



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 03:04 PM EDT

PDB ID : 3EJZ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

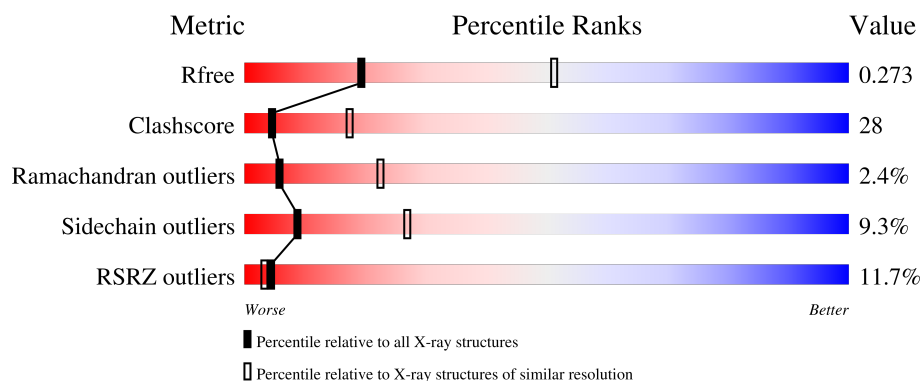
1 Overall quality at a glance

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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	<div> <div>9%</div> <div>53%</div> <div>34%</div> <div>7%</div> <div>6%</div> </div>
1	B	473	<div> <div>11%</div> <div>52%</div> <div>34%</div> <div>7%</div> <div>7%</div> </div>
2	C	221	<div> <div>7%</div> <div>63%</div> <div>32%</div> <div>5%</div> </div>
2	E	221	<div> <div>9%</div> <div>65%</div> <div>31%</div> <div>.</div> </div>
3	D	211	<div> <div>20%</div> <div>45%</div> <div>45%</div> <div>9%</div> </div>

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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 (three-letter code: BR) (formula: Br).

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

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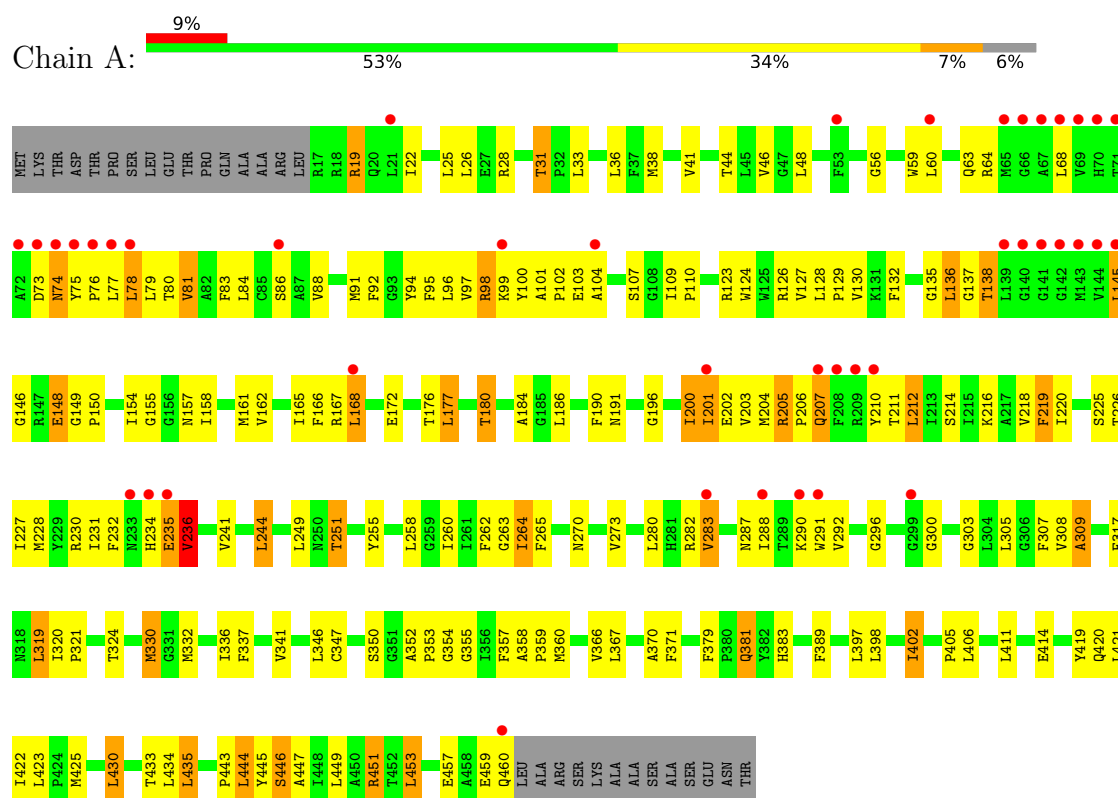
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Br	0	0
			2	2		

