



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:05 AM UTC

PDB ID : 3EJZ / pdb_00003ejz
Title : Structure of E203V mutant E.coli Cl⁻/H⁺ exchanger, CLC-ec1
Authors : Lim, H.-H.; Miller, C.
Deposited on : 2008-09-18
Resolution : 2.90 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

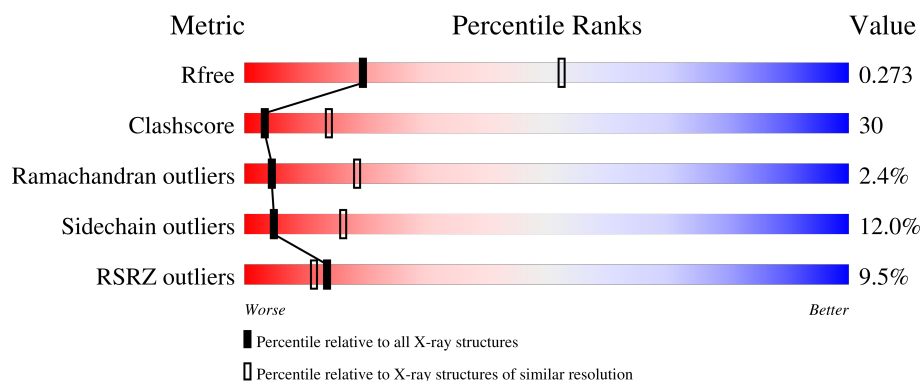
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	6% 48% 36% 9% 6%
1	B	473	9% 48% 37% 8% 7%
2	C	221	10% 60% 33% 5%
2	E	221	12% 61% 34%
3	D	211	19% 42% 44% 12%

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Mol	Chain	Length	Quality of chain
3	F	211	

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
4	BR	A	474	-	-	X	-

2 Entry composition

There are 4 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
			3331	2190	560	561	20			
1	B	441	Total	C	N	O	S	0	0	0
			3302	2174	553	555	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	VAL	GLU	engineered mutation	UNP P37019
B	203	VAL	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			

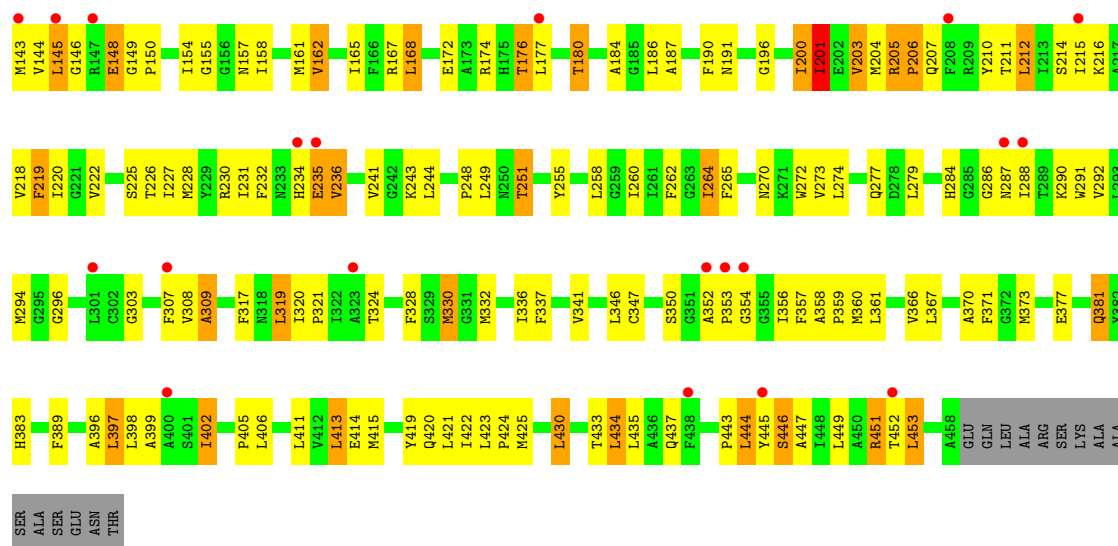
- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Br	0	0
			2	2		

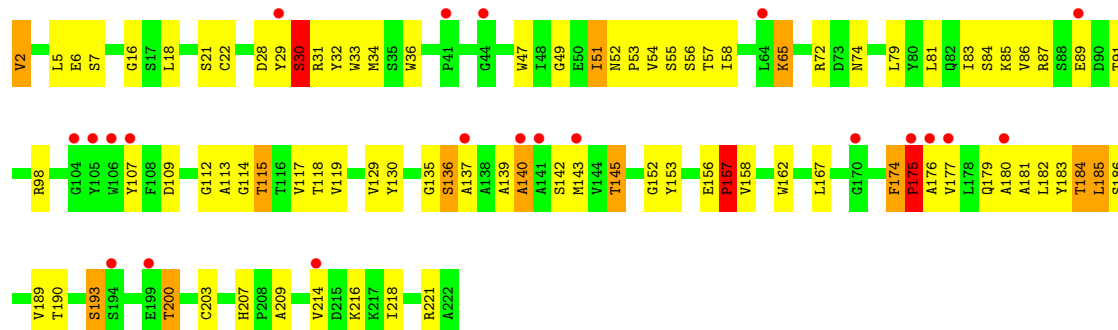
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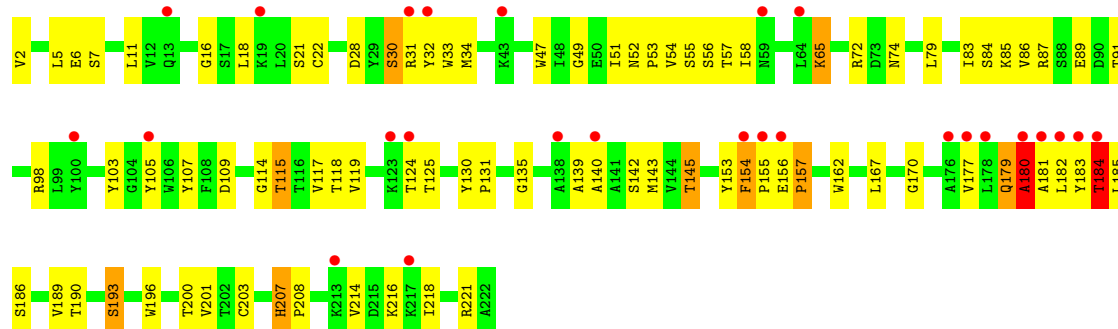
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Br	0	0
			2	2		



• Molecule 2: Fab fragment, Heavy chain

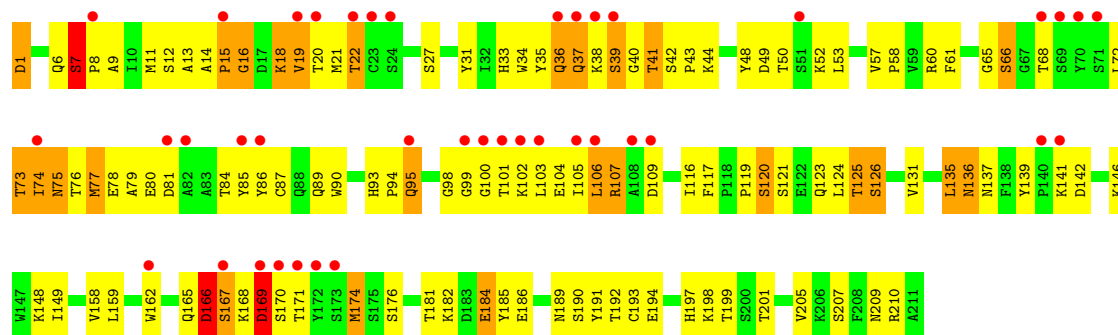


• Molecule 2: Fab fragment, Heavy chain

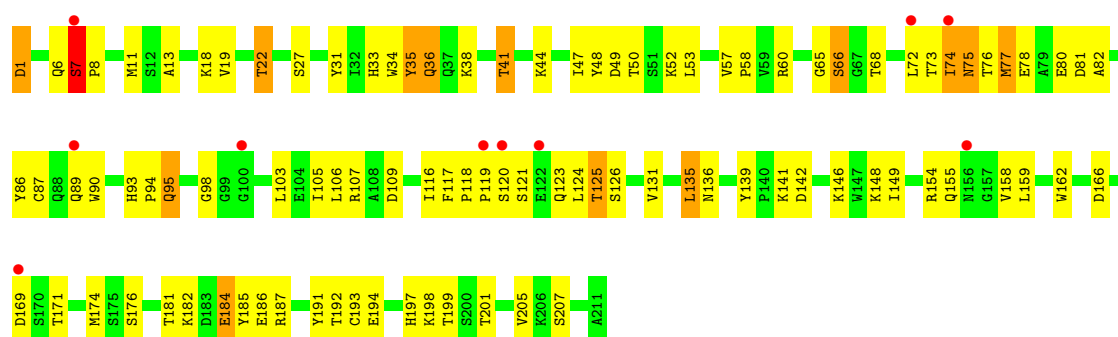


• Molecule 3: Fab fragment, Light chain





● 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	231.26Å 96.42Å 170.15Å 90.00° 131.78° 90.00°	Depositor
Resolution (Å)	58.76 – 2.90 58.76 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (58.76-2.90) 99.3 (58.76-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, R_{free}	0.252 , 0.281 0.246 , 0.273	Depositor DCC
R_{free} test set	3094 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	89.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 85.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

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

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	0.53	0/3403	0.86	2/4619 (0.0%)
1	B	0.51	0/3374	0.84	1/4581 (0.0%)
2	C	0.64	0/1721	1.03	5/2355 (0.2%)
2	E	0.65	1/1721 (0.1%)	0.98	5/2355 (0.2%)
3	D	0.59	2/1660 (0.1%)	1.02	12/2257 (0.5%)
3	F	0.68	2/1660 (0.1%)	0.94	4/2257 (0.2%)
All	All	0.58	5/13539 (0.0%)	0.92	29/18424 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	107	ARG	N-CA	6.09	1.53	1.45
2	E	184	THR	N-CA	5.88	1.53	1.46
3	F	35	TYR	C-N	-5.67	1.25	1.33
3	D	74	ILE	N-CA	5.56	1.53	1.46
3	D	74	ILE	CA-CB	5.21	1.60	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	140	ALA	CB-CA-C	10.01	122.11	109.80
2	E	207	HIS	CA-C-N	7.93	129.76	119.84
2	E	207	HIS	C-N-CA	7.93	129.76	119.84
1	A	176	THR	N-CA-C	7.66	119.26	111.07
2	C	140	ALA	N-CA-C	-7.29	99.85	110.64
3	D	169	ASP	CB-CA-C	7.19	124.73	110.42
2	E	154	PHE	N-CA-C	-6.80	101.55	110.39
3	D	20	THR	N-CA-C	6.52	119.08	107.80
3	D	136	ASN	N-CA-C	6.43	119.42	109.07
3	F	7	SER	CA-C-N	-6.35	112.42	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	SER	C-N-CA	-6.35	112.42	120.23
2	C	136	SER	CB-CA-C	6.31	122.97	110.42
3	D	7	SER	CA-C-N	-6.26	112.53	120.23
3	D	7	SER	C-N-CA	-6.26	112.53	120.23
3	D	167	SER	N-CA-C	6.21	118.98	111.40
3	D	19	VAL	O-C-N	6.09	129.39	122.93
3	F	136	ASN	N-CA-C	6.04	118.79	109.07
3	D	166	ASP	N-CA-C	5.61	117.77	110.53
3	D	73	THR	N-CA-C	5.59	117.60	108.55
3	D	18	LYS	N-CA-C	-5.46	100.33	109.24
2	C	30	SER	N-CA-C	-5.42	101.33	109.79
2	E	180	ALA	N-CA-C	5.32	122.13	110.80
1	A	144	VAL	CB-CA-C	-5.28	107.30	113.22
2	C	174	PHE	CB-CA-C	5.21	116.07	110.08
2	E	177	VAL	N-CA-C	5.20	116.15	108.45
1	B	144	VAL	N-CA-C	5.19	111.76	106.21
3	D	99	GLY	N-CA-C	-5.18	108.65	114.40
3	F	18	LYS	N-CA-C	-5.11	100.91	109.24
3	D	78	GLU	N-CA-C	-5.09	104.14	110.41

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	3331	0	3486	225	0
1	B	3302	0	3459	216	0
2	C	1672	0	1654	75	0
2	E	1672	0	1654	70	0
3	D	1621	0	1546	160	0
3	F	1621	0	1546	110	0
4	A	2	0	0	3	0
4	B	2	0	0	1	0
All	All	13223	0	13345	805	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 30.

