



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:33 AM UTC

PDB ID : 2FEE / pdb_00002fee
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

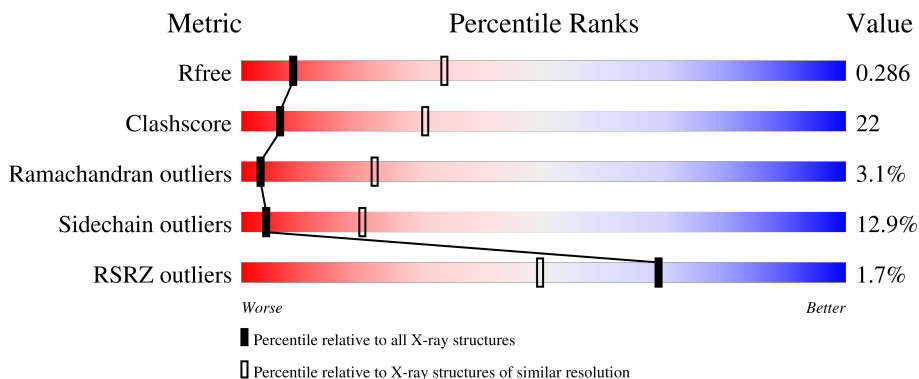
1 Overall quality at a glance i

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.



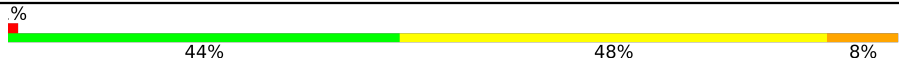
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	465	
1	B	465	
2	I	222	
2	J	222	
3	L	211	

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Mol	Chain	Length	Quality of chain
3	O	211	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a green segment on the left labeled '44%', a yellow segment in the middle labeled '48%', and a red segment on the right labeled '8%'. A small red square is positioned at the beginning of the bar, and a '%' symbol is located above the bar.</p>

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
			Total	C	N	O	S			
1	A	444	3333	2190	560	563	20	0	0	0
1	B	441	3304	2174	553	557	20	0	0	0

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

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

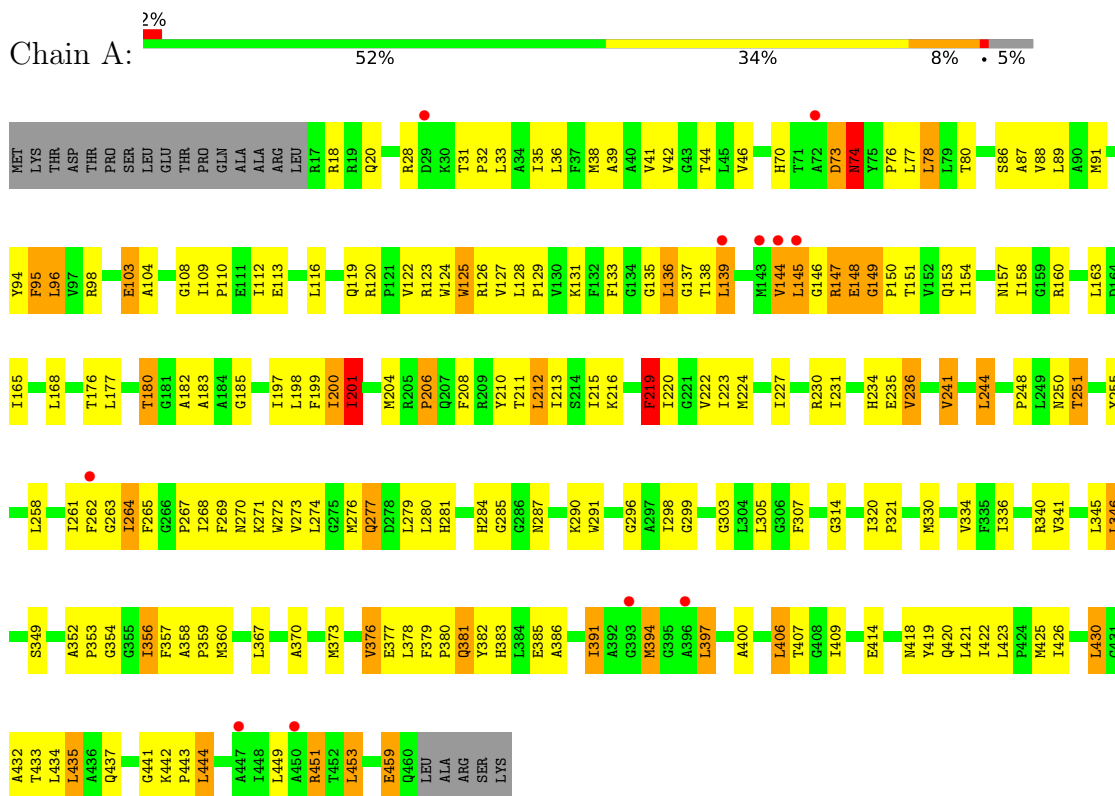
- Molecule 3 is a protein called Fab fragment, light chain.