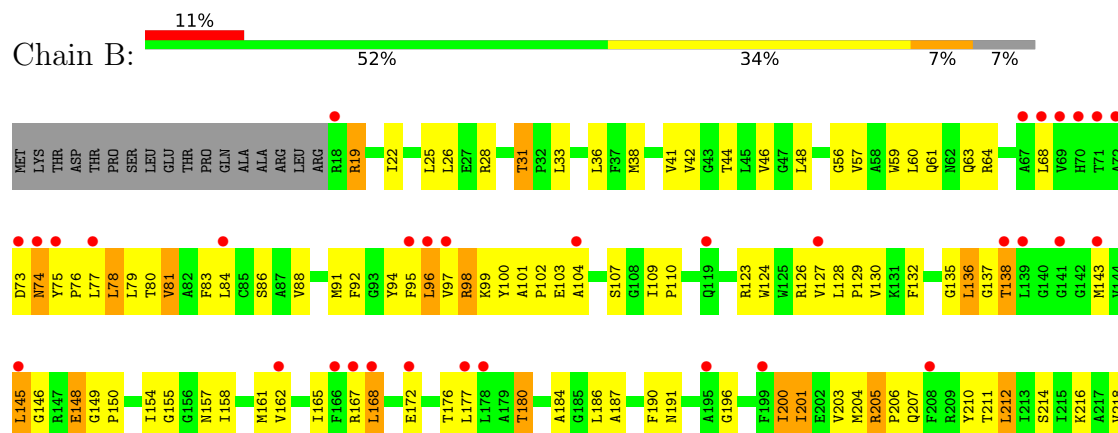
3 Residue-property plots

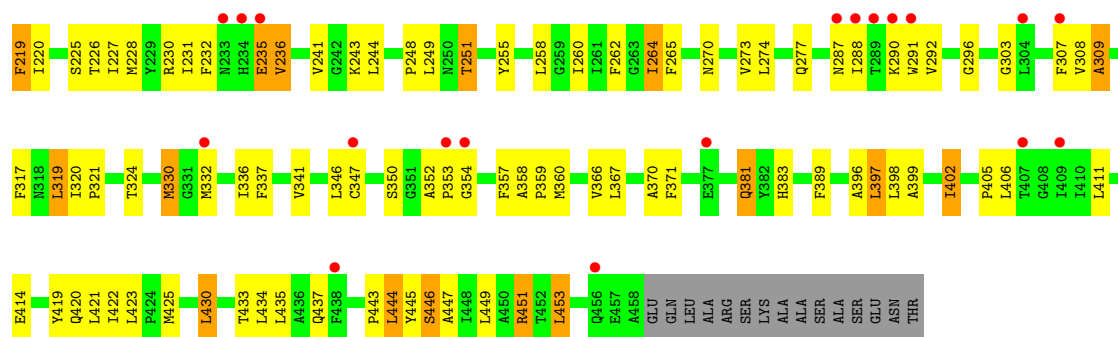
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