All (805) 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:105:ILE:HB	3:D:170:SER:OG	1.43	1.18
1:A:19:ARG:HG2	1:A:19:ARG:HH11	1.11	1.14
1:B:235:GLU:O	1:B:236:VAL:HG23	1.46	1.14
3:D:95:GLN:CD	3:D:95:GLN:H	1.59	1.09
3:F:95:GLN:H	3:F:95:GLN:CD	1.62	1.08
3:D:36:GLN:HG3	3:D:37:GLN:N	1.69	1.08
1:B:19:ARG:HG2	1:B:19:ARG:HH11	1.09	1.07
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.38	1.06
3:F:34:TRP:CG	3:F:72:LEU:HD12	1.92	1.04
3:D:36:GLN:HG3	3:D:37:GLN:H	1.21	1.03
3:D:80:GLU:O	3:D:81:ASP:OD2	1.78	1.00
3:D:19:VAL:O	3:D:73:THR:HG23	1.60	1.00
1:A:176:THR:O	1:A:180:THR:HG23	1.62	1.00
3:F:77:MET:HE2	3:F:103:LEU:HD21	1.44	1.00
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.45	0.97
1:B:104:ALA:HB2	1:B:127:VAL:HG13	1.47	0.96
3:D:14:ALA:HA	3:D:106:LEU:HB2	1.47	0.96
3:D:6:GLN:NE2	3:D:100:GLY:H	1.65	0.95
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.46	0.94
1:A:154:ILE:O	1:A:158:ILE:HG12	1.69	0.93
3:F:19:VAL:HG21	3:F:77:MET:HE3	1.51	0.92
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.48	0.92
1:A:104:ALA:HB2	1:A:127:VAL:HG13	1.47	0.92
1:B:154:ILE:O	1:B:158:ILE:HG12	1.69	0.92
2:C:152:GLY:HA2	2:C:182:LEU:HB3	1.49	0.91
3:D:86:TYR:CD2	3:D:100:GLY:HA3	2.07	0.90
1:A:381:GLN:HE21	1:A:381:GLN:N	1.70	0.90
3:D:105:ILE:CB	3:D:170:SER:OG	2.18	0.89
1:B:381:GLN:H	1:B:381:GLN:HE21	0.94	0.89
2:C:51:ILE:HD13	2:C:72:ARG:HG2	1.53	0.89
1:A:381:GLN:H	1:A:381:GLN:NE2	1.71	0.87
3:F:73:THR:HG22	3:F:74:ILE:N	1.90	0.87
3:D:95:GLN:CD	3:D:95:GLN:N	2.29	0.87
2:E:51:ILE:HD13	2:E:72:ARG:HG2	1.57	0.87
3:D:168:LYS:O	3:D:169:ASP:HB3	1.71	0.86
1:B:235:GLU:O	1:B:236:VAL:CG2	2.25	0.85
3:D:15:PRO:HA	3:D:77:MET:O	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:73:THR:CG2	3:F:74:ILE:N	2.39	0.85
1:B:381:GLN:H	1:B:381:GLN:NE2	1.75	0.84
3:F:95:GLN:CD	3:F:95:GLN:N	2.29	0.84
1:B:381:GLN:HE21	1:B:381:GLN:N	1.74	0.83
3:D:80:GLU:C	3:D:81:ASP:OD2	2.21	0.83
2:C:135:GLY:HA2	2:C:221:ARG:HD3	1.62	0.82
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.61	0.82
1:A:381:GLN:HE21	1:A:381:GLN:H	0.88	0.82
1:A:443:PRO:HB2	1:A:446:SER:HB2	1.62	0.82
3:D:14:ALA:CA	3:D:106:LEU:HB2	2.10	0.81
2:C:32:TYR:CE2	2:C:98:ARG:HD3	2.15	0.81
3:D:36:GLN:CG	3:D:37:GLN:N	2.43	0.81
3:D:192:THR:HG22	3:D:207:SER:CB	2.11	0.81
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.64	0.80
3:F:73:THR:CG2	3:F:74:ILE:H	1.94	0.80
3:F:76:THR:HG22	3:F:76:THR:O	1.82	0.80
1:A:205:ARG:O	1:A:205:ARG:HG3	1.81	0.80
2:E:32:TYR:CE2	2:E:98:ARG:HD3	2.17	0.80
2:E:135:GLY:HA2	2:E:221:ARG:HD3	1.64	0.79
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.64	0.79
3:F:34:TRP:CG	3:F:72:LEU:CD1	2.66	0.79
1:B:19:ARG:HG2	1:B:19:ARG:NH1	1.89	0.78
2:C:51:ILE:HG13	2:C:58:ILE:HG12	1.64	0.78
3:D:107:ARG:HD3	3:D:139:TYR:HB2	1.64	0.78
2:C:153:TYR:CZ	2:C:183:TYR:HB3	2.18	0.77
1:B:243:LYS:HG2	2:E:31:ARG:HH21	1.48	0.77
3:F:125:THR:O	3:F:125:THR:HG22	1.84	0.77
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.00	0.77
3:F:7:SER:HB2	3:F:22:THR:HB	1.67	0.77
1:A:98:ARG:HE	1:A:98:ARG:HA	1.50	0.76
3:F:95:GLN:H	3:F:95:GLN:NE2	1.82	0.76
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.68	0.76
2:C:174:PHE:O	2:C:175:PRO:O	2.04	0.76
3:F:192:THR:HG22	3:F:207:SER:CB	2.15	0.76
1:B:19:ARG:HH11	1:B:19:ARG:CG	1.96	0.76
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.21	0.76
2:C:174:PHE:O	2:C:175:PRO:C	2.28	0.75
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.68	0.75
3:F:7:SER:HB3	3:F:8:PRO:CD	2.15	0.75
3:D:125:THR:HG22	3:D:125:THR:O	1.86	0.75
1:B:98:ARG:HE	1:B:98:ARG:HA	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:38:LYS:O	3:D:40:GLY:N	2.19	0.75
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.68	0.74
3:D:6:GLN:NE2	3:D:100:GLY:N	2.34	0.74
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.67	0.74
3:F:106:LEU:HD23	3:F:139:TYR:OH	1.88	0.74
1:A:19:ARG:HH11	1:A:19:ARG:CG	1.97	0.74
1:B:212:LEU:HD12	1:B:212:LEU:H	1.53	0.74
3:D:95:GLN:H	3:D:95:GLN:NE2	1.87	0.73
3:D:86:TYR:CD2	3:D:100:GLY:CA	2.71	0.73
3:D:7:SER:HB2	3:D:22:THR:HB	1.71	0.73
3:F:34:TRP:CD2	3:F:72:LEU:HD12	2.24	0.72
3:D:77:MET:HE2	3:D:103:LEU:HD21	1.70	0.72
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.70	0.72
2:C:174:PHE:C	2:C:175:PRO:O	2.32	0.72
2:E:143:MET:HE3	2:E:190:THR:HG22	1.72	0.72
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.72	0.72
3:D:105:ILE:HG22	3:D:106:LEU:N	2.05	0.72
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.05	0.72
2:C:143:MET:HE3	2:C:190:THR:HG22	1.72	0.71
3:D:13:ALA:HB3	3:D:77:MET:CE	2.19	0.71
1:A:262:PHE:CZ	1:A:367:LEU:HD23	2.25	0.71
1:B:98:ARG:NH1	1:B:291:TRP:CZ3	2.57	0.71
3:D:166:ASP:CG	3:D:167:SER:N	2.49	0.71
2:E:30:SER:O	2:E:31:ARG:HB2	1.89	0.71
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.74	0.70
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.27	0.70
2:C:162:TRP:CZ3	2:C:203:CYS:HB3	2.27	0.70
2:C:30:SER:O	2:C:31:ARG:HB2	1.92	0.70
3:D:19:VAL:HG21	3:D:77:MET:HE3	1.74	0.70
1:A:212:LEU:HD12	1:A:212:LEU:H	1.55	0.70
3:D:21:MET:SD	3:D:101:THR:HG21	2.32	0.70
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.73	0.70
3:D:21:MET:CB	3:D:101:THR:HG21	2.21	0.70
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.74	0.69
2:C:130:TYR:CE2	3:D:123:GLN:HG3	2.27	0.69
3:D:19:VAL:O	3:D:73:THR:CG2	2.41	0.69
3:D:192:THR:HG22	3:D:207:SER:HB2	1.73	0.69
3:F:77:MET:HE2	3:F:103:LEU:CD2	2.21	0.69
3:D:61:PHE:CE2	3:D:74:ILE:HG12	2.28	0.68
2:E:124:THR:HG22	2:E:125:THR:N	2.08	0.68
2:E:51:ILE:HG13	2:E:58:ILE:HG12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:105:ILE:HB	3:D:170:SER:HG	1.55	0.68
3:F:34:TRP:CD2	3:F:72:LEU:CD1	2.77	0.68
3:F:34:TRP:CD1	3:F:72:LEU:HD12	2.29	0.68
1:B:243:LYS:CG	2:E:31:ARG:NH2	2.57	0.68
3:F:192:THR:HG22	3:F:207:SER:HB2	1.74	0.68
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.75	0.68
3:D:7:SER:HB3	3:D:8:PRO:CD	2.22	0.68
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.28	0.67
3:F:73:THR:HG23	3:F:74:ILE:H	1.58	0.67
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.76	0.67
1:A:172:GLU:HA	1:A:212:LEU:HB2	1.77	0.67
1:B:91:MET:HG2	1:B:292:VAL:O	1.94	0.67
1:B:212:LEU:HD12	1:B:212:LEU:N	2.09	0.67
2:E:52:ASN:ND2	2:E:57:THR:HB	2.09	0.67
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.29	0.67
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.77	0.67
1:B:172:GLU:HA	1:B:212:LEU:HB2	1.77	0.67
3:D:6:GLN:HE21	3:D:100:GLY:H	1.42	0.67
1:A:204:MET:O	1:A:205:ARG:C	2.37	0.67
2:C:177:VAL:CG2	2:C:184:THR:O	2.43	0.66
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.77	0.66
1:A:98:ARG:NH1	1:A:291:TRP:CZ3	2.63	0.66
3:D:19:VAL:O	3:D:73:THR:HA	1.96	0.66
3:F:7:SER:CB	3:F:22:THR:HB	2.25	0.66
1:A:212:LEU:HD12	1:A:212:LEU:N	2.12	0.65
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.78	0.65
1:A:211:THR:HG22	1:A:212:LEU:H	1.61	0.65
1:B:148:GLU:CD	1:B:148:GLU:H	2.04	0.65
1:A:19:ARG:HG2	1:A:19:ARG:NH1	1.91	0.65
1:A:109:ILE:HG23	1:A:204:MET:HE1	1.77	0.65
1:B:44:THR:O	1:B:48:LEU:HG	1.97	0.65
1:A:148:GLU:CD	1:A:148:GLU:H	2.05	0.65
3:D:105:ILE:CG2	3:D:170:SER:OG	2.44	0.65
2:E:105:TYR:CE1	3:F:31:TYR:CD1	2.85	0.65
3:F:7:SER:CB	3:F:8:PRO:HD3	2.21	0.65