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

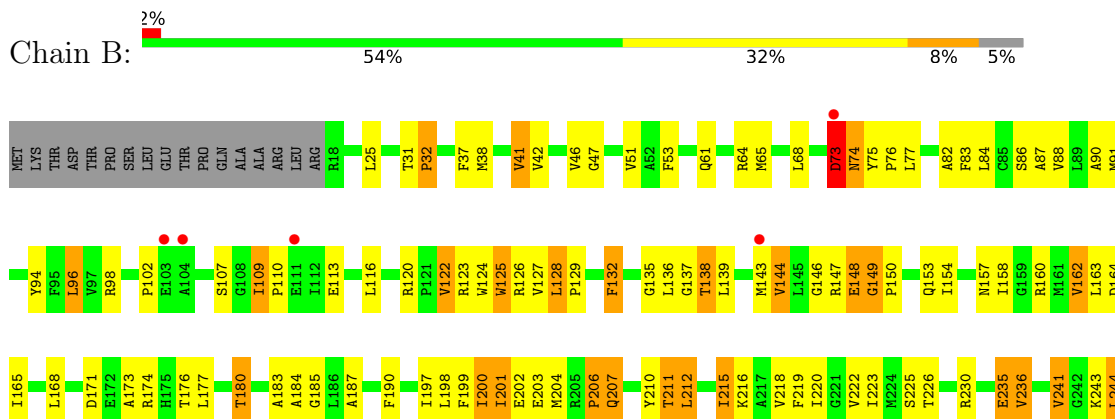
3 Residue-property plots i

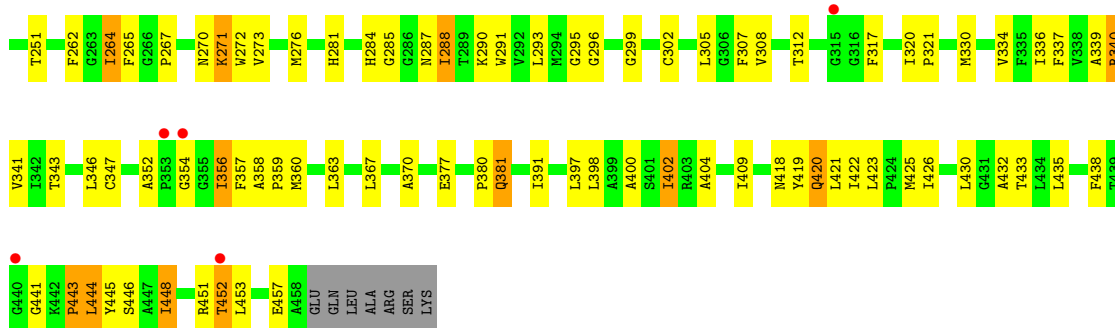
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

