



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:21 pm BST

PDB ID : 2FEE
Title : Structure of the Cl⁻/H⁺ exchanger CLC-ec1 from E.Coli in NaBr
Authors : Accardi, A.; Walden, M.P.; Nguitragool, W.; Jayaram, H.; Williams, C.;
Miller, C.
Deposited on : 2005-12-15
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

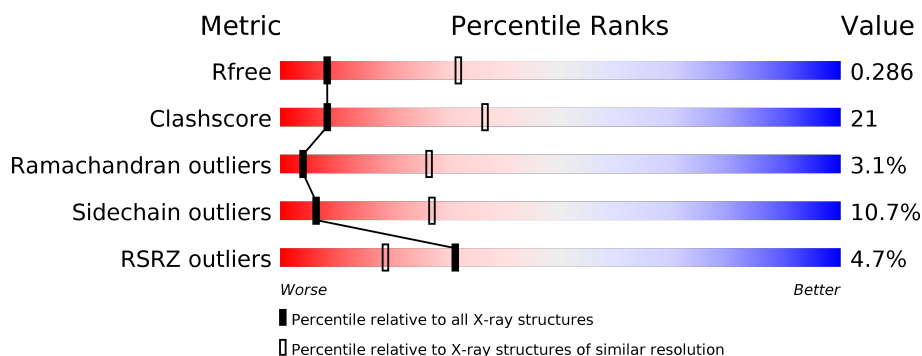
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	465	<div> <div>2%</div> <div>56% 34% 5% 5%</div> </div>
1	B	465	<div> <div>5%</div> <div>55% 32% 7% 5%</div> </div>
2	I	222	<div> <div>2%</div> <div>62% 35% .</div> </div>
2	J	222	<div> <div>3%</div> <div>53% 41% 5%</div> </div>
3	L	211	<div> <div>12%</div> <div>57% 38% .</div> </div>
3	O	211	<div> <div>6%</div> <div>45% 49% 6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13223 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	560	563	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	553	557	20			

- Molecule 2 is a protein called Fab fragment, heavy chain.

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

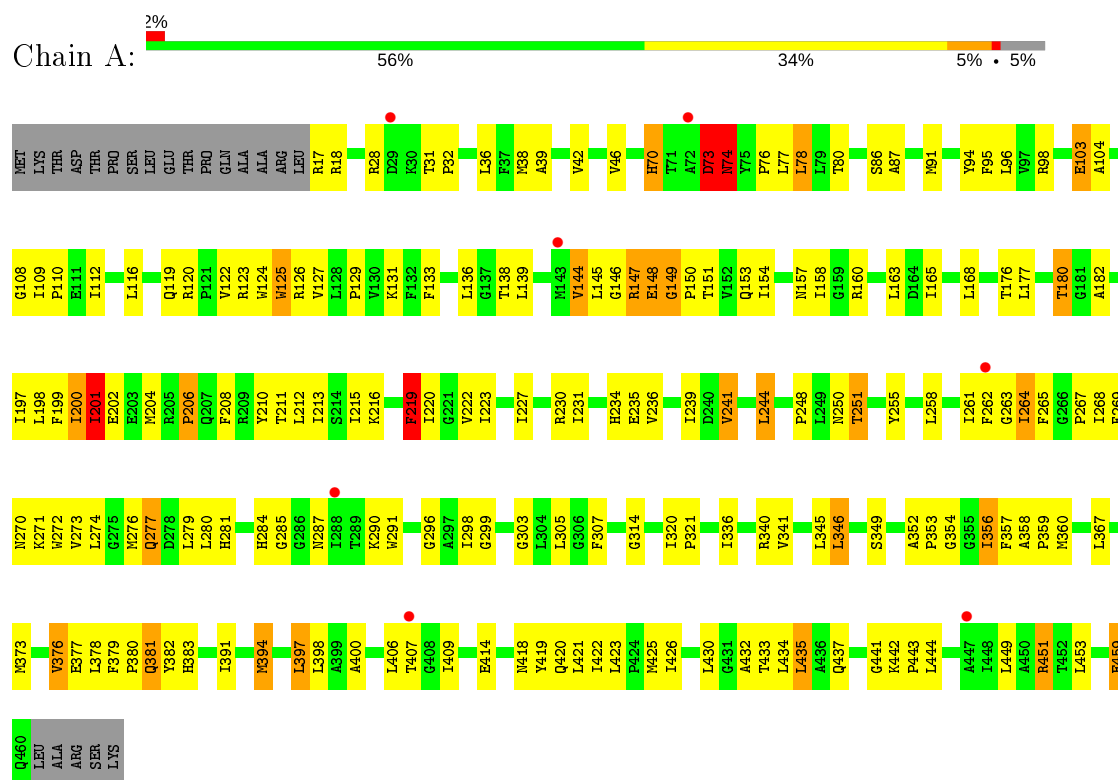
- Molecule 3 is a protein called Fab fragment, light chain.

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

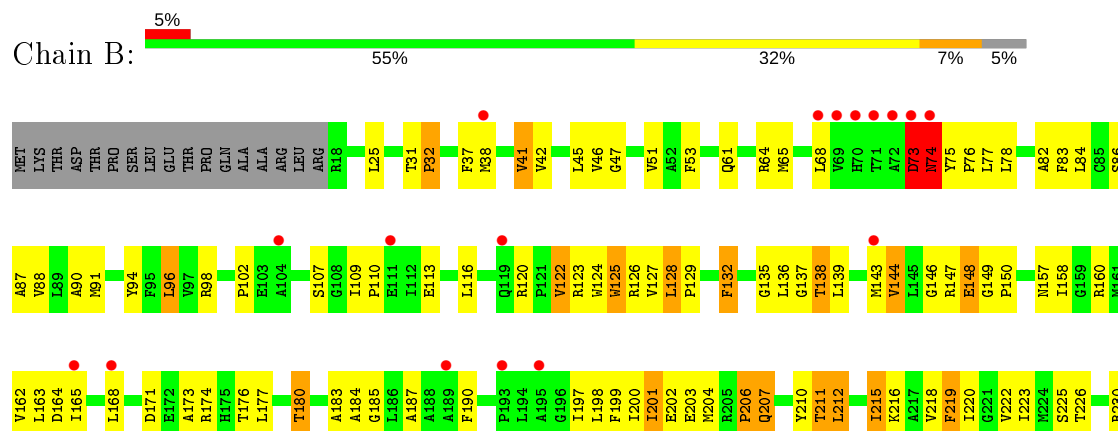
3 Residue-property plots

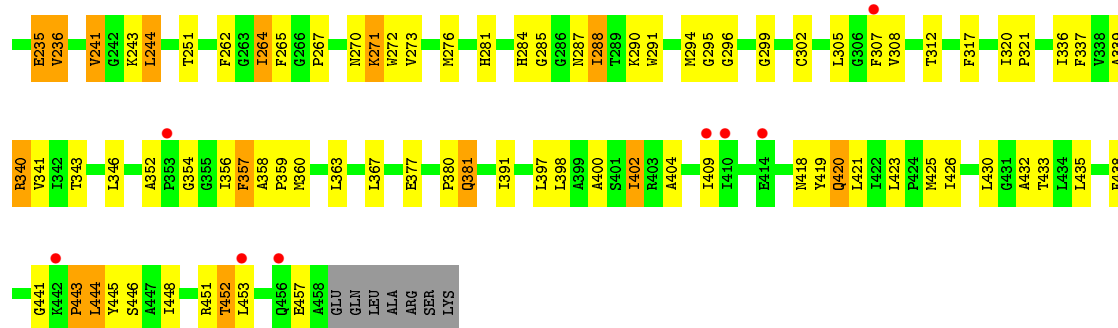
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