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.61	0.65
1:B:264:ILE:HG13	1:B:265:PHE:N	2.11	0.64
3:D:84:THR:HG21	3:D:86:TYR:CZ	2.32	0.64
1:B:211:THR:HG22	1:B:212:LEU:H	1.60	0.64
1:B:422:ILE:HA	1:B:425:MET:HE3	1.78	0.64
3:D:158:VAL:O	3:D:159:LEU:HD23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:109:ASP:HB3	3:D:199:THR:HG22	1.79	0.64
2:C:145:THR:HG22	3:D:117:PHE:HZ	1.62	0.64
1:A:124:TRP:CZ3	1:A:161:MET:HG3	2.32	0.64
1:A:56:GLY:HA3	1:A:136:LEU:HD11	1.80	0.64
1:A:176:THR:O	1:A:180:THR:CG2	2.42	0.64
3:D:1:ASP:OD2	3:D:1:ASP:N	2.29	0.63
3:F:34:TRP:CE2	3:F:72:LEU:HB2	2.33	0.63
1:A:91:MET:HG2	1:A:292:VAL:O	1.98	0.63
1:A:264:ILE:HG13	1:A:265:PHE:N	2.13	0.63
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.65	0.63
3:F:116:ILE:HD12	3:F:193:CYS:HB2	1.81	0.63
3:D:86:TYR:HA	3:D:100:GLY:HA2	1.81	0.63
1:B:124:TRP:CZ3	1:B:161:MET:HG3	2.34	0.63
3:D:7:SER:CB	3:D:22:THR:HB	2.27	0.63
3:D:135:LEU:N	3:D:135:LEU:HD23	2.14	0.63
1:A:414:GLU:HG2	1:B:419:TYR:OH	1.98	0.63
3:D:169:ASP:O	3:D:170:SER:HB2	1.98	0.63
1:A:249:LEU:HD13	1:B:231:ILE:HD13	1.80	0.63
3:D:79:ALA:O	3:D:81:ASP:N	2.28	0.63
1:A:459:GLU:HG3	1:A:459:GLU:O	1.99	0.62
2:C:177:VAL:HG22	2:C:184:THR:O	1.99	0.62
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.63	0.62
3:D:107:ARG:HD3	3:D:139:TYR:CB	2.29	0.62
3:D:119:PRO:HD3	3:D:131:VAL:HG22	1.82	0.62
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.98	0.62
3:F:1:ASP:OD2	3:F:1:ASP:N	2.30	0.62
3:F:6:GLN:HE21	3:F:98:GLY:C	2.07	0.62
1:B:56:GLY:HA3	1:B:136:LEU:HD11	1.80	0.62
2:C:176:ALA:HA	2:C:185:LEU:HB3	1.82	0.62
3:D:182:LYS:HE2	3:D:186:GLU:OE1	1.99	0.62
1:B:357:PHE:CE2	1:B:398:LEU:HD11	2.35	0.61
2:C:98:ARG:NH1	2:C:109:ASP:OD2	2.33	0.61
2:C:52:ASN:ND2	2:C:57:THR:HB	2.14	0.61
3:D:60:ARG:HB2	3:D:75:ASN:H	1.65	0.61
1:A:414:GLU:HG2	1:B:419:TYR:CZ	2.35	0.61
1:B:204:MET:O	1:B:205:ARG:C	2.44	0.61
3:D:79:ALA:C	3:D:81:ASP:H	2.09	0.61
1:A:124:TRP:CE3	1:A:161:MET:HG3	2.35	0.61
1:B:124:TRP:CE3	1:B:161:MET:HG3	2.35	0.61
2:C:153:TYR:CE1	2:C:183:TYR:CB	2.83	0.61
1:A:330:MET:HE1	1:A:370:ALA:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:MET:HE1	1:B:370:ALA:HA	1.82	0.61
1:A:98:ARG:HA	1:A:98:ARG:NE	2.15	0.60
1:A:270:ASN:O	1:A:273:VAL:HG12	2.01	0.60
1:B:101:ALA:HB3	1:B:130:VAL:HG11	1.83	0.60
1:B:123:ARG:O	1:B:127:VAL:HG23	2.00	0.60
2:C:139:ALA:O	2:C:140:ALA:C	2.44	0.60
3:D:36:GLN:O	3:D:37:GLN:HB2	2.01	0.60
3:D:14:ALA:N	3:D:106:LEU:HG	2.16	0.60
3:D:166:ASP:OD1	3:D:168:LYS:N	2.34	0.60
3:D:194:GLU:HG2	3:D:205:VAL:CG1	2.27	0.60
2:E:16:GLY:O	2:E:86:VAL:HG23	2.01	0.60
3:D:107:ARG:HB2	3:D:107:ARG:CZ	2.32	0.60
2:C:153:TYR:CE1	2:C:183:TYR:HB3	2.36	0.60
3:D:7:SER:CB	3:D:8:PRO:HD3	2.28	0.60
3:D:79:ALA:C	3:D:81:ASP:N	2.59	0.60
3:F:148:LYS:HB2	3:F:192:THR:OG1	2.02	0.60
1:B:243:LYS:CG	2:E:31:ARG:HH21	2.14	0.60
1:B:75:TYR:CE2	1:B:79:LEU:HD11	2.37	0.60
3:D:166:ASP:OD1	3:D:167:SER:N	2.35	0.60
1:A:123:ARG:O	1:A:127:VAL:HG23	2.02	0.60
3:F:146:LYS:HB3	3:F:194:GLU:HB2	1.83	0.60
1:A:422:ILE:HA	1:A:425:MET:HE3	1.82	0.60
3:D:19:VAL:CG2	3:D:77:MET:HB2	2.32	0.60
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.84	0.59
1:A:357:PHE:CE2	1:A:398:LEU:HD11	2.37	0.59
3:F:182:LYS:HE2	3:F:186:GLU:OE1	2.01	0.59
1:A:101:ALA:HB3	1:A:130:VAL:HG11	1.84	0.59
1:A:258:LEU:HD13	1:A:371:PHE:CG	2.38	0.59
3:D:19:VAL:HG23	3:D:77:MET:HB2	1.83	0.59
1:A:75:TYR:CE2	1:A:79:LEU:HD11	2.37	0.59
3:D:86:TYR:CE2	3:D:100:GLY:HA3	2.36	0.59
3:D:95:GLN:N	3:D:95:GLN:OE1	2.35	0.59
3:F:27:SER:O	3:F:68:THR:HG22	2.03	0.59
1:A:109:ILE:HG23	1:A:204:MET:CE	2.32	0.59
3:D:27:SER:O	3:D:68:THR:HG22	2.02	0.59
2:E:153:TYR:HD1	2:E:155:PRO:O	1.84	0.59
3:D:11:MET:HG3	3:D:103:LEU:HD12	1.84	0.59
3:D:36:GLN:HA	3:D:85:TYR:HA	1.85	0.59
3:D:90:TRP:CZ2	3:D:95:GLN:NE2	2.69	0.59
1:A:132:PHE:O	1:A:136:LEU:HB2	2.03	0.59
1:A:126:ARG:O	1:A:129:PRO:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:105:ILE:CG2	3:D:106:LEU:N	2.66	0.59
1:A:44:THR:O	1:A:48:LEU:HG	2.03	0.58
3:D:36:GLN:O	3:D:43:PRO:HA	2.03	0.58
2:E:105:TYR:CE1	3:F:31:TYR:HD1	2.20	0.58
3:D:146:LYS:HB3	3:D:194:GLU:HB2	1.85	0.58
1:A:235:GLU:O	1:A:236:VAL:HG23	2.03	0.58
1:B:83:PHE:CD1	1:B:83:PHE:C	2.80	0.58
3:F:60:ARG:NH2	3:F:81:ASP:OD2	2.36	0.58
2:E:52:ASN:HD22	2:E:57:THR:HB	1.69	0.58
1:A:180:THR:HB	1:A:218:VAL:HA	1.85	0.58
2:C:179:GLN:O	2:C:180:ALA:C	2.46	0.58
2:E:91:THR:HG23	2:E:118:THR:HA	1.85	0.58
3:D:77:MET:HE2	3:D:103:LEU:CD2	2.34	0.58
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.36	0.58
3:F:124:LEU:C	3:F:126:SER:H	2.11	0.58
1:A:330:MET:HA	1:A:330:MET:CE	2.34	0.58
1:A:234:HIS:CD2	1:A:235:GLU:HG3	2.38	0.58
1:A:411:LEU:HG	1:A:415:MET:HE2	1.85	0.57
3:F:72:LEU:O	3:F:72:LEU:HD23	2.04	0.57
1:A:453:LEU:HB3	1:B:22:ILE:HD11	1.85	0.57
1:B:98:ARG:HA	1:B:98:ARG:NE	2.17	0.57
1:B:227:ILE:O	1:B:231:ILE:HG12	2.04	0.57
1:B:451:ARG:HH11	1:B:451:ARG:CG	2.17	0.57
2:C:18:LEU:HD11	2:C:117:VAL:HG22	1.86	0.57
2:C:16:GLY:O	2:C:86:VAL:HG23	2.03	0.57
2:C:153:TYR:CD2	2:C:183:TYR:O	2.56	0.57
2:E:145:THR:HG22	3:F:117:PHE:HZ	1.69	0.57
2:E:124:THR:CG2	2:E:125:THR:N	2.67	0.57
2:E:124:THR:O	2:E:125:THR:OG1	2.17	0.57
1:A:38:MET:HG3	1:A:168:LEU:CD1	2.33	0.57
3:D:116:ILE:HD12	3:D:193:CYS:HB2	1.85	0.57
1:A:231:ILE:HD13	1:B:249:LEU:HD13	1.86	0.57
1:A:78:LEU:HD13	1:A:79:LEU:N	2.19	0.57
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.34	0.57
1:A:86:SER:OG	1:A:303:GLY:HA3	2.04	0.57
1:B:127:VAL:HB	1:B:157:ASN:HD21	1.69	0.57
3:D:6:GLN:HE21	3:D:98:GLY:HA3	1.70	0.57
3:F:90:TRP:CE2	3:F:95:GLN:NE2	2.67	0.57
2:C:181:ALA:O	2:C:182:LEU:HD23	2.05	0.57
1:B:48:LEU:HD21	1:B:228:MET:SD	2.45	0.56
2:C:91:THR:HG23	2:C:118:THR:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:61:PHE:HA	3:D:73:THR:O	2.05	0.56
3:D:192:THR:HG22	3:D:207:SER:HB3	1.85	0.56
1:B:78:LEU:HD13	1:B:79:LEU:N	2.19	0.56
1:B:411:LEU:HG	1:B:415:MET:HE2	1.86	0.56
3:F:135:LEU:N	3:F:135:LEU:HD23	2.20	0.56
3:F:158:VAL:O	3:F:159:LEU:HD23	2.05	0.56
3:F:169:ASP:OD1	3:F:171:THR:HG23	2.06	0.56
3:F:95:GLN:N	3:F:95:GLN:OE1	2.39	0.56
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.88	0.56
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.86	0.56
3:F:125:THR:O	3:F:125:THR:CG2	2.54	0.56
3:F:194:GLU:HG2	3:F:205:VAL:CG1	2.29	0.56
1:B:91:MET:HG3	1:B:296:GLY:HA3	1.86	0.56
1:B:205:ARG:HG3	1:B:205:ARG:O	2.05	0.56
3:F:11:MET:HE2	3:F:19:VAL:HG13	1.88	0.56
1:B:38:MET:HG3	1:B:168:LEU:CD1	2.36	0.56
1:B:109:ILE:HG23	1:B:204:MET:HE1	1.87	0.56
3:D:162:TRP:CD1	3:D:174:MET:HG3	2.41	0.55
3:D:169:ASP:OD1	3:D:171:THR:HG23	2.06	0.55
2:E:18:LEU:HD11	2:E:117:VAL:HG22	1.88	0.55
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.14	0.55
3:F:75:ASN:O	3:F:76:THR:HB	2.06	0.55
1:B:258:LEU:HD13	1:B:371:PHE:CG	2.41	0.55
1:B:132:PHE:O	1:B:136:LEU:HB2	2.06	0.55
3:D:65:GLY:O	3:D:66:SER:HB3	2.06	0.55
1:A:78:LEU:HD21	1:A:307:PHE:CE1	2.42	0.55
1:A:83:PHE:CD1	1:A:83:PHE:C	2.84	0.55
1:A:98:ARG:HE	1:A:98:ARG:CA	2.18	0.55
1:B:75:TYR:HA	1:B:78:LEU:HD12	1.89	0.55
3:D:37:GLN:HG3	3:D:41:THR:O	2.06	0.55
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.89	0.55
1:A:145:LEU:HD21	1:A:347:CYS:HB3	1.89	0.55
1:B:19:ARG:NH1	1:B:19:ARG:CG	2.63	0.55
2:C:113:ALA:HA	3:D:42:SER:OG	2.07	0.55
3:D:13:ALA:C	3:D:106:LEU:HG	2.32	0.55