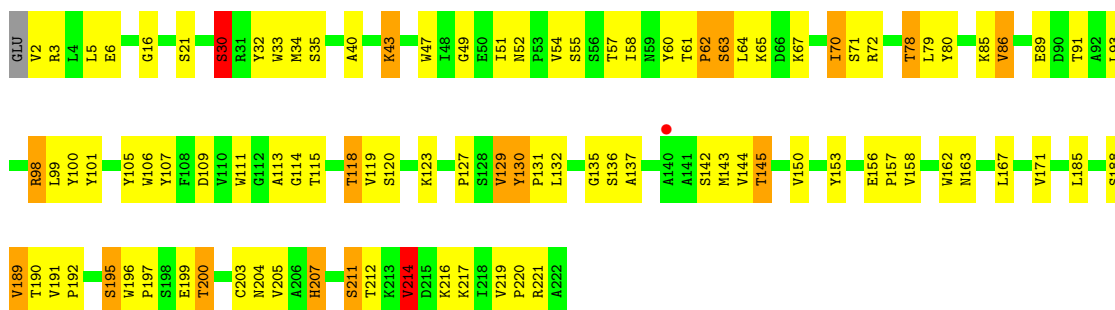


- Molecule 1: H(+)/Cl(-) exchange transporter *clcA*

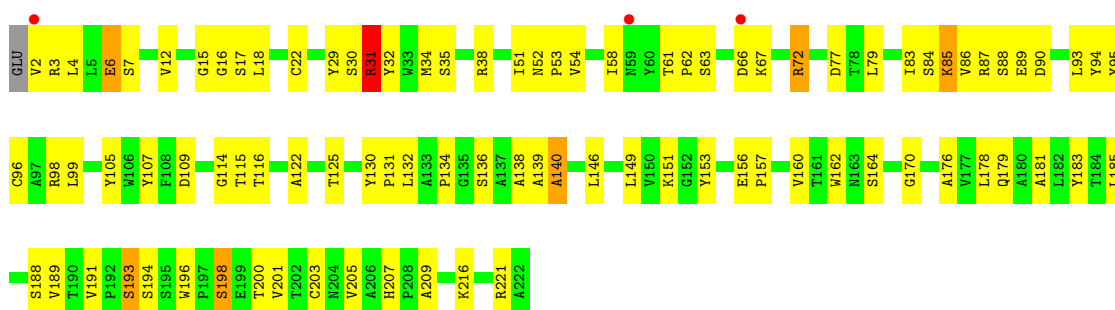




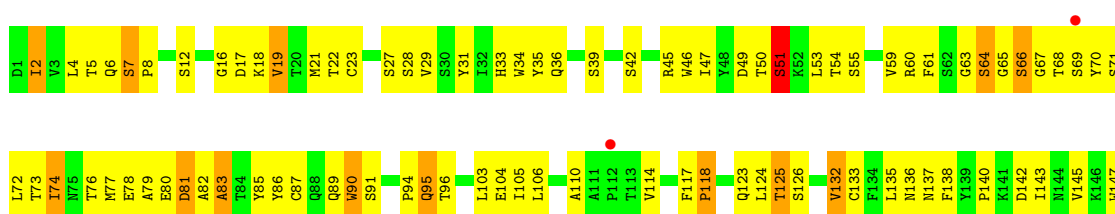
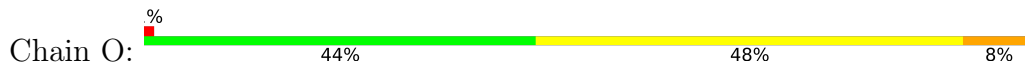
• Molecule 2: Fab fragment, heavy chain



• Molecule 2: Fab fragment, heavy chain

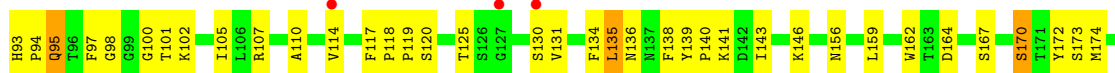
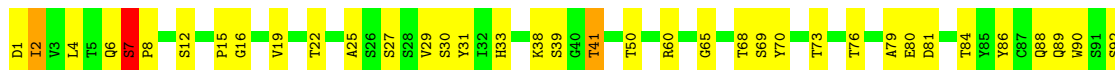


• Molecule 3: Fab fragment, light chain





- Molecule 3: Fab fragment, light chain



4 Data and refinement statistics i

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 – 3.20 128.04 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (128.04-3.20) 97.8 (128.04-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.19Å)	Xtrriage
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 (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	109.4	Xtrriage
Anisotropy	0.386	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtrriage'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 i

5.1 Standard geometry i

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	0.70	0/3405	1.00	0/4621
1	B	0.80	2/3376 (0.1%)	1.02	1/4583 (0.0%)
2	I	0.76	0/1721	0.98	2/2355 (0.1%)
2	J	0.82	1/1721 (0.1%)	1.00	4/2355 (0.2%)
3	L	0.79	0/1660	0.99	4/2257 (0.2%)
3	O	0.70	0/1660	1.07	8/2257 (0.4%)
All	All	0.76	3/13543 (0.0%)	1.01	19/18428 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	LYS	CD-CE	10.88	1.85	1.52
2	J	195	SER	CB-OG	8.18	1.58	1.42
1	B	271	LYS	CE-NZ	7.91	1.73	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	7	SER	CA-C-N	-7.21	112.55	119.76
3	L	7	SER	C-N-CA	-7.21	112.55	119.76
3	O	7	SER	CA-C-N	-7.17	112.08	119.83
3	O	7	SER	C-N-CA	-7.17	112.08	119.83
3	O	114	VAL	N-CA-C	6.10	116.93	109.30
2	J	130	TYR	CA-C-N	5.89	125.86	120.03
2	J	130	TYR	C-N-CA	5.89	125.86	120.03
3	L	202	SER	CA-C-N	5.73	127.00	119.84
3	L	202	SER	C-N-CA	5.73	127.00	119.84
2	I	66	ASP	N-CA-C	-5.65	103.66	110.44
1	B	271	LYS	CG-CD-CE	-5.55	98.53	111.30
3	O	51	SER	N-CA-C	5.50	122.53	110.80
2	I	7	SER	N-CA-C	5.48	115.78	108.38
3	O	90	TRP	N-CA-C	-5.46	104.88	112.03
3	O	66	SER	N-CA-C	5.35	116.57	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	118	PRO	CA-C-N	5.15	125.15	119.90
3	O	118	PRO	C-N-CA	5.15	125.15	119.90
2	J	214	VAL	N-CA-C	5.09	115.99	108.45
2	J	207	HIS	N-CA-C	-5.03	97.68	108.64

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	3333	0	3484	174	0
1	B	3304	0	3457	167	0
2	I	1672	0	1654	51	0
2	J	1672	0	1654	66	0
3	L	1621	0	1546	75	0
3	O	1621	0	1546	92	0
All	All	13223	0	13341	585	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 22.