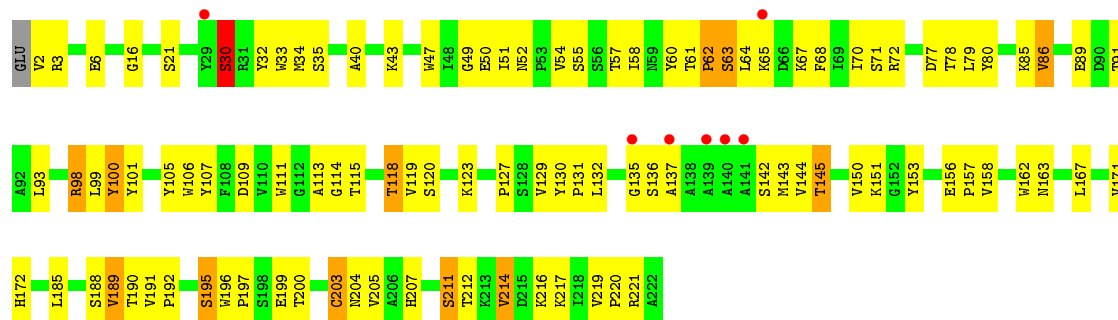


- Molecule 1: H(+)/Cl(-) exchange transporter clcA

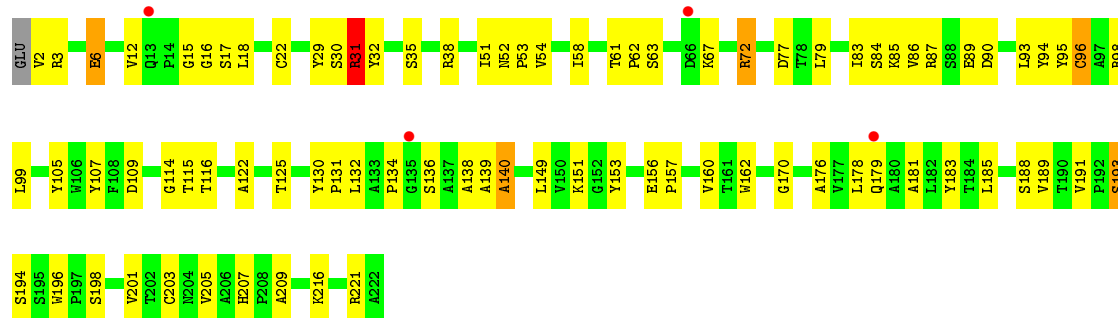




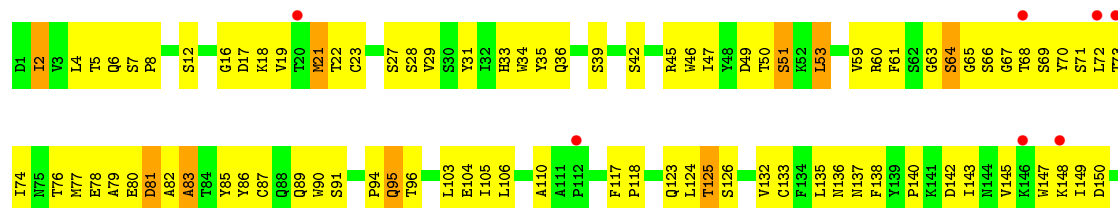
• Molecule 2: Fab fragment, heavy chain

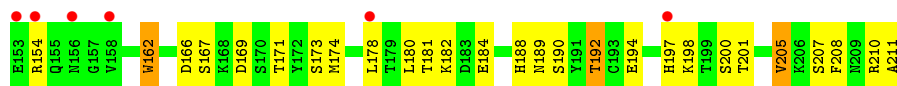


• Molecule 2: Fab fragment, heavy chain

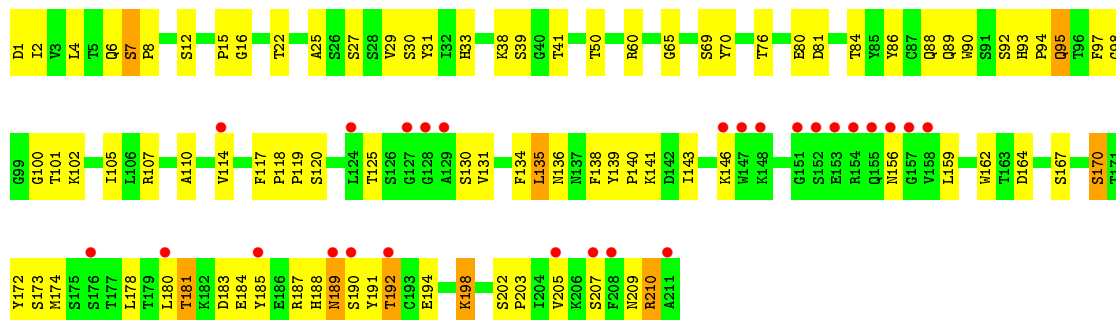


• Molecule 3: Fab fragment, light chain





- 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	230.82Å 97.68Å 170.20Å 90.00° 131.11° 90.00°	Depositor
Resolution (Å)	128.04 – 3.20 44.36 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (128.04-3.20) 97.8 (44.36-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.251 , 0.293 0.248 , 0.286	Depositor DCC
R_{free} test set	2341 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	109.4	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 77.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 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)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.57	0/3405	0.67	1/4621 (0.0%)
1	B	0.69	2/3376 (0.1%)	0.70	3/4583 (0.1%)
2	I	0.60	0/1721	0.72	0/2355
2	J	0.70	1/1721 (0.1%)	0.75	0/2355
3	L	0.60	0/1660	0.72	0/2257
3	O	0.56	0/1660	0.73	1/2257 (0.0%)
All	All	0.62	3/13543 (0.0%)	0.71	5/18428 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	LYS	CD-CE	13.54	1.85	1.51
2	J	195	SER	CB-OG	12.51	1.58	1.42
1	B	271	LYS	CE-NZ	9.61	1.73	1.49

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	LEU	CA-CB-CG	6.14	129.42	115.30
1	A	398	LEU	CA-CB-CG	5.31	127.50	115.30
1	B	177	LEU	CA-CB-CG	5.12	127.07	115.30
3	O	53	LEU	CA-CB-CG	5.10	127.04	115.30
1	B	45	LEU	CA-CB-CG	5.08	126.97	115.30

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	3333	0	3484	160	0
1	B	3304	0	3457	158	0
2	I	1672	0	1654	49	0
2	J	1672	0	1654	68	0
3	L	1621	0	1546	72	0
3	O	1621	0	1546	91	0
All	All	13223	0	13341	556	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 21.

