HG22	2:C:125:THR:N	2.06	0.70
2:C:72:ARG:NH1	2:C:74:ASN:OD1	2.24	0.70
1:A:451:ARG:CB	1:A:451:ARG:HH11	2.04	0.70
1:B:206:PRO:HG2	1:B:211:THR:OG1	1.91	0.70
2:C:45:LEU:HD12	2:C:45:LEU:N	2.03	0.70
1:A:108:GLY:HA2	1:A:153:GLN:NE2	2.06	0.70
1:B:144:VAL:HG21	1:B:343:THR:HB	1.73	0.70
2:C:12:VAL:HG23	2:C:119:VAL:HG22	1.72	0.70
1:A:216:LYS:HD3	1:B:434:LEU:CD2	2.22	0.70
1:A:239:ILE:HD12	1:A:415:MET:HE3	1.74	0.70
3:F:2:ILE:HD11	3:F:27:SER:HB2	1.74	0.70
1:A:144:VAL:HG21	1:A:343:THR:HB	1.73	0.69
1:B:182:ALA:HB1	1:B:204:MET:CE	2.22	0.69
1:B:381:GLN:H	1:B:381:GLN:HE21	0.80	0.69
1:A:22:ILE:HD13	1:B:454:ALA:HB2	1.73	0.69
1:A:123:ARG:HH21	1:A:126:ARG:HH11	1.36	0.69
1:B:274:LEU:HA	1:B:277:GLN:NE2	2.07	0.69
2:E:39:GLN:O	2:E:92:ALA:HB1	1.92	0.69
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.75	0.69
1:A:18:ARG:NH2	1:B:456:GLN:HE21	1.90	0.69
1:A:109:ILE:HD12	1:A:445:TYR:CE2	2.28	0.69
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.92	0.69
2:E:91:THR:OG1	2:E:119:VAL:HG23	1.91	0.69
1:A:79:LEU:H	1:A:79:LEU:CD2	2.06	0.69
1:A:426:ILE:CG2	1:B:223:ILE:HD11	2.22	0.69
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.28	0.69
1:A:207:GLN:CG	1:B:28:ARG:HD2	2.21	0.69
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.74	0.69
2:C:39:GLN:O	2:C:92:ALA:HB1	1.93	0.69
3:F:7:SER:HB2	3:F:22:THR:HB	1.75	0.69
1:B:37:PHE:CD2	1:B:38:MET:HE2	2.27	0.68
1:B:274:LEU:HD12	1:B:277:GLN:NE2	2.07	0.68
1:B:358:ALA:O	1:B:361:LEU:HB2	1.91	0.68
2:E:18:LEU:HD23	2:E:18:LEU:H	1.57	0.68
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.27	0.68
2:C:129:VAL:HG21	2:C:214:VAL:CG2	2.23	0.68
3:F:111:ALA:HB2	3:F:199:THR:HB	1.75	0.68
1:A:163:LEU:HD21	1:A:174:ARG:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HB3	1:B:98:ARG:NH1	2.05	0.68
1:A:79:LEU:H	1:A:79:LEU:HD22	1.58	0.68
1:A:320:ILE:HD13	1:A:394:MET:HE2	1.75	0.68
1:B:274:LEU:HD12	1:B:277:GLN:HE22	1.59	0.68
1:B:282:ARG:O	1:B:284:HIS:N	2.26	0.68
1:B:79:LEU:H	1:B:79:LEU:HD22	1.57	0.68
3:F:192:THR:HA	3:F:207:SER:CB	2.19	0.68
1:B:284:HIS:HA	1:B:290:LYS:HB3	1.75	0.68
3:D:7:SER:HB3	3:D:8:PRO:CD	2.23	0.68
1:A:182:ALA:HB1	1:A:204:MET:CE	2.24	0.68
1:A:380:PRO:HD2	1:A:381:GLN:HE22	1.59	0.67
1:A:458:ALA:N	1:A:460:GLN:HE22	1.91	0.67
1:B:172:GLU:O	1:B:176:THR:HB	1.93	0.67
2:C:204:ASN:HB3	2:C:215:ASP:OD1	1.93	0.67
1:B:79:LEU:H	1:B:79:LEU:CD2	2.07	0.67
1:B:374:VAL:HG12	1:B:378:LEU:HD11	1.77	0.67
1:A:120:ARG:HB3	1:A:120:ARG:NH1	2.09	0.67
1:A:421:LEU:O	1:A:424:PRO:HD2	1.95	0.67
1:A:199:PHE:HA	1:A:407:THR:OG1	1.95	0.67
1:B:451:ARG:HH11	1:B:451:ARG:HB3	1.59	0.66
2:E:129:VAL:HG21	2:E:214:VAL:CG2	2.25	0.66
3:F:7:SER:CB	3:F:8:PRO:HD3	2.22	0.66
1:A:458:ALA:H	1:A:460:GLN:HE22	1.43	0.66
3:D:13:ALA:HB3	3:D:77:MET:CE	2.25	0.66
1:A:143:MET:HE2	1:A:347:CYS:SG	2.35	0.66
1:A:97:VAL:HG22	1:A:104:ALA:HB3	1.76	0.66
1:A:434:LEU:CD2	1:B:216:LYS:HD3	2.25	0.66
1:B:143:MET:HE2	1:B:347:CYS:SG	2.35	0.66
1:A:403:ARG:NH2	1:A:437:GLN:HB2	2.10	0.66
2:C:18:LEU:HD23	2:C:18:LEU:N	2.08	0.66
2:C:41:PRO:HD3	2:C:92:ALA:HA	1.78	0.66
3:F:148:LYS:HA	3:F:152:SER:O	1.96	0.66
1:A:172:GLU:O	1:A:176:THR:HB	1.95	0.66
3:D:148:LYS:HA	3:D:152:SER:O	1.95	0.66
2:E:192:PRO:O	2:E:195:SER:HB3	1.95	0.66
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.76	0.66
2:C:30:SER:C	2:C:32:TYR:H	2.04	0.66
1:A:403:ARG:HH22	1:A:437:GLN:HB2	1.60	0.66
1:A:266:GLY:HA3	1:A:400:ALA:HB1	1.78	0.66
3:D:192:THR:CA	3:D:207:SER:HB3	2.25	0.66
1:A:282:ARG:O	1:A:284:HIS:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:MET:O	1:A:336:ILE:HG13	1.95	0.65
1:A:403:ARG:HH22	1:A:437:GLN:CB	2.09	0.65
2:C:45:LEU:HD11	3:D:86:TYR:CD1	2.31	0.65
1:A:122:VAL:HG11	1:A:160:ARG:CB	2.26	0.65
1:A:166:PHE:HB2	1:A:168:LEU:HD11	1.77	0.65
1:A:374:VAL:HG12	1:A:378:LEU:HD11	1.79	0.65
2:C:129:VAL:HG21	2:C:214:VAL:HG21	1.78	0.65
2:E:6:GLU:HA	2:E:22:CYS:HA	1.78	0.65
2:E:172:HIS:HB2	2:E:188:SER:HB3	1.77	0.65
1:A:411:LEU:O	1:A:414:GLU:HB2	1.97	0.65
2:E:207:HIS:ND1	2:E:210:SER:HB3	2.12	0.65
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.32	0.65
1:B:108:GLY:HA2	1:B:153:GLN:NE2	2.12	0.65
1:B:423:LEU:HB3	1:B:424:PRO:HD3	1.79	0.65
3:F:22:THR:HG22	3:F:23:CYS:N	2.12	0.65
1:A:374:VAL:HG12	1:A:378:LEU:HD12	1.79	0.65
3:D:22:THR:HG22	3:D:23:CYS:N	2.12	0.65
1:A:250:ASN:OD1	1:A:251:THR:HG23	1.96	0.65
1:B:23:ARG:O	1:B:27:GLU:HB2	1.97	0.65
1:B:114:GLY:HA2	1:B:449:LEU:HD21	1.79	0.65
2:E:35:SER:HB2	2:E:49:GLY:O	1.97	0.65
3:F:95:GLN:H	3:F:95:GLN:CD	2.05	0.65
1:A:114:GLY:HA2	1:A:449:LEU:HD21	1.79	0.64
1:A:168:LEU:HD12	1:A:168:LEU:H	1.61	0.64
1:A:357:PHE:CE1	1:A:398:LEU:HD22	2.31	0.64
1:B:227:ILE:HG22	1:B:228:MET:HE2	1.79	0.64
3:F:134:PHE:O	3:F:135:LEU:HD23	1.97	0.64
3:D:182:LYS:HG2	3:D:186:GLU:OE1	1.97	0.64
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.78	0.64
1:A:318:ASN:N	1:A:318:ASN:HD22	1.95	0.64
2:E:2:VAL:HG23	2:E:2:VAL:O	1.96	0.64
2:E:146:LEU:HD12	2:E:201:VAL:HG11	1.79	0.64
1:A:220:ILE:CG1	1:B:430:LEU:HD21	2.26	0.64
1:B:119:GLN:O	1:B:120:ARG:HD2	1.98	0.64
1:B:410:ILE:O	1:B:414:GLU:HG2	1.98	0.64
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.62	0.64
1:B:250:ASN:OD1	1:B:251:THR:HG23	1.97	0.64
1:A:227:ILE:HG22	1:A:228:MET:HE2	1.80	0.64
1:B:270:ASN:ND2	1:B:444:LEU:HD23	2.12	0.64
2:E:189:VAL:HG13	2:E:189:VAL:O	1.95	0.64
1:A:120:ARG:HH11	1:A:120:ARG:CB	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:TRP:H	2:E:106:TRP:CD1	2.16	0.64
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.63	0.63
1:B:239:ILE:HD12	1:B:415:MET:HE3	1.80	0.63
3:D:205:VAL:O	3:D:206:LYS:HG2	1.98	0.63
2:E:24:ALA:HB1	2:E:27:PHE:HE1	1.63	0.63
2:E:132:LEU:HB2	2:E:147:GLY:O	1.99	0.63
3:F:58:PRO:C	3:F:60:ARG:H	2.05	0.63
1:A:443:PRO:HB2	1:A:446:SER:HB2	1.80	0.63
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.80	0.63
1:A:454:ALA:HB2	1:B:22:ILE:HD13	1.79	0.63
1:B:166:PHE:HB2	1:B:168:LEU:CD1	2.29	0.63
2:C:192:PRO:O	2:C:195:SER:HB3	1.98	0.63
3:D:179:THR:O	3:D:180:LEU:HD23	1.97	0.63
2:E:207:HIS:CE1	2:E:209:ALA:HB3	2.34	0.63
3:D:95:GLN:CD	3:D:95:GLN:H	2.06	0.63
3:D:114:VAL:O	3:D:206:LYS:HD2	1.98	0.63
3:F:11:MET:HE2	3:F:19:VAL:HG23	1.80	0.63
2:C:51:ILE:CD1	2:C:72:ARG:HD2	2.29	0.63
3:F:72:LEU:C	3:F:72:LEU:HD23	2.24	0.63
1:A:138:THR:HG22	1:A:143:MET:SD	2.38	0.63
1:B:163:LEU:HD21	1:B:174:ARG:HG3	1.81	0.63
2:E:30:SER:C	2:E:32:TYR:H	2.07	0.62
1:A:269:PHE:O	1:A:273:VAL:HG12	1.99	0.62
1:A:320:ILE:HG21	1:A:394:MET:CE	2.29	0.62
1:B:266:GLY:HA3	1:B:400:ALA:HB1	1.81	0.62
2:E:45:LEU:H	2:E:45:LEU:CD1	2.09	0.62
3:F:20:THR:HG23	3:F:73:THR:OG1	1.99	0.62
1:B:63:GLN:C	1:B:65:MET:H	2.08	0.62
3:F:190:SER:HA	3:F:209:ASN:OD1	1.99	0.62
1:A:287:ASN:ND2	1:A:290:LYS:HG3	2.14	0.62
1:B:374:VAL:HG12	1:B:378:LEU:HD12	1.81	0.62
1:A:86:SER:OG	1:A:303:GLY:HA3	1.99	0.62
3:D:7:SER:CB	3:D:8:PRO:HD3	2.25	0.62
1:A:71:THR:HB	1:A:77:LEU:HD23	1.81	0.62
1:A:410:ILE:O	1:A:414:GLU:HG2	1.99	0.62
2:C:185:LEU:C	2:C:185:LEU:HD12	2.24	0.62
3:F:111:ALA:HB2	3:F:199:THR:CB	2.30	0.62