All (585) 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:CE	1:B:271:LYS:CD	1.85	1.54
1:B:271:LYS:CE	1:B:271:LYS:NZ	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:O:95:GLN:CD	3:O:95:GLN:H	1.59	1.10
3:L:194:GLU:HG2	3:L:205:VAL:HG12	1.37	1.06
1:A:381:GLN:HE21	1:A:381:GLN:N	1.53	1.05
1:A:381:GLN:H	1:A:381:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:GLN:H	1:B:381:GLN:HE21	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:CE	1.98	0.93
3:O:95:GLN:CD	3:O:95:GLN:N	2.23	0.93
1:A:409:ILE:HD11	1:A:426:ILE:HA	1.51	0.91
1:B:356:ILE:HG23	1:B:360:MET:HE2	1.54	0.90
1:B:143:MET:HE2	1:B:347:CYS:SG	2.13	0.88
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:A:356:ILE:HG23	1:A:360:MET:HE2	1.60	0.83
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
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:HE21	1:B:381:GLN:N	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:H	1:B:381:GLN:NE2	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
3:L:95:GLN:CD	3:L:95:GLN:H	1.91	0.77
2:J:189:VAL:O	2:J:189:VAL:HG13	1.83	0.77
1:B:271:LYS:CE	1:B:271:LYS:CG	2.62	0.77
1:A:320:ILE:HD13	1:A:394:MET:HE3	1.67	0.76
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
1:B:148:GLU:CD	1:B:148:GLU:H	1.93	0.74
3:O:189:ASN:HD21	3:O:211:ALA:H	1.31	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HE3	3:O:162:TRP:H	1.36	0.71
3:O:124:LEU:C	3:O:126:SER:H	1.97	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:HA	2:I:31:ARG:HH11	1.54	0.71
1:B:337:PHE:O	1:B:341:VAL:HG23	1.91	0.71
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
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
3:L:95:GLN:CD	3:L:95:GLN:N	2.51	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
1:A:74:ASN:HD22	1:A:74:ASN:C	2.02	0.67
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:201:ILE:HG13	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:J:91:THR:HG23	2:J:118:THR:HA	1.80	0.63
2:I:132:LEU:HD11	2:I:149:LEU:HB2	1.78	0.63
1:B:98:ARG:HB3	1:B:288:ILE:HG13	1.80	0.63
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:192:THR:HB	3:O:207:SER:HB3	1.81	0.62
2:J:195:SER:O	2:J:199:GLU:HB2	1.98	0.62
2:I:156:GLU:OE1	2:I:157:PRO:HA	2.00	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
3:O:125:THR:HG22	3:O:125:THR:O	1.99	0.62
2:I:67:LYS:NZ	2:I:90:ASP:OD2	2.28	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: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
2:J:30:SER:C	2:J:32:TYR:H	2.09	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:O:95:GLN:H	3:O:95:GLN:NE2	1.96	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:61:THR:HG23	2:J:63:SER:HB2	1.83	0.59
2:I:134:PRO:O	2:I:221:ARG:HG3	2.03	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:HG12	1:A:144:VAL:O	2.03	0.58
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
1:A:148:GLU:CD	1:A:357:PHE:HB3	2.29	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
1:A:356:ILE:HG23	1:A:360:MET:HE3	1.81	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:HG3	1:A:459:GLU:O	2.05	0.57
1:A:451:ARG:HH11	1:A:451:ARG:HB3	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
2:J:135:GLY:C	2:J:137:ALA:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:O:149:ILE:HD12	3:O:154:ARG:HH11	1.69	0.56
2:I:6:GLU:HA	2:I:22:CYS:HA	1.86	0.56
1:A:356:ILE:CG2	1:A:360:MET:HE2	2.34	0.56
1:A:274:LEU:HA	1:A:277:GLN:NE2	2.20	0.56
2:J:43:LYS:HB3	2:J:43:LYS:HZ2	1.71	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
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:86:VAL:HG12	2:J:119:VAL:HG21	1.89	0.55
2:J:129:VAL:HG21	2:J:214:VAL:HG12	1.88	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: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:L:95:GLN:N	3:L:95:GLN:OE1	2.38	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