1:A:419:TYR:CZ	1:B:414:GLU:HG2	2.41	0.55
1:A:430:LEU:CD1	1:B:219:PHE:HB3	2.37	0.55
1:B:109:ILE:N	1:B:110:PRO:CD	2.69	0.55
1:A:447:ALA:O	1:A:451:ARG:HG2	2.06	0.54
3:F:73:THR:C	3:F:74:ILE:HG13	2.30	0.54
1:B:180:THR:HB	1:B:218:VAL:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:THR:O	1:B:180:THR:HG23	2.08	0.54
1:B:243:LYS:HG2	2:E:31:ARG:NH2	2.16	0.54
1:A:330:MET:HA	1:A:330:MET:HE2	1.90	0.54
1:B:126:ARG:O	1:B:129:PRO:HG2	2.07	0.54
1:A:451:ARG:CG	1:A:451:ARG:HH11	2.20	0.54
1:A:459:GLU:O	1:A:460:GLN:HG2	2.08	0.54
1:B:235:GLU:O	1:B:236:VAL:CB	2.55	0.54
3:D:72:LEU:HD23	3:D:73:THR:N	2.23	0.54
3:D:125:THR:O	3:D:125:THR:CG2	2.55	0.54
3:F:197:HIS:CE1	3:F:199:THR:HG23	2.43	0.54
1:A:328:PHE:O	1:A:373:MET:HE1	2.08	0.54
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.07	0.54
3:D:124:LEU:HD22	3:D:182:LYS:HG3	1.88	0.54
3:F:162:TRP:CD1	3:F:174:MET:HG3	2.43	0.54
1:B:78:LEU:HD21	1:B:307:PHE:CE1	2.43	0.54
3:D:6:GLN:HE21	3:D:98:GLY:C	2.15	0.54
3:D:6:GLN:NE2	3:D:100:GLY:CA	2.71	0.54
3:F:38:LYS:O	3:F:41:THR:HG22	2.08	0.54
2:C:112:GLY:O	3:D:42:SER:OG	2.25	0.53
1:A:75:TYR:HA	1:A:78:LEU:HD12	1.89	0.53
1:B:92:PHE:CD1	1:B:92:PHE:C	2.86	0.53
3:F:60:ARG:HD2	3:F:81:ASP:OD1	2.08	0.53
1:B:330:MET:CE	1:B:330:MET:HA	2.37	0.53
3:D:34:TRP:CG	3:D:72:LEU:HD12	2.44	0.53
1:A:433:THR:HG21	1:B:216:LYS:HE2	1.91	0.53
1:B:186:LEU:HD23	1:B:196:GLY:HA2	1.91	0.53
3:D:6:GLN:HE21	3:D:98:GLY:CA	2.22	0.53
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.44	0.53
1:A:48:LEU:HD21	1:A:228:MET:SD	2.49	0.53
1:A:214:SER:O	1:A:218:VAL:HG23	2.09	0.53
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.44	0.53
3:D:166:ASP:OD1	3:D:166:ASP:C	2.51	0.53
1:A:449:LEU:HD23	1:B:25:LEU:HD11	1.90	0.53
3:F:13:ALA:HB3	3:F:77:MET:HE1	1.90	0.53
1:A:150:PRO:CD	1:A:354:GLY:HA2	2.37	0.53
2:C:153:TYR:CE1	2:C:183:TYR:HB2	2.43	0.53
1:A:419:TYR:OH	1:B:414:GLU:HG2	2.09	0.53
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.91	0.53
3:D:9:ALA:O	3:D:102:LYS:HB3	2.08	0.53
1:A:191:ASN:OD1	1:A:230:ARG:NH1	2.42	0.52
3:F:192:THR:HG22	3:F:207:SER:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ARG:HE	1:B:98:ARG:CA	2.21	0.52
1:B:249:LEU:C	1:B:251:THR:H	2.17	0.52
1:A:204:MET:O	1:A:205:ARG:O	2.26	0.52
1:B:100:TYR:O	1:B:126:ARG:HD3	2.09	0.52
3:D:124:LEU:C	3:D:126:SER:H	2.16	0.52
3:D:197:HIS:CE1	3:D:199:THR:HG23	2.44	0.52
1:A:92:PHE:CD1	1:A:92:PHE:C	2.87	0.52
1:A:100:TYR:O	1:A:126:ARG:HD3	2.10	0.52
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.09	0.52
2:C:185:LEU:C	2:C:185:LEU:HD12	2.35	0.52
3:D:104:GLU:HB3	3:D:165:GLN:OE1	2.08	0.52
3:D:104:GLU:CB	3:D:165:GLN:OE1	2.57	0.52
1:B:270:ASN:O	1:B:273:VAL:HG12	2.09	0.52
1:B:145:LEU:HD21	1:B:347:CYS:HB3	1.92	0.52
2:C:153:TYR:CD1	2:C:183:TYR:HB2	2.45	0.52
3:D:14:ALA:HB2	3:D:106:LEU:HD12	1.91	0.52
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.92	0.52
1:B:158:ILE:O	1:B:162:VAL:HG13	2.10	0.52
1:B:330:MET:HA	1:B:330:MET:HE2	1.91	0.52
3:F:7:SER:CB	3:F:8:PRO:CD	2.86	0.52
3:F:73:THR:C	3:F:74:ILE:CG1	2.82	0.52
1:A:186:LEU:HD23	1:A:196:GLY:HA2	1.91	0.52
1:A:219:PHE:HB3	1:B:430:LEU:CD1	2.40	0.52
1:A:109:ILE:N	1:A:110:PRO:CD	2.72	0.52
2:C:7:SER:HA	2:C:115:THR:HG21	1.92	0.52
2:E:125:THR:N	2:E:154:PHE:O	2.43	0.52
3:F:60:ARG:HG3	3:F:74:ILE:CG2	2.40	0.52
1:A:249:LEU:C	1:A:251:THR:H	2.17	0.51
1:A:433:THR:CG2	1:B:216:LYS:HE2	2.40	0.51
1:B:138:THR:HG21	1:B:353:PRO:HD2	1.92	0.51
2:C:32:TYR:CD2	2:C:98:ARG:HD3	2.45	0.51
2:C:84:SER:O	2:C:85:LYS:C	2.53	0.51
2:E:107:TYR:CD1	2:E:107:TYR:C	2.89	0.51
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.46	0.51
3:F:194:GLU:CG	3:F:205:VAL:HG12	2.32	0.51
2:C:130:TYR:HB3	3:D:120:SER:OG	2.10	0.51
2:C:177:VAL:HG23	2:C:184:THR:O	2.09	0.51
3:D:168:LYS:O	3:D:169:ASP:CB	2.45	0.51
3:F:191:TYR:O	3:F:207:SER:HB2	2.10	0.51
1:A:107:SER:N	4:A:475:BR:BR	2.95	0.51
1:A:227:ILE:O	1:A:231:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:GLU:OE2	2:C:176:ALA:HB3	2.11	0.51
1:B:86:SER:OG	1:B:303:GLY:HA3	2.10	0.51
3:F:13:ALA:HB3	3:F:77:MET:CE	2.41	0.51
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.45	0.51
1:B:332:MET:O	1:B:336:ILE:HG13	2.11	0.51
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.92	0.51
1:B:361:LEU:HD13	1:B:415:MET:HE1	1.93	0.51
3:D:35:TYR:HA	3:D:44:LYS:O	2.11	0.51
1:B:78:LEU:HD13	1:B:79:LEU:H	1.75	0.51
1:B:447:ALA:O	1:B:451:ARG:HG2	2.10	0.51
1:A:146:GLY:HA3	1:A:148:GLU:OE2	2.10	0.50
3:D:60:ARG:O	3:D:75:ASN:N	2.44	0.50
3:F:11:MET:CE	3:F:19:VAL:HG13	2.41	0.50
1:A:22:ILE:HD11	1:B:453:LEU:HB3	1.93	0.50
2:C:72:ARG:HD3	2:C:74:ASN:OD1	2.11	0.50
3:D:181:THR:OG1	3:D:184:GLU:HB3	2.11	0.50
1:A:73:ASP:OD1	1:A:73:ASP:N	2.41	0.50
1:A:78:LEU:HD13	1:A:79:LEU:H	1.77	0.50
1:B:260:ILE:O	1:B:264:ILE:HG23	2.11	0.50
1:B:451:ARG:HH11	1:B:451:ARG:HG3	1.76	0.50
1:A:138:THR:HG21	1:A:352:ALA:HB1	1.93	0.50
1:B:138:THR:HG22	1:B:143:MET:SD	2.51	0.50
1:A:59:TRP:O	1:A:63:GLN:HG2	2.11	0.50
1:A:22:ILE:O	1:A:26:LEU:HD12	2.12	0.50
1:A:33:LEU:C	1:A:33:LEU:HD23	2.37	0.50
1:B:68:LEU:HD22	1:B:78:LEU:HD23	1.94	0.50
2:E:6:GLU:CD	2:E:114:GLY:H	2.19	0.50
1:A:127:VAL:HB	1:A:157:ASN:HD21	1.74	0.50
2:C:52:ASN:HD22	2:C:57:THR:HB	1.75	0.50
2:E:52:ASN:HB2	2:E:53:PRO:CD	2.42	0.50
3:F:77:MET:HG2	3:F:78:GLU:N	2.26	0.50
1:A:184:ALA:HB1	1:A:225:SER:HB3	1.95	0.49
1:B:68:LEU:HD13	1:B:307:PHE:CD1	2.47	0.49
3:D:105:ILE:CG2	3:D:106:LEU:H	2.24	0.49
1:A:68:LEU:HD13	1:A:307:PHE:CD1	2.47	0.49
1:A:413:LEU:HD12	1:A:425:MET:HE1	1.93	0.49
1:B:73:ASP:OD1	1:B:73:ASP:N	2.41	0.49
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.47	0.49
3:D:34:TRP:CZ3	3:D:87:CYS:HB3	2.48	0.49
3:D:98:GLY:C	3:D:100:GLY:H	2.19	0.49
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:TYR:O	2:C:183:TYR:N	2.39	0.49
3:D:84:THR:HG22	3:D:86:TYR:CE1	2.46	0.49
1:A:230:ARG:NH2	1:B:423:LEU:HD13	2.27	0.49
1:A:91:MET:HG3	1:A:296:GLY:CA	2.43	0.49
1:A:457:GLU:C	1:A:459:GLU:H	2.19	0.49
1:B:270:ASN:HA	1:B:273:VAL:HG12	1.95	0.49
3:D:19:VAL:O	3:D:73:THR:CA	2.60	0.49
3:D:34:TRP:CD2	3:D:72:LEU:HD12	2.48	0.49
3:D:194:GLU:CG	3:D:205:VAL:HG12	2.32	0.49
2:E:52:ASN:ND2	2:E:57:THR:H	2.11	0.49
1:A:158:ILE:O	1:A:162:VAL:HG13	2.12	0.49
3:D:90:TRP:CG	3:D:95:GLN:HB3	2.47	0.49
1:A:83:PHE:HD1	1:A:84:LEU:HD23	1.77	0.49
1:A:216:LYS:HE2	1:B:433:THR:HG21	1.94	0.49
3:D:191:TYR:O	3:D:207:SER:HB2	2.12	0.49
2:E:52:ASN:ND2	2:E:57:THR:N	2.60	0.49
3:D:77:MET:HE2	3:D:103:LEU:CG	2.43	0.49
2:E:11:LEU:HD23	2:E:124:THR:OG1	2.13	0.49
3:F:34:TRP:CD2	3:F:72:LEU:HD13	2.46	0.49
1:B:191:ASN:OD1	1:B:230:ARG:NH1	2.42	0.49
2:C:135:GLY:C	2:C:137:ALA:H	2.21	0.49
3:D:13:ALA:HB3	3:D:77:MET:HE3	1.95	0.49
3:D:90:TRP:CE2	3:D:95:GLN:NE2	2.67	0.49
3:F:124:LEU:HD22	3:F:182:LYS:HG3	1.93	0.49
1:A:216:LYS:HD3	1:B:434:LEU:HD23	1.94	0.48
1:B:346:LEU:O	1:B:350:SER:HB3	2.13	0.48
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.95	0.48
2:C:87:ARG:HE	2:C:89:GLU:HB2	1.78	0.48
1:A:148:GLU:OE1	1:A:357:PHE:CB	2.61	0.48
2:C:52:ASN:HB2	2:C:53:PRO:CD	2.44	0.48
1:A:203:VAL:HA	1:B:28:ARG:NH2	2.28	0.48
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.48	0.48
3:D:84:THR:CG2	3:D:86:TYR:CE1	2.95	0.48
3:F:34:TRP:CZ2	3:F:72:LEU:HB2	2.48	0.48