All (556) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LYS:CD	1:B:271:LYS:CE	1.85	1.54
1:B:271:LYS:NZ	1:B:271:LYS:CE	1.73	1.46
2:J:60:TYR:HE2	2:J:70:ILE:HG13	1.04	1.14
2:J:135:GLY:HA2	2:J:221:ARG:HD3	1.31	1.11
3:L:194:GLU:HG2	3:L:205:VAL:HG12	1.37	1.06
3:O:95:GLN:CD	3:O:95:GLN:H	1.59	1.05
1:A:381:GLN:N	1:A:381:GLN:HE21	1.53	1.05
1:A:381:GLN:NE2	1:A:381:GLN:H	1.54	1.04
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.20	1.03
2:J:60:TYR:CE2	2:J:70:ILE:HG13	1.94	1.01
1:B:381:GLN:HE21	1:B:381:GLN:H	1.08	1.01
3:L:7:SER:HB2	3:L:22:THR:HB	1.37	1.01
1:A:18:ARG:NH1	1:B:457:GLU:HB3	1.79	0.98
3:L:7:SER:HB3	3:L:8:PRO:HD3	1.43	0.97
1:A:356:ILE:HG23	1:A:360:MET:HE2	1.46	0.94
1:A:356:ILE:HG23	1:A:360:MET:CE	1.98	0.93
1:A:409:ILE:HD11	1:A:426:ILE:HA	1.51	0.91
3:O:95:GLN:CD	3:O:95:GLN:N	2.23	0.89
2:I:30:SER:O	2:I:31:ARG:HB2	1.76	0.86
3:L:7:SER:HB3	3:L:8:PRO:CD	2.05	0.85
3:L:16:GLY:HA2	3:L:76:THR:HG23	1.58	0.85
3:L:6:GLN:HE21	3:L:98:GLY:HA3	1.40	0.84
1:B:358:ALA:HB3	1:B:359:PRO:HD3	1.59	0.84
1:B:150:PRO:HD3	1:B:354:GLY:HA2	1.57	0.83
3:L:7:SER:CB	3:L:8:PRO:HD3	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:HA	1:A:204:MET:HB2	1.59	0.82
1:B:38:MET:HG3	1:B:168:LEU:HD11	1.60	0.82
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.62	0.81
3:O:6:GLN:HE22	3:O:86:TYR:HA	1.43	0.80
1:B:381:GLN:N	1:B:381:GLN:HE21	1.78	0.80
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.64	0.80
1:A:150:PRO:HD3	1:A:354:GLY:HA2	1.63	0.80
1:B:381:GLN:NE2	1:B:381:GLN:H	1.79	0.80
1:A:86:SER:HB3	1:A:299:GLY:O	1.82	0.79
3:O:31:TYR:HB3	3:O:49:ASP:HA	1.64	0.79
1:A:360:MET:HG2	1:A:397:LEU:HD12	1.64	0.79
1:B:123:ARG:HE	1:B:126:ARG:HD2	1.47	0.79
3:O:95:GLN:N	3:O:95:GLN:OE1	2.15	0.79
2:J:52:ASN:ND2	2:J:57:THR:HB	1.98	0.79
1:B:86:SER:HB3	1:B:299:GLY:O	1.84	0.78
2:J:189:VAL:HG13	2:J:189:VAL:O	1.83	0.77
1:B:271:LYS:CE	1:B:271:LYS:CG	2.62	0.77
1:A:380:PRO:HD2	1:A:381:GLN:HE22	1.51	0.75
1:A:148:GLU:OE1	1:A:357:PHE:CB	2.34	0.75
3:O:194:GLU:HG2	3:O:205:VAL:HG12	1.69	0.75
3:O:189:ASN:HD21	3:O:211:ALA:H	1.31	0.74
2:J:100:TYR:HD2	2:J:101:TYR:H	1.35	0.74
1:A:227:ILE:O	1:A:231:ILE:HG12	1.87	0.74
3:O:22:THR:HG22	3:O:23:CYS:N	2.03	0.74
1:A:146:GLY:HA3	1:A:148:GLU:OE2	1.88	0.74
1:A:123:ARG:HE	1:A:126:ARG:HD2	1.52	0.73
2:I:51:ILE:HG13	2:I:58:ILE:HG12	1.69	0.73
3:L:95:GLN:H	3:L:95:GLN:CD	1.91	0.73
3:O:36:GLN:HB2	3:O:85:TYR:HE2	1.53	0.73
1:A:148:GLU:OE1	1:A:357:PHE:HB3	1.88	0.72
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.72	0.72
3:O:162:TRP:H	3:O:162:TRP:HE3	1.36	0.71
2:I:32:TYR:O	2:I:72:ARG:NH2	2.22	0.71
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.06	0.71
2:I:31:ARG:HH11	2:I:31:ARG:HA	1.54	0.71
1:B:337:PHE:O	1:B:341:VAL:HG23	1.91	0.71
1:B:148:GLU:CD	1:B:148:GLU:H	1.93	0.70
1:B:98:ARG:HD2	1:B:291:TRP:CD2	2.25	0.70
1:A:379:PHE:HB3	1:A:382:TYR:CD1	2.26	0.70
2:I:98:ARG:NH1	2:I:109:ASP:OD2	2.25	0.70
2:J:51:ILE:HG13	2:J:58:ILE:HG12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:160:VAL:HG22	2:I:205:VAL:HG22	1.75	0.69
1:B:47:GLY:O	1:B:51:VAL:HG23	1.93	0.69
1:A:38:MET:HB3	1:A:177:LEU:HD11	1.75	0.68
1:B:138:THR:HG22	1:B:143:MET:SD	2.33	0.68
2:I:16:GLY:O	2:I:86:VAL:HG23	1.93	0.68
1:B:200:ILE:HG22	1:B:201:ILE:HG23	1.73	0.68
3:O:12:SER:HB3	3:O:106:LEU:HB2	1.76	0.68
1:A:28:ARG:NH2	1:B:203:GLU:OE1	2.25	0.68
3:O:66:SER:HA	3:O:70:TYR:CZ	2.29	0.67
1:A:274:LEU:HA	1:A:277:GLN:HE21	1.59	0.67
2:J:127:PRO:HB3	2:J:153:TYR:HB3	1.75	0.67
2:J:130:TYR:CE2	3:O:123:GLN:HG3	2.30	0.67
3:L:90:TRP:CZ2	3:L:95:GLN:NE2	2.63	0.67
2:I:51:ILE:HD13	2:I:72:ARG:HG2	1.76	0.67
3:O:124:LEU:C	3:O:126:SER:H	1.97	0.67
1:A:78:LEU:HD21	1:A:307:PHE:CZ	2.31	0.66
1:B:241:VAL:HG11	1:B:391:ILE:HD11	1.76	0.66
3:O:124:LEU:HD22	3:O:182:LYS:HG3	1.76	0.66
2:J:33:TRP:HB2	2:J:99:LEU:HB2	1.78	0.66
1:A:358:ALA:HB3	1:A:359:PRO:HD3	1.77	0.66
3:L:4:LEU:HD23	3:L:25:ALA:HB2	1.78	0.66
1:A:409:ILE:CD1	1:A:426:ILE:HA	2.24	0.66
3:O:189:ASN:ND2	3:O:211:ALA:H	1.93	0.65
1:B:109:ILE:N	1:B:110:PRO:HD2	2.11	0.65
1:B:150:PRO:CD	1:B:354:GLY:HA2	2.27	0.65
3:L:90:TRP:CG	3:L:95:GLN:HB3	2.31	0.65
1:B:144:VAL:HG12	1:B:144:VAL:O	1.95	0.65
2:J:40:ALA:O	2:J:43:LYS:HB2	1.97	0.65
2:I:179:GLN:OE1	3:L:159:LEU:HD11	1.96	0.64
1:A:201:ILE:HG13	1:A:201:ILE:O	1.96	0.64
3:L:119:PRO:HD3	3:L:131:VAL:HG22	1.79	0.64
2:I:30:SER:O	2:I:31:ARG:CB	2.46	0.64
2:J:132:LEU:O	3:O:117:PHE:CE2	2.51	0.64
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.33	0.63
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.32	0.63
3:L:7:SER:HB2	3:L:22:THR:CB	2.22	0.63
1:A:223:ILE:HD12	1:B:430:LEU:HD22	1.80	0.63
2:I:132:LEU:HD11	2:I:149:LEU:HB2	1.78	0.63
2:J:91:THR:HG23	2:J:118:THR:HA	1.80	0.63
3:L:95:GLN:N	3:L:95:GLN:CD	2.51	0.63
1:B:98:ARG:HB3	1:B:288:ILE:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.33	0.63
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.34	0.63
1:B:272:TRP:O	1:B:276:MET:HB2	1.98	0.63
3:O:95:GLN:H	3:O:95:GLN:NE2	1.96	0.62
3:O:192:THR:HB	3:O:207:SER:HB3	1.81	0.62
2:I:156:GLU:OE1	2:I:157:PRO:HA	2.00	0.62
2:J:195:SER:O	2:J:199:GLU:HB2	1.98	0.62
2:J:129:VAL:HG21	2:J:214:VAL:CG1	2.29	0.62
1:B:200:ILE:HA	1:B:204:MET:HB2	1.81	0.62
2:I:67:LYS:NZ	2:I:90:ASP:OD2	2.28	0.62
3:O:125:THR:O	3:O:125:THR:HG22	1.99	0.62
1:B:190:PHE:HE2	1:B:317:PHE:HZ	1.46	0.62
1:B:146:GLY:HA3	1:B:148:GLU:OE2	2.00	0.62
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.35	0.62
3:O:22:THR:HG22	3:O:23:CYS:H	1.64	0.62
3:O:60:ARG:HD2	3:O:76:THR:O	2.00	0.62
1:A:74:ASN:HD22	1:A:74:ASN:C	2.02	0.61
1:A:262:PHE:CE2	1:A:367:LEU:HD23	2.35	0.61
2:J:171:VAL:HG22	2:J:189:VAL:HG23	1.81	0.61
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.81	0.61
1:A:269:PHE:HE1	1:A:341:VAL:HG13	1.66	0.60
1:B:90:ALA:HB3	1:B:296:GLY:HA2	1.83	0.60
2:J:197:PRO:HB3	2:J:220:PRO:HG3	1.83	0.60
3:L:31:TYR:HA	3:L:50:THR:OG1	2.00	0.60
2:J:51:ILE:HD13	2:J:72:ARG:HG2	1.83	0.60
1:B:202:GLU:OE1	1:B:404:ALA:HB1	2.02	0.60
1:B:243:LYS:HG2	2:I:31:ARG:HH21	1.65	0.60
1:A:248:PRO:O	1:A:251:THR:HB	2.01	0.59
1:A:423:LEU:HD13	1:B:230:ARG:NH2	2.18	0.59
1:A:38:MET:HG3	1:A:168:LEU:HD11	1.84	0.59
2:I:130:TYR:HD2	2:I:149:LEU:HD23	1.67	0.59
1:B:143:MET:HA	1:B:302:CYS:SG	2.42	0.59
2:I:134:PRO:O	2:I:221:ARG:HG3	2.03	0.59
2:J:61:THR:HG23	2:J:63:SER:HB2	1.83	0.59
3:L:136:ASN:HD22	3:L:173:SER:HB3	1.67	0.59
1:B:176:THR:O	1:B:180:THR:HG23	2.02	0.59
1:A:219:PHE:HB3	1:B:430:LEU:HD13	1.85	0.59
3:O:19:VAL:HG11	3:O:103:LEU:HD11	1.85	0.59
1:A:200:ILE:HG22	1:A:201:ILE:HG22	1.85	0.58
2:I:221:ARG:HH22	3:L:120:SER:HA	1.67	0.58
1:A:144:VAL:O	1:A:144:VAL:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:52:ASN:HB2	2:I:53:PRO:CD	2.33	0.58
3:L:1:ASP:HB3	3:L:94:PRO:HD2	1.85	0.58
1:A:154:ILE:O	1:A:158:ILE:HG12	2.04	0.58
1:A:287:ASN:ND2	1:A:290:LYS:HG3	2.17	0.58
3:O:194:GLU:HG2	3:O:205:VAL:CG1	2.32	0.58
1:B:98:ARG:HD2	1:B:291:TRP:CE3	2.39	0.58
3:O:148:LYS:HB2	3:O:192:THR:OG1	2.03	0.58
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.69	0.58
2:I:162:TRP:CZ3	2:I:203:CYS:HB3	2.38	0.58
3:L:189:ASN:HA	3:L:210:ARG:HD3	1.86	0.58
3:O:12:SER:HA	3:O:104:GLU:O	2.04	0.58
1:A:198:LEU:HD12	1:A:406:LEU:HG	1.84	0.57
3:O:19:VAL:HB	3:O:74:ILE:HD12	1.87	0.57
1:A:74:ASN:ND2	1:A:76:PRO:HD2	2.19	0.57
2:I:107:TYR:HB3	3:L:33:HIS:CD2	2.40	0.57
1:A:459:GLU:O	1:A:459:GLU:HG3	2.05	0.57
1:A:451:ARG:HB3	1:A:451:ARG:HH11	1.70	0.57
2:J:143:MET:HB3	2:J:190:THR:HG22	1.87	0.57
1:B:201:ILE:HD13	1:B:215:ILE:HD11	1.85	0.57
1:B:305:LEU:HD23	1:B:308:VAL:HG23	1.87	0.57
1:A:270:ASN:HA	1:A:273:VAL:CG1	2.35	0.56
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.87	0.56
2:I:6:GLU:HA	2:I:22:CYS:HA	1.86	0.56
3:O:149:ILE:HD12	3:O:154:ARG:HH11	1.69	0.56
1:A:274:LEU:HA	1:A:277:GLN:NE2	2.20	0.56
1:B:187:ALA:CB	1:B:222:VAL:HG13	2.36	0.56
3:O:162:TRP:N	3:O:162:TRP:CE3	2.73	0.56
2:J:30:SER:C	2:J:32:TYR:H	2.09	0.56
1:B:264:ILE:O	1:B:267:PRO:HD2	2.06	0.56
3:O:47:ILE:HD12	3:O:72:LEU:HG	1.88	0.56
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.88	0.56
2:J:34:MET:HB3	2:J:79:LEU:HD22	1.88	0.56
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.37	0.55
1:A:235:GLU:O	1:A:236:VAL:HG22	2.06	0.55
1:B:122:VAL:HB	1:B:160:ARG:HG2	1.89	0.55
2:J:129:VAL:HG21	2:J:214:VAL:HG12	1.88	0.55
2:J:86:VAL:HG12	2:J:119:VAL:HG21	1.89	0.55