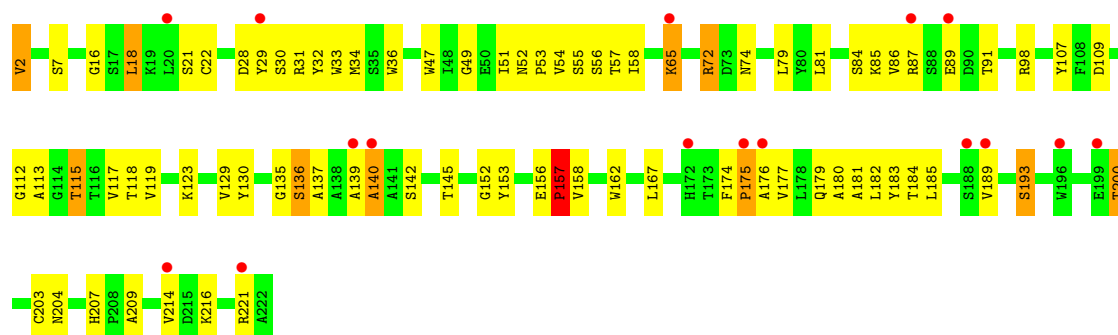


- Molecule 1: H(+)/Cl(-) exchange transporter clcA

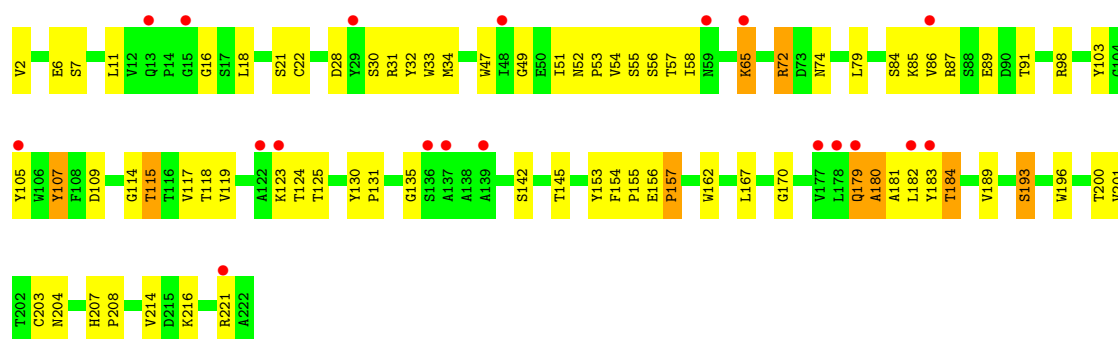




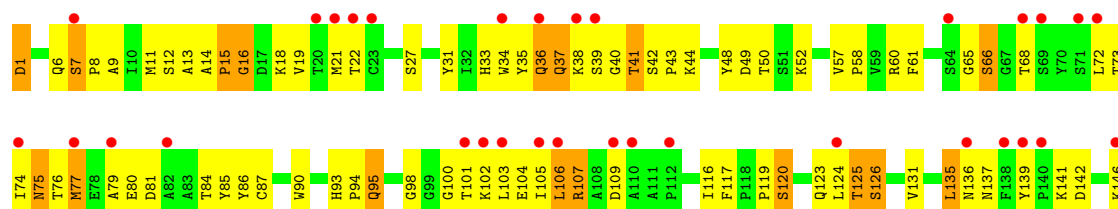
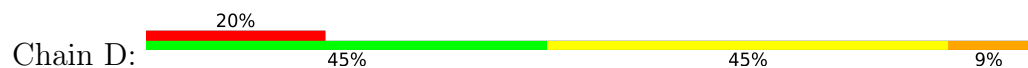
• Molecule 2: Fab fragment, Heavy chain

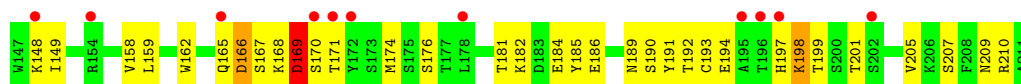


• Molecule 2: Fab fragment, Heavy chain

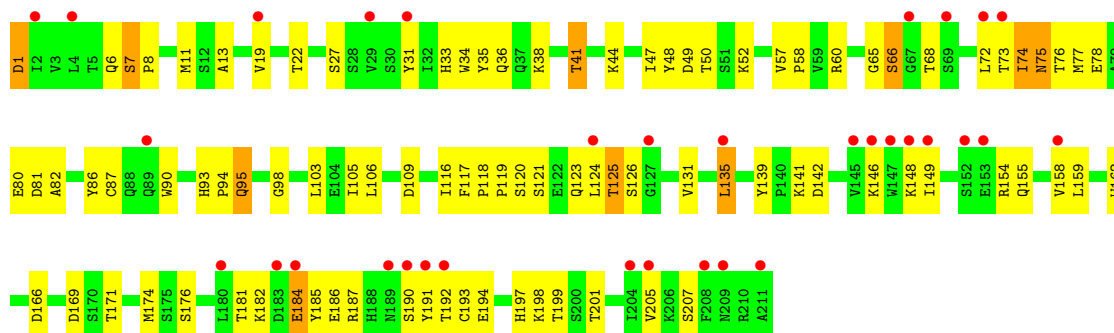


• Molecule 3: Fab fragment, Light chain





- 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	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 (5.01%)	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 , 80.1	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 [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/3403	0.55	0/4619
1	B	0.40	0/3374	0.54	0/4581
2	C	0.52	0/1721	0.73	2/2355 (0.1%)
2	E	0.53	0/1721	0.68	0/2355
3	D	0.46	0/1660	0.69	1/2257 (0.0%)
3	F	0.53	0/1660	0.67	0/2257
All	All	0.46	0/13539	0.63	3/18424 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	140	ALA	CB-CA-C	8.01	122.11	110.10
3	D	169	ASP	CB-CA-C	7.16	124.73	110.40
2	C	136	SER	CB-CA-C	6.77	122.97	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	209	0
1	B	3302	0	3459	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1672	0	1654	73	0
2	E	1672	0	1654	65	0
3	D	1621	0	1546	151	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	754	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 28.