1:B:305:LEU:C	1:B:307:PHE:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:SER:OG	1:A:303:GLY:HA3	2.08	0.53
1:A:200:ILE:HG22	1:A:201:ILE:CG2	2.38	0.53
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.73	0.53
3:O:124:LEU:C	3:O:126:SER:N	2.65	0.53
3:O:17:ASP:H	3:O:77:MET:H	1.57	0.53
1:A:305:LEU:C	1:A:307:PHE:H	2.16	0.53
1:B:402:ILE:O	1:B:402:ILE:HG13	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:42:VAL:O	1:A:46:VAL:HG23	2.07	0.53
1:A:78:LEU:HD21	1:A:307:PHE:CE2	2.45	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:360:MET:HE1	1:B:402:ILE:HG22	1.90	0.52
1:B:38:MET:O	1:B:42:VAL:HG23	2.09	0.52
3:O:133:CYS:HB2	3:O:147:TRP:CH2	2.45	0.52
3:L:194:GLU:CG	3:L:205:VAL:HG12	2.26	0.52
1:A:87:ALA:O	1:A:91:MET:HG3	2.10	0.52
1:A:108:GLY:O	1:A:112:ILE:HG12	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
1:A:88:VAL:HA	1:A:91:MET:HE2	1.93	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
3:L:189:ASN:C	3:L:189:ASN:HD22	2.17	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:J:156:GLU:OE1	2:J:157:PRO:HA	2.11	0.51
2:I:31:ARG:HH11	2:I:31:ARG:CA	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:83:PHE:CD1	1:B:83:PHE:C	2.90	0.50
3:O:118:PRO:HB3	3:O:208:PHE:CE1	2.47	0.50
1:B:91:MET:HG3	1:B:296:GLY:HA3	1.93	0.50
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.77	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:74:ASN:ND2	1:A:77:LEU:H	2.10	0.49
1:A:116:LEU:HB3	1:A:206:PRO:HD3	1.94	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
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:O:36:GLN:HB2	3:O:85:TYR:CE2	2.40	0.49
3:L:188:HIS:O	3:L:210:ARG:NE	2.46	0.49
1:A:330:MET:HE1	1:A:370:ALA:CB	2.42	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:CD	1:B:271:LYS:NZ	2.74	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
2:J:105:TYR:CD2	3:O:91:SER:HA	2.47	0.48
3:O:79:ALA:C	3:O:81:ASP:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.95	0.48
1:A:269:PHE:O	1:A:273:VAL:HG12	2.13	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:O:7:SER:HB3	3:O:8:PRO:HD3	1.96	0.48
3:L:90:TRP:CE2	3:L:95:GLN:NE2	2.81	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:148:GLU:CD	1:A:148:GLU:H	2.21	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:2:ILE:HG23	3:L:27:SER:H	1.77	0.48
3:L:114:VAL:HG13	3:L:135:LEU:HD23	1.96	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:O	1:A:444:LEU:HD22	2.14	0.47
1:B:243:LYS:CG	2:I:31:ARG:HH21	2.27	0.47
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:O:136:ASN:HB3	3:O:137:ASN:ND2	2.30	0.47
3:L:65:GLY:HA3	3:L:70:TYR:HA	1.95	0.47
3:L:139:TYR:CD2	3:L:140:PRO:HA	2.49	0.47
1:A:265:PHE:HA	1:A:268:ILE:HD12	1.96	0.47
1:B:183:ALA:C	1:B:185:GLY:N	2.72	0.47
3:O:162:TRP:CG	3:O:174:MET:HG3	2.49	0.47
2:I:131:PRO:HD3	2:I:216:LYS:HG2	1.95	0.47
1:A:147:ARG:O	1:A:151:THR:HG23	2.14	0.47
3:L:130:SER:HA	3:L:178:LEU:O	2.15	0.47
2:I:105:TYR:CD1	3:L:31:TYR:HD1	2.32	0.47
3:L:107:ARG:HD3	3:L:170:SER:O	2.13	0.47
2:J:78:THR:HG22	2:J:80:TYR:CZ	2.49	0.47
2:J:150:VAL:HG11	2:J:205:VAL:HG11	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD11	1:A:145:LEU:O	2.15	0.47
3:O:2:ILE:O	3:O:96:THR:HG21	2.15	0.47
3:O:192:THR:HA	3:O:207:SER:CB	2.44	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:O:16:GLY:HA2	3:O:76:THR:HG23	1.96	0.47
3:L:185:TYR:HD1	3:L:191:TYR:CZ	2.33	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
2:I:29:TYR:HE1	2:I:34:MET:HE2	1.80	0.46
3:O:125:THR:O	3:O:125:THR:CG2	2.63	0.46
1:A:153:GLN:O	1:A:154:ILE:C	2.57	0.46
1:A:70:HIS:O	1:A:70:HIS:ND1	2.48	0.46
1:A:119:GLN:O	1:A:120:ARG:HD2	2.15	0.46
1:B:207:GLN:HA	1:B:207:GLN:HE21	1.81	0.46
3:O:21:MET:O	3:O:71:SER:HB2	2.16	0.46
3:L:29:VAL:HG11	3:L:89:GLN:HG2	1.96	0.46