2:J:129:VAL:CG2	2:J:214:VAL:HG11	2.37	0.55
2:J:135:GLY:CA	2:J:221:ARG:HD3	2.21	0.55
1:A:250:ASN:ND2	1:A:382:TYR:HE2	2.05	0.55
3:L:95:GLN:OE1	3:L:95:GLN:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:22:THR:CG2	3:O:23:CYS:N	2.70	0.55
3:L:141:LYS:HB3	3:L:172:TYR:CE1	2.42	0.55
1:A:380:PRO:HD2	1:A:381:GLN:NE2	2.22	0.55
1:B:109:ILE:N	1:B:110:PRO:CD	2.70	0.55
3:O:140:PRO:HD2	3:O:197:HIS:HE2	1.72	0.55
3:O:169:ASP:OD1	3:O:171:THR:OG1	2.24	0.55
1:B:158:ILE:O	1:B:162:VAL:HG13	2.07	0.54
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.89	0.54
2:J:158:VAL:HG12	2:J:207:HIS:HB2	1.88	0.54
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.22	0.54
3:O:6:GLN:NE2	3:O:86:TYR:HA	2.18	0.54
2:J:93:LEU:HD11	2:J:114:GLY:HA3	1.90	0.54
3:O:194:GLU:CG	3:O:205:VAL:HG12	2.35	0.54
1:A:216:LYS:O	1:A:220:ILE:HG13	2.08	0.54
1:A:258:LEU:HA	1:A:261:ILE:HD12	1.88	0.54
3:O:2:ILE:HD13	3:O:2:ILE:N	2.23	0.54
1:A:77:LEU:O	1:A:80:THR:HB	2.07	0.54
1:A:430:LEU:CD1	1:B:219:PHE:HB3	2.38	0.54
1:B:94:TYR:CZ	1:B:295:GLY:HA2	2.43	0.54
3:O:2:ILE:HB	3:O:89:GLN:HE21	1.72	0.53
1:A:200:ILE:HG22	1:A:201:ILE:CG2	2.38	0.53
1:A:86:SER:OG	1:A:303:GLY:HA3	2.08	0.53
1:A:148:GLU:CD	1:A:357:PHE:HB3	2.29	0.53
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.73	0.53
3:O:17:ASP:H	3:O:77:MET:H	1.57	0.53
1:B:402:ILE:HG13	1:B:402:ILE:O	2.07	0.53
1:A:148:GLU:OE1	1:A:357:PHE:HB2	2.06	0.53
3:O:50:THR:O	3:O:51:SER:HB3	2.09	0.53
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.91	0.53
1:B:68:LEU:HD21	1:B:82:ALA:HB2	1.91	0.53
1:A:78:LEU:HD21	1:A:307:PHE:CE2	2.45	0.53
1:A:42:VAL:O	1:A:46:VAL:HG23	2.07	0.53
1:B:409:ILE:HD11	1:B:426:ILE:HA	1.92	0.53
2:I:35:SER:HB2	2:I:99:LEU:HD11	1.90	0.52
3:L:110:ALA:O	3:L:138:PHE:HA	2.09	0.52
3:O:28:SER:HA	3:O:67:GLY:O	2.08	0.52
1:B:38:MET:O	1:B:42:VAL:HG23	2.09	0.52
2:J:135:GLY:C	2:J:137:ALA:H	2.12	0.52
2:J:63:SER:HG	2:J:68:PHE:HE1	1.57	0.52
3:L:194:GLU:CG	3:L:205:VAL:HG12	2.26	0.52
3:O:133:CYS:HB2	3:O:147:TRP:CH2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLY:O	1:A:112:ILE:HG12	2.10	0.52
1:A:87:ALA:O	1:A:91:MET:HG3	2.10	0.52
2:I:196:TRP:HD1	2:I:201:VAL:HG23	1.74	0.52
3:L:146:LYS:HB3	3:L:194:GLU:HB2	1.90	0.52
1:A:274:LEU:O	1:A:277:GLN:HB2	2.10	0.51
2:J:172:HIS:CD2	3:O:173:SER:HG	2.28	0.51
1:A:138:THR:HG21	1:A:353:PRO:HD2	1.92	0.51
1:B:187:ALA:HB2	1:B:222:VAL:HG13	1.91	0.51
2:I:17:SER:HB2	2:I:83:ILE:O	2.10	0.51
1:B:53:PHE:CD1	1:B:136:LEU:HD12	2.46	0.51
1:A:272:TRP:O	1:A:276:MET:HB2	2.10	0.51
3:L:60:ARG:NH2	3:L:81:ASP:OD2	2.43	0.51
1:A:430:LEU:HD13	1:B:219:PHE:HB3	1.92	0.51
1:B:116:LEU:HB3	1:B:206:PRO:HD3	1.93	0.51
1:B:421:LEU:O	1:B:425:MET:HG3	2.10	0.51
2:I:31:ARG:HH11	2:I:31:ARG:CA	2.21	0.51
2:J:156:GLU:OE1	2:J:157:PRO:HA	2.11	0.51
3:L:6:GLN:NE2	3:L:100:GLY:H	2.08	0.51
1:A:78:LEU:HD11	1:A:307:PHE:CZ	2.46	0.51
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.26	0.51
1:B:264:ILE:HG13	1:B:265:PHE:N	2.25	0.50
2:J:61:THR:OG1	2:J:62:PRO:HD2	2.11	0.50
1:A:263:GLY:HA3	1:A:435:LEU:HB2	1.92	0.50
3:O:118:PRO:HB3	3:O:208:PHE:CE1	2.47	0.50
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.77	0.50
1:B:91:MET:HG3	1:B:296:GLY:HA3	1.93	0.50
1:B:305:LEU:C	1:B:307:PHE:H	2.15	0.50
3:O:17:ASP:OD1	3:O:18:LYS:N	2.44	0.50
1:A:211:THR:HG22	1:A:212:LEU:H	1.76	0.50
1:A:423:LEU:HD11	1:B:226:THR:HG21	1.92	0.50
2:I:61:THR:O	2:I:63:SER:N	2.44	0.50
1:A:434:LEU:HD23	1:B:216:LYS:HD3	1.94	0.50
1:B:199:PHE:CE1	1:B:203:GLU:HG2	2.47	0.50
3:L:30:SER:HA	3:L:70:TYR:OH	2.11	0.50
1:A:116:LEU:HB3	1:A:206:PRO:HD3	1.94	0.49
1:A:74:ASN:ND2	1:A:77:LEU:H	2.10	0.49
1:B:180:THR:HG22	1:B:218:VAL:HG22	1.93	0.49
3:O:154:ARG:HH12	3:O:180:LEU:CD2	2.25	0.49
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.93	0.49
1:A:200:ILE:HG22	1:A:201:ILE:N	2.27	0.49
1:A:314:GLY:O	1:A:340:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASN:HA	1:B:273:VAL:HG12	1.93	0.49
3:L:6:GLN:HA	3:L:22:THR:O	2.13	0.49
1:A:109:ILE:N	1:A:110:PRO:CD	2.75	0.49
1:B:74:ASN:HB3	1:B:77:LEU:HD23	1.95	0.49
3:L:188:HIS:O	3:L:210:ARG:NE	2.46	0.49
3:O:36:GLN:HB2	3:O:85:TYR:CE2	2.40	0.49
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.93	0.49
3:O:31:TYR:HA	3:O:50:THR:OG1	2.13	0.49
1:B:271:LYS:NZ	1:B:271:LYS:CD	2.74	0.49
3:O:124:LEU:C	3:O:126:SER:N	2.65	0.49
3:O:22:THR:CG2	3:O:23:CYS:H	2.25	0.49
1:A:437:GLN:NE2	1:B:31:THR:H	2.10	0.48
2:J:98:ARG:HG2	2:J:109:ASP:HB3	1.93	0.48
1:A:356:ILE:CG2	1:A:360:MET:HE2	2.31	0.48
2:J:105:TYR:CD2	3:O:91:SER:HA	2.47	0.48
1:B:212:LEU:HD12	1:B:212:LEU:N	2.28	0.48
3:O:47:ILE:HG23	3:O:51:SER:HA	1.94	0.48
1:A:305:LEU:C	1:A:307:PHE:H	2.16	0.48
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.95	0.48
1:B:356:ILE:HG23	1:B:360:MET:CE	2.43	0.48
1:A:269:PHE:O	1:A:273:VAL:HG12	2.13	0.48
2:J:43:LYS:HB3	2:J:43:LYS:HZ2	1.79	0.48
3:O:34:TRP:HB2	3:O:47:ILE:HB	1.95	0.48
1:A:98:ARG:HA	1:A:98:ARG:NE	2.29	0.48
2:J:127:PRO:HD2	2:J:212:THR:HG21	1.94	0.48
2:J:129:VAL:HG21	2:J:214:VAL:HG11	1.94	0.48
3:L:90:TRP:CE2	3:L:95:GLN:NE2	2.81	0.48
3:O:7:SER:HB3	3:O:8:PRO:HD3	1.96	0.48
2:I:193:SER:O	2:I:196:TRP:O	2.32	0.48
3:L:93:HIS:CG	3:L:94:PRO:HA	2.48	0.48
1:B:128:LEU:HB2	1:B:129:PRO:HD3	1.96	0.48
1:A:377:GLU:HG3	1:A:378:LEU:N	2.29	0.48
2:J:192:PRO:HD2	2:J:195:SER:OG	2.14	0.48
3:L:114:VAL:HG13	3:L:135:LEU:HD23	1.96	0.48
3:L:2:ILE:HG23	3:L:27:SER:H	1.77	0.48
1:A:281:HIS:O	1:A:285:GLY:N	2.44	0.48
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.49	0.48
3:L:8:PRO:O	3:L:101:THR:HG23	2.14	0.48
1:A:379:PHE:CB	1:A:382:TYR:CD1	2.96	0.47
1:A:444:LEU:HD22	1:A:444:LEU:O	2.14	0.47
1:B:243:LYS:CG	2:I:31:ARG:HH21	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:6:GLN:HE21	3:L:98:GLY:CA	2.19	0.47
3:L:7:SER:CB	3:L:8:PRO:CD	2.72	0.47
1:A:414:GLU:HG2	1:B:419:TYR:CZ	2.50	0.47
3:L:139:TYR:CD2	3:L:140:PRO:HA	2.49	0.47
3:L:65:GLY:HA3	3:L:70:TYR:HA	1.95	0.47
3:O:136:ASN:HB3	3:O:137:ASN:ND2	2.30	0.47
1:A:265:PHE:HA	1:A:268:ILE:HD12	1.96	0.47
2:I:131:PRO:HD3	2:I:216:LYS:HG2	1.95	0.47
3:O:162:TRP:CG	3:O:174:MET:HG3	2.49	0.47
1:A:147:ARG:O	1:A:151:THR:HG23	2.14	0.47
1:A:239:ILE:HD13	1:A:394:MET:HE3	1.96	0.47
3:L:130:SER:HA	3:L:178:LEU:O	2.15	0.47
3:L:107:ARG:HD3	3:L:170:SER:O	2.13	0.47
2:I:105:TYR:CD1	3:L:31:TYR:HD1	2.32	0.47
2:J:150:VAL:HG11	2:J:205:VAL:HG11	1.96	0.47
2:J:78:THR:HG22	2:J:80:TYR:CZ	2.49	0.47
1:B:171:ASP:HA	1:B:174:ARG:HH12	1.80	0.47
1:B:271:LYS:CE	1:B:271:LYS:HG3	2.44	0.47
3:O:150:ASP:N	3:O:190:SER:O	2.45	0.47
1:A:139:LEU:HD11	1:A:145:LEU:O	2.15	0.47
3:O:192:THR:HA	3:O:207:SER:CB	2.44	0.47
3:O:2:ILE:O	3:O:96:THR:HG21	2.15	0.47
1:A:104:ALA:HB1	1:A:131:LYS:HD3	1.97	0.47
1:B:357:PHE:CE2	1:B:398:LEU:HD11	2.50	0.47
3:L:185:TYR:HD1	3:L:191:TYR:CZ	2.33	0.47
3:O:16:GLY:HA2	3:O:76:THR:HG23	1.96	0.47
1:A:449:LEU:HD23	1:B:25:LEU:HD11	1.96	0.46
1:B:98:ARG:HB3	1:B:288:ILE:CG1	2.45	0.46
2:J:167:LEU:HD21	2:J:191:VAL:HG11	1.97	0.46
3:L:189:ASN:C	3:L:189:ASN:HD22	2.17	0.46
3:O:125:THR:CG2	3:O:125:THR:O	2.63	0.46
1:A:119:GLN:O	1:A:120:ARG:HD2	2.15	0.46
1:A:70:HIS:O	1:A:70:HIS:ND1	2.48	0.46
1:B:207:GLN:HA	1:B:207:GLN:HE21	1.81	0.46
3:L:29:VAL:HG11	3:L:89:GLN:HG2	1.96	0.46
3:O:21:MET:O	3:O:71:SER:HB2	2.16	0.46
2:J:143:MET:HB3	2:J:190:THR:CG2	2.46	0.46
2:J:51:ILE:HD12	2:J:71:SER:HA	1.97	0.46
1:B:180:THR:HG22	1:B:218:VAL:HA	1.97	0.46
3:L:135:LEU:HD13	3:L:143:ILE:HD13	1.97	0.46
1:B:171:ASP:HB3	1:B:212:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ALA:HB3	1:B:359:PRO:CD	2.36	0.46
1:B:42:VAL:O	1:B:46:VAL:HG23	2.16	0.46
1:B:84:LEU:O	1:B:88:VAL:HG23	2.14	0.46
2:J:189:VAL:CG1	2:J:189:VAL:O	2.54	0.46
1:A:91:MET:CG	1:A:296:GLY:HA3	2.46	0.46
3:L:187:ARG:O	3:L:187:ARG:HG3	2.16	0.46
2:J:145:THR:HG22	3:O:117:PHE:HZ	1.81	0.46
1:A:263:GLY:HA3	1:A:435:LEU:CB	2.46	0.46
3:O:189:ASN:HD22	3:O:210:ARG:HB2	1.81	0.46
1:B:83:PHE:C	1:B:83:PHE:CD1	2.90	0.45
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.99	0.45
1:B:138:THR:O	1:B:143:MET:HB2	2.16	0.45
2:I:29:TYR:CD2	2:I:77:ASP:HA	2.51	0.45
2:J:52:ASN:HD22	2:J:57:THR:HB	1.80	0.45
3:O:53:LEU:HD21	3:O:61:PHE:O	2.17	0.45
1:B:110:PRO:HG3	1:B:448:ILE:HG21	1.99	0.45
2:I:170:GLY:O	2:I:189:VAL:HA	2.16	0.45
2:J:131:PRO:HD3	2:J:216:LYS:HG2	1.99	0.45
3:O:138:PHE:CE1	3:O:143:ILE:HB	2.51	0.45
1:B:87:ALA:HA	1:B:296:GLY:O	2.16	0.45