1:B:199:PHE:HA	1:B:407:THR:OG1	2.00	0.61
1:B:279:LEU:O	1:B:279:LEU:HD23	1.98	0.61
3:F:13:ALA:HB3	3:F:77:MET:CE	2.29	0.61
1:A:437:GLN:NE2	1:B:31:THR:H	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:196:TRP:O	2:C:197:PRO:C	2.40	0.61
1:A:31:THR:H	1:B:437:GLN:NE2	1.97	0.61
3:F:7:SER:CB	3:F:22:THR:HB	2.30	0.61
1:A:23:ARG:O	1:A:27:GLU:HB2	2.00	0.61
1:A:75:TYR:HB3	1:A:76:PRO:CD	2.29	0.61
1:A:357:PHE:CE1	1:A:398:LEU:HD13	2.35	0.61
1:A:358:ALA:O	1:A:361:LEU:HB2	1.99	0.61
1:B:243:LYS:HE2	1:B:420:GLN:OE1	2.00	0.61
1:A:216:LYS:HD3	1:B:434:LEU:HD22	1.82	0.61
1:A:287:ASN:ND2	1:A:290:LYS:N	2.47	0.61
2:E:18:LEU:HD23	2:E:18:LEU:N	2.15	0.61
1:A:99:LYS:HB2	1:A:288:ILE:HD11	1.83	0.61
1:B:147:ARG:HG3	1:B:147:ARG:HH11	1.65	0.61
2:C:129:VAL:CG2	2:C:214:VAL:HG21	2.30	0.61
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.83	0.61
1:A:148:GLN:HE22	1:A:189:ALA:HB1	1.66	0.61
1:A:166:PHE:HB2	1:A:168:LEU:CD1	2.30	0.61
1:B:72:ALA:HA	1:B:78:LEU:HD21	1.81	0.61
1:A:72:ALA:HA	1:A:78:LEU:HD21	1.83	0.61
1:A:413:LEU:HD11	1:A:419:TYR:HD1	1.65	0.60
1:A:298:ILE:CG2	1:A:346:LEU:HG	2.31	0.60
1:A:101:ALA:C	1:A:103:GLU:H	2.09	0.60
1:B:176:THR:O	1:B:180:THR:HG23	2.01	0.60
1:B:403:ARG:NH2	1:B:437:GLN:HB2	2.15	0.60
3:F:182:LYS:HG2	3:F:186:GLU:OE1	2.00	0.60
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.66	0.60
3:F:77:MET:SD	3:F:103:LEU:HD21	2.41	0.60
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.83	0.60
3:F:194:GLU:CG	3:F:205:VAL:HG12	2.24	0.60
2:C:185:LEU:HD12	2:C:185:LEU:O	2.00	0.60
1:A:284:HIS:HA	1:A:290:LYS:HB3	1.84	0.60
2:C:6:GLU:HA	2:C:22:CYS:HA	1.82	0.60
1:A:190:PHE:CE2	1:A:411:LEU:HD21	2.37	0.60
1:A:148:GLN:NE2	1:A:189:ALA:HB1	2.16	0.60
1:A:243:LYS:HE2	1:A:420:GLN:OE1	2.01	0.60
3:F:179:THR:O	3:F:180:LEU:HD23	2.01	0.60
1:A:53:PHE:HE2	1:A:147:ARG:HB2	1.66	0.59
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.36	0.59
1:B:369:THR:HG22	1:B:373:MET:HE3	1.83	0.59
2:E:207:HIS:HE1	2:E:209:ALA:HB3	1.67	0.59
1:B:357:PHE:CE1	1:B:398:LEU:HD13	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:129:VAL:CG2	2:E:214:VAL:HG21	2.32	0.59
3:F:34:TRP:CZ3	3:F:87:CYS:HB3	2.37	0.59
3:F:114:VAL:HG12	3:F:115:SER:N	2.17	0.59
3:F:116:ILE:HD13	3:F:193:CYS:HB2	1.84	0.59
2:C:51:ILE:HD13	2:C:72:ARG:HD2	1.84	0.59
1:B:318:ASN:HD22	1:B:319:LEU:H	1.49	0.59
1:A:122:VAL:HG11	1:A:160:ARG:HB3	1.84	0.59
1:A:434:LEU:HD22	1:B:216:LYS:HD3	1.84	0.59
1:B:86:SER:OG	1:B:303:GLY:HA3	2.03	0.59
1:A:198:LEU:HG	1:A:410:ILE:CD1	2.32	0.59
1:B:71:THR:HB	1:B:77:LEU:HD23	1.85	0.59
1:A:63:GLN:C	1:A:65:MET:H	2.11	0.59
1:A:212:LEU:HD12	1:A:212:LEU:H	1.67	0.59
3:D:153:GLU:HG3	3:D:154:ARG:H	1.67	0.59
2:E:49:GLY:HA3	2:E:70:ILE:CD1	2.33	0.59
2:E:185:LEU:HD12	2:E:185:LEU:O	2.03	0.59
3:F:15:PRO:HD3	3:F:105:ILE:HG22	1.83	0.59
1:A:451:ARG:HH11	1:A:451:ARG:HB3	1.66	0.59
1:B:97:VAL:HG22	1:B:104:ALA:HB3	1.85	0.59
1:B:171:ASP:HB2	1:B:212:LEU:HD22	1.83	0.59
2:E:121:SER:O	2:E:122:ALA:O	2.21	0.59
1:A:23:ARG:HG3	1:A:23:ARG:HH11	1.66	0.59
1:A:60:LEU:O	1:A:64:ARG:HG3	2.02	0.59
1:B:287:ASN:ND2	1:B:290:LYS:HG3	2.18	0.59
2:C:35:SER:HB2	2:C:49:GLY:O	2.02	0.59
1:A:17:ARG:HD2	1:A:17:ARG:O	2.02	0.58
1:A:385:GLU:O	1:A:387:GLY:N	2.36	0.58
1:A:270:ASN:ND2	1:A:444:LEU:HD23	2.16	0.58
1:A:356:ILE:O	1:A:360:MET:HG3	2.03	0.58
1:B:252:LEU:HD11	1:B:423:LEU:HD23	1.84	0.58
1:B:267:PRO:O	1:B:270:ASN:HB2	2.02	0.58
2:E:196:TRP:O	2:E:197:PRO:C	2.46	0.58
1:B:413:LEU:HD11	1:B:419:TYR:HD1	1.69	0.58
2:C:106:TRP:H	2:C:106:TRP:CD1	2.19	0.58
2:C:127:PRO:HB3	2:C:153:TYR:CB	2.31	0.58
2:C:146:LEU:HD12	2:C:201:VAL:HG11	1.86	0.58
1:A:266:GLY:N	1:A:267:PRO:HD2	2.18	0.58
2:C:132:LEU:HD21	3:D:132:VAL:HG21	1.86	0.58
2:E:129:VAL:HG21	2:E:214:VAL:HG21	1.83	0.58
1:A:98:ARG:NH1	1:A:98:ARG:CB	2.67	0.58
1:A:122:VAL:HG12	1:A:122:VAL:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ILE:O	1:B:340:ARG:HG3	2.03	0.58
1:B:457:GLU:O	1:B:458:ALA:HB3	2.04	0.58
3:D:158:VAL:O	3:D:159:LEU:HD23	2.03	0.58
3:F:153:GLU:HG3	3:F:154:ARG:H	1.68	0.58
1:B:403:ARG:HH22	1:B:437:GLN:CB	2.16	0.58
2:E:40:ALA:HA	2:E:92:ALA:CB	2.33	0.58
1:A:403:ARG:HH22	1:A:437:GLN:CA	2.17	0.58
1:B:148:GLN:HG3	1:B:190:PHE:CZ	2.39	0.58
1:B:227:ILE:O	1:B:231:ILE:HG12	2.03	0.58
2:E:61:THR:HB	2:E:62:PRO:CD	2.34	0.58
3:F:111:ALA:H	3:F:199:THR:HG21	1.69	0.58
1:B:122:VAL:HG11	1:B:160:ARG:CB	2.33	0.58
3:D:117:PHE:CD1	3:D:117:PHE:N	2.72	0.58
3:D:189:ASN:ND2	3:D:211:ALA:H	2.01	0.58
1:B:19:ARG:HG2	1:B:19:ARG:HH11	1.69	0.58
1:B:122:VAL:HG12	1:B:122:VAL:O	2.03	0.58
2:C:100:TYR:HB3	2:C:107:TYR:CE1	2.39	0.58
3:D:58:PRO:C	3:D:60:ARG:H	2.12	0.58
1:A:305:LEU:HA	1:A:308:VAL:CG2	2.32	0.57
1:A:336:ILE:O	1:A:340:ARG:HG3	2.04	0.57
1:A:402:ILE:HD12	1:A:445:TYR:CE1	2.39	0.57
2:E:39:GLN:C	2:E:92:ALA:HB1	2.29	0.57
1:B:99:LYS:HB2	1:B:288:ILE:HD11	1.86	0.57
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.18	0.57
1:A:79:LEU:HD22	1:A:79:LEU:N	2.19	0.57
1:B:403:ARG:HH22	1:B:437:GLN:HB2	1.69	0.57
2:C:39:GLN:C	2:C:92:ALA:HB1	2.29	0.57
2:C:124:THR:HG22	2:C:125:THR:H	1.68	0.57
1:A:23:ARG:HG3	1:A:23:ARG:NH1	2.19	0.57
1:A:252:LEU:HD22	1:A:427:ILE:CD1	2.31	0.57
1:B:75:TYR:O	1:B:79:LEU:HD23	2.04	0.57
1:B:90:ALA:O	1:B:94:TYR:HD1	1.87	0.57
3:D:134:PHE:O	3:D:135:LEU:HD23	2.04	0.57
1:A:31:THR:H	1:B:437:GLN:HE22	1.52	0.57
1:B:74:ASN:CG	1:B:77:LEU:HB2	2.29	0.57
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.40	0.57
1:A:148:GLN:HB3	1:A:190:PHE:HE1	1.68	0.57
1:A:287:ASN:HD22	1:A:290:LYS:N	1.99	0.57
1:A:170:GLY:O	1:A:172:GLU:N	2.37	0.57
2:E:91:THR:HG23	2:E:118:THR:HA	1.86	0.57
1:A:74:ASN:CG	1:A:77:LEU:HB2	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:THR:HG22	2:C:200:THR:O	2.05	0.57
1:B:266:GLY:N	1:B:267:PRO:HD2	2.20	0.57
3:D:114:VAL:HG22	3:D:135:LEU:CD2	2.34	0.57
1:A:186:LEU:O	1:A:186:LEU:HG	2.05	0.56
1:B:318:ASN:HD22	1:B:318:ASN:N	2.02	0.56
1:A:206:PRO:HG2	1:A:211:THR:OG1	2.04	0.56
1:A:369:THR:HG22	1:A:373:MET:HE3	1.87	0.56
2:E:49:GLY:HA3	2:E:70:ILE:HD12	1.87	0.56
1:A:148:GLN:HG3	1:A:190:PHE:CZ	2.40	0.56
1:A:252:LEU:HD11	1:A:423:LEU:HD23	1.87	0.56
1:A:437:GLN:HE22	1:B:31:THR:H	1.51	0.56
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.88	0.56
3:D:190:SER:HA	3:D:209:ASN:OD1	2.06	0.56
1:B:101:ALA:C	1:B:103:GLU:H	2.14	0.56
1:A:419:TYR:CE1	1:B:414:GLU:OE1	2.59	0.56
1:B:298:ILE:CG2	1:B:346:LEU:HG	2.35	0.56
1:B:357:PHE:CE1	1:B:398:LEU:HD22	2.40	0.56
3:D:125:THR:HG22	3:D:125:THR:O	2.03	0.56
1:A:200:ILE:CG2	1:A:201:ILE:N	2.67	0.56
2:C:40:ALA:HA	2:C:92:ALA:HB2	1.86	0.56
2:E:171:VAL:C	2:E:172:HIS:HD1	2.14	0.56
2:E:196:TRP:HB3	2:E:197:PRO:HD3	1.88	0.56
1:B:170:GLY:O	1:B:172:GLU:N	2.39	0.56
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.29	0.56
1:A:75:TYR:O	1:A:79:LEU:HD23	2.05	0.56
1:B:79:LEU:HD22	1:B:79:LEU:N	2.21	0.56
1:B:190:PHE:CE2	1:B:411:LEU:HD21	2.40	0.56
3:F:82:ALA:HB2	3:F:105:ILE:CD1	2.32	0.56
1:B:356:ILE:O	1:B:360:MET:HG3	2.06	0.56
2:E:40:ALA:HA	2:E:92:ALA:HB2	1.86	0.56
2:E:107:TYR:HB3	3:F:33:HIS:NE2	2.21	0.56