1:A:73:ASP:O	1:A:74:ASN:C	2.59	0.46
1:A:74:ASN:C	1:A:74:ASN:ND2	2.73	0.46
1:B:135:GLY:C	1:B:137:GLY:N	2.74	0.46
2:J:51:ILE:HD12	2:J:71:SER:HA	1.97	0.46
2:J:143:MET:HB3	2:J:190:THR:CG2	2.46	0.46
1:A:148:GLU:O	1:A:149:GLY:C	2.59	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
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:O	2:J:189:VAL:CG1	2.54	0.46
1:A:91:MET:CG	1:A:296:GLY:HA3	2.46	0.46
1:B:330:MET:HE3	1:B:330:MET:HA	1.98	0.46
2:J:145:THR:HG22	3:O:117:PHE:HZ	1.81	0.46
3:L:187:ARG:O	3:L:187:ARG:HG3	2.16	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:A:330:MET:HE1	1:A:370:ALA:HB1	1.98	0.45
1:B:73:ASP:O	1:B:74:ASN:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:52:ASN:HD22	2:J:57:THR:HB	1.80	0.45
2:I:29:TYR:CD2	2:I:77:ASP:HA	2.51	0.45
3:O:53:LEU:HD21	3:O:61:PHE:O	2.17	0.45
3:L:60:ARG:HH21	3:L:81:ASP:CG	2.24	0.45
1:B:110:PRO:HG3	1:B:448:ILE:HG21	1.99	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
2:I:170:GLY:O	2:I:189:VAL:HA	2.16	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:O:166:ASP:OD1	3:O:167:SER:N	2.49	0.45
3:L:2:ILE:H	3:L:2:ILE:HG12	1.54	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: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
2:J:163:ASN:HD22	2:J:167:LEU:CB	2.29	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:127:VAL:O	1:B:128:LEU:C	2.59	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:HD3	2:I:216:LYS:HA	1.88	0.44
1:A:383:HIS:ND1	2:J:106:TRP:CD1	2.86	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
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:O:2:ILE:HB	3:O:89:GLN:NE2	2.33	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
1:B:235:GLU:O	1:B:236:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:421:LEU:HD23	1:A:421:LEU:HA	1.78	0.44
1:A:437:GLN:HE22	1:B:31:THR:H	1.66	0.44
1:B:171:ASP:HA	1:B:174:ARG:NH1	2.32	0.44
1:B:243:LYS:HD3	1:B:420:GLN:OE1	2.16	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:53:PHE:CE1	1:B:136:LEU:HD12	2.53	0.43
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.83	0.43
2:J:132:LEU:CD2	3:O:132:VAL:HG21	2.48	0.43
3:O:77:MET:HE3	3:O:78:GLU:O	2.17	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:95:PHE:O	1:A:96:LEU:C	2.61	0.43
1:A:280:LEU:O	1:A:284:HIS:CD2	2.71	0.43
3:L:6:GLN:HE22	3:L:86:TYR:HA	1.83	0.43
3:L:181:THR:OG1	3:L:184:GLU:HB3	2.18	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
1:B:422:ILE:HD12	1:B:425:MET:HE3	2.00	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
2:J:16:GLY:C	2:J:86:VAL:HG23	2.44	0.43
3:O:29:VAL:HG23	3:O:70:TYR:CE1	2.53	0.43
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.54	0.43
1:B:148:GLU:HG2	1:B:357:PHE:HB3	2.01	0.43
3:O:6:GLN:NE2	3:O:87:CYS:H	2.15	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
1:A:31:THR:HA	1:A:32:PRO:HD2	1.89	0.43
1:A:78:LEU:HD11	1:A:307:PHE:CE1	2.54	0.43
1:A:163:LEU:HD12	1:A:168:LEU:HB2	2.00	0.43
1:A:356:ILE:CG2	1:A:360:MET:CE	2.85	0.43
1:B:148:GLU:O	1:B:149:GLY:C	2.62	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:O:143:ILE:HG13	3:O:197:HIS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:188:SER:HB3	3:L:134:PHE:CE2	2.53	0.43
3:L:84:THR:HA	3:L:102:LYS:HA	2.01	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:110:ALA:O	3:O:197:HIS:CE1	2.72	0.43
3:O:154:ARG:HH12	3:O:180:LEU:HD22	1.84	0.43
1:A:127:VAL:O	1:A:128:LEU:C	2.61	0.42
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
3:O:4:LEU:HD21	3:O:89:GLN:HG2	2.00	0.42
2:I:94:TYR:O	2:I:114:GLY:HA2	2.18	0.42
1:A:124:TRP:C	1:A:126:ARG:N	2.76	0.42
1:A:422:ILE:HA	1:A:425:MET:HE3	2.01	0.42
1:B:270:ASN:ND2	1:B:444:LEU:HG	2.34	0.42
2:J:144:VAL:N	2:J:191:VAL:O	2.47	0.42
2:J:162:TRP:CZ3	2:J:203:CYS:HB3	2.54	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:A:385:GLU:O	1:A:386:ALA:C	2.63	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:183:ALA:C	1:A:185:GLY:N	2.77	0.42