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.97	0.45
3:L:2:ILE:H	3:L:2:ILE:HG12	1.54	0.45
3:O:166:ASP:OD1	3:O:167:SER:N	2.49	0.45
1:A:18:ARG:NH1	1:B:457:GLU:CB	2.67	0.45
1:A:345:LEU:O	1:A:349:SER:HB2	2.17	0.45
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.82	0.45
1:B:357:PHE:CE2	1:B:398:LEU:CD1	2.99	0.45
2:J:163:ASN:HD22	2:J:167:LEU:CB	2.29	0.45
2:J:47:TRP:CZ2	2:J:49:GLY:HA2	2.52	0.45
2:J:67:LYS:NZ	2:J:85:LYS:O	2.50	0.45
3:O:63:GLY:O	3:O:64:SER:HB3	2.17	0.45
2:I:52:ASN:HB2	2:I:53:PRO:HD3	1.99	0.45
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.99	0.45
1:A:414:GLU:HG2	1:B:419:TYR:CE1	2.52	0.45
1:B:132:PHE:O	1:B:136:LEU:HD13	2.17	0.45
1:B:281:HIS:O	1:B:285:GLY:N	2.43	0.45
2:I:216:LYS:HA	2:I:216:LYS:HD3	1.88	0.44
1:B:336:ILE:O	1:B:340:ARG:HB2	2.17	0.44
2:I:176:ALA:HB2	2:I:185:LEU:HD23	1.99	0.44
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.52	0.44
3:O:35:TYR:CD2	3:O:45:ARG:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:HIS:O	1:A:287:ASN:HB3	2.17	0.44
1:A:376:VAL:CG1	1:A:377:GLU:N	2.81	0.44
2:J:107:TYR:HB3	3:O:33:HIS:CD2	2.52	0.44
1:A:264:ILE:HG13	1:A:265:PHE:N	2.31	0.44
1:A:336:ILE:O	1:A:340:ARG:HB2	2.17	0.44
3:L:136:ASN:HD22	3:L:173:SER:CB	2.30	0.44
3:L:136:ASN:ND2	3:L:173:SER:HB3	2.30	0.44
3:O:2:ILE:HB	3:O:89:GLN:NE2	2.33	0.44
1:B:235:GLU:O	1:B:236:VAL:HG23	2.17	0.44
2:I:15:GLY:O	2:I:85:LYS:HA	2.18	0.44
2:I:207:HIS:CE1	2:I:209:ALA:HB3	2.53	0.44
3:O:79:ALA:C	3:O:81:ASP:H	2.21	0.44
1:A:421:LEU:HA	1:A:421:LEU:HD23	1.78	0.44
1:B:171:ASP:HA	1:B:174:ARG:NH1	2.32	0.44
1:B:183:ALA:C	1:B:185:GLY:N	2.72	0.44
1:B:243:LYS:HD3	1:B:420:GLN:OE1	2.16	0.44
1:A:437:GLN:HE22	1:B:31:THR:H	1.66	0.44
3:O:82:ALA:O	3:O:83:ALA:HB2	2.18	0.44
1:A:123:ARG:NE	1:A:126:ARG:HD2	2.27	0.44
1:B:125:TRP:HD1	1:B:126:ARG:HG3	1.82	0.44
3:L:88:GLN:HB2	3:L:97:PHE:CD1	2.52	0.44
1:A:124:TRP:O	1:A:126:ARG:N	2.50	0.43
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.83	0.43
1:B:53:PHE:CE1	1:B:136:LEU:HD12	2.53	0.43
2:J:132:LEU:CD2	3:O:132:VAL:HG21	2.48	0.43
3:O:180:LEU:HB3	3:O:184:GLU:HG3	2.00	0.43
3:O:188:HIS:O	3:O:210:ARG:NE	2.51	0.43
1:A:280:LEU:O	1:A:284:HIS:CD2	2.71	0.43
3:L:181:THR:OG1	3:L:184:GLU:HB3	2.18	0.43
3:L:6:GLN:HE22	3:L:86:TYR:HA	1.83	0.43
1:A:129:PRO:O	1:A:133:PHE:HD2	2.02	0.43
1:A:244:LEU:HB2	1:A:418:ASN:OD1	2.18	0.43
2:I:38:ARG:NH1	2:I:90:ASP:HA	2.34	0.43
1:B:402:ILE:HD12	1:B:445:TYR:CD1	2.54	0.43
3:O:29:VAL:HG23	3:O:70:TYR:CE1	2.53	0.43
1:A:148:GLU:H	1:A:148:GLU:CD	2.21	0.43
1:B:148:GLU:HG2	1:B:357:PHE:HB3	2.01	0.43
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.54	0.43
2:I:153:TYR:CE1	2:I:183:TYR:HB2	2.54	0.43
3:L:190:SER:HA	3:L:209:ASN:OD1	2.18	0.43
3:O:6:GLN:NE2	3:O:87:CYS:H	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HD12	1:A:168:LEU:HB2	2.00	0.43
1:A:31:THR:HA	1:A:32:PRO:HD2	1.89	0.43
1:A:356:ILE:CG2	1:A:360:MET:CE	2.85	0.43
1:A:78:LEU:HD11	1:A:307:PHE:CE1	2.54	0.43
1:B:216:LYS:O	1:B:220:ILE:HG13	2.19	0.43
1:B:400:ALA:HB2	1:B:432:ALA:HB1	2.00	0.43
3:L:84:THR:HA	3:L:102:LYS:HA	2.01	0.43
2:I:188:SER:HB3	3:L:134:PHE:CE2	2.53	0.43
3:O:143:ILE:HG13	3:O:197:HIS:HB2	2.00	0.43
1:A:210:TYR:N	1:B:210:TYR:HB2	2.34	0.43
1:B:262:PHE:CE1	1:B:367:LEU:HD23	2.53	0.43
3:O:154:ARG:HH12	3:O:180:LEU:HD22	1.84	0.43
3:O:110:ALA:O	3:O:197:HIS:CE1	2.72	0.43
1:A:199:PHE:HA	1:A:407:THR:OG1	2.19	0.42
1:A:449:LEU:O	1:A:453:LEU:HB2	2.19	0.42
2:I:94:TYR:O	2:I:114:GLY:HA2	2.18	0.42
3:O:4:LEU:HD21	3:O:89:GLN:HG2	2.00	0.42
1:B:270:ASN:ND2	1:B:444:LEU:HG	2.34	0.42
2:J:162:TRP:CZ3	2:J:203:CYS:HB3	2.54	0.42
2:J:144:VAL:N	2:J:191:VAL:O	2.47	0.42
3:L:117:PHE:HA	3:L:118:PRO:HD3	1.83	0.42
1:A:103:GLU:OE1	1:A:123:ARG:HB2	2.19	0.42
1:A:125:TRP:NE1	1:A:126:ARG:HG3	2.34	0.42
1:B:150:PRO:HD3	1:B:354:GLY:CA	2.39	0.42
1:A:39:ALA:O	1:A:42:VAL:HB	2.20	0.42
1:A:208:PHE:HE1	1:B:25:LEU:HD23	1.84	0.42
1:B:339:ALA:O	1:B:343:THR:HG23	2.19	0.42
1:B:124:TRP:O	1:B:126:ARG:N	2.52	0.42
2:J:6:GLU:HA	2:J:21:SER:O	2.19	0.42
3:L:80:GLU:HA	3:L:167:SER:O	2.19	0.42
3:O:90:TRP:CG	3:O:95:GLN:HB3	2.55	0.42
1:A:251:THR:HG22	1:A:255:TYR:HE1	1.83	0.42
1:B:109:ILE:HG21	1:B:445:TYR:CD1	2.54	0.42
1:A:223:ILE:CD1	1:B:430:LEU:HD22	2.47	0.42
3:L:185:TYR:O	3:L:191:TYR:OH	2.37	0.42
3:L:192:THR:CB	3:L:207:SER:HB3	2.50	0.42
1:B:299:GLY:O	1:B:302:CYS:HB2	2.20	0.42
1:B:37:PHE:O	1:B:41:VAL:HG12	2.19	0.42
2:I:87:ARG:HH21	2:I:89:GLU:HG2	1.85	0.42
2:J:113:ALA:HA	3:O:42:SER:OG	2.19	0.42
3:L:15:PRO:HD3	3:L:105:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:HIS:ND1	2:J:106:TRP:CD1	2.86	0.42
1:B:212:LEU:H	1:B:212:LEU:HD12	1.84	0.42
1:A:219:PHE:HD2	1:B:430:LEU:HD13	1.84	0.42
3:L:180:LEU:HB3	3:L:184:GLU:HG3	2.00	0.42
1:A:153:GLN:O	1:A:154:ILE:C	2.57	0.41
1:A:250:ASN:ND2	1:A:382:TYR:CE2	2.87	0.41
1:A:267:PRO:HB3	1:A:441:GLY:HA3	2.02	0.41
3:L:202:SER:HA	3:L:203:PRO:HD2	1.68	0.41
1:A:150:PRO:O	1:A:154:ILE:HG13	2.20	0.41
1:A:426:ILE:HG22	1:B:223:ILE:HD11	2.03	0.41
3:O:2:ILE:HD12	3:O:27:SER:HB2	2.02	0.41
1:A:126:ARG:HH11	1:A:126:ARG:HG2	1.85	0.41
1:A:73:ASP:O	1:A:74:ASN:C	2.59	0.41
1:B:135:GLY:C	1:B:137:GLY:N	2.74	0.41
1:B:198:LEU:HA	1:B:198:LEU:HD13	1.94	0.41
1:B:211:THR:HG22	1:B:212:LEU:H	1.85	0.41
1:B:312:THR:HB	1:B:339:ALA:HB1	2.03	0.41
3:L:162:TRP:CD1	3:L:174:MET:HG3	2.54	0.41
1:A:148:GLU:O	1:A:149:GLY:C	2.59	0.41
1:A:274:LEU:HD23	1:A:277:GLN:HE22	1.86	0.41
1:A:400:ALA:HB2	1:A:432:ALA:HB1	2.02	0.41
1:B:120:ARG:NH1	1:B:452:THR:HG23	2.36	0.41
1:B:163:LEU:HD13	1:B:173:ALA:O	2.20	0.41
2:J:196:TRP:CD1	2:J:197:PRO:HA	2.55	0.41
2:J:217:LYS:HE2	2:J:219:VAL:CG1	2.50	0.41
3:L:90:TRP:CE3	3:L:95:GLN:HG3	2.56	0.41
3:O:19:VAL:HG11	3:O:103:LEU:CD1	2.48	0.41
1:A:284:HIS:HA	1:A:290:LYS:HB3	2.03	0.41
1:A:383:HIS:NE2	2:J:50:GLU:OE1	2.54	0.41
1:B:98:ARG:HH22	1:B:102:PRO:HB3	1.82	0.41
1:B:147:ARG:N	1:B:148:GLU:OE2	2.53	0.41
1:B:91:MET:CG	1:B:296:GLY:HA3	2.51	0.41
2:I:138:ALA:O	2:I:140:ALA:N	2.48	0.41
2:I:17:SER:HB3	2:I:84:SER:HA	2.03	0.41
1:B:124:TRP:CE3	1:B:125:TRP:N	2.89	0.41
2:I:84:SER:HB3	2:I:85:LYS:HE2	2.03	0.41
2:I:79:LEU:HD23	2:I:96:CYS:HB2	2.02	0.41
2:J:30:SER:O	2:J:32:TYR:N	2.51	0.41
3:O:60:ARG:CZ	3:O:78:GLU:HG3	2.51	0.41
1:A:176:THR:O	1:A:180:THR:HG23	2.20	0.41
1:A:197:ILE:HG13	1:A:222:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:178:LEU:HD11	2:I:181:ALA:HA	2.01	0.41
2:J:200:THR:HG22	2:J:200:THR:O	2.20	0.41
1:A:201:ILE:CG1	1:A:201:ILE:O	2.66	0.41
1:A:298:ILE:HG12	1:A:346:LEU:HD23	2.03	0.41
1:A:421:LEU:O	1:A:425:MET:HG3	2.21	0.41
1:B:31:THR:HA	1:B:32:PRO:HD2	1.87	0.41
3:L:192:THR:HB	3:L:207:SER:HB3	2.03	0.41
3:O:65:GLY:O	3:O:66:SER:HB3	2.21	0.41
1:A:104:ALA:HB2	1:A:127:VAL:HG13	2.02	0.41
1:A:210:TYR:H	1:B:210:TYR:HB2	1.85	0.41
1:B:61:GLN:HA	1:B:64:ARG:HE	1.85	0.41
2:I:134:PRO:HB2	2:I:138:ALA:HB2	2.03	0.41
2:I:93:LEU:HD23	2:I:95:TYR:OH	2.20	0.41
3:L:185:TYR:CD1	3:L:191:TYR:CZ	3.09	0.41
1:A:36:LEU:HD12	1:B:438:PHE:HZ	1.86	0.41
1:A:419:TYR:CE1	1:A:422:ILE:HB	2.56	0.41
1:A:264:ILE:HG22	1:A:435:LEU:HD12	2.02	0.41
1:B:218:VAL:O	1:B:222:VAL:HG23	2.21	0.41
1:B:73:ASP:O	1:B:74:ASN:C	2.59	0.41
3:L:194:GLU:HG2	3:L:205:VAL:CG1	2.26	0.41
1:A:182:ALA:HB1	1:A:204:MET:CE	2.52	0.40
1:A:377:GLU:CG	1:A:378:LEU:N	2.84	0.40
1:B:267:PRO:HB3	1:B:441:GLY:HA3	2.03	0.40
3:L:60:ARG:HH21	3:L:81:ASP:CG	2.24	0.40
2:J:111:TRP:N	2:J:111:TRP:CD1	2.90	0.40
3:L:38:LYS:O	3:L:41:THR:HG22	2.22	0.40
1:B:113:GLU:HA	1:B:116:LEU:HD12	2.03	0.40
1:B:244:LEU:HB2	1:B:418:ASN:OD1	2.21	0.40
2:J:192:PRO:O	2:J:195:SER:HB2	2.21	0.40
2:J:43:LYS:HB3	2:J:43:LYS:NZ	2.36	0.40
3:O:181:THR:OG1	3:O:184:GLU:HB3	2.20	0.40
2:J:33:TRP:CH2	2:J:52:ASN:HB3	2.56	0.40
3:L:140:PRO:HD3	3:L:198:LYS:HD3	2.04	0.40
3:O:77:MET:SD	3:O:103:LEU:HD21	2.61	0.40
3:O:79:ALA:O	3:O:81:ASP:N	2.55	0.40
1:A:201:ILE:HD13	1:A:201:ILE:HG21	1.91	0.40
1:B:53:PHE:CE2	1:B:139:LEU:HD12	2.56	0.40
2:J:16:GLY:O	2:J:86:VAL:HG23	2.21	0.40
3:O:94:PRO:HB2	3:O:95:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/465 (95%)	377 (85%)	52 (12%)	13 (3%)	4	28
1	B	439/465 (94%)	369 (84%)	54 (12%)	16 (4%)	3	23
2	I	219/222 (99%)	190 (87%)	21 (10%)	8 (4%)	3	22
2	J	219/222 (99%)	186 (85%)	26 (12%)	7 (3%)	4	26
3	L	209/211 (99%)	183 (88%)	24 (12%)	2 (1%)	15	54
3	O	209/211 (99%)	180 (86%)	21 (10%)	8 (4%)	3	22
All	All	1737/1796 (97%)	1485 (86%)	198 (11%)	54 (3%)	4	26