2:E:146:LEU:HD13	2:E:218:ILE:HG21	1.87	0.56
3:D:32:ILE:HG22	3:D:33:HIS:N	2.22	0.55
1:A:18:ARG:HH21	1:B:456:GLN:NE2	2.03	0.55
1:B:64:ARG:NH1	1:B:64:ARG:HB3	2.21	0.55
2:E:127:PRO:HB3	2:E:153:TYR:CB	2.35	0.55
3:F:114:VAL:HG22	3:F:135:LEU:CD2	2.35	0.55
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.87	0.55
3:D:192:THR:HA	3:D:207:SER:CB	2.30	0.55
1:A:35:ILE:CG2	1:A:176:THR:HG21	2.36	0.55
1:A:212:LEU:HD12	1:A:212:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ILE:CG2	1:B:201:ILE:N	2.69	0.55
1:B:269:PHE:O	1:B:273:VAL:HG12	2.06	0.55
1:B:318:ASN:HD22	1:B:319:LEU:N	2.04	0.55
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.89	0.55
1:A:318:ASN:HD22	1:A:319:LEU:H	1.55	0.55
1:B:243:LYS:HE2	1:B:420:GLN:CG	2.36	0.55
3:F:111:ALA:CA	3:F:199:THR:HG21	2.36	0.55
2:C:109:ASP:OD2	2:C:110:VAL:HG23	2.07	0.55
2:C:156:GLU:HG2	2:C:183:TYR:CE1	2.41	0.55
1:B:294:MET:HG2	1:B:294:MET:O	2.06	0.55
2:E:100:TYR:HB3	2:E:107:TYR:CE1	2.42	0.55
1:A:17:ARG:HH21	1:B:119:GLN:NE2	2.03	0.55
1:B:123:ARG:HA	1:B:125:TRP:CH2	2.42	0.55
1:A:59:TRP:CZ3	1:A:60:LEU:HD23	2.42	0.55
1:A:199:PHE:CD1	1:A:407:THR:HG21	2.42	0.55
1:B:398:LEU:O	1:B:402:ILE:HG23	2.06	0.54
2:C:127:PRO:CB	2:C:153:TYR:HB3	2.32	0.54
2:E:132:LEU:HD21	3:F:132:VAL:CG2	2.35	0.54
1:B:305:LEU:C	1:B:307:PHE:H	2.16	0.54
3:D:105:ILE:HB	3:D:170:SER:OG	2.07	0.54
3:D:110:ALA:C	3:D:199:THR:HG21	2.33	0.54
1:B:320:ILE:HG21	1:B:394:MET:HE3	1.89	0.54
1:B:380:PRO:HD2	1:B:381:GLN:NE2	2.20	0.54
1:A:92:PHE:O	1:A:96:LEU:HD23	2.07	0.54
1:A:457:GLU:HB3	1:B:18:ARG:NH1	2.22	0.54
3:F:29:VAL:CG2	3:F:32:ILE:HD11	2.37	0.54
1:A:33:LEU:C	1:A:33:LEU:HD23	2.32	0.54
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.43	0.54
1:A:267:PRO:O	1:A:270:ASN:HB2	2.06	0.54
1:B:332:MET:O	1:B:336:ILE:HG13	2.08	0.54
2:C:30:SER:C	2:C:32:TYR:N	2.64	0.54
3:F:29:VAL:O	3:F:67:GLY:HA2	2.08	0.54
1:A:17:ARG:C	1:A:19:ARG:H	2.16	0.54
1:A:243:LYS:HE2	1:A:420:GLN:CG	2.38	0.54
1:B:212:LEU:HD12	1:B:212:LEU:N	2.23	0.54
2:C:24:ALA:HB1	2:C:27:PHE:HE1	1.72	0.54
2:E:10:GLY:N	2:E:116:THR:O	2.41	0.54
1:A:90:ALA:O	1:A:94:TYR:HD1	1.91	0.54
1:A:457:GLU:O	1:A:458:ALA:HB3	2.08	0.54
1:B:176:THR:HG22	1:B:177:LEU:N	2.22	0.54
1:B:197:ILE:HG13	1:B:222:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:HA	1:B:345:LEU:HD22	1.89	0.54
3:F:197:HIS:ND1	3:F:198:LYS:N	2.56	0.54
1:A:101:ALA:O	1:A:103:GLU:N	2.41	0.53
3:D:12:SER:HB3	3:D:106:LEU:HB2	1.90	0.53
3:D:197:HIS:ND1	3:D:198:LYS:N	2.55	0.53
2:E:51:ILE:HD11	2:E:55:SER:HB3	1.89	0.53
2:C:18:LEU:N	2:C:18:LEU:CD2	2.71	0.53
2:C:40:ALA:HA	2:C:92:ALA:CB	2.37	0.53
1:A:21:LEU:HD11	1:B:117:GLU:OE1	2.09	0.53
1:A:430:LEU:C	1:A:432:ALA:N	2.64	0.53
1:B:183:ALA:O	1:B:184:ALA:C	2.51	0.53
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.43	0.53
3:F:210:ARG:HH11	3:F:210:ARG:HG2	1.73	0.53
1:A:452:THR:HG22	1:A:452:THR:O	2.07	0.53
1:B:92:PHE:O	1:B:96:LEU:HD23	2.07	0.53
1:B:108:GLY:O	1:B:153:GLN:HB2	2.09	0.53
1:A:99:LYS:O	1:A:99:LYS:HG3	2.08	0.53
1:A:443:PRO:O	1:A:446:SER:N	2.28	0.53
1:B:59:TRP:CE3	1:B:60:LEU:HD23	2.43	0.53
2:C:149:LEU:HD12	2:C:150:VAL:N	2.24	0.53
3:D:8:PRO:O	3:D:101:THR:HG23	2.09	0.53
2:E:38:ARG:HE	2:E:46:LYS:HZ1	1.55	0.53
1:A:62:ASN:O	1:A:65:MET:N	2.41	0.53
1:B:98:ARG:NH1	1:B:98:ARG:CB	2.72	0.53
2:C:91:THR:HG23	2:C:118:THR:HA	1.91	0.53
2:C:150:VAL:HG22	2:C:205:VAL:HG21	1.89	0.53
1:B:33:LEU:HD23	1:B:33:LEU:C	2.34	0.53
1:B:198:LEU:HD12	1:B:406:LEU:HG	1.90	0.53
3:D:3:VAL:HB	3:D:26:SER:HB3	1.90	0.53
3:F:32:ILE:HG22	3:F:33:HIS:N	2.24	0.53
1:A:108:GLY:O	1:A:153:GLN:HB2	2.08	0.53
1:B:136:LEU:HD12	1:B:136:LEU:H	1.73	0.53
1:B:187:ALA:O	1:B:189:ALA:N	2.42	0.53
1:B:443:PRO:O	1:B:445:TYR:N	2.41	0.53
3:D:22:THR:HG22	3:D:23:CYS:H	1.72	0.53
1:A:38:MET:HG3	1:A:168:LEU:HD21	1.91	0.53
1:B:202:GLU:O	1:B:202:GLU:HG2	2.09	0.53
2:C:30:SER:O	2:C:32:TYR:N	2.42	0.53
3:D:153:GLU:HG3	3:D:154:ARG:N	2.23	0.53
2:E:30:SER:C	2:E:32:TYR:N	2.67	0.53
1:A:131:LYS:HE2	1:A:150:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TYR:HB3	1:B:76:PRO:CD	2.33	0.52
1:B:122:VAL:HG11	1:B:160:ARG:HB3	1.91	0.52
1:B:148:GLN:NE2	1:B:189:ALA:HB1	2.24	0.52
3:F:79:ALA:HA	3:F:105:ILE:HD13	1.90	0.52
1:B:272:TRP:O	1:B:276:MET:HB2	2.09	0.52
2:E:72:ARG:HG3	2:E:74:ASN:OD1	2.09	0.52
1:A:91:MET:C	1:A:93:GLY:N	2.67	0.52
1:A:248:PRO:HG2	1:A:251:THR:HG23	1.92	0.52
1:A:343:THR:O	1:A:347:CYS:HB2	2.10	0.52
1:B:385:GLU:O	1:B:386:ALA:C	2.51	0.52
3:F:164:ASP:O	3:F:165:GLN:C	2.52	0.52
1:B:25:LEU:C	1:B:27:GLU:H	2.18	0.52
1:B:171:ASP:CB	1:B:212:LEU:HD22	2.39	0.52
2:C:6:GLU:CD	2:C:114:GLY:HA2	2.35	0.52
2:E:5:LEU:HD13	2:E:5:LEU:C	2.34	0.52
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.37	0.52
1:B:109:ILE:CD1	1:B:445:TYR:HE2	2.17	0.52
1:A:109:ILE:CD1	1:A:445:TYR:HE2	2.21	0.52
1:A:192:ALA:HB1	1:A:414:GLU:HG3	1.92	0.52
1:B:101:ALA:O	1:B:103:GLU:N	2.43	0.52
3:D:88:GLN:HB2	3:D:97:PHE:CD1	2.44	0.52
3:F:115:SER:HB3	3:F:117:PHE:CE1	2.44	0.52
2:C:49:GLY:HA3	2:C:70:ILE:CD1	2.40	0.52
2:E:67:LYS:HE2	2:E:85:LYS:O	2.10	0.52
1:B:159:GLY:O	1:B:162:VAL:HG22	2.10	0.52
1:B:442:LYS:O	1:B:444:LEU:N	2.43	0.52
3:D:107:ARG:NE	3:D:108:ALA:O	2.41	0.51
1:A:284:HIS:C	1:A:286:GLY:H	2.19	0.51
2:C:120:SER:OG	2:C:121:SER:N	2.43	0.51
3:D:89:GLN:CD	3:D:89:GLN:C	2.78	0.51
3:F:153:GLU:HG3	3:F:154:ARG:N	2.25	0.51
3:F:158:VAL:O	3:F:159:LEU:HD23	2.11	0.51
1:A:18:ARG:HB2	1:B:119:GLN:OE1	2.10	0.51
1:A:65:MET:O	1:A:67:ALA:N	2.42	0.51
1:A:201:ILE:O	1:A:201:ILE:HG13	2.10	0.51
1:B:91:MET:O	1:B:93:GLY:N	2.44	0.51
1:B:370:ALA:O	1:B:374:VAL:HG23	2.11	0.51
1:B:411:LEU:O	1:B:414:GLU:HB2	2.11	0.51
2:C:32:TYR:CE2	2:C:98:ARG:HD3	2.45	0.51
1:A:119:GLN:O	1:A:120:ARG:HD2	2.11	0.51
1:A:198:LEU:HD12	1:A:406:LEU:HG	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ASN:N	1:A:318:ASN:ND2	2.55	0.51
2:C:163:ASN:ND2	2:C:167:LEU:HD23	2.26	0.51
2:E:38:ARG:HE	2:E:46:LYS:NZ	2.07	0.51
1:A:59:TRP:CE3	1:A:60:LEU:HD23	2.44	0.51
1:A:64:ARG:HB3	1:A:64:ARG:NH1	2.25	0.51
1:A:293:LEU:C	1:A:295:GLY:H	2.18	0.51
1:B:21:LEU:HD22	1:B:25:LEU:HG	1.93	0.51
1:B:152:VAL:CG1	1:B:204:MET:HE1	2.41	0.51
2:E:185:LEU:HD12	2:E:185:LEU:C	2.35	0.51
3:F:29:VAL:HG21	3:F:32:ILE:HD11	1.93	0.51
3:F:75:ASN:O	3:F:76:THR:HB	2.11	0.51
1:A:28:ARG:CD	1:B:207:GLN:HG2	2.28	0.51
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.41	0.51
1:A:220:ILE:HG12	1:B:430:LEU:CD2	2.36	0.51
1:B:91:MET:C	1:B:93:GLY:N	2.66	0.51
2:C:156:GLU:OE2	2:C:176:ALA:HB3	2.11	0.51
2:E:24:ALA:HB1	2:E:27:PHE:CE1	2.44	0.51
1:A:25:LEU:C	1:A:27:GLU:H	2.19	0.51
1:A:437:GLN:C	1:A:439:THR:H	2.18	0.51
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.41	0.51
2:C:38:ARG:HE	2:C:46:LYS:HZ1	1.59	0.51
2:C:67:LYS:HE2	2:C:85:LYS:O	2.10	0.51
3:D:7:SER:CB	3:D:8:PRO:CD	2.88	0.51
1:A:18:ARG:NH1	1:B:457:GLU:CB	2.71	0.51
1:A:357:PHE:CZ	1:A:398:LEU:HD13	2.46	0.51
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.46	0.51
3:D:210:ARG:HG2	3:D:210:ARG:HH11	1.74	0.51
1:A:191:ASN:O	1:A:191:ASN:ND2	2.44	0.50