1:A:355:GLY:HA2	4:A:474:BR:BR	2.68	0.48
1:B:413:LEU:HD12	1:B:425:MET:HE1	1.95	0.48
1:B:451:ARG:HG3	1:B:451:ARG:NH1	2.28	0.48
3:D:12:SER:HA	3:D:104:GLU:O	2.13	0.48
2:E:72:ARG:HD3	2:E:74:ASN:OD1	2.13	0.48
3:F:181:THR:OG1	3:F:184:GLU:HB3	2.13	0.48
1:A:216:LYS:HE2	1:B:433:THR:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:HIS:HD2	1:A:235:GLU:HG3	1.78	0.48
1:A:346:LEU:O	1:A:350:SER:HB3	2.14	0.48
1:A:355:GLY:CA	4:A:474:BR:BR	3.17	0.48
1:A:430:LEU:HD11	1:B:219:PHE:HB3	1.94	0.48
1:B:91:MET:HG3	1:B:296:GLY:CA	2.44	0.48
1:B:190:PHE:HE2	1:B:317:PHE:HZ	1.61	0.48
1:A:135:GLY:C	1:A:137:GLY:N	2.70	0.48
1:B:88:VAL:HA	1:B:91:MET:HE2	1.94	0.48
1:B:109:ILE:HG23	1:B:204:MET:CE	2.43	0.48
1:B:214:SER:O	1:B:218:VAL:HG23	2.14	0.48
1:A:38:MET:HA	1:A:41:VAL:HG13	1.95	0.48
1:B:201:ILE:O	1:B:201:ILE:HG13	2.13	0.48
1:B:402:ILE:HD13	1:B:445:TYR:CD1	2.49	0.48
2:C:32:TYR:O	2:C:72:ARG:NH2	2.41	0.48
2:E:181:ALA:O	2:E:182:LEU:HD23	2.13	0.48
1:A:91:MET:CG	1:A:296:GLY:HA3	2.43	0.48
1:B:91:MET:CG	1:B:296:GLY:HA3	2.44	0.48
3:D:6:GLN:HE22	3:D:100:GLY:HA2	1.79	0.48
2:E:47:TRP:CZ2	2:E:49:GLY:HA2	2.48	0.48
1:B:38:MET:HA	1:B:41:VAL:HG13	1.95	0.48
3:F:31:TYR:HA	3:F:50:THR:OG1	2.13	0.48
1:B:328:PHE:O	1:B:373:MET:HE1	2.13	0.47
3:F:34:TRP:CZ3	3:F:87:CYS:HB3	2.49	0.47
1:A:219:PHE:HB3	1:B:430:LEU:HD11	1.96	0.47
1:A:282:ARG:O	1:A:283:VAL:C	2.57	0.47
3:D:18:LYS:HE3	3:D:75:ASN:OD1	2.14	0.47
1:A:205:ARG:HD3	1:A:207:GLN:OE1	2.14	0.47
3:F:35:TYR:CD1	3:F:35:TYR:N	2.82	0.47
1:A:361:LEU:HD13	1:A:415:MET:HE1	1.95	0.47
1:B:186:LEU:O	1:B:187:ALA:C	2.57	0.47
2:E:30:SER:C	2:E:32:TYR:H	2.22	0.47
3:F:73:THR:O	3:F:74:ILE:HG12	2.14	0.47
1:A:68:LEU:HD22	1:A:78:LEU:HD23	1.96	0.47
1:B:294:MET:HE2	1:B:294:MET:HB3	1.82	0.47
1:A:270:ASN:ND2	1:A:444:LEU:HG	2.30	0.47
1:B:184:ALA:HB1	1:B:225:SER:HB3	1.97	0.47
3:D:14:ALA:O	3:D:16:GLY:N	2.42	0.47
3:D:21:MET:HB3	3:D:101:THR:HG21	1.93	0.47
3:D:36:GLN:O	3:D:37:GLN:CB	2.63	0.47
3:D:84:THR:CG2	3:D:86:TYR:CZ	2.97	0.47
2:E:84:SER:O	2:E:85:LYS:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:107:TYR:CD1	2:C:107:TYR:C	2.92	0.47
1:B:78:LEU:C	1:B:78:LEU:HD22	2.39	0.47
1:B:107:SER:HB3	4:B:475:BR:BR	2.70	0.47
2:E:7:SER:HA	2:E:115:THR:HG21	1.97	0.47
1:A:46:VAL:HG22	1:A:155:GLY:HA2	1.97	0.47
1:A:421:LEU:O	1:A:425:MET:HG3	2.14	0.47
1:B:200:ILE:HA	1:B:204:MET:HB2	1.96	0.47
1:A:98:ARG:NE	1:A:98:ARG:CA	2.78	0.46
2:C:107:TYR:HB3	3:D:33:HIS:NE2	2.30	0.46
3:D:13:ALA:HB3	3:D:77:MET:HE1	1.96	0.46
2:E:32:TYR:O	2:E:72:ARG:NH2	2.44	0.46
1:A:148:GLU:OE1	1:A:357:PHE:HB3	2.15	0.46
1:B:22:ILE:O	1:B:26:LEU:HD12	2.15	0.46
1:B:38:MET:O	1:B:42:VAL:HG23	2.16	0.46
2:E:32:TYR:CD2	2:E:98:ARG:HD3	2.50	0.46
1:B:148:GLU:OE1	1:B:357:PHE:CB	2.63	0.46
1:A:88:VAL:HA	1:A:91:MET:HE2	1.97	0.46
1:B:83:PHE:HD1	1:B:84:LEU:HD23	1.80	0.46
1:B:97:VAL:HG21	1:B:353:PRO:HG3	1.98	0.46
2:C:87:ARG:HG3	2:C:89:GLU:OE1	2.15	0.46
2:E:54:VAL:HG23	2:E:56:SER:HB3	1.96	0.46
2:E:153:TYR:O	2:E:183:TYR:HB2	2.15	0.46
1:A:405:PRO:HG2	1:A:406:LEU:H	1.80	0.46
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.81	0.46
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.63	0.46
2:E:130:TYR:CE2	3:F:123:GLN:HG3	2.51	0.46
1:A:260:ILE:O	1:A:264:ILE:HG23	2.16	0.46
1:A:357:PHE:HE2	1:A:411:LEU:HD22	1.81	0.46
1:A:201:ILE:O	1:A:201:ILE:HG13	2.16	0.46
1:B:231:ILE:HB	1:B:232:PHE:CD1	2.51	0.46
3:D:21:MET:HB2	3:D:101:THR:HG21	1.96	0.46
1:A:234:HIS:CD2	1:A:235:GLU:CG	2.99	0.46
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.98	0.46
1:B:33:LEU:HD23	1:B:33:LEU:C	2.40	0.46
2:C:22:CYS:HB3	2:C:79:LEU:HB3	1.98	0.46
2:C:86:VAL:HG12	2:C:119:VAL:HG21	1.98	0.46
2:E:52:ASN:HD21	2:E:57:THR:N	2.13	0.46
3:F:89:GLN:C	3:F:89:GLN:CD	2.84	0.46
3:D:36:GLN:HA	3:D:84:THR:O	2.16	0.45
3:F:65:GLY:O	3:F:66:SER:HB3	2.15	0.45
1:B:31:THR:HB	1:B:36:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:156:GLU:HB3	2:E:157:PRO:HA	1.98	0.45
1:A:31:THR:HB	1:A:36:LEU:HD21	1.98	0.45
1:A:234:HIS:HD2	1:A:235:GLU:CG	2.30	0.45
1:A:337:PHE:O	1:A:341:VAL:HG23	2.17	0.45
1:B:77:LEU:O	1:B:80:THR:HB	2.17	0.45
1:B:135:GLY:C	1:B:137:GLY:N	2.73	0.45
2:C:30:SER:C	2:C:32:TYR:H	2.24	0.45
1:A:28:ARG:NH2	1:B:203:VAL:HA	2.31	0.45
1:A:200:ILE:HA	1:A:204:MET:HB2	1.99	0.45
3:F:34:TRP:CE3	3:F:72:LEU:HD13	2.51	0.45
1:A:332:MET:O	1:A:336:ILE:HG13	2.17	0.45
3:F:49:ASP:O	3:F:50:THR:HB	2.15	0.45
1:A:241:VAL:CG2	1:A:324:THR:HG21	2.47	0.45
3:F:103:LEU:HD12	3:F:103:LEU:HA	1.61	0.45
3:F:197:HIS:HE1	3:F:199:THR:HG23	1.81	0.45
1:A:78:LEU:C	1:A:78:LEU:HD22	2.42	0.45
1:A:99:LYS:HB3	1:A:100:TYR:CD1	2.52	0.45
1:A:226:THR:O	1:A:230:ARG:HG2	2.17	0.45
1:A:74:ASN:HD22	1:A:74:ASN:C	2.25	0.45
3:D:89:GLN:CD	3:D:89:GLN:C	2.85	0.45
3:F:109:ASP:HB3	3:F:199:THR:HG22	1.99	0.45
3:F:154:ARG:HD2	3:F:155:GLN:H	1.81	0.45
1:B:59:TRP:O	1:B:63:GLN:HG2	2.17	0.45
3:F:124:LEU:C	3:F:126:SER:N	2.75	0.45
3:D:7:SER:CB	3:D:8:PRO:CD	2.91	0.45
3:D:21:MET:SD	3:D:101:THR:CG2	3.05	0.45
3:D:31:TYR:HB3	3:D:49:ASP:HA	1.99	0.45
1:A:135:GLY:O	1:A:137:GLY:N	2.50	0.44
1:B:165:ILE:O	1:B:165:ILE:CG2	2.65	0.44
1:B:422:ILE:HA	1:B:425:MET:CE	2.46	0.44
3:D:31:TYR:HA	3:D:50:THR:OG1	2.17	0.44
1:A:75:TYR:HE2	1:A:79:LEU:HD11	1.80	0.44
1:A:241:VAL:HG21	1:A:324:THR:HG21	1.98	0.44
1:A:451:ARG:HH11	1:A:451:ARG:HG3	1.82	0.44
1:B:308:VAL:O	1:B:309:ALA:HB2	2.16	0.44
1:B:319:LEU:HD11	1:B:366:VAL:CG2	2.47	0.44
2:E:153:TYR:HE1	2:E:156:GLU:HA	1.83	0.44
1:A:190:PHE:HE2	1:A:317:PHE:HZ	1.64	0.44
1:A:402:ILE:HD13	1:A:445:TYR:CD1	2.52	0.44
3:F:6:GLN:HE21	3:F:98:GLY:CA	2.30	0.44
1:A:124:TRP:HA	1:A:157:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:174:MET:HE2	3:D:174:MET:HB3	1.84	0.44
1:A:78:LEU:HD21	1:A:307:PHE:CZ	2.53	0.44
1:A:135:GLY:C	1:A:137:GLY:H	2.25	0.44
1:B:75:TYR:HE2	1:B:79:LEU:HD11	1.80	0.44
1:B:95:PHE:O	1:B:97:VAL:N	2.50	0.44
1:B:357:PHE:HE2	1:B:411:LEU:HD22	1.82	0.44
3:D:210:ARG:HG2	3:D:210:ARG:HH11	1.83	0.44
3:F:124:LEU:O	3:F:126:SER:N	2.45	0.44
1:A:263:GLY:HA3	1:A:435:LEU:HB2	2.00	0.44
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.34	0.44
1:B:279:LEU:C	1:B:279:LEU:HD23	2.43	0.44
1:B:405:PRO:HG2	1:B:406:LEU:H	1.82	0.44
2:E:207:HIS:HA	2:E:208:PRO:HD2	1.69	0.44
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.73	0.44
1:A:330:MET:O	1:A:330:MET:HG3	2.17	0.44
1:B:421:LEU:C	1:B:424:PRO:HD2	2.42	0.44
1:B:444:LEU:HD22	1:B:444:LEU:O	2.18	0.44
2:E:179:GLN:O	2:E:180:ALA:HB3	2.17	0.44
3:F:105:ILE:HG22	3:F:106:LEU:N	2.32	0.44
1:A:451:ARG:HG3	1:A:451:ARG:NH1	2.32	0.44
2:C:36:TRP:CE2	2:C:81:LEU:HB2	2.52	0.44
3:F:6:GLN:HE22	3:F:86:TYR:HA	1.83	0.44
3:F:38:LYS:HE2	3:F:80:GLU:O	2.18	0.44
1:B:211:THR:HG22	1:B:212:LEU:N	2.31	0.44
2:E:87:ARG:HE	2:E:89:GLU:HB2	1.83	0.44
1:A:444:LEU:O	1:A:444:LEU:HD22	2.18	0.43
1:A:60:LEU:O	1:A:64:ARG:HG3	2.18	0.43
1:A:78:LEU:C	1:A:80:THR:N	2.76	0.43
1:A:136:LEU:HD12	1:A:136:LEU:HA	1.81	0.43
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.83	0.43
3:F:36:GLN:NE2	3:F:38:LYS:HG3	2.33	0.43
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.82	0.43
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.33	0.43
1:A:451:ARG:HH11	1:A:451:ARG:CB	2.31	0.43
2:C:54:VAL:HG23	2:C:56:SER:HB3	2.01	0.43
3:D:80:GLU:C	3:D:81:ASP:CG	2.86	0.43