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	125	TRP
2	J	65	LYS
3	O	51	SER
3	O	125	THR
3	O	200	SER
2	I	62	PRO
3	L	7	SER
3	L	198	LYS
1	A	74	ASN
1	A	125	TRP
1	B	74	ASN
1	B	96	LEU
1	B	149	GLY
2	J	189	VAL
3	O	80	GLU
3	O	83	ALA
3	O	105	ILE
3	O	198	LYS
2	I	31	ARG
2	I	136	SER

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Mol	Chain	Res	Type
2	I	140	ALA
1	A	96	LEU
1	B	132	PHE
2	J	62	PRO
2	J	136	SER
2	J	211	SER
2	I	139	ALA
2	I	194	SER
2	I	198	SER
1	A	73	ASP
1	A	95	PHE
1	A	149	GLY
1	A	443	PRO
1	B	73	ASP
1	B	165	ILE
1	B	184	ALA
1	B	443	PRO
2	I	122	ALA
1	A	165	ILE
1	A	219	PHE
1	A	234	HIS
1	B	164	ASP
2	J	30	SER
1	B	128	LEU
1	B	144	VAL
2	J	55	SER
3	O	64	SER
1	A	201	ILE
1	B	201	ILE
1	B	236	VAL
1	A	206	PRO
1	B	206	PRO
1	A	144	VAL
1	B	32	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	335/353 (95%)	298 (89%)	37 (11%)	6	26
1	B	332/353 (94%)	293 (88%)	39 (12%)	5	23
2	I	181/182 (100%)	166 (92%)	15 (8%)	11	40
2	J	181/182 (100%)	156 (86%)	25 (14%)	3	16
3	L	185/185 (100%)	170 (92%)	15 (8%)	11	42
3	O	185/185 (100%)	166 (90%)	19 (10%)	7	29
All	All	1399/1440 (97%)	1249 (89%)	150 (11%)	6	27