1:A:459:GLU:O	1:A:459:GLU:HG2	2.10	0.50
2:E:66:ASP:O	2:E:67:LYS:C	2.54	0.50
1:A:123:ARG:HD2	1:A:125:TRP:CZ2	2.46	0.50
1:A:293:LEU:C	1:A:295:GLY:N	2.67	0.50
1:B:95:PHE:O	1:B:97:VAL:N	2.44	0.50
1:B:99:LYS:C	1:B:100:TYR:CD1	2.90	0.50
3:F:205:VAL:O	3:F:206:LYS:HG2	2.11	0.50
1:A:197:ILE:HG13	1:A:222:VAL:HG21	1.92	0.50
1:B:284:HIS:HA	1:B:290:LYS:CB	2.40	0.50
3:D:86:TYR:CE2	3:D:100:GLY:HA3	2.46	0.50
3:F:116:ILE:CD1	3:F:193:CYS:HB2	2.41	0.50
3:F:114:VAL:HG13	3:F:135:LEU:HD23	1.92	0.50
3:F:116:ILE:HD13	3:F:193:CYS:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:SER:HB2	3:D:22:THR:HB	1.92	0.50
1:A:298:ILE:HG21	1:A:346:LEU:HG	1.92	0.50
1:A:320:ILE:HG21	1:A:394:MET:HE2	1.92	0.50
1:B:53:PHE:HE2	1:B:147:ARG:HB2	1.77	0.50
1:B:413:LEU:CD1	1:B:422:ILE:HD13	2.41	0.50
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.93	0.50
1:A:139:LEU:HD13	1:A:147:ARG:HB3	1.93	0.50
1:A:385:GLU:O	1:A:386:ALA:C	2.55	0.50
1:B:358:ALA:N	1:B:359:PRO:HD2	2.27	0.50
2:C:12:VAL:CG2	2:C:119:VAL:HG22	2.40	0.50
2:E:200:THR:HG22	2:E:200:THR:O	2.11	0.50
1:B:65:MET:O	1:B:67:ALA:N	2.44	0.50
1:B:197:ILE:HD13	1:B:219:PHE:CD1	2.46	0.50
1:B:212:LEU:HD12	1:B:212:LEU:H	1.77	0.50
2:C:109:ASP:CG	2:C:110:VAL:HG23	2.37	0.50
2:E:64:LEU:O	2:E:65:LYS:C	2.55	0.50
3:F:58:PRO:C	3:F:60:ARG:N	2.70	0.49
1:A:123:ARG:HA	1:A:125:TRP:CZ3	2.47	0.49
1:A:138:THR:O	1:A:143:MET:HG3	2.13	0.49
1:A:190:PHE:HD1	1:A:190:PHE:H	1.59	0.49
1:A:255:TYR:HB3	1:A:428:THR:OG1	2.12	0.49
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.94	0.49
1:A:361:LEU:HD23	1:A:394:MET:O	2.13	0.49
1:B:35:ILE:CG2	1:B:176:THR:HG21	2.42	0.49
1:B:412:VAL:O	1:B:416:THR:HG23	2.12	0.49
3:D:11:MET:HE2	3:D:19:VAL:HG23	1.94	0.49
1:A:176:THR:HG22	1:A:177:LEU:N	2.27	0.49
1:A:203:GLU:CD	1:B:28:ARG:HH22	2.20	0.49
2:C:111:TRP:N	2:C:111:TRP:CD1	2.80	0.49
2:E:132:LEU:CD2	3:F:132:VAL:HG21	2.40	0.49
1:A:274:LEU:CA	1:A:277:GLN:HE21	2.18	0.49
1:A:356:ILE:O	1:A:356:ILE:HG12	2.13	0.49
1:B:241:VAL:HG12	1:B:244:LEU:HD21	1.95	0.49
2:E:207:HIS:CE1	2:E:210:SER:H	2.30	0.49
1:B:135:GLY:O	1:B:136:LEU:C	2.54	0.49
3:D:77:MET:SD	3:D:103:LEU:HD21	2.52	0.49
3:D:107:ARG:NH2	3:D:108:ALA:O	2.43	0.49
3:D:194:GLU:CG	3:D:205:VAL:HG12	2.29	0.49
2:E:30:SER:O	2:E:32:TYR:N	2.46	0.49
2:E:79:LEU:HD23	2:E:96:CYS:HB2	1.94	0.49
2:E:108:PHE:CD1	3:F:88:GLN:NE2	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:VAL:HG11	1:B:344:THR:OG1	2.12	0.49
1:B:148:GLN:HE22	1:B:189:ALA:HB1	1.77	0.49
1:B:183:ALA:C	1:B:185:GLY:N	2.68	0.49
1:B:223:ILE:O	1:B:227:ILE:HD13	2.12	0.49
1:B:357:PHE:CZ	1:B:398:LEU:HD13	2.47	0.49
1:B:437:GLN:C	1:B:439:THR:H	2.21	0.49
2:C:124:THR:CG2	2:C:125:THR:N	2.74	0.49
3:D:19:VAL:HG12	3:D:74:ILE:HB	1.94	0.49
1:A:176:THR:O	1:A:180:THR:HG23	2.11	0.49
2:C:196:TRP:O	2:C:199:GLU:N	2.45	0.49
1:A:284:HIS:HA	1:A:290:LYS:CB	2.43	0.49
1:B:318:ASN:N	1:B:318:ASN:ND2	2.60	0.49
1:B:403:ARG:HH22	1:B:437:GLN:CA	2.26	0.49
2:C:29:TYR:OH	2:C:34:MET:HG3	2.13	0.49
2:E:38:ARG:NE	2:E:46:LYS:HZ1	2.09	0.49
2:E:72:ARG:HG3	2:E:72:ARG:HH11	1.78	0.49
2:E:178:LEU:HD12	2:E:182:LEU:O	2.12	0.49
1:A:84:LEU:O	1:A:88:VAL:HG23	2.12	0.49
1:A:171:ASP:HB2	1:A:212:LEU:HD22	1.94	0.49
1:A:380:PRO:HD2	1:A:381:GLN:NE2	2.26	0.49
3:D:29:VAL:CG2	3:D:32:ILE:HD11	2.43	0.49
1:A:241:VAL:HG12	1:A:244:LEU:HD21	1.95	0.49
1:A:294:MET:O	1:A:298:ILE:HG13	2.13	0.49
1:B:59:TRP:CZ3	1:B:60:LEU:HD23	2.48	0.49
1:B:148:GLN:HB3	1:B:190:PHE:HE1	1.77	0.49
2:C:24:ALA:HB1	2:C:27:PHE:CE1	2.46	0.49
1:A:18:ARG:CZ	1:B:456:GLN:HE21	2.25	0.48
1:A:337:PHE:CE1	1:A:363:LEU:HD12	2.48	0.48
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.31	0.48
1:A:402:ILE:HD12	1:A:445:TYR:CD1	2.48	0.48
1:B:100:TYR:O	1:B:101:ALA:HB2	2.12	0.48
1:B:220:ILE:O	1:B:224:MET:HG2	2.12	0.48
1:B:239:ILE:HD13	1:B:394:MET:HE1	1.95	0.48
2:E:163:ASN:ND2	2:E:167:LEU:HD23	2.28	0.48
3:F:153:GLU:O	3:F:154:ARG:HB2	2.12	0.48
1:B:23:ARG:HG3	1:B:23:ARG:HH11	1.78	0.48
2:E:98:ARG:O	2:E:109:ASP:HB3	2.13	0.48
1:A:202:GLU:HG2	1:A:202:GLU:O	2.13	0.48
1:A:270:ASN:HA	1:A:273:VAL:CG1	2.43	0.48
1:B:148:GLN:O	1:B:149:GLY:C	2.56	0.48
1:B:437:GLN:C	1:B:439:THR:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:SER:O	2:C:122:ALA:C	2.56	0.48
3:F:8:PRO:O	3:F:101:THR:HG23	2.13	0.48
3:F:189:ASN:ND2	3:F:211:ALA:H	2.05	0.48
1:A:99:LYS:C	1:A:100:TYR:CD1	2.91	0.48
1:A:109:ILE:HG21	1:A:445:TYR:CD2	2.48	0.48
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.48	0.48
2:C:107:TYR:HB3	3:D:33:HIS:NE2	2.29	0.48
3:D:153:GLU:O	3:D:154:ARG:HB2	2.12	0.48
2:C:72:ARG:O	2:C:72:ARG:HG2	2.12	0.48
3:D:178:LEU:HD12	3:D:179:THR:N	2.29	0.48
1:B:78:LEU:HD13	1:B:307:PHE:CZ	2.49	0.48
2:C:37:VAL:HG22	2:C:47:TRP:HA	1.96	0.48
2:E:16:GLY:O	2:E:86:VAL:HG13	2.14	0.48
1:B:131:LYS:HE2	1:B:150:PRO:HA	1.95	0.48
2:C:185:LEU:C	2:C:185:LEU:CD1	2.87	0.48
2:E:144:VAL:O	2:E:144:VAL:HG13	2.14	0.48
3:F:79:ALA:O	3:F:105:ILE:HD11	2.14	0.48
1:A:128:LEU:CB	1:A:129:PRO:CD	2.91	0.48
1:A:228:MET:O	1:A:232:PHE:HD1	1.97	0.48
1:A:414:GLU:OE1	1:B:419:TYR:CE1	2.67	0.48
1:B:250:ASN:ND2	2:E:105:TYR:CD1	2.80	0.48
2:E:69:ILE:HG22	2:E:69:ILE:O	2.14	0.48
1:B:124:TRP:HA	1:B:157:ASN:ND2	2.19	0.48
1:B:270:ASN:ND2	1:B:444:LEU:CD2	2.77	0.48
2:C:38:ARG:HE	2:C:46:LYS:NZ	2.12	0.48
1:A:100:TYR:O	1:A:101:ALA:HB2	2.14	0.48
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.96	0.48
1:B:402:ILE:HD12	1:B:445:TYR:CD1	2.49	0.48
2:E:106:TRP:H	2:E:106:TRP:HD1	1.61	0.48
1:A:28:ARG:HH22	1:B:203:GLU:CD	2.22	0.47
1:A:35:ILE:HG23	1:A:176:THR:HG21	1.96	0.47
1:A:305:LEU:C	1:A:307:PHE:H	2.22	0.47
1:B:84:LEU:O	1:B:88:VAL:HG23	2.13	0.47
1:B:312:THR:HG22	1:B:339:ALA:HB3	1.96	0.47
2:C:49:GLY:HA3	2:C:70:ILE:HD12	1.96	0.47
2:C:196:TRP:HB3	2:C:197:PRO:HD3	1.95	0.47
3:D:6:GLN:OE1	3:D:86:TYR:HA	2.14	0.47
3:F:11:MET:HE2	3:F:19:VAL:CG2	2.43	0.47
1:A:279:LEU:HA	1:A:282:ARG:NH1	2.22	0.47
1:A:308:VAL:O	1:A:309:ALA:HB2	2.14	0.47
1:B:23:ARG:HG3	1:B:23:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LYS:HG3	1:B:99:LYS:O	2.13	0.47
1:B:187:ALA:C	1:B:189:ALA:N	2.72	0.47
1:B:284:HIS:C	1:B:286:GLY:H	2.21	0.47
1:B:402:ILE:HD12	1:B:445:TYR:CE1	2.49	0.47
1:B:441:GLY:O	1:B:442:LYS:HG3	2.14	0.47
1:A:17:ARG:C	1:A:17:ARG:CD	2.86	0.47
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.29	0.47
1:B:92:PHE:CD1	1:B:92:PHE:C	2.93	0.47
1:B:128:LEU:CB	1:B:129:PRO:CD	2.92	0.47
3:F:89:GLN:C	3:F:89:GLN:CD	2.82	0.47
1:B:293:LEU:C	1:B:295:GLY:H	2.22	0.47
1:B:294:MET:O	1:B:298:ILE:HG13	2.15	0.47
2:C:22:CYS:O	2:C:78:THR:HG23	2.13	0.47
2:C:38:ARG:NE	2:C:46:LYS:HZ1	2.12	0.47
2:E:87:ARG:HG3	2:E:89:GLU:OE2	2.15	0.47
1:A:182:ALA:HB1	1:A:204:MET:HE2	1.94	0.47
1:B:38:MET:HG3	1:B:168:LEU:HD21	1.95	0.47
1:B:241:VAL:HG12	1:B:241:VAL:O	2.13	0.47
1:A:65:MET:C	1:A:67:ALA:N	2.60	0.47
1:A:370:ALA:O	1:A:374:VAL:HG23	2.15	0.47
1:B:182:ALA:HB1	1:B:204:MET:HE3	1.94	0.47
2:C:126:PRO:CB	2:C:210:SER:OG	2.59	0.47
2:C:221:ARG:CZ	3:D:118:PRO:HG2	2.44	0.47
2:E:18:LEU:N	2:E:18:LEU:CD2	2.78	0.47
1:A:17:ARG:C	1:A:19:ARG:N	2.73	0.47