1:A:208:PHE:HE1	1:B:25:LEU:HD23	1.84	0.42
1:B:124:TRP:C	1:B:126:ARG:N	2.77	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:O:90:TRP:CG	3:O:95:GLN:HB3	2.55	0.42
3:L:80:GLU:HA	3:L:167:SER:O	2.19	0.42
1:A:223:ILE:CD1	1:B:430:LEU:HD22	2.47	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
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:37:PHE:O	1:B:41:VAL:HG12	2.19	0.42
1:B:299:GLY:O	1:B:302:CYS:HB2	2.20	0.42
1:B:330:MET:HE1	1:B:370:ALA:HB1	2.02	0.42
2:J:113:ALA:HA	3:O:42:SER:OG	2.19	0.42
2:I:87:ARG:HH21	2:I:89:GLU:HG2	1.85	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:219:PHE:HD2	1:B:430:LEU:HD13	1.84	0.42
1:B:212:LEU:HD12	1:B:212:LEU:H	1.84	0.42
3:L:180:LEU:HB3	3:L:184:GLU:HG3	2.00	0.42
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:135:GLY:O	1:A:136:LEU:C	2.63	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
3:O:54:THR:O	3:O:55:SER:C	2.63	0.41
1:A:126:ARG:HG2	1:A:126:ARG:HH11	1.85	0.41
1:B:198:LEU:HD13	1:B:198:LEU:HA	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:60:ARG:NH2	3:L:81:ASP:CG	2.79	0.41
3:L:162:TRP:CD1	3:L:174:MET:HG3	2.54	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:O:19:VAL:HG11	3:O:103:LEU:CD1	2.48	0.41
3:L:79:ALA:C	3:L:81:ASP:H	2.28	0.41
3:L:90:TRP:CE3	3:L:95:GLN:HG3	2.56	0.41
1:A:284:HIS:HA	1:A:290:LYS:HB3	2.03	0.41
1:B:91:MET:CG	1:B:296:GLY:HA3	2.51	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
2:I:17:SER:HB3	2:I:84:SER:HA	2.03	0.41
2:I:138:ALA:O	2:I:140:ALA:N	2.48	0.41
1:B:124:TRP:CE3	1:B:125:TRP:N	2.89	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
2:I:79:LEU:HD23	2:I:96:CYS:HB2	2.02	0.41
2:I:84:SER:HB3	2:I:85:LYS:HE2	2.03	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
2:J:200:THR:O	2:J:200:THR:HG22	2.20	0.41
2:I:178:LEU:HD11	2:I:181:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ILE:O	1:A:201:ILE:CG1	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:O:65:GLY:O	3:O:66:SER:HB3	2.21	0.41
3:L:192:THR:HB	3:L:207:SER:HB3	2.03	0.41
1:A:33:LEU:HD23	1:A:33:LEU:C	2.46	0.41
1:A:36:LEU:HD12	1:B:438:PHE:HZ	1.86	0.41
1:A:104:ALA:HB2	1:A:127:VAL:HG13	2.02	0.41
1:A:135:GLY:C	1:A:137:GLY:N	2.75	0.41
1:A:210:TYR:H	1:B:210:TYR:HB2	1.85	0.41
1:A:264:ILE:HG22	1:A:435:LEU:HD12	2.02	0.41
1:A:419:TYR:CE1	1:A:422:ILE:HB	2.56	0.41
1:B:61:GLN:HA	1:B:64:ARG:HE	1.85	0.41
1:B:218:VAL:O	1:B:222:VAL:HG23	2.21	0.41
2:I:93:LEU:HD23	2:I:95:TYR:OH	2.20	0.41
2:I:134:PRO:HB2	2:I:138:ALA:HB2	2.03	0.41
3:L:185:TYR:CD1	3:L:191:TYR:CZ	3.09	0.41
1:B:83:PHE:C	1:B:83:PHE:HD1	2.29	0.41
3:L:189:ASN:C	3:L:189:ASN:ND2	2.79	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
2:J:111:TRP:CD1	2:J:111:TRP:N	2.90	0.40
2:I:88:SER:C	2:I:90:ASP:N	2.78	0.40
3:L:38:LYS:O	3:L:41:THR:HG22	2.22	0.40
1:A:224:MET:HA	1:A:224:MET:HE3	2.03	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:43:LYS:HB3	2:J:43:LYS:NZ	2.36	0.40
2:J:192:PRO:O	2:J:195:SER:HB2	2.21	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: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
3:L:140:PRO:HD3	3:L:198:LYS:HD3	2.04	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
1:B:153:GLN:O	1:B:154:ILE:C	2.64	0.40
2:J:16:GLY:O	2:J:86:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:94:PRO:HB2	3:O:95:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/465 (95%)	377 (85%)	52 (12%)	13 (3%)	3	24
1	B	439/465 (94%)	369 (84%)	54 (12%)	16 (4%)	2	19
2	I	219/222 (99%)	190 (87%)	21 (10%)	8 (4%)	2	18
2	J	219/222 (99%)	186 (85%)	26 (12%)	7 (3%)	3	21
3	L	209/211 (99%)	183 (88%)	24 (12%)	2 (1%)	12	45
3	O	209/211 (99%)	180 (86%)	21 (10%)	8 (4%)	2	18
All	All	1737/1796 (97%)	1485 (86%)	198 (11%)	54 (3%)	3	22