All (754) 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: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:D:95:GLN:CD	3:D:95:GLN:H	1.59	1.04
3:F:34:TRP:CG	3:F:72:LEU:HD12	1.92	1.04
3:F:95:GLN:H	3:F:95:GLN:CD	1.62	1.03
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:D:13:ALA:HB3	3:D:77:MET:HE3	1.44	0.99
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:77:MET:HE2	3:F:103:LEU:HD21	1.54	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
3:F:13:ALA:HB3	3:F:77:MET:HE3	1.57	0.86
3:D:95:GLN:CD	3:D:95:GLN:N	2.29	0.85
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
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
1:B:381:GLN:HE21	1:B:381:GLN:N	1.74	0.83
2:C:135:GLY:HA2	2:C:221:ARG:HD3	1.62	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
3:D:80:GLU:C	3:D:81:ASP:OD2	2.21	0.78
3:F:95:GLN:CD	3:F:95:GLN:N	2.29	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:D:77:MET:HE2	3:D:103:LEU:HD21	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:125:THR:HG22	3:D:125:THR:O	1.86	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
1:B:98:ARG:HE	1:B:98:ARG:HA	1.52	0.75
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
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
1:B:422:ILE:HA	1:B:425:MET:HE2	1.71	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
2:E:30:SER:O	2:E:31:ARG:HB2	1.89	0.71
2:C:174:PHE:O	2:C:175:PRO:C	2.28	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:13:ALA:HB3	3:D:77:MET:CE	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:192:THR:HG22	3:D:207:SER:HB2	1.73	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
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
1:A:422:ILE:HA	1:A:425:MET:HE2	1.75	0.68
2:C:174:PHE:C	2:C:175:PRO:O	2.32	0.67
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
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:166:ASP:CG	3:D:167:SER:N	2.49	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:A:19:ARG:HG2	1:A:19:ARG:NH1	1.91	0.65
1:B:44:THR:O	1:B:48:LEU:HG	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:THR:HG22	1:B:212:LEU:H	1.60	0.64
3:D:158:VAL:O	3:D:159:LEU:HD23	1.97	0.64
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: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
1:A:204:MET:O	1:A:205:ARG:C	2.37	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:A:330:MET:HE2	1:A:330:MET:HA	1.82	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: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:98:ARG:HA	1:A:98:ARG:NE	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:148:GLU:CD	1:B:148:GLU:H	2.04	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:1:ASP:OD2	3:D:1:ASP:N	2.29	0.60
3:D:107:ARG:HB2	3:D:107:ARG:CZ	2.32	0.60
1:A:148:GLU:CD	1:A:148:GLU:H	2.05	0.60
1:A:330:MET:HE1	1:A:370:ALA:HA	1.81	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: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
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
3:D:105:ILE:CG2	3:D:106:LEU:N	2.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:330:MET:HE1	1:B:370:ALA:HA	1.83	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:E:91:THR:HG23	2:E:118:THR:HA	1.85	0.58
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.36	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
3:F:6:GLN:HE21	3:F:98:GLY:C	2.07	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
1:B:204:MET:O	1:B:205:ARG:C	2.44	0.56
1:B:205:ARG:HG3	1:B:205:ARG:O	2.05	0.56
3:D:61:PHE:HA	3:D:73:THR:O	2.05	0.56
3:D:79:ALA:C	3:D:81:ASP:H	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:139:ALA:O	2:C:140:ALA:C	2.44	0.56
3:D:79:ALA:C	3:D:81:ASP:N	2.59	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:38:MET:HG3	1:B:168:LEU:CD1	2.36	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: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: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
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
1:B:180:THR:HB	1:B:218:VAL:HA	1.88	0.54
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:83:PHE:CD1	1:B:83:PHE:C	2.80	0.54
3:D:109:ASP:OD2	3:D:198:LYS:NZ	2.29	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
1:A:75:TYR:HA	1:A:78:LEU:HD12	1.89	0.53
3:F:60:ARG:HD2	3:F:81:ASP:OD1	2.08	0.53
2:C:179:GLN:O	2:C:180:ALA:C	2.46	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
3:F:124:LEU:C	3:F:126:SER:H	2.11	0.53
1:A:360:MET:HE3	1:A:398:LEU:HD23	1.90	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
1:A:449:LEU:HD23	1:B:25:LEU:HD11	1.90	0.53
3:D:168:LYS:O	3:D:169:ASP:CB	2.45	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:77:MET:CE	3:F:103:LEU:HD21	2.36	0.52
3:F:192:THR:HG22	3:F:207:SER:HB3	1.90	0.52
1:B:98:ARG:HE	1:B:98:ARG:CA	2.21	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:197:HIS:CE1	3:D:199:THR:HG23	2.44	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
3:D:104:GLU:HB3	3:D:165:GLN:OE1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:360:MET:HE3	1:B:398:LEU:HD23	1.92	0.52
3:F:7:SER:CB	3:F:8:PRO:CD	2.86	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: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
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: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
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
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
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
3:F:60:ARG:HH21	3:F:81:ASP:CG	2.14	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
1:A:83:PHE:CD1	1:A:83:PHE:C	2.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:13:ALA:C	3:D:106:LEU:HG	2.32	0.50
1:A:109:ILE:HG23	1:A:204:MET:HE2	1.92	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:B:68:LEU:HD22	1:B:78:LEU:HD23	1.94	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: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:F:19:VAL:HG21	3:F:77:MET:CE	2.42	0.49
3:F:73:THR:C	3:F:74:ILE:HG13	2.30	0.49