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	70	HIS
1	A	73	ASP
1	A	74	ASN
1	A	78	LEU
1	A	103	GLU
1	A	136	LEU
1	A	147	ARG
1	A	148	GLU
1	A	180	THR
1	A	200	ILE
1	A	201	ILE
1	A	202	GLU
1	A	213	ILE
1	A	215	ILE
1	A	219	PHE
1	A	230	ARG
1	A	241	VAL
1	A	244	LEU
1	A	251	THR
1	A	264	ILE
1	A	271	LYS
1	A	277	GLN
1	A	279	LEU
1	A	346	LEU
1	A	356	ILE
1	A	373	MET
1	A	376	VAL
1	A	381	GLN
1	A	394	MET

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Mol	Chain	Res	Type
1	A	397	LEU
1	A	420	GLN
1	A	433	THR
1	A	435	LEU
1	A	442	LYS
1	A	451	ARG
1	A	459	GLU
1	B	41	VAL
1	B	65	MET
1	B	73	ASP
1	B	74	ASN
1	B	96	LEU
1	B	107	SER
1	B	122	VAL
1	B	138	THR
1	B	148	GLU
1	B	180	THR
1	B	207	GLN
1	B	211	THR
1	B	212	LEU
1	B	215	ILE
1	B	219	PHE
1	B	225	SER
1	B	235	GLU
1	B	241	VAL
1	B	244	LEU
1	B	251	THR
1	B	264	ILE
1	B	288	ILE
1	B	294	MET
1	B	340	ARG
1	B	346	LEU
1	B	357	PHE
1	B	363	LEU
1	B	377	GLU
1	B	381	GLN
1	B	397	LEU
1	B	402	ILE
1	B	420	GLN
1	B	423	LEU
1	B	433	THR
1	B	435	LEU