3:F:82:ALA:HB2	3:F:105:ILE:CG1	2.49	0.43
3:D:168:LYS:HA	3:D:168:LYS:HD3	1.92	0.43
3:F:31:TYR:HB3	3:F:49:ASP:HA	2.00	0.43
1:A:19:ARG:CG	1:A:19:ARG:NH1	2.64	0.43
1:A:205:ARG:O	1:A:206:PRO:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:O	1:A:309:ALA:HB2	2.18	0.43
1:A:422:ILE:HG23	1:A:423:LEU:N	2.32	0.43
3:D:38:LYS:O	3:D:39:SER:C	2.60	0.43
3:D:136:ASN:O	3:D:137:ASN:HB2	2.18	0.43
1:A:95:PHE:O	1:A:97:VAL:N	2.52	0.43
1:B:60:LEU:O	1:B:64:ARG:HG3	2.18	0.43
1:B:234:HIS:C	1:B:235:GLU:HG2	2.41	0.43
1:B:241:VAL:HG21	1:B:324:THR:HG21	2.01	0.43
3:F:35:TYR:HA	3:F:44:LYS:O	2.18	0.43
1:A:231:ILE:HB	1:A:232:PHE:CD1	2.54	0.43
1:B:148:GLU:OE1	1:B:357:PHE:HB3	2.18	0.43
3:D:149:ILE:HG12	3:D:191:TYR:CE2	2.54	0.43
2:E:189:VAL:O	2:E:189:VAL:HG13	2.18	0.43
3:F:47:ILE:HD12	3:F:72:LEU:HG	1.99	0.43
3:F:93:HIS:CG	3:F:94:PRO:HA	2.54	0.43
1:A:210:TYR:N	1:B:210:TYR:HB2	2.33	0.43
1:A:210:TYR:HB2	1:B:210:TYR:N	2.32	0.43
1:A:319:LEU:HD11	1:A:366:VAL:CG2	2.48	0.43
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.49	0.43
1:B:205:ARG:O	1:B:206:PRO:C	2.61	0.43
1:A:74:ASN:HD22	1:A:76:PRO:HD2	1.82	0.43
1:A:77:LEU:O	1:A:81:VAL:HG13	2.19	0.43
1:B:212:LEU:H	1:B:212:LEU:CD1	2.27	0.43
1:B:422:ILE:HG23	1:B:423:LEU:N	2.33	0.43
2:C:153:TYR:CE1	2:C:158:VAL:HG13	2.54	0.43
3:D:185:TYR:CE1	3:D:191:TYR:CE1	3.07	0.43
2:E:185:LEU:C	2:E:185:LEU:HD12	2.44	0.43
1:A:98:ARG:NH2	1:A:102:PRO:HB3	2.34	0.43
1:A:200:ILE:HA	1:A:200:ILE:HD12	1.74	0.43
1:B:78:LEU:HD21	1:B:307:PHE:CZ	2.54	0.43
3:F:187:ARG:O	3:F:187:ARG:HG3	2.19	0.43
1:A:166:PHE:O	1:A:168:LEU:N	2.52	0.42
1:A:298:ILE:O	1:A:299:GLY:C	2.62	0.42
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.78	0.42
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.34	0.42
2:C:189:VAL:O	2:C:189:VAL:HG13	2.19	0.42
2:C:200:THR:O	2:C:200:THR:HG22	2.18	0.42
2:E:86:VAL:HG12	2:E:119:VAL:HG21	2.00	0.42
3:F:60:ARG:HG3	3:F:74:ILE:HG22	2.01	0.42
1:A:184:ALA:HB1	1:A:225:SER:CB	2.49	0.42
1:B:74:ASN:HD22	1:B:76:PRO:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.37	0.42
1:B:398:LEU:HD23	1:B:398:LEU:HA	1.93	0.42
2:C:142:SER:O	2:C:193:SER:HB2	2.19	0.42
1:A:118:ASP:CG	1:A:174:ARG:HH21	2.28	0.42
1:B:421:LEU:O	1:B:425:MET:HG3	2.19	0.42
2:C:6:GLU:CD	2:C:114:GLY:H	2.25	0.42
3:D:197:HIS:HE1	3:D:199:THR:HG23	1.84	0.42
1:B:451:ARG:CG	1:B:451:ARG:NH1	2.80	0.42
3:D:124:LEU:O	3:D:126:SER:N	2.46	0.42
2:E:11:LEU:HD12	2:E:11:LEU:HA	1.86	0.42
1:A:172:GLU:N	1:A:212:LEU:HD22	2.35	0.42
2:C:162:TRP:CH2	2:C:203:CYS:HB3	2.53	0.42
2:E:107:TYR:C	2:E:107:TYR:HD1	2.28	0.42
3:F:57:VAL:HA	3:F:58:PRO:HD2	1.82	0.42
1:A:25:LEU:HD11	1:B:449:LEU:HD23	2.02	0.42
1:B:46:VAL:HG22	1:B:155:GLY:HA2	2.01	0.42
1:B:118:ASP:CG	1:B:174:ARG:HH21	2.28	0.42
1:B:150:PRO:O	1:B:154:ILE:HG13	2.20	0.42
2:C:2:VAL:O	2:C:2:VAL:HG22	2.18	0.42
3:D:14:ALA:N	3:D:106:LEU:HB2	2.35	0.42
1:A:279:LEU:HD23	1:A:279:LEU:C	2.45	0.42
1:B:99:LYS:HB3	1:B:100:TYR:CD1	2.55	0.42
3:D:35:TYR:O	3:D:85:TYR:HA	2.20	0.42
2:E:170:GLY:O	2:E:189:VAL:HA	2.20	0.42
3:F:185:TYR:CE1	3:F:191:TYR:CE1	3.07	0.42
1:A:126:ARG:HG2	1:A:126:ARG:HH11	1.85	0.42
1:B:77:LEU:O	1:B:81:VAL:HG13	2.19	0.42
1:B:248:PRO:O	1:B:251:THR:HB	2.20	0.42
2:C:29:TYR:CE1	2:C:34:MET:HG3	2.55	0.42
2:C:52:ASN:ND2	2:C:57:THR:H	2.17	0.42
2:E:196:TRP:HD1	2:E:201:VAL:HG23	1.85	0.42
3:D:98:GLY:C	3:D:100:GLY:N	2.76	0.42
2:E:87:ARG:HG3	2:E:89:GLU:OE1	2.20	0.42
2:E:162:TRP:CH2	2:E:203:CYS:HB3	2.55	0.42
3:F:34:TRP:CB	3:F:72:LEU:CD1	2.97	0.42
1:A:272:TRP:O	1:A:273:VAL:C	2.62	0.41
1:A:457:GLU:OE1	1:B:19:ARG:HG3	2.21	0.41
1:B:78:LEU:C	1:B:80:THR:N	2.77	0.41
1:B:272:TRP:O	1:B:273:VAL:C	2.62	0.41
3:F:6:GLN:HE21	3:F:98:GLY:HA3	1.84	0.41
1:A:150:PRO:O	1:A:154:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:C	1:A:424:PRO:HD2	2.45	0.41
1:B:337:PHE:O	1:B:341:VAL:HG23	2.19	0.41
2:E:28:ASP:O	2:E:30:SER:O	2.38	0.41
2:E:142:SER:O	2:E:193:SER:HB2	2.19	0.41
1:A:77:LEU:O	1:A:80:THR:HB	2.20	0.41
1:A:183:ALA:O	1:A:184:ALA:C	2.63	0.41
1:B:396:ALA:O	1:B:399:ALA:HB3	2.20	0.41
3:D:93:HIS:CG	3:D:94:PRO:HA	2.56	0.41
1:B:74:ASN:HD22	1:B:74:ASN:C	2.28	0.41
1:B:135:GLY:O	1:B:137:GLY:N	2.54	0.41
2:E:107:TYR:HB3	3:F:33:HIS:NE2	2.35	0.41
1:B:135:GLY:C	1:B:137:GLY:H	2.28	0.41
1:B:184:ALA:HB1	1:B:225:SER:CB	2.50	0.41
1:B:201:ILE:O	1:B:201:ILE:CG1	2.68	0.41
2:E:124:THR:C	2:E:125:THR:HG1	2.19	0.41
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.80	0.41
1:A:294:MET:HE2	1:A:294:MET:HB3	1.81	0.41
1:B:127:VAL:O	1:B:128:LEU:C	2.62	0.41
1:B:231:ILE:O	1:B:231:ILE:HG22	2.21	0.41
1:B:236:VAL:O	1:B:236:VAL:HG12	2.19	0.41
2:C:28:ASP:O	2:C:30:SER:O	2.38	0.41
2:C:52:ASN:ND2	2:C:57:THR:N	2.68	0.41
2:E:131:PRO:HD3	2:E:216:LYS:HG2	2.03	0.41
1:A:244:LEU:N	1:A:244:LEU:CD2	2.84	0.41
2:C:153:TYR:CE2	2:C:183:TYR:O	2.74	0.41
3:D:166:ASP:CG	3:D:167:SER:H	2.26	0.41
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.50	0.41
1:B:241:VAL:CG2	1:B:324:THR:HG21	2.51	0.41
1:B:255:TYR:CE2	1:B:389:PHE:CD2	3.09	0.41
3:D:6:GLN:HA	3:D:22:THR:O	2.21	0.41
2:E:103:TYR:HD2	3:F:31:TYR:CE2	2.39	0.41
1:A:127:VAL:O	1:A:128:LEU:C	2.63	0.41
1:A:211:THR:HG22	1:A:212:LEU:N	2.33	0.41
1:A:212:LEU:H	1:A:212:LEU:CD1	2.30	0.41
1:A:422:ILE:HA	1:A:422:ILE:HD12	1.96	0.41
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.84	0.41
1:B:57:VAL:HG12	1:B:61:GLN:OE1	2.21	0.41
1:B:95:PHE:C	1:B:97:VAL:N	2.79	0.41
1:B:126:ARG:HH11	1:B:126:ARG:HG2	1.85	0.41
1:B:249:LEU:C	1:B:251:THR:N	2.79	0.41
2:C:174:PHE:HA	2:C:175:PRO:HD2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:125:THR:HB	2:E:154:PHE:H	1.85	0.41
3:F:73:THR:O	3:F:74:ILE:CG1	2.68	0.41
3:F:149:ILE:HG12	3:F:191:TYR:CE2	2.55	0.41
1:A:33:LEU:HD23	1:A:33:LEU:O	2.20	0.41
1:A:62:ASN:O	1:A:63:GLN:C	2.63	0.41
1:A:148:GLU:O	1:A:149:GLY:C	2.62	0.41
1:A:255:TYR:CE2	1:A:389:PHE:CD2	3.10	0.41
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.70	0.41
3:D:6:GLN:NE2	3:D:100:GLY:HA2	2.36	0.41
3:D:57:VAL:HA	3:D:58:PRO:HD2	1.85	0.41
3:D:189:ASN:O	3:D:209:ASN:HA	2.21	0.41
1:A:216:LYS:NZ	1:B:437:GLN:NE2	2.69	0.40
1:B:59:TRP:CZ3	1:B:63:GLN:HG3	2.56	0.40
1:B:136:LEU:HD12	1:B:136:LEU:HA	1.76	0.40
1:B:284:HIS:C	1:B:286:GLY:H	2.29	0.40
1:B:451:ARG:HH11	1:B:451:ARG:CB	2.34	0.40
2:C:7:SER:HA	2:C:115:THR:CG2	2.51	0.40
2:C:129:VAL:O	2:C:216:LYS:HE3	2.21	0.40
3:D:12:SER:HB3	3:D:106:LEU:HD23	2.02	0.40
2:E:183:TYR:HB3	2:E:184:THR:H	1.75	0.40
1:A:86:SER:HB2	1:A:300:GLY:HA2	2.03	0.40
1:A:176:THR:HG22	1:A:177:LEU:N	2.37	0.40
1:A:186:LEU:O	1:A:187:ALA:C	2.65	0.40
1:A:434:LEU:HD23	1:A:434:LEU:HA	1.65	0.40
1:B:274:LEU:O	1:B:277:GLN:HB3	2.22	0.40
1:A:379:PHE:HA	1:A:381:GLN:HE22	1.86	0.40
1:A:423:LEU:HD11	1:B:226:THR:HG21	2.04	0.40
2:E:22:CYS:HB3	2:E:79:LEU:HB3	2.04	0.40
2:E:139:ALA:O	2:E:140:ALA:C	2.64	0.40
1:B:58:ALA:O	1:B:59:TRP:C	2.65	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%)	382 (86%)	50 (11%)	10 (2%)	5	19
1	B	439/473 (93%)	382 (87%)	48 (11%)	9 (2%)	5	21
2	C	219/221 (99%)	197 (90%)	18 (8%)	4 (2%)	6	25
2	E	219/221 (99%)	195 (89%)	21 (10%)	3 (1%)	9	30
3	D	209/211 (99%)	173 (83%)	26 (12%)	10 (5%)	2	7
3	F	209/211 (99%)	184 (88%)	20 (10%)	5 (2%)	4	18
All	All	1737/1810 (96%)	1513 (87%)	183 (10%)	41 (2%)	4	18