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.46	0.49
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:B:270:ASN:HA	1:B:273:VAL:HG12	1.95	0.49
3:D:6:GLN:HE21	3:D:98:GLY:C	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:92:PHE:CD1	1:B:92:PHE:C	2.86	0.49
1:B:191:ASN:OD1	1:B:230:ARG:NH1	2.42	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: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
3:D:166:ASP:OD1	3:D:166:ASP:C	2.51	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:31:TYR:HA	3:F:50:THR:OG1	2.13	0.48
3:F:34:TRP:CZ3	3:F:87:CYS:HB3	2.49	0.47
1:A:92:PHE:CD1	1:A:92:PHE:C	2.87	0.47
2:C:185:LEU:C	2:C:185:LEU:HD12	2.35	0.47
1:A:219:PHE:HB3	1:B:430:LEU:HD11	1.96	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
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:A:109:ILE:HG23	1:A:204:MET:HE1	1.95	0.47
3:D:124:LEU:C	3:D:126:SER:H	2.16	0.47
3:F:11:MET:HE2	3:F:19:VAL:HG13	1.97	0.47
1:A:249:LEU:C	1:A:251:THR:H	2.17	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
1:B:249:LEU:C	1:B:251:THR:H	2.17	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
3:F:73:THR:C	3:F:74:ILE:CG1	2.82	0.47
2:C:84:SER:O	2:C:85:LYS:C	2.53	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
2:E:107:TYR:CD1	2:E:107:TYR:C	2.89	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
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
1:B:88:VAL:HA	1:B:91:MET:HE2	1.96	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
3:F:65:GLY:O	3:F:66:SER:HB3	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:330:MET:HA	1:B:330:MET:HE2	1.97	0.45
3:D:36:GLN:HA	3:D:84:THR:O	2.16	0.45
1:B:31:THR:HB	1:B:36:LEU:HD21	1.98	0.45
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:33:LEU:C	1:A:33:LEU:HD23	2.37	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: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:D:98:GLY:C	3:D:100:GLY:H	2.19	0.45
3:F:34:TRP:CE3	3:F:72:LEU:HD13	2.51	0.45
3:F:106:LEU:HD23	3:F:139:TYR:HH	1.82	0.45
1:A:332:MET:O	1:A:336:ILE:HG13	2.17	0.45
2:E:6:GLU:CD	2:E:114:GLY:H	2.19	0.45
3:F:49:ASP:O	3:F:50:THR:HB	2.15	0.45
1:A:88:VAL:HA	1:A:91:MET:HE2	1.98	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: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
3:F:109:ASP:HB3	3:F:199:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:457:GLU:C	1:A:459:GLU:H	2.19	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
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
1:B:422:ILE:HG23	1:B:423:LEU:N	2.33	0.44
1:A:78:LEU:HD21	1:A:307:PHE:CZ	2.53	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:405:PRO:HG2	1:B:406:LEU:H	1.82	0.44
2:C:135:GLY:C	2:C:137:ALA:H	2.21	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:444:LEU:HD22	1:B:444:LEU:O	2.18	0.44
2:C:112:GLY:O	3:D:42:SER:OG	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:GLY:C	1:A:137:GLY:N	2.70	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: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: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: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: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:HG13	2:E:189:VAL:O	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: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
2:C:107:TYR:CD1	2:C:107:TYR:C	2.92	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:O	1:A:283:VAL:C	2.57	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: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:HG13	2:C:189:VAL:O	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
1:B:109:ILE:HG23	1:B:204:MET:HE2	2.01	0.42
1:B:186:LEU:O	1:B:187:ALA:C	2.57	0.42
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:B:421:LEU:O	1:B:425:MET:HG3	2.19	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
2:E:84:SER:O	2:E:85:LYS:C	2.57	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
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:78:LEU:C	1:B:78:LEU:HD22	2.39	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
2:E:30:SER:C	2:E:32:TYR:H	2.22	0.42
1:B:99:LYS:HB3	1:B:100:TYR:CD1	2.55	0.42
1:B:422:ILE:HA	1:B:425:MET:CE	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:457:GLU:OE1	1:B:19:ARG:HG3	2.21	0.41
1:B:135:GLY:C	1:B:137:GLY:N	2.73	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
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: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: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: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
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.80	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:33:LEU:HD23	1:A:33:LEU:O	2.20	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
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.50	0.41
1:B:33:LEU:HD23	1:B:33:LEU:C	2.40	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:165:ILE:O	1:A:165:ILE:CG2	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ARG:HH11	1:B:126:ARG:HG2	1.85	0.41
2:C:30:SER:C	2:C:32:TYR:H	2.24	0.41
2:C:174:PHE:HA	2:C:175:PRO:HD2	1.95	0.41
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: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: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
3:F:19:VAL:HG21	3:F:77:MET:HE3	2.03	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: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:78:LEU:C	1:A:78:LEU:HD22	2.42	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
1:A:74:ASN:HD22	1:A:74:ASN:C	2.25	0.40
3:F:124:LEU:C	3:F:126:SER:N	2.75	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%)	6	23
1	B	439/473 (93%)	382 (87%)	48 (11%)	9 (2%)	7	26
2	C	219/221 (99%)	197 (90%)	18 (8%)	4 (2%)	8	29
2	E	219/221 (99%)	195 (89%)	21 (10%)	3 (1%)	11	36
3	D	209/211 (99%)	173 (83%)	26 (12%)	10 (5%)	2	8
3	F	209/211 (99%)	184 (88%)	20 (10%)	5 (2%)	6	22
All	All	1737/1810 (96%)	1513 (87%)	183 (10%)	41 (2%)	6	22