1:A:200:ILE:HA	1:A:204:MET:HB2	1.95	0.47
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.96	0.47
1:B:385:GLU:O	1:B:387:GLY:N	2.48	0.47
1:A:122:VAL:HG21	1:A:178:LEU:HD11	1.96	0.47
1:A:150:PRO:CG	1:A:354:GLY:HA2	2.45	0.47
1:A:422:ILE:HG23	1:A:423:LEU:N	2.29	0.47
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.50	0.47
3:F:34:TRP:CE2	3:F:72:LEU:HB2	2.50	0.47
1:A:160:ARG:HD3	1:A:163:LEU:HD23	1.97	0.47
3:F:3:VAL:HB	3:F:26:SER:HB3	1.97	0.47
2:C:12:VAL:O	2:C:119:VAL:HA	2.14	0.47
3:F:73:THR:HG22	3:F:74:ILE:N	2.29	0.47
2:E:76:LYS:O	2:E:77:ASP:C	2.58	0.46
1:A:109:ILE:HG21	1:A:445:TYR:HD2	1.80	0.46
1:A:241:VAL:HG12	1:A:241:VAL:O	2.14	0.46
1:A:451:ARG:O	1:A:455:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:O	1:B:96:LEU:C	2.58	0.46
2:C:103:TYR:HD2	3:D:31:TYR:CE2	2.33	0.46
3:D:106:LEU:HD23	3:D:107:ARG:N	2.30	0.46
3:F:36:GLN:HG3	3:F:85:TYR:CE2	2.50	0.46
1:A:22:ILE:HD13	1:B:454:ALA:CB	2.44	0.46
1:A:144:VAL:O	1:A:145:LEU:HD23	2.15	0.46
1:A:150:PRO:HG2	1:A:354:GLY:HA2	1.97	0.46
1:B:318:ASN:ND2	1:B:319:LEU:N	2.64	0.46
1:A:28:ARG:NH2	1:B:443:PRO:HB3	2.31	0.46
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.50	0.46
2:C:144:VAL:O	2:C:144:VAL:HG13	2.15	0.46
3:F:88:GLN:HB2	3:F:97:PHE:HD1	1.78	0.46
1:A:109:ILE:HG12	1:A:152:VAL:HG11	1.97	0.46
1:A:270:ASN:ND2	1:A:444:LEU:HG	2.31	0.46
1:B:198:LEU:HG	1:B:410:ILE:CD1	2.38	0.46
1:B:331:GLY:O	1:B:333:LEU:N	2.48	0.46
2:C:4:LEU:HD12	2:C:4:LEU:HA	1.72	0.46
3:F:49:ASP:O	3:F:50:THR:HB	2.16	0.46
1:A:78:LEU:O	1:A:79:LEU:C	2.59	0.46
1:A:248:PRO:HG2	1:A:251:THR:CG2	2.46	0.46
1:A:272:TRP:O	1:A:276:MET:HB2	2.15	0.46
1:A:295:GLY:C	1:A:297:ALA:N	2.73	0.46
1:A:444:LEU:O	1:A:444:LEU:HD13	2.16	0.46
1:B:218:VAL:O	1:B:219:PHE:C	2.58	0.46
2:C:66:ASP:O	2:C:67:LYS:C	2.58	0.46
3:D:46:TRP:HA	3:D:46:TRP:CE3	2.51	0.46
3:D:73:THR:HG22	3:D:74:ILE:N	2.30	0.46
3:F:7:SER:CB	3:F:8:PRO:CD	2.85	0.46
3:F:116:ILE:HD12	3:F:133:CYS:HB2	1.98	0.46
1:A:287:ASN:HD22	1:A:290:LYS:CG	2.25	0.46
1:B:138:THR:HG22	1:B:143:MET:SD	2.54	0.46
1:B:282:ARG:O	1:B:285:GLY:N	2.49	0.46
1:A:148:GLN:O	1:A:149:GLY:C	2.59	0.46
1:A:430:LEU:O	1:A:431:GLY:C	2.57	0.46
1:B:35:ILE:HG23	1:B:176:THR:HG21	1.97	0.46
1:B:440:GLY:O	1:B:441:GLY:O	2.34	0.46
1:B:452:THR:HG22	1:B:452:THR:O	2.15	0.46
2:C:189:VAL:O	2:C:189:VAL:CG1	2.59	0.46
2:C:210:SER:O	2:C:212:THR:HG23	2.15	0.46
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.51	0.46
1:A:358:ALA:N	1:A:359:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:ILE:HG22	2:E:49:GLY:N	2.31	0.46
3:F:29:VAL:HG23	3:F:70:TYR:CE1	2.50	0.46
1:A:47:GLY:O	1:A:48:LEU:C	2.58	0.46
1:A:136:LEU:HD12	1:A:136:LEU:N	2.31	0.46
1:A:358:ALA:HB3	1:A:359:PRO:CD	2.46	0.46
1:B:139:LEU:HD13	1:B:147:ARG:HB3	1.97	0.46
1:B:293:LEU:C	1:B:295:GLY:N	2.72	0.46
2:C:162:TRP:C	2:C:164:SER:N	2.71	0.46
3:D:105:ILE:HD12	3:D:170:SER:OG	2.16	0.46
3:F:82:ALA:HB2	3:F:105:ILE:CG1	2.45	0.46
1:B:94:TYR:HE2	1:B:350:SER:O	1.99	0.45
1:B:305:LEU:HA	1:B:308:VAL:CG2	2.37	0.45
1:B:312:THR:HG22	1:B:339:ALA:CB	2.46	0.45
2:E:4:LEU:HD12	2:E:4:LEU:HA	1.73	0.45
3:F:64:SER:OG	3:F:65:GLY:N	2.49	0.45
3:F:79:ALA:CA	3:F:105:ILE:HD13	2.46	0.45
1:A:359:PRO:O	1:A:363:LEU:HD23	2.17	0.45
1:B:109:ILE:HB	1:B:445:TYR:CE2	2.51	0.45
2:C:196:TRP:HD1	2:C:201:VAL:HG23	1.81	0.45
3:D:29:VAL:HG23	3:D:70:TYR:CE1	2.50	0.45
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.97	0.45
1:A:97:VAL:HG12	1:A:98:ARG:N	2.31	0.45
1:A:430:LEU:HD21	1:B:220:ILE:CG1	2.38	0.45
2:C:107:TYR:CD1	2:C:107:TYR:C	2.93	0.45
3:F:19:VAL:HG12	3:F:74:ILE:HB	1.99	0.45
1:A:192:ALA:HB1	1:A:414:GLU:CG	2.46	0.45
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.97	0.45
2:C:45:LEU:H	2:C:45:LEU:CD1	2.07	0.45
2:C:196:TRP:CG	2:C:197:PRO:N	2.84	0.45
3:D:22:THR:CG2	3:D:23:CYS:N	2.77	0.45
2:E:196:TRP:CG	2:E:197:PRO:N	2.85	0.45
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.84	0.45
1:A:200:ILE:HG22	1:A:201:ILE:H	1.80	0.45
1:A:318:ASN:HD22	1:A:319:LEU:N	2.13	0.45
1:B:136:LEU:HD12	1:B:136:LEU:N	2.31	0.45
1:B:166:PHE:C	1:B:167:ARG:HG2	2.42	0.45
1:B:279:LEU:HD23	1:B:279:LEU:C	2.41	0.45
1:B:287:ASN:HD22	1:B:290:LYS:CG	2.30	0.45
3:D:65:GLY:CA	3:D:70:TYR:HA	2.44	0.45
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.51	0.45
1:A:282:ARG:C	1:A:284:HIS:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:CD1	1:A:422:ILE:HD13	2.46	0.45
1:B:270:ASN:ND2	1:B:444:LEU:CG	2.79	0.45
2:C:64:LEU:N	2:C:64:LEU:HD23	2.32	0.45
2:E:207:HIS:ND1	2:E:210:SER:CB	2.79	0.45
3:F:22:THR:CG2	3:F:23:CYS:N	2.78	0.45
1:B:116:LEU:HD23	1:B:178:LEU:HD23	1.99	0.45
1:B:402:ILE:HG12	1:B:402:ILE:O	2.16	0.45
3:D:13:ALA:O	3:D:77:MET:HE3	2.17	0.45
2:E:45:LEU:HD11	3:F:86:TYR:CE1	2.51	0.45
2:E:107:TYR:CD1	2:E:107:TYR:C	2.95	0.45
1:A:123:ARG:HD2	1:A:125:TRP:HZ2	1.82	0.45
1:A:298:ILE:HG23	1:A:346:LEU:HG	1.98	0.45
1:A:423:LEU:HB3	1:A:424:PRO:CD	2.44	0.45
1:B:123:ARG:HD2	1:B:125:TRP:CZ2	2.52	0.45
1:B:270:ASN:ND2	1:B:444:LEU:HG	2.31	0.45
2:C:2:VAL:O	2:C:2:VAL:HG13	2.16	0.45
1:A:116:LEU:HD23	1:A:178:LEU:HD23	1.98	0.45
1:B:90:ALA:CB	1:B:299:GLY:HA3	2.46	0.45
1:B:298:ILE:HG21	1:B:346:LEU:HG	1.98	0.45
3:D:58:PRO:C	3:D:60:ARG:N	2.74	0.45
3:D:201:THR:CG2	3:D:202:SER:N	2.79	0.45
2:E:149:LEU:HD12	2:E:150:VAL:N	2.32	0.45
1:A:81:VAL:C	1:A:83:PHE:H	2.25	0.45
1:A:399:ALA:O	1:A:403:ARG:HA	2.17	0.45
1:A:420:GLN:H	1:A:420:GLN:HG3	1.49	0.45
1:B:343:THR:O	1:B:347:CYS:HB2	2.17	0.45
1:B:359:PRO:O	1:B:363:LEU:HD23	2.17	0.45
2:C:146:LEU:HD13	2:C:218:ILE:HG21	1.98	0.45
2:E:131:PRO:HB3	2:E:216:LYS:HG3	1.99	0.45
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.52	0.45
3:F:149:ILE:HG12	3:F:191:TYR:CE2	2.52	0.45
1:A:167:ARG:HG2	1:A:167:ARG:HH11	1.82	0.44
1:A:208:PHE:O	1:A:209:ARG:HB3	2.17	0.44
1:A:270:ASN:ND2	1:A:444:LEU:CD2	2.79	0.44
1:B:37:PHE:CD2	1:B:37:PHE:O	2.71	0.44
1:B:421:LEU:O	1:B:424:PRO:CD	2.59	0.44
1:B:441:GLY:C	1:B:442:LYS:HG3	2.43	0.44
2:C:99:LEU:HD21	2:C:108:PHE:CD2	2.52	0.44
3:D:32:ILE:HG12	3:D:70:TYR:CE2	2.52	0.44
1:A:219:PHE:HB3	1:B:430:LEU:HD13	1.99	0.44
1:A:357:PHE:HE1	1:A:398:LEU:HD22	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ALA:HB3	1:B:200:ILE:HD11	1.98	0.44
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.17	0.44
2:E:162:TRP:CZ3	2:E:203:CYS:CB	3.00	0.44
1:A:210:TYR:CE1	1:B:208:PHE:HA	2.52	0.44
3:D:139:TYR:HA	3:D:140:PRO:C	2.42	0.44
3:F:189:ASN:ND2	3:F:210:ARG:N	2.65	0.44
1:A:21:LEU:HD22	1:A:25:LEU:HG	1.99	0.44
1:B:272:TRP:N	1:B:272:TRP:CD1	2.83	0.44
2:E:69:ILE:HB	2:E:82:GLN:HB2	1.99	0.44
2:E:167:LEU:HD21	2:E:191:VAL:HG11	1.97	0.44
2:E:178:LEU:HD12	2:E:179:GLN:H	1.82	0.44
3:F:187:ARG:HG3	3:F:187:ARG:O	2.17	0.44
1:A:63:GLN:C	1:A:65:MET:N	2.74	0.44
1:A:160:ARG:CD	1:A:163:LEU:HD23	2.47	0.44
1:A:250:ASN:CG	2:C:104:GLY:HA3	2.43	0.44
1:A:442:LYS:O	1:A:444:LEU:N	2.51	0.44
1:B:163:LEU:CD2	1:B:174:ARG:HA	2.47	0.44
1:B:218:VAL:O	1:B:221:GLY:N	2.50	0.44
1:B:411:LEU:O	1:B:415:MET:HG2	2.17	0.44
2:C:171:VAL:C	2:C:172:HIS:HD1	2.26	0.44