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ARG
1	A	205	ARG
1	A	236	VAL
1	B	236	VAL
2	C	157	PRO
2	C	175	PRO
3	D	7	SER
3	D	37	GLN
3	D	39	SER
2	E	184	THR
3	F	7	SER
1	A	96	LEU
1	B	96	LEU
1	B	136	LEU
1	B	167	ARG
2	C	65	LYS
3	D	125	THR
3	D	169	ASP
3	F	74	ILE
3	F	125	THR
3	F	198	LYS
2	C	136	SER
3	D	66	SER
2	E	65	LYS
2	E	180	ALA
3	F	66	SER
1	A	136	LEU

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Mol	Chain	Res	Type
1	A	149	GLY
1	B	309	ALA
3	D	198	LYS
1	A	309	ALA
1	B	205	ARG
3	D	16	GLY
3	D	126	SER
1	A	201	ILE
1	A	206	PRO
1	B	149	GLY
1	B	201	ILE
1	B	206	PRO
3	D	15	PRO
1	A	283	VAL

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%)	288 (86%)	47 (14%)	3	11
1	B	332/358 (93%)	287 (86%)	45 (14%)	3	12
2	C	181/181 (100%)	161 (89%)	20 (11%)	6	20
2	E	181/181 (100%)	163 (90%)	18 (10%)	7	24
3	D	185/185 (100%)	164 (89%)	21 (11%)	5	18
3	F	185/185 (100%)	168 (91%)	17 (9%)	8	27
All	All	1399/1448 (97%)	1231 (88%)	168 (12%)	5	16