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%)	299 (89%)	36 (11%)	6	20
1	B	332/358 (93%)	297 (90%)	35 (10%)	7	21
2	C	181/181 (100%)	167 (92%)	14 (8%)	13	35
2	E	181/181 (100%)	166 (92%)	15 (8%)	11	32
3	D	185/185 (100%)	169 (91%)	16 (9%)	10	30
3	F	185/185 (100%)	171 (92%)	14 (8%)	13	36
All	All	1399/1448 (97%)	1269 (91%)	130 (9%)	9	27

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

Mol	Chain	Res	Type
1	A	19	ARG
1	A	31	THR
1	A	74	ASN
1	A	78	LEU

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Mol	Chain	Res	Type
1	A	81	VAL
1	A	98	ARG
1	A	103	GLU
1	A	138	THR
1	A	145	LEU
1	A	148	GLU
1	A	168	LEU
1	A	177	LEU
1	A	180	THR
1	A	200	ILE
1	A	202	GLU
1	A	207	GLN
1	A	212	LEU
1	A	219	PHE
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	381	GLN
1	A	397	LEU
1	A	402	ILE
1	A	420	GLN
1	A	430	LEU
1	A	435	LEU
1	A	444	LEU
1	A	446	SER
1	A	451	ARG
1	A	453	LEU
1	B	19	ARG
1	B	31	THR
1	B	74	ASN
1	B	78	LEU
1	B	81	VAL
1	B	96	LEU
1	B	98	ARG
1	B	103	GLU
1	B	138	THR
1	B	145	LEU

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Mol	Chain	Res	Type
1	B	148	GLU
1	B	168	LEU
1	B	177	LEU
1	B	180	THR
1	B	200	ILE
1	B	207	GLN
1	B	212	LEU
1	B	219	PHE
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	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	430	LEU
1	B	435	LEU
1	B	444	LEU
1	B	446	SER
1	B	451	ARG
1	B	453	LEU
2	C	2	VAL
2	C	18	LEU
2	C	21	SER
2	C	55	SER
2	C	65	LYS
2	C	72	ARG
2	C	115	THR
2	C	123	LYS
2	C	157	PRO
2	C	167	LEU
2	C	193	SER
2	C	200	THR
2	C	204	ASN
2	C	214	VAL
3	D	1	ASP
3	D	36	GLN
3	D	41	THR