3:F:33:HIS:CE1	3:F:49:ASP:H	2.35	0.44
1:A:294:MET:O	1:A:294:MET:HG2	2.16	0.44
1:A:437:GLN:C	1:A:439:THR:N	2.73	0.44
1:A:437:GLN:O	1:A:439:THR:N	2.51	0.44
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.36	0.44
2:C:29:TYR:CZ	2:C:34:MET:HG3	2.52	0.44
2:C:60:TYR:CD1	2:C:60:TYR:N	2.85	0.44
3:F:86:TYR:HE2	3:F:100:GLY:HA3	1.83	0.44
3:F:95:GLN:C	3:F:96:THR:HG23	2.42	0.44
3:F:143:ILE:CG2	3:F:174:MET:HE3	2.47	0.44
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.99	0.44
1:A:382:TYR:HB3	1:A:384:LEU:HD21	1.99	0.44
1:B:331:GLY:C	1:B:333:LEU:N	2.75	0.44
3:F:35:TYR:CD1	3:F:35:TYR:N	2.85	0.44
3:F:119:PRO:CD	3:F:131:VAL:HG22	2.48	0.44
1:A:101:ALA:C	1:A:103:GLU:N	2.76	0.44
1:A:109:ILE:HB	1:A:445:TYR:CE2	2.53	0.44
1:A:150:PRO:HD3	1:A:355:GLY:N	2.33	0.44
1:A:404:ALA:O	1:A:405:PRO:C	2.61	0.44
1:B:272:TRP:CD1	1:B:272:TRP:H	2.34	0.44
2:C:5:LEU:HD13	2:C:5:LEU:C	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:165:GLY:C	2:C:167:LEU:N	2.74	0.44
3:D:7:SER:CB	3:D:22:THR:HB	2.47	0.44
3:D:53:LEU:HB3	3:D:57:VAL:HB	1.99	0.44
1:A:270:ASN:ND2	1:A:444:LEU:CG	2.81	0.44
1:A:270:ASN:CG	1:A:444:LEU:HD23	2.42	0.44
1:B:248:PRO:HG2	1:B:251:THR:HG23	2.00	0.44
2:C:67:LYS:HA	2:C:67:LYS:HD3	1.77	0.44
3:D:162:TRP:CD1	3:D:174:MET:HB2	2.53	0.44
2:E:61:THR:HB	2:E:62:PRO:HD2	1.99	0.44
1:A:69:VAL:CG1	1:A:70:HIS:N	2.81	0.43
1:A:155:GLY:HA3	1:A:181:GLY:O	2.17	0.43
1:A:211:THR:HG22	1:A:212:LEU:N	2.33	0.43
1:A:280:LEU:O	1:A:284:HIS:CE1	2.71	0.43
1:A:307:PHE:O	1:A:307:PHE:CG	2.71	0.43
1:B:64:ARG:HB3	1:B:64:ARG:HH11	1.82	0.43
2:C:40:ALA:HB3	2:C:43:LYS:HB2	2.00	0.43
3:D:6:GLN:HG3	3:D:100:GLY:H	1.82	0.43
1:B:224:MET:O	1:B:228:MET:HG2	2.18	0.43
1:B:282:ARG:C	1:B:284:HIS:H	2.26	0.43
2:C:210:SER:OG	2:C:212:THR:HG23	2.17	0.43
3:F:60:ARG:NH1	3:F:81:ASP:OD1	2.51	0.43
1:A:32:PRO:O	1:A:33:LEU:C	2.61	0.43
1:A:135:GLY:O	1:A:136:LEU:C	2.61	0.43
1:A:138:THR:HG21	1:A:352:ALA:HB1	2.00	0.43
1:A:166:PHE:C	1:A:167:ARG:HG2	2.43	0.43
1:A:454:ALA:O	1:A:458:ALA:HB3	2.18	0.43
1:B:109:ILE:HG21	1:B:445:TYR:CD2	2.53	0.43
1:B:215:ILE:HG22	1:B:216:LYS:N	2.32	0.43
2:E:67:LYS:HA	2:E:67:LYS:HD3	1.65	0.43
1:A:128:LEU:HB2	1:A:129:PRO:HD2	2.00	0.43
1:A:136:LEU:HD12	1:A:136:LEU:H	1.82	0.43
1:A:398:LEU:O	1:A:402:ILE:HG23	2.18	0.43
1:B:148:GLN:HG2	1:B:358:ALA:HB2	1.99	0.43
1:B:302:CYS:C	1:B:304:LEU:N	2.76	0.43
1:B:446:SER:O	1:B:449:LEU:N	2.51	0.43
1:A:250:ASN:ND2	2:C:105:TYR:CD1	2.82	0.43
1:A:266:GLY:HA3	1:A:400:ALA:CB	2.47	0.43
1:A:372:GLY:O	1:A:376:VAL:HG23	2.18	0.43
1:A:446:SER:C	1:A:448:ILE:N	2.77	0.43
1:B:116:LEU:CD2	1:B:178:LEU:HD23	2.48	0.43
1:B:136:LEU:H	1:B:136:LEU:CD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PHE:CE1	1:B:363:LEU:HD12	2.54	0.43
1:A:279:LEU:HD23	1:A:279:LEU:O	2.18	0.43
1:B:126:ARG:O	1:B:130:VAL:HG23	2.19	0.43
1:A:90:ALA:CB	1:A:299:GLY:HA3	2.49	0.43
1:A:136:LEU:O	1:A:140:GLY:N	2.51	0.43
1:A:148:GLN:HB3	1:A:190:PHE:CE1	2.51	0.43
1:A:426:ILE:C	1:A:428:THR:N	2.76	0.43
1:B:47:GLY:O	1:B:48:LEU:C	2.61	0.43
1:A:243:LYS:HE2	1:A:420:GLN:CD	2.44	0.43
1:B:21:LEU:CD2	1:B:25:LEU:HG	2.49	0.43
1:B:32:PRO:O	1:B:33:LEU:C	2.62	0.43
1:B:298:ILE:HG23	1:B:346:LEU:HG	1.99	0.43
1:B:369:THR:CG2	1:B:373:MET:HE3	2.49	0.43
1:B:457:GLU:O	1:B:458:ALA:CB	2.66	0.43
2:C:167:LEU:HD21	2:C:191:VAL:HG11	2.00	0.43
2:E:4:LEU:HB3	2:E:112:GLY:CA	2.48	0.43
3:F:82:ALA:CB	3:F:105:ILE:HD11	2.41	0.43
1:A:362:ALA:O	1:A:363:LEU:C	2.61	0.43
1:A:367:LEU:HD12	1:A:367:LEU:O	2.19	0.43
1:A:380:PRO:CD	1:A:381:GLN:HE22	2.30	0.43
1:B:37:PHE:CD2	1:B:37:PHE:C	2.96	0.43
1:B:63:GLN:C	1:B:65:MET:N	2.71	0.43
1:B:223:ILE:HG22	1:B:227:ILE:HD13	2.01	0.43
1:B:250:ASN:HD22	2:E:105:TYR:HE1	1.62	0.43
1:B:264:ILE:HG13	1:B:265:PHE:N	2.33	0.43
1:B:330:MET:HE1	1:B:374:VAL:CG2	2.49	0.43
2:C:16:GLY:O	2:C:86:VAL:HG13	2.18	0.43
3:D:106:LEU:HD23	3:D:106:LEU:C	2.44	0.43
2:E:125:THR:HA	2:E:126:PRO:HD2	1.94	0.43
3:F:79:ALA:O	3:F:105:ILE:CD1	2.66	0.43
1:B:78:LEU:HD13	1:B:307:PHE:CE2	2.54	0.43
1:B:91:MET:C	1:B:93:GLY:H	2.26	0.43
1:B:308:VAL:O	1:B:309:ALA:HB2	2.19	0.43
2:E:178:LEU:HB2	2:E:183:TYR:CE2	2.54	0.43
1:A:210:TYR:N	1:B:210:TYR:HB2	2.34	0.42
1:A:210:TYR:HB2	1:B:210:TYR:N	2.33	0.42
1:A:330:MET:HE1	1:A:374:VAL:HG22	2.00	0.42
1:A:430:LEU:O	1:A:432:ALA:N	2.52	0.42
1:B:307:PHE:O	1:B:307:PHE:CG	2.71	0.42
1:B:394:MET:O	1:B:394:MET:HG2	2.19	0.42
1:B:430:LEU:C	1:B:432:ALA:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:TYR:OH	2:E:34:MET:HG3	2.18	0.42
1:A:256:LEU:HD12	1:A:256:LEU:HA	1.86	0.42
1:B:187:ALA:O	1:B:188:ALA:C	2.62	0.42
2:C:131:PRO:HB3	2:C:216:LYS:HG3	2.01	0.42
2:E:51:ILE:CD1	2:E:72:ARG:HD2	2.49	0.42
2:E:165:GLY:C	2:E:167:LEU:N	2.76	0.42
1:A:78:LEU:HD13	1:A:307:PHE:CZ	2.55	0.42
1:B:58:ALA:O	1:B:59:TRP:C	2.62	0.42
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.92	0.42
1:B:443:PRO:O	1:B:444:LEU:C	2.62	0.42
1:B:444:LEU:HD13	1:B:444:LEU:O	2.20	0.42
1:A:83:PHE:CD1	1:A:83:PHE:C	2.97	0.42
1:A:282:ARG:O	1:A:285:GLY:N	2.52	0.42
1:A:282:ARG:C	1:A:284:HIS:N	2.77	0.42
1:A:302:CYS:C	1:A:304:LEU:N	2.76	0.42
1:B:60:LEU:C	1:B:62:ASN:N	2.76	0.42
3:D:79:ALA:C	3:D:81:ASP:H	2.27	0.42
3:D:185:TYR:HD1	3:D:191:TYR:HH	1.68	0.42
2:E:27:PHE:HE2	2:E:98:ARG:HG3	1.85	0.42
3:F:84:THR:OG1	3:F:102:LYS:HG3	2.19	0.42
1:A:190:PHE:HE2	1:A:361:LEU:HD11	1.84	0.42
1:A:234:HIS:NE2	3:F:52:LYS:NZ	2.67	0.42
1:A:317:PHE:HD2	1:A:317:PHE:HA	1.71	0.42
1:B:413:LEU:O	1:B:414:GLU:C	2.61	0.42
3:D:112:PRO:HB3	3:D:138:PHE:HB3	2.01	0.42
3:D:118:PRO:HB3	3:D:208:PHE:CE1	2.55	0.42
2:E:33:TRP:CE2	2:E:52:ASN:HB2	2.55	0.42
1:A:171:ASP:CB	1:A:212:LEU:HD22	2.49	0.42
1:B:128:LEU:HB2	1:B:129:PRO:HD2	2.02	0.42
1:B:207:GLN:HB3	1:B:208:PHE:CE1	2.54	0.42
1:B:276:MET:O	1:B:280:LEU:HB2	2.20	0.42
2:E:126:PRO:CB	2:E:210:SER:OG	2.62	0.42
1:A:434:LEU:HD22	1:A:434:LEU:HA	1.92	0.42
1:B:155:GLY:O	1:B:158:ILE:N	2.50	0.42
2:E:107:TYR:C	2:E:107:TYR:HD1	2.27	0.42
3:F:90:TRP:CH2	3:F:95:GLN:NE2	2.88	0.42
3:F:162:TRP:CD2	3:F:174:MET:HG3	2.54	0.42
1:A:95:PHE:O	1:A:97:VAL:N	2.53	0.42
1:A:159:GLY:O	1:A:162:VAL:HG22	2.19	0.42
1:A:167:ARG:O	1:A:168:LEU:C	2.62	0.42
1:A:395:GLY:O	1:A:398:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ILE:CG2	1:A:423:LEU:N	2.83	0.42
3:D:116:ILE:HD12	3:D:193:CYS:HB2	2.02	0.42
2:E:64:LEU:N	2:E:64:LEU:HD23	2.34	0.42
1:A:116:LEU:HD23	1:A:178:LEU:CD2	2.50	0.42
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.55	0.42
1:A:441:GLY:C	1:A:442:LYS:HG3	2.45	0.42
1:B:228:MET:O	1:B:232:PHE:HD1	2.03	0.42
1:B:446:SER:C	1:B:448:ILE:N	2.78	0.42
2:C:53:PRO:C	2:C:55:SER:H	2.28	0.42
3:F:114:VAL:CG1	3:F:115:SER:N	2.83	0.42
3:F:181:THR:O	3:F:182:LYS:C	2.62	0.42
3:F:192:THR:CB	3:F:207:SER:HB3	2.48	0.42
1:A:91:MET:O	1:A:93:GLY:N	2.53	0.42
1:A:95:PHE:O	1:A:96:LEU:C	2.62	0.42
1:A:187:ALA:C	1:A:189:ALA:N	2.78	0.42
1:A:190:PHE:CD1	1:A:190:PHE:N	2.87	0.42
1:A:190:PHE:HD2	1:A:415:MET:SD	2.42	0.42
1:A:270:ASN:HA	1:A:270:ASN:HD22	1.58	0.42
1:A:276:MET:O	1:A:280:LEU:HB2	2.20	0.42
1:A:380:PRO:CD	1:A:381:GLN:NE2	2.83	0.42