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Mol	Chain	Res	Type
1	B	444	LEU
1	B	451	ARG
1	B	452	THR
1	B	453	LEU
2	J	2	VAL
2	J	3	ARG
2	J	30	SER
2	J	35	SER
2	J	54	VAL
2	J	63	SER
2	J	64	LEU
2	J	77	ASP
2	J	86	VAL
2	J	89	GLU
2	J	98	ARG
2	J	100	TYR
2	J	115	THR
2	J	118	THR
2	J	120	SER
2	J	123	LYS
2	J	142	SER
2	J	145	THR
2	J	151	LYS
2	J	185	LEU
2	J	188	SER
2	J	203	CYS
2	J	204	ASN
2	J	211	SER
2	J	214	VAL
3	O	2	ILE
3	O	5	THR
3	O	21	MET
3	O	39	SER
3	O	46	TRP
3	O	59	VAL
3	O	68	THR
3	O	69	SER
3	O	73	THR
3	O	81	ASP
3	O	95	GLN
3	O	135	LEU
3	O	142	ASP

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Mol	Chain	Res	Type
3	O	145	VAL
3	O	162	TRP
3	O	178	LEU
3	O	192	THR
3	O	201	THR
3	O	205	VAL
2	I	2	VAL
2	I	3	ARG
2	I	6	GLU
2	I	12	VAL
2	I	18	LEU
2	I	31	ARG
2	I	54	VAL
2	I	72	ARG
2	I	96	CYS
2	I	115	THR
2	I	116	THR
2	I	125	THR
2	I	151	LYS
2	I	191	VAL
2	I	193	SER
3	L	12	SER
3	L	39	SER
3	L	69	SER
3	L	92	SER
3	L	95	GLN
3	L	125	THR
3	L	135	LEU
3	L	156	ASN
3	L	164	ASP
3	L	170	SER
3	L	181	THR
3	L	183	ASP
3	L	189	ASN
3	L	192	THR
3	L	210	ARG

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

Mol	Chain	Res	Type
1	A	74	ASN
1	A	153	GLN

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Mol	Chain	Res	Type
1	A	157	ASN
1	A	270	ASN
1	A	277	GLN
1	A	327	ASN
1	A	381	GLN
1	A	437	GLN
1	B	62	ASN
1	B	74	ASN
1	B	157	ASN
1	B	270	ASN
1	B	277	GLN
1	B	287	ASN
1	B	327	ASN
1	B	381	GLN
1	B	437	GLN
2	J	39	GLN
2	J	163	ASN
3	O	6	GLN
3	O	36	GLN
3	O	37	GLN
3	O	136	ASN
3	O	137	ASN
3	O	189	ASN
3	L	6	GLN
3	L	136	ASN
3	L	155	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	444/465 (95%)	0.15	7 (1%) 72 59	94, 117, 145, 163	0
1	B	441/465 (94%)	0.31	25 (5%) 23 13	94, 116, 145, 162	0
2	I	221/222 (99%)	0.06	4 (1%) 68 55	92, 118, 143, 162	0
2	J	221/222 (99%)	0.16	7 (3%) 47 31	90, 117, 142, 162	0
3	L	211/211 (100%)	0.47	26 (12%) 4 2	82, 112, 145, 154	0
3	O	211/211 (100%)	0.22	13 (6%) 20 11	96, 126, 145, 153	0
All	All	1749/1796 (97%)	0.23	82 (4%) 31 19	82, 118, 145, 163	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	ASP	6.6
1	B	72	ALA	4.7
2	J	139	ALA	4.6
3	L	155	GLN	4.2
3	L	158	VAL	4.2
3	L	146	LYS	4.1
1	B	104	ALA	4.1
3	L	147	TRP	3.9
2	J	135	GLY	3.7
3	O	112	PRO	3.6
2	I	66	ASP	3.6
3	L	156	ASN	3.5
3	L	151	GLY	3.4
1	B	71	THR	3.4
1	B	165	ILE	3.3
1	B	119	GLN	3.3
3	L	153	GLU	3.2
3	L	157	GLY	3.2
2	J	140	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	29	ASP	3.0
3	L	207	SER	3.0
3	O	154	ARG	3.0
3	L	127	GLY	3.0
1	A	447	ALA	3.0
3	L	180	LEU	2.9
1	B	74	ASN	2.8
3	O	153	GLU	2.8
2	J	137	ALA	2.8
1	B	456	GLN	2.8
2	I	135	GLY	2.8
3	O	148	LYS	2.8
3	O	72	LEU	2.8
3	L	189	ASN	2.7
3	L	152	SER	2.7
1	B	307	PHE	2.6
3	L	192	THR	2.6
1	B	453	LEU	2.6
1	B	410	ILE	2.6
3	L	128	GLY	2.6
1	B	70	HIS	2.6
3	O	178	LEU	2.6
3	L	211	ALA	2.6
1	B	442	LYS	2.5
1	B	195	ALA	2.5
3	L	154	ARG	2.5
3	O	197	HIS	2.5
2	J	29	TYR	2.5
1	B	168	LEU	2.5
3	O	73	THR	2.4
1	B	111	GLU	2.4
3	L	185	TYR	2.4
1	A	262	PHE	2.4
3	L	176	SER	2.4
3	L	124	LEU	2.4
3	L	205	VAL	2.3
3	O	146	LYS	2.3
1	B	143	MET	2.3
3	O	20	THR	2.3
3	O	158	VAL	2.3
1	A	143	MET	2.3
2	J	141	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	O	156	ASN	2.3
3	L	114	VAL	2.2
1	B	68	LEU	2.2
1	B	353	PRO	2.2
3	L	190	SER	2.2
3	O	68	THR	2.2
3	L	148	LYS	2.2
1	B	189	ALA	2.1
1	B	69	VAL	2.1
1	A	407	THR	2.1
1	B	38	MET	2.1
1	B	193	PRO	2.1
1	B	414	GLU	2.1
3	L	208	PHE	2.1
2	I	13	GLN	2.1
3	L	129	ALA	2.1
2	J	65	LYS	2.1
1	A	288	ILE	2.0
1	A	72	ALA	2.0
1	B	409	ILE	2.0
2	I	179	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.