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Mol	Chain	Res	Type
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	135	LEU
3	D	141	LYS
3	D	142	ASP
3	D	166	ASP
3	D	176	SER
3	D	190	SER
3	D	201	THR
2	E	2	VAL
2	E	21	SER
2	E	55	SER
2	E	65	LYS
2	E	72	ARG
2	E	107	TYR
2	E	115	THR
2	E	123	LYS
2	E	157	PRO
2	E	167	LEU
2	E	179	GLN
2	E	193	SER
2	E	200	THR
2	E	204	ASN
2	E	214	VAL
3	F	1	ASP
3	F	41	THR
3	F	75	ASN
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	190	SER
3	F	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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	284	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	284	HIS
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	437	GLN
3	D	6	GLN
3	D	136	ASN
3	F	6	GLN
3	F	36	GLN
3	F	136	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 monosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	0.77	42 (9%) 8 6	61, 93, 155, 219	0
1	B	441/473 (93%)	0.84	52 (11%) 4 3	58, 96, 168, 244	0
2	C	221/221 (100%)	0.45	16 (7%) 15 11	49, 83, 136, 237	0
2	E	221/221 (100%)	0.54	19 (8%) 10 8	55, 86, 154, 215	0
3	D	211/211 (100%)	0.97	43 (20%) 1 0	63, 101, 148, 189	0
3	F	211/211 (100%)	0.97	33 (15%) 2 1	54, 77, 136, 186	0
All	All	1749/1810 (96%)	0.77	205 (11%) 4 3	49, 91, 154, 244	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	208	PHE	10.5
1	A	72	ALA	10.4
1	B	73	ASP	8.8
3	F	211	ALA	8.6
2	E	178	LEU	8.4
1	B	72	ALA	8.1
1	B	70	HIS	7.8
1	B	353	PRO	7.5
1	B	307	PHE	6.6
1	B	71	THR	6.0
1	B	104	ALA	5.4
1	A	73	ASP	5.3
1	B	143	MET	5.1
1	B	74	ASN	5.1
1	A	235	GLU	5.1
1	A	71	THR	4.8
3	D	170	SER	4.8
1	B	177	LEU	4.6
3	F	209	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	234	HIS	4.6
1	B	168	LEU	4.5
2	C	139	ALA	4.3
3	D	172	TYR	4.3
3	F	124	LEU	4.3
1	B	288	ILE	4.3
3	F	2	ILE	4.3
3	D	23	CYS	4.2
3	F	153	GLU	4.1
1	A	78	LEU	4.1
3	D	82	ALA	4.1
1	B	75	TYR	4.1
3	D	39	SER	4.1
1	A	288	ILE	4.1
3	F	152	SER	4.1
3	D	138	PHE	4.0
2	E	15	GLY	4.0
1	B	304	LEU	4.0
3	D	22	THR	3.9
1	B	234	HIS	3.9
1	A	75	TYR	3.8
3	D	110	ALA	3.8
3	D	20	THR	3.7
1	A	69	VAL	3.7
3	D	101	THR	3.7
3	D	197	HIS	3.6
1	B	167	ARG	3.6
1	A	283	VAL	3.6
1	B	138	THR	3.6
2	E	13	GLN	3.6
1	A	291	TRP	3.6
1	A	208	PHE	3.5
2	C	140	ALA	3.5
2	E	182	LEU	3.5
1	B	67	ALA	3.5
2	E	86	VAL	3.5
1	B	354	GLY	3.4
1	A	76	PRO	3.4
1	B	68	LEU	3.4
1	B	69	VAL	3.4
3	F	190	SER	3.4
3	F	189	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	290	LYS	3.3
3	F	69	SER	3.3
1	A	67	ALA	3.3
1	A	74	ASN	3.3
3	D	171	THR	3.3
1	A	209	ARG	3.3
1	A	144	VAL	3.3
3	F	147	TRP	3.2
3	D	140	PRO	3.2
2	C	65	LYS	3.2
2	C	199	GLU	3.2