1:B:69:VAL:CG1	1:B:70:HIS:N	2.83	0.42
1:B:80:THR:O	1:B:83:PHE:HB3	2.20	0.42
1:B:190:PHE:HE2	1:B:361:LEU:HD11	1.85	0.42
1:B:208:PHE:O	1:B:209:ARG:HB3	2.19	0.42
2:E:179:GLN:O	2:E:180:ALA:HB3	2.20	0.42
3:F:82:ALA:O	3:F:83:ALA:HB2	2.19	0.42
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.79	0.42
1:A:294:MET:HE2	1:A:294:MET:HB3	1.94	0.41
1:B:81:VAL:C	1:B:83:PHE:H	2.28	0.41
1:B:98:ARG:HH11	1:B:98:ARG:CB	2.15	0.41
1:B:172:GLU:HG2	1:B:212:LEU:O	2.20	0.41
1:B:187:ALA:C	1:B:189:ALA:H	2.28	0.41
2:C:181:ALA:O	2:C:182:LEU:HD23	2.20	0.41
1:A:215:ILE:HG22	1:A:216:LYS:N	2.35	0.41
1:B:83:PHE:CD1	1:B:83:PHE:C	2.98	0.41
1:B:239:ILE:HD13	1:B:394:MET:CE	2.50	0.41
1:B:258:LEU:O	1:B:258:LEU:HG	2.20	0.41
1:B:283:VAL:HG12	1:B:283:VAL:O	2.19	0.41
2:C:29:TYR:CD2	2:C:77:ASP:HA	2.56	0.41
2:C:107:TYR:C	2:C:107:TYR:HD1	2.27	0.41
2:C:176:ALA:HA	2:C:185:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:35:TYR:HE1	3:D:88:GLN:HB3	1.86	0.41
2:E:99:LEU:HD21	2:E:108:PHE:CD2	2.55	0.41
2:E:131:PRO:HD3	2:E:216:LYS:HG2	2.01	0.41
3:F:6:GLN:HE21	3:F:6:GLN:HB3	1.64	0.41
1:A:337:PHE:HE1	1:A:363:LEU:HD12	1.84	0.41
1:B:255:TYR:CG	1:B:424:PRO:HB3	2.55	0.41
2:C:196:TRP:O	2:C:198:SER:N	2.52	0.41
2:E:32:TYR:O	2:E:72:ARG:NH2	2.53	0.41
2:E:107:TYR:CB	3:F:33:HIS:CD2	2.95	0.41
2:E:151:LYS:HB2	2:E:151:LYS:HE3	1.78	0.41
3:F:73:THR:CG2	3:F:74:ILE:N	2.83	0.41
1:A:223:ILE:CG2	1:A:227:ILE:HD13	2.51	0.41
1:B:42:VAL:O	1:B:43:GLY:C	2.62	0.41
1:B:167:ARG:HG2	1:B:167:ARG:HH11	1.85	0.41
2:C:132:LEU:HD21	3:D:132:VAL:CG2	2.50	0.41
3:D:22:THR:CG2	3:D:23:CYS:H	2.32	0.41
3:F:33:HIS:O	3:F:87:CYS:HA	2.20	0.41
3:F:47:ILE:HG22	3:F:48:TYR:N	2.35	0.41
3:F:115:SER:CB	3:F:117:PHE:HE1	2.34	0.41
1:A:443:PRO:O	1:A:445:TYR:N	2.54	0.41
1:B:110:PRO:HG2	1:B:448:ILE:HG21	2.02	0.41
1:B:198:LEU:CD1	1:B:406:LEU:HG	2.51	0.41
1:B:199:PHE:CD1	1:B:407:THR:HG21	2.55	0.41
2:E:72:ARG:NH1	2:E:72:ARG:HG3	2.35	0.41
3:F:86:TYR:CE2	3:F:100:GLY:HA3	2.54	0.41
1:A:30:LYS:NZ	1:B:442:LYS:HE2	2.35	0.41
1:A:96:LEU:O	1:A:100:TYR:HB2	2.20	0.41
1:A:250:ASN:ND2	2:C:105:TYR:HD1	2.17	0.41
1:A:427:ILE:O	1:A:427:ILE:HG22	2.20	0.41
1:B:148:GLN:HB3	1:B:190:PHE:CE1	2.56	0.41
1:B:420:GLN:HE21	1:B:420:GLN:HB2	1.62	0.41
3:D:189:ASN:ND2	3:D:210:ARG:N	2.68	0.41
3:F:4:LEU:HD11	3:F:89:GLN:HG3	2.03	0.41
1:A:250:ASN:HD22	2:C:105:TYR:HD1	1.61	0.41
1:B:47:GLY:C	1:B:49:ALA:N	2.78	0.41
1:B:380:PRO:CD	1:B:381:GLN:NE2	2.82	0.41
2:C:76:LYS:O	2:C:77:ASP:C	2.63	0.41
2:E:109:ASP:OD2	2:E:110:VAL:HG23	2.21	0.41
1:A:223:ILE:O	1:A:224:MET:C	2.64	0.41
1:B:191:ASN:ND2	1:B:191:ASN:O	2.53	0.41
1:B:243:LYS:HE2	1:B:420:GLN:CD	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:PRO:O	1:B:270:ASN:N	2.53	0.41
1:B:273:VAL:HG11	1:B:444:LEU:HD21	2.03	0.41
1:B:330:MET:HE1	1:B:374:VAL:HG22	2.03	0.41
2:C:99:LEU:HD21	2:C:108:PHE:CE2	2.55	0.41
3:D:127:GLY:HA2	3:D:182:LYS:HB2	2.02	0.41
2:E:134:PRO:HD3	2:E:146:LEU:CD2	2.51	0.41
3:F:57:VAL:HA	3:F:58:PRO:HD3	1.95	0.41
1:A:62:ASN:O	1:A:63:GLN:C	2.62	0.41
1:A:63:GLN:N	1:A:63:GLN:OE1	2.53	0.41
1:A:86:SER:HB2	1:A:300:GLY:HA2	2.02	0.41
1:A:205:ARG:HA	1:A:206:PRO:HD2	1.92	0.41
1:A:295:GLY:C	1:A:297:ALA:H	2.28	0.41
1:A:394:MET:O	1:A:394:MET:HG2	2.21	0.41
1:B:78:LEU:O	1:B:79:LEU:C	2.62	0.41
1:B:91:MET:HG3	1:B:296:GLY:HA3	2.02	0.41
1:B:191:ASN:O	1:B:191:ASN:CG	2.63	0.41
1:B:247:ALA:HA	1:B:248:PRO:HD2	1.76	0.41
1:B:402:ILE:O	1:B:402:ILE:CG1	2.69	0.41
2:C:124:THR:CG2	2:C:125:THR:H	2.32	0.41
3:D:86:TYR:HE2	3:D:100:GLY:HA3	1.83	0.41
2:E:18:LEU:HD11	2:E:117:VAL:CG1	2.51	0.41
2:E:38:ARG:HE	2:E:46:LYS:HE3	1.86	0.41
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.56	0.41
3:F:202:SER:HA	3:F:203:PRO:HD2	1.92	0.41
1:A:21:LEU:CD2	1:A:25:LEU:HG	2.51	0.41
1:A:75:TYR:CB	1:A:76:PRO:HD3	2.37	0.41
1:A:413:LEU:HB2	1:A:425:MET:HE1	2.03	0.41
1:B:270:ASN:HA	1:B:273:VAL:CG1	2.51	0.41
1:B:270:ASN:CG	1:B:444:LEU:HD23	2.46	0.41
1:B:287:ASN:HB3	1:B:290:LYS:HB2	2.02	0.41
1:B:295:GLY:C	1:B:297:ALA:N	2.78	0.41
3:D:7:SER:O	3:D:8:PRO:C	2.63	0.41
3:F:125:THR:O	3:F:125:THR:HG22	2.21	0.41
1:A:25:LEU:C	1:A:27:GLU:N	2.78	0.40
1:A:198:LEU:CD1	1:A:406:LEU:HG	2.51	0.40
1:A:330:MET:HE1	1:A:374:VAL:CG2	2.51	0.40
1:B:150:PRO:CG	1:B:354:GLY:HA2	2.51	0.40
1:B:221:GLY:O	1:B:222:VAL:C	2.62	0.40
1:B:227:ILE:O	1:B:228:MET:C	2.64	0.40
1:B:270:ASN:HA	1:B:273:VAL:HG12	2.02	0.40
1:B:337:PHE:O	1:B:341:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:66:SER:O	3:D:68:THR:N	2.54	0.40
3:D:149:ILE:HG12	3:D:191:TYR:CE2	2.56	0.40
2:E:33:TRP:CZ2	2:E:52:ASN:HB2	2.57	0.40
2:E:185:LEU:C	2:E:185:LEU:CD1	2.94	0.40
2:E:193:SER:C	2:E:195:SER:H	2.28	0.40
1:A:33:LEU:HD23	1:A:33:LEU:O	2.21	0.40
1:A:183:ALA:O	1:A:184:ALA:C	2.64	0.40
1:A:210:TYR:H	1:B:210:TYR:HB2	1.87	0.40
1:A:312:THR:HG22	1:A:339:ALA:HB3	2.02	0.40
1:B:91:MET:O	1:B:92:PHE:C	2.64	0.40
1:B:211:THR:HG22	1:B:212:LEU:H	1.86	0.40
1:B:437:GLN:O	1:B:439:THR:N	2.54	0.40
2:C:103:TYR:CD2	3:D:31:TYR:CE2	3.09	0.40
3:D:149:ILE:O	3:D:150:ASP:C	2.64	0.40
2:E:174:PHE:HA	2:E:175:PRO:HD3	1.96	0.40
3:F:59:VAL:HG12	3:F:59:VAL:O	2.21	0.40
3:F:125:THR:O	3:F:126:SER:HB3	2.22	0.40
3:F:178:LEU:HD12	3:F:179:THR:N	2.36	0.40
1:A:191:ASN:O	1:A:191:ASN:CG	2.61	0.40
1:A:193:PRO:HA	1:A:222:VAL:CG1	2.52	0.40
1:B:109:ILE:HG21	1:B:445:TYR:HD2	1.85	0.40
1:B:148:GLN:O	1:B:151:THR:N	2.51	0.40
2:C:165:GLY:C	2:C:167:LEU:H	2.28	0.40
3:D:11:MET:HE2	3:D:19:VAL:CG2	2.51	0.40
3:D:74:ILE:CG2	3:D:77:MET:HA	2.51	0.40
3:D:184:GLU:O	3:D:187:ARG:HG2	2.22	0.40
2:E:51:ILE:HD13	2:E:72:ARG:HD2	2.02	0.40
3:F:113:THR:HG22	3:F:113:THR:O	2.21	0.40
1:A:223:ILE:HG22	1:A:227:ILE:HD13	2.02	0.40
1:B:95:PHE:C	1:B:97:VAL:N	2.78	0.40
1:B:197:ILE:CG1	1:B:222:VAL:HG21	2.51	0.40
1:B:250:ASN:ND2	2:E:105:TYR:HD1	2.19	0.40
1:B:270:ASN:HA	1:B:270:ASN:HD22	1.57	0.40
3:D:64:SER:OG	3:D:65:GLY:N	2.54	0.40
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.86	0.40
1:A:109:ILE:CG2	1:A:445:TYR:HD2	2.34	0.40
1:A:136:LEU:H	1:A:136:LEU:CD1	2.34	0.40
1:B:139:LEU:O	1:B:142:GLY:N	2.50	0.40
1:B:451:ARG:O	1:B:455:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	442/473 (93%)	311 (70%)	103 (23%)	28 (6%)	1	6
1	B	439/473 (93%)	296 (67%)	111 (25%)	32 (7%)	1	5
2	C	219/222 (99%)	174 (80%)	35 (16%)	10 (5%)	2	12
2	E	219/222 (99%)	180 (82%)	28 (13%)	11 (5%)	1	11
3	D	209/211 (99%)	169 (81%)	27 (13%)	13 (6%)	1	7
3	F	209/211 (99%)	165 (79%)	36 (17%)	8 (4%)	2	15
All	All	1737/1812 (96%)	1295 (75%)	340 (20%)	102 (6%)	1	8

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	PHE
1	A	171	ASP
1	A	201	ILE
1	A	283	VAL
1	A	307	PHE
1	A	309	ALA
1	A	386	ALA
1	B	132	PHE
1	B	171	ASP
1	B	201	ILE
1	B	283	VAL
1	B	309	ALA
1	B	441	GLY
1	B	444	LEU
2	C	65	LYS
2	C	106	TRP
2	C	140	ALA
3	D	7	SER
3	D	67	GLY
3	D	126	SER

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Mol	Chain	Res	Type
3	D	153	GLU
2	E	65	LYS
2	E	106	TRP
2	E	122	ALA
2	E	140	ALA
3	F	7	SER
3	F	67	GLY
3	F	112	PRO
3	F	126	SER
1	A	102	PRO
1	A	314	GLY
1	A	441	GLY