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	31	THR
1	A	41	VAL
1	A	69	VAL

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Mol	Chain	Res	Type
1	A	78	LEU
1	A	81	VAL
1	A	96	LEU
1	A	103	GLU
1	A	138	THR
1	A	145	LEU
1	A	148	GLU
1	A	162	VAL
1	A	168	LEU
1	A	176	THR
1	A	177	LEU
1	A	180	THR
1	A	200	ILE
1	A	201	ILE
1	A	203	VAL
1	A	207	GLN
1	A	212	LEU
1	A	215	ILE
1	A	219	PHE
1	A	222	VAL
1	A	235	GLU
1	A	236	VAL
1	A	244	LEU
1	A	251	THR
1	A	264	ILE
1	A	288	ILE
1	A	319	LEU
1	A	330	MET
1	A	356	ILE
1	A	377	GLU
1	A	381	GLN
1	A	397	LEU
1	A	402	ILE
1	A	413	LEU
1	A	420	GLN
1	A	430	LEU
1	A	434	LEU
1	A	435	LEU
1	A	444	LEU
1	A	446	SER
1	A	451	ARG
1	A	452	THR

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Mol	Chain	Res	Type
1	A	453	LEU
1	B	19	ARG
1	B	31	THR
1	B	41	VAL
1	B	69	VAL
1	B	78	LEU
1	B	81	VAL
1	B	96	LEU
1	B	103	GLU
1	B	138	THR
1	B	145	LEU
1	B	148	GLU
1	B	162	VAL
1	B	168	LEU
1	B	176	THR
1	B	177	LEU
1	B	180	THR
1	B	200	ILE
1	B	201	ILE
1	B	203	VAL
1	B	207	GLN
1	B	212	LEU
1	B	215	ILE
1	B	219	PHE
1	B	222	VAL
1	B	235	GLU
1	B	244	LEU
1	B	251	THR
1	B	264	ILE
1	B	288	ILE
1	B	319	LEU
1	B	330	MET
1	B	377	GLU
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	413	LEU
1	B	420	GLN
1	B	430	LEU
1	B	434	LEU
1	B	435	LEU
1	B	444	LEU

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Mol	Chain	Res	Type
1	B	446	SER
1	B	451	ARG
1	B	452	THR
1	B	453	LEU
2	C	2	VAL
2	C	5	LEU
2	C	21	SER
2	C	30	SER
2	C	51	ILE
2	C	55	SER
2	C	65	LYS
2	C	83	ILE
2	C	115	THR
2	C	145	THR
2	C	157	PRO
2	C	167	LEU
2	C	175	PRO
2	C	184	THR
2	C	185	LEU
2	C	186	SER
2	C	193	SER
2	C	200	THR
2	C	214	VAL
2	C	218	ILE
3	D	1	ASP
3	D	22	THR
3	D	36	GLN
3	D	41	THR
3	D	53	LEU
3	D	75	ASN
3	D	77	MET
3	D	95	GLN
3	D	106	LEU
3	D	107	ARG
3	D	120	SER
3	D	121	SER
3	D	135	LEU
3	D	141	LYS
3	D	142	ASP
3	D	166	ASP
3	D	174	MET
3	D	176	SER

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Mol	Chain	Res	Type
3	D	184	GLU
3	D	190	SER
3	D	201	THR
2	E	2	VAL
2	E	5	LEU
2	E	21	SER
2	E	30	SER
2	E	55	SER
2	E	65	LYS
2	E	83	ILE
2	E	115	THR
2	E	145	THR
2	E	157	PRO
2	E	167	LEU
2	E	179	GLN
2	E	184	THR
2	E	186	SER
2	E	193	SER
2	E	200	THR
2	E	214	VAL
2	E	218	ILE
3	F	1	ASP
3	F	22	THR
3	F	36	GLN
3	F	41	THR
3	F	53	LEU
3	F	75	ASN
3	F	77	MET
3	F	95	GLN
3	F	120	SER
3	F	121	SER
3	F	135	LEU
3	F	141	LYS
3	F	142	ASP
3	F	166	ASP
3	F	176	SER
3	F	184	GLU
3	F	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	153	GLN
1	A	157	ASN
1	A	270	ASN
1	A	281	HIS
1	A	287	ASN
1	A	327	ASN
1	A	381	GLN
1	A	437	GLN
1	B	74	ASN
1	B	153	GLN
1	B	157	ASN
1	B	270	ASN
1	B	281	HIS
1	B	284	HIS
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	437	GLN
3	D	6	GLN
3	D	88	GLN
3	F	6	GLN
3	F	36	GLN
3	F	88	GLN
3	F	136	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	444/473 (93%)	0.63	29 (6%)	25	20	61, 93, 155, 219	0
1	B	441/473 (93%)	0.75	41 (9%)	14	12	58, 96, 168, 244	0
2	C	221/221 (100%)	0.80	21 (9%)	14	11	49, 83, 136, 237	0
2	E	221/221 (100%)	0.83	26 (11%)	9	7	55, 86, 154, 215	0
3	D	211/211 (100%)	1.13	40 (18%)	3	3	63, 101, 148, 189	0
3	F	211/211 (100%)	0.49	10 (4%)	36	28	54, 77, 136, 186	0
All	All	1749/1810 (96%)	0.75	167 (9%)	14	11	49, 91, 154, 244	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	PRO	8.7
1	B	307	PHE	8.3
3	D	36	GLN	6.9
1	B	104	ALA	6.6
2	E	178	LEU	6.3
3	D	101	THR	6.3
2	E	182	LEU	6.0
1	B	72	ALA	5.6
2	E	183	TYR	5.3
1	A	72	ALA	5.2
3	D	82	ALA	5.2
3	D	22	THR	5.0
1	B	288	ILE	4.9
1	A	283	VAL	4.7
3	D	69	SER	4.7
2	E	177	VAL	4.6
3	D	20	THR	4.6
1	B	452	THR	4.4
2	E	31	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
2	E	140	ALA	4.2
2	C	175	PRO	4.1
2	E	155	PRO	4.0
3	D	106	LEU	3.9
2	E	13	GLN	3.8
2	E	64	LEU	3.8
2	C	64	LEU	3.8
1	B	147	ARG	3.7
2	C	199	GLU	3.5
2	E	156	GLU	3.4
3	D	71	SER	3.4
3	D	23	CYS	3.4
2	E	32	TYR	3.4
1	B	69	VAL	3.3
2	C	141	ALA	3.3
1	B	119	GLN	3.3
1	B	138	THR	3.3
1	A	73	ASP	3.3
2	C	106	TRP	3.3
3	D	74	ILE	3.3
1	A	168	LEU	3.2
1	B	97	VAL	3.2
2	C	170	GLY	3.2
3	D	95	GLN	3.2
1	B	139	LEU	3.2
1	B	28	ARG	3.2
1	B	445	TYR	3.1
3	F	100	GLY	3.1
1	A	235	GLU	3.1
2	C	177	VAL	3.1
1	B	105	GLY	3.1
1	A	386	ALA	3.1
1	B	73	ASP	3.1
1	A	111	GLU	3.1
3	D	37	GLN	3.0
3	D	86	TYR	3.0
1	A	67	ALA	3.0
2	C	140	ALA	3.0
1	A	69	VAL	3.0
2	E	123	LYS	3.0
1	A	288	ILE	2.9
3	D	85	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	235	GLU	2.9
1	A	234	HIS	2.9
2	E	213	LYS	2.9
1	B	135	GLY	2.9
2	C	214	VAL	2.9
1	B	53	PHE	2.9
2	C	176	ALA	2.8
3	D	167	SER	2.8
1	B	354	GLY	2.8
1	A	115	ALA	2.8
2	E	138	ALA	2.8
2	E	124	THR	2.8
2	E	181	ALA	2.7
3	D	141	LYS	2.7
2	E	176	ALA	2.7
1	B	143	MET	2.7
1	B	145	LEU	2.7
1	B	215	ILE	2.7
3	D	51	SER	2.7
1	B	177	LEU	2.7
3	D	24	SER	2.7
3	D	170	SER	2.6
2	C	104	GLY	2.6
2	E	154	PHE	2.6
1	A	380	PRO	2.6
2	E	184	THR	2.6
3	F	72	LEU	2.6
1	A	17	ARG	2.5
3	F	7	SER	2.5
2	C	41	PRO	2.5
1	A	445	TYR	2.5
3	F	156	ASN	2.5
3	D	70	TYR	2.5
1	A	71	THR	2.5
1	B	67	ALA	2.5
1	A	84	LEU	2.4
1	A	207	GLN	2.4
1	A	140	GLY	2.4
3	D	38	LYS	2.4
2	E	105	TYR	2.4
3	F	74	ILE	2.4
3	D	81	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	100	GLY	2.4
3	D	173	SER	2.4
1	B	82	ALA	2.4
3	D	8	PRO	2.4
3	D	102	LYS	2.4
1	A	438	PHE	2.4
2	C	107	TYR	2.4
3	D	172	TYR	2.4
3	D	19	VAL	2.3
2	E	59	ASN	2.3
1	B	323	ALA	2.3
3	F	89	GLN	2.3
1	B	136	LEU	2.3
1	A	291	TRP	2.3
3	D	39	SER	2.3
2	C	105	TYR	2.3
2	C	44	GLY	2.3
2	C	137	ALA	2.3
2	C	143	MET	2.3
1	B	70	HIS	2.3
3	D	162	TRP	2.3
3	D	103	LEU	2.2
3	D	169	ASP	2.2
1	A	120	ARG	2.2
1	A	57	VAL	2.2
2	C	29	TYR	2.2
3	F	120	SER	2.2
1	B	208	PHE	2.2
3	D	105	ILE	2.2
3	F	169	ASP	2.2
1	B	85	CYS	2.2
3	F	119	PRO	2.2
1	B	75	TYR	2.2
2	E	180	ALA	2.2
1	B	234	HIS	2.2
3	D	171	THR	2.2
1	B	301	LEU	2.2
1	A	338	VAL	2.2
3	D	68	THR	2.2
2	E	43	LYS	2.2
3	D	99	GLY	2.2
2	C	194	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	180	ALA	2.2
3	D	108	ALA	2.2
1	A	344	THR	2.1
1	A	178	LEU	2.1
1	B	438	PHE	2.1
2	C	89	GLU	2.1
1	B	103	GLU	2.1
1	B	287	ASN	2.1
2	E	19	LYS	2.1
2	E	217	LYS	2.1
1	A	156	GLY	2.1
1	A	401	SER	2.1
3	D	140	PRO	2.1
2	E	100	TYR	2.1
1	B	71	THR	2.0
3	F	122	GLU	2.0
3	D	15	PRO	2.0
1	A	205	ARG	2.0
1	B	352	ALA	2.0
1	B	400	ALA	2.0
3	D	109	ASP	2.0
1	B	94	TYR	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](#)

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
4	BR	A	475	1/1	0.85	0.37	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BR	B	475	1/1	0.90	0.35	100,100,100,100	0
4	BR	B	474	1/1	0.91	0.33	100,100,100,100	0
4	BR	A	474	1/1	0.96	0.29	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.