3	F	149	ILE	3.2
1	A	68	LEU	3.1
3	D	165	GLN	3.1
1	A	207	GLN	3.0
1	B	291	TRP	3.0
1	B	456	GLN	3.0
3	F	89	GLN	3.0
1	A	65	MET	3.0
2	E	179	GLN	2.9
1	B	119	GLN	2.9
3	D	109	ASP	2.9
1	A	99	LYS	2.9
2	C	29	TYR	2.8
1	B	145	LEU	2.8
1	A	290	LYS	2.8
3	D	105	ILE	2.8
1	B	235	GLU	2.8
3	D	103	LEU	2.8
2	E	65	LYS	2.8
1	B	18	ARG	2.8
3	D	38	LYS	2.7
1	B	178	LEU	2.7
1	A	168	LEU	2.7
1	B	95	PHE	2.7
1	B	139	LEU	2.7
1	B	347	CYS	2.7
1	A	60	LEU	2.7
1	B	172	GLU	2.7
3	F	72	LEU	2.7
3	D	146	LYS	2.7
1	A	299	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	143	MET	2.6
2	E	183	TYR	2.6
3	F	192	THR	2.6
3	F	148	LYS	2.6
1	A	139	LEU	2.6
1	B	141	GLY	2.6
1	B	287	ASN	2.6
2	C	176	ALA	2.6
2	E	59	ASN	2.6
1	A	21	LEU	2.6
3	F	4	LEU	2.6
2	E	105	TYR	2.6
1	A	70	HIS	2.5
3	D	36	GLN	2.5
1	B	84	LEU	2.5
3	F	127	GLY	2.5
1	A	104	ALA	2.5
3	D	77	MET	2.5
3	F	29	VAL	2.5
3	F	145	VAL	2.5
3	F	180	LEU	2.5
1	A	77	LEU	2.5
3	D	7	SER	2.5
3	D	71	SER	2.5
1	B	332	MET	2.5
1	A	140	GLY	2.4
3	D	72	LEU	2.4
3	F	191	TYR	2.4
3	F	158	VAL	2.4
3	D	68	THR	2.4
3	D	196	THR	2.4
3	D	69	SER	2.4
1	B	409	ILE	2.4
1	B	162	VAL	2.4
2	C	175	PRO	2.4
2	E	177	VAL	2.4
2	C	189	VAL	2.4
3	F	208	PHE	2.3
2	C	188	SER	2.3
1	B	233	ASN	2.3
1	A	233	ASN	2.3
2	C	214	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	29	TYR	2.3
3	F	31	TYR	2.3
1	B	195	ALA	2.3
3	D	79	ALA	2.3
3	F	205	VAL	2.3
1	A	53	PHE	2.3
3	D	195	ALA	2.3
1	A	66	GLY	2.3
3	D	64	SER	2.3
3	F	184	GLU	2.3
2	E	221	ARG	2.3
1	B	166	PHE	2.3
1	A	145	LEU	2.2
1	B	96	LEU	2.2
2	E	136	SER	2.2
3	F	146	LYS	2.2
1	B	438	PHE	2.2
2	C	172	HIS	2.2
3	D	202	SER	2.2
2	E	139	ALA	2.2
1	B	77	LEU	2.2
3	D	34	TRP	2.2
1	A	141	GLY	2.2
1	A	142	GLY	2.2
1	B	289	THR	2.2
2	E	137	ALA	2.2
3	D	21	MET	2.2
3	D	112	PRO	2.2
1	B	407	THR	2.2
2	E	48	ILE	2.1
2	C	221	ARG	2.1
1	B	199	PHE	2.1
1	A	201	ILE	2.1
2	C	89	GLU	2.1
1	B	377	GLU	2.1
3	D	106	LEU	2.1
2	C	20	LEU	2.1
3	D	124	LEU	2.1
3	F	135	LEU	2.1
2	E	122	ALA	2.1
3	F	204	ILE	2.1
3	D	74	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	19	VAL	2.1
1	A	86	SER	2.1
3	D	139	TYR	2.1
3	F	73	THR	2.1
2	C	196	TRP	2.1
2	C	87	ARG	2.0
3	D	102	LYS	2.0
3	D	136	ASN	2.0
3	F	183	ASP	2.0
3	F	67	GLY	2.0
1	A	460	GLN	2.0
3	D	154	ARG	2.0
3	D	148	LYS	2.0
1	A	210	TYR	2.0
1	B	97	VAL	2.0
1	B	127	VAL	2.0
2	E	123	LYS	2.0
3	D	178	LEU	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 monosaccharides 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	0.91	0.68	100,100,100,100	0
4	BR	B	474	1/1	0.93	0.16	100,100,100,100	0
4	BR	B	475	1/1	0.93	0.29	100,100,100,100	0
4	BR	A	474	1/1	0.97	0.18	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.