1	A	444	LEU
1	B	102	PRO
1	B	307	PHE
1	B	314	GLY
1	B	332	MET
1	B	351	GLY
1	B	386	ALA
1	B	443	PRO
2	C	9	GLY
3	D	105	ILE
2	E	9	GLY
3	F	153	GLU
1	A	96	LEU
1	A	189	ALA
1	A	337	PHE
1	A	438	PHE
1	A	443	PRO
1	A	447	ALA
1	B	92	PHE
1	B	96	LEU
1	B	188	ALA
2	C	31	ARG
2	C	53	PRO
2	C	109	ASP
2	C	196	TRP
3	D	154	ARG
3	F	113	THR
3	F	154	ARG
1	A	107	SER
1	A	419	TYR

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Mol	Chain	Res	Type
1	B	95	PHE
1	B	107	SER
1	B	128	LEU
1	B	447	ALA
2	C	157	PRO
3	D	15	PRO
3	D	55	SER
3	D	83	ALA
3	D	199	THR
2	E	31	ARG
2	E	64	LEU
1	A	95	PHE
1	A	128	LEU
1	B	26	LEU
1	B	64	ARG
1	B	285	GLY
1	B	337	PHE
1	B	405	PRO
3	D	51	SER
3	D	137	ASN
2	E	53	PRO
2	E	196	TRP
1	A	242	GLY
1	A	412	VAL
1	B	59	TRP
1	B	101	ALA
1	B	422	ILE
3	D	80	GLU
3	F	15	PRO
1	A	376	VAL
1	B	200	ILE
2	C	54	VAL
1	A	200	ILE
1	B	121	PRO
1	A	101	ALA
1	A	285	GLY
2	E	14	PRO
1	A	405	PRO
1	B	338	VAL
2	E	157	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	335/358 (94%)	299 (89%)	36 (11%)	6	25
1	B	332/358 (93%)	297 (90%)	35 (10%)	6	26
2	C	181/182 (100%)	162 (90%)	19 (10%)	6	26
2	E	181/182 (100%)	162 (90%)	19 (10%)	6	26
3	D	185/185 (100%)	177 (96%)	8 (4%)	26	57
3	F	185/185 (100%)	172 (93%)	13 (7%)	14	41
All	All	1399/1450 (96%)	1269 (91%)	130 (9%)	8	31

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	21	LEU
1	A	35	ILE
1	A	48	LEU
1	A	63	GLN
1	A	79	LEU
1	A	98	ARG
1	A	120	ARG
1	A	138	THR
1	A	167	ARG
1	A	172	GLU
1	A	176	THR
1	A	178	LEU
1	A	180	THR
1	A	198	LEU
1	A	200	ILE
1	A	207	GLN
1	A	208	PHE
1	A	212	LEU
1	A	215	ILE
1	A	274	LEU
1	A	292	VAL

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Mol	Chain	Res	Type
1	A	304	LEU
1	A	317	PHE
1	A	318	ASN
1	A	340	ARG
1	A	347	CYS
1	A	356	ILE
1	A	379	PHE
1	A	381	GLN
1	A	391	ILE
1	A	397	LEU
1	A	415	MET
1	A	420	GLN
1	A	434	LEU
1	A	451	ARG
1	B	21	LEU
1	B	35	ILE
1	B	48	LEU
1	B	63	GLN
1	B	79	LEU
1	B	98	ARG
1	B	103	GLU
1	B	120	ARG
1	B	138	THR
1	B	167	ARG
1	B	172	GLU
1	B	176	THR
1	B	178	LEU
1	B	180	THR
1	B	198	LEU
1	B	200	ILE
1	B	207	GLN
1	B	208	PHE
1	B	212	LEU
1	B	215	ILE
1	B	274	LEU
1	B	292	VAL
1	B	304	LEU
1	B	317	PHE
1	B	318	ASN
1	B	340	ARG
1	B	347	CYS
1	B	356	ILE

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Mol	Chain	Res	Type
1	B	379	PHE
1	B	381	GLN
1	B	391	ILE
1	B	397	LEU
1	B	420	GLN
1	B	434	LEU
1	B	451	ARG
2	C	4	LEU
2	C	14	PRO
2	C	18	LEU
2	C	41	PRO
2	C	45	LEU
2	C	53	PRO
2	C	61	THR
2	C	67	LYS
2	C	72	ARG
2	C	98	ARG
2	C	107	TYR
2	C	115	THR
2	C	157	PRO
2	C	167	LEU
2	C	185	LEU
2	C	200	THR
2	C	203	CYS
2	C	204	ASN
2	C	221	ARG
3	D	28	SER
3	D	30	SER
3	D	41	THR
3	D	46	TRP
3	D	77	MET
3	D	88	GLN
3	D	117	PHE
3	D	146	LYS
2	E	4	LEU
2	E	14	PRO
2	E	27	PHE
2	E	45	LEU
2	E	61	THR
2	E	67	LYS
2	E	72	ARG
2	E	98	ARG

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Mol	Chain	Res	Type
2	E	107	TYR
2	E	119	VAL
2	E	124	THR
2	E	127	PRO
2	E	157	PRO
2	E	167	LEU
2	E	185	LEU
2	E	186	SER
2	E	200	THR
2	E	203	CYS
2	E	204	ASN
3	F	1	ASP
3	F	2	ILE
3	F	6	GLN
3	F	15	PRO
3	F	28	SER
3	F	46	TRP
3	F	77	MET
3	F	88	GLN
3	F	102	LYS
3	F	105	ILE
3	F	119	PRO
3	F	146	LYS
3	F	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	62	ASN
1	A	148	GLN
1	A	157	ASN
1	A	207	GLN
1	A	270	ASN
1	A	277	GLN
1	A	287	ASN
1	A	318	ASN
1	A	327	ASN
1	A	381	GLN
1	A	383	HIS
1	A	437	GLN
1	A	460	GLN

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Mol	Chain	Res	Type
1	B	24	GLN
1	B	62	ASN
1	B	119	GLN
1	B	148	GLN
1	B	157	ASN
1	B	175	HIS
1	B	207	GLN
1	B	270	ASN
1	B	277	GLN
1	B	287	ASN
1	B	318	ASN
1	B	327	ASN
1	B	381	GLN
1	B	383	HIS
1	B	437	GLN
1	B	456	GLN
2	C	39	GLN
3	D	37	GLN
3	D	93	HIS
3	D	136	ASN
3	D	189	ASN
2	E	163	ASN
3	F	136	ASN
3	F	189	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	121:SER	C	122:ALA	N	1.19

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	444/473 (93%)	0.74	34 (7%)	19 10	50, 77, 100, 111	0
1	B	441/473 (93%)	0.68	26 (5%)	28 15	46, 76, 103, 121	0
2	C	221/222 (99%)	1.01	25 (11%)	10 5	43, 74, 94, 125	0
2	E	221/222 (99%)	1.12	29 (13%)	7 4	40, 75, 95, 116	0
3	D	211/211 (100%)	1.10	19 (9%)	15 8	57, 85, 98, 103	0
3	F	211/211 (100%)	1.10	21 (9%)	12 6	40, 71, 99, 110	0
All	All	1749/1812 (96%)	0.90	154 (8%)	15 9	40, 77, 99, 125	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ALA	6.0
3	D	167	SER	4.9
2	C	105	TYR	4.5
1	A	235	GLU	4.4
2	C	136	SER	4.3
1	B	235	GLU	4.2
2	E	29	TYR	4.2
2	E	16	GLY	4.0
3	F	190	SER	4.0
3	F	153	GLU	3.9
1	A	19	ARG	3.8
2	E	133	ALA	3.7
2	E	134	PRO	3.7
3	F	192	THR	3.6
1	B	75	TYR	3.5
1	B	23	ARG	3.5
3	D	64	SER	3.5
2	E	179	GLN	3.5
2	C	199	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	87	ARG	3.4
2	C	166	SER	3.3
2	E	196	TRP	3.3
3	F	207	SER	3.3
2	C	140	ALA	3.3
1	A	183	ALA	3.2
2	E	188	SER	3.2
1	B	61	GLN	3.2
2	C	201	VAL	3.2
1	A	460	GLN	3.2
2	E	2	VAL	3.2
3	F	169	ASP	3.2
1	A	170	GLY	3.2
1	A	234	HIS	3.2
2	C	139	ALA	3.1
1	A	29	ASP	3.1
1	B	458	ALA	3.1
1	A	73	ASP	3.1
3	F	208	PHE	3.0
3	D	24	SER	3.0
3	D	152	SER	3.0
2	E	105	TYR	3.0
1	B	18	ARG	3.0
3	F	211	ALA	2.9
2	E	77	ASP	2.9
3	D	183	ASP	2.9
2	E	44	GLY	2.9
2	E	96	CYS	2.9
3	F	142	ASP	2.9
2	E	94	TYR	2.9
3	D	157	GLY	2.9
2	E	35	SER	2.8
1	B	240	ASP	2.8
1	A	302	CYS	2.8
2	E	31	ARG	2.8
3	F	120	SER	2.8
3	F	170	SER	2.8
1	A	212	LEU	2.8
1	B	189	ALA	2.8
2	C	133	ALA	2.7
1	B	234	HIS	2.7
2	E	141	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	28	SER	2.7
3	F	22	THR	2.7
2	C	31	ARG	2.7
2	C	103	TYR	2.7
1	A	172	GLU	2.7
2	E	221	ARG	2.7
3	F	141	LYS	2.7
2	C	89	GLU	2.7
1	B	125	TRP	2.7
1	A	25	LEU	2.7
1	A	292	VAL	2.7
3	D	59	VAL	2.6
2	C	217	LYS	2.6
1	B	452	THR	2.6
1	A	30	LYS	2.6
1	B	212	LEU	2.5
2	E	210	SER	2.5
1	A	17	ARG	2.5
1	A	90	ALA	2.5
2	C	2	VAL	2.5
2	C	196	TRP	2.5
1	A	456	GLN	2.5
3	D	190	SER	2.4
1	B	96	LEU	2.4
2	E	137	ALA	2.4
1	B	86	SER	2.4
1	B	401	SER	2.4
3	D	115	SER	2.4
1	B	290	LYS	2.4
2	E	216	LYS	2.4
2	E	66	ASP	2.4
2	C	67	LYS	2.4
2	E	166	SER	2.4
1	A	429	GLY	2.4
3	D	102	LYS	2.4
2	C	146	LEU	2.4
2	C	186	SER	2.4
2	C	202	THR	2.4
2	E	86	VAL	2.4
3	F	183	ASP	2.4
1	A	238	LEU	2.4
3	F	191	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	307	PHE	2.3
1	A	125	TRP	2.3
1	A	167	ARG	2.3
3	F	32	ILE	2.3
1	B	296	GLY	2.3
3	D	103	LEU	2.3
3	D	180	LEU	2.3
1	B	233	ASN	2.3
1	B	347	CYS	2.3
2	C	77	ASP	2.3
2	C	142	SER	2.3
3	F	189	ASN	2.3
1	B	94	TYR	2.2
2	C	216	LYS	2.2
3	F	149	ILE	2.2
1	A	184	ALA	2.2
3	F	157	GLY	2.2
1	A	457	GLU	2.2
1	A	296	GLY	2.2
1	B	316	GLY	2.2
2	E	42	GLY	2.2
1	A	138	THR	2.2
1	A	20	GLN	2.2
1	A	441	GLY	2.2
1	B	73	ASP	2.2
2	C	33	TRP	2.2
1	B	72	ALA	2.2
3	D	87	CYS	2.2
1	B	127	VAL	2.1
1	A	205	ARG	2.1
1	B	170	GLY	2.1
3	D	151	GLY	2.1
1	A	31	THR	2.1
3	F	179	THR	2.1
1	A	189	ALA	2.1
2	E	140	ALA	2.1
2	E	135	GLY	2.1
1	A	283	VAL	2.1
1	A	303	GLY	2.1
2	E	211	SER	2.1
2	C	222	ALA	2.1
3	D	112	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	33	TRP	2.1
1	A	348	PHE	2.1
2	E	139	ALA	2.0
3	F	110	ALA	2.0
3	D	208	PHE	2.0
2	C	211	SER	2.0
3	D	74	ILE	2.0
3	D	126	SER	2.0
3	F	16	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.