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	B	32	PRO

5.3.2 Protein sidechains [i](#)

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%)	286 (85%)	49 (15%)	3	16
1	B	332/353 (94%)	289 (87%)	43 (13%)	4	20
2	I	181/182 (100%)	161 (89%)	20 (11%)	6	26
2	J	181/182 (100%)	154 (85%)	27 (15%)	3	15
3	L	185/185 (100%)	166 (90%)	19 (10%)	7	28
3	O	185/185 (100%)	162 (88%)	23 (12%)	4	21
All	All	1399/1440 (97%)	1218 (87%)	181 (13%)	4	20

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	35	ILE
1	A	41	VAL
1	A	44	THR
1	A	74	ASN
1	A	78	LEU
1	A	89	LEU
1	A	103	GLU
1	A	113	GLU
1	A	136	LEU
1	A	139	LEU
1	A	145	LEU
1	A	147	ARG
1	A	148	GLU
1	A	180	THR
1	A	200	ILE
1	A	201	ILE

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Mol	Chain	Res	Type
1	A	212	LEU
1	A	213	ILE
1	A	215	ILE
1	A	219	PHE
1	A	230	ARG
1	A	236	VAL
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	334	VAL
1	A	346	LEU
1	A	356	ILE
1	A	373	MET
1	A	376	VAL
1	A	381	GLN
1	A	391	ILE
1	A	394	MET
1	A	397	LEU
1	A	406	LEU
1	A	420	GLN
1	A	430	LEU
1	A	433	THR
1	A	435	LEU
1	A	442	LYS
1	A	444	LEU
1	A	451	ARG
1	A	453	LEU
1	A	459	GLU
1	B	41	VAL
1	B	65	MET
1	B	73	ASP
1	B	96	LEU
1	B	107	SER
1	B	109	ILE
1	B	122	VAL
1	B	138	THR
1	B	148	GLU
1	B	162	VAL

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Mol	Chain	Res	Type
1	B	177	LEU
1	B	180	THR
1	B	200	ILE
1	B	207	GLN
1	B	211	THR
1	B	212	LEU
1	B	215	ILE
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	293	LEU
1	B	334	VAL
1	B	340	ARG
1	B	346	LEU
1	B	356	ILE
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
1	B	444	LEU
1	B	448	ILE
1	B	451	ARG
1	B	452	THR
1	B	453	LEU
2	J	2	VAL
2	J	3	ARG
2	J	5	LEU
2	J	30	SER
2	J	35	SER
2	J	43	LYS
2	J	54	VAL
2	J	63	SER
2	J	64	LEU

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Mol	Chain	Res	Type
2	J	70	ILE
2	J	78	THR
2	J	86	VAL
2	J	89	GLU
2	J	98	ARG
2	J	115	THR
2	J	118	THR
2	J	120	SER
2	J	123	LYS
2	J	129	VAL
2	J	142	SER
2	J	145	THR
2	J	185	LEU
2	J	188	SER
2	J	200	THR
2	J	204	ASN
2	J	211	SER
2	J	214	VAL
3	O	2	ILE
3	O	5	THR
3	O	19	VAL
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	74	ILE
3	O	81	ASP
3	O	95	GLN
3	O	132	VAL
3	O	135	LEU
3	O	142	ASP
3	O	145	VAL
3	O	155	GLN
3	O	162	TRP
3	O	178	LEU
3	O	192	THR
3	O	201	THR
3	O	205	VAL
3	O	206	LYS
2	I	2	VAL

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Mol	Chain	Res	Type
2	I	3	ARG
2	I	4	LEU
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	85	LYS
2	I	115	THR
2	I	116	THR
2	I	125	THR
2	I	146	LEU
2	I	151	LYS
2	I	164	SER
2	I	191	VAL
2	I	193	SER
2	I	198	SER
2	I	200	THR
3	L	2	ILE
3	L	12	SER
3	L	19	VAL
3	L	39	SER
3	L	41	THR
3	L	68	THR
3	L	69	SER
3	L	73	THR
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	192	THR
3	L	204	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) 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	277	GLN
1	A	281	HIS
1	A	284	HIS
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	163	ASN
3	O	6	GLN
3	O	36	GLN
3	O	136	ASN
3	O	137	ASN
3	O	189	ASN
2	I	59	ASN
3	L	6	GLN
3	L	36	GLN
3	L	136	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	-0.03	11 (2%) 58 39	94, 117, 145, 163	0
1	B	441/465 (94%)	0.03	10 (2%) 61 41	94, 116, 145, 162	0
2	I	221/222 (99%)	-0.05	3 (1%) 73 54	92, 118, 143, 162	0
2	J	221/222 (99%)	0.04	1 (0%) 87 76	90, 117, 142, 162	0
3	L	211/211 (100%)	-0.08	3 (1%) 73 54	82, 112, 145, 154	0
3	O	211/211 (100%)	-0.00	2 (0%) 81 64	96, 126, 145, 153	0
All	All	1749/1796 (97%)	-0.01	30 (1%) 69 49	82, 118, 145, 163	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	ALA	4.5
1	A	29	ASP	4.5
1	A	143	MET	4.1
1	B	104	ALA	3.9
3	O	112	PRO	3.6
1	A	144	VAL	3.2
2	J	140	ALA	2.9
2	I	66	ASP	2.7
3	L	127	GLY	2.7
1	B	73	ASP	2.7
1	A	396	ALA	2.6
1	A	450	ALA	2.6
1	B	452	THR	2.5
1	A	72	ALA	2.4
1	B	111	GLU	2.4
1	B	315	GLY	2.4
3	O	69	SER	2.4
1	A	145	LEU	2.4
1	B	353	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	262	PHE	2.4
1	B	440	GLY	2.3
3	L	114	VAL	2.3
1	B	354	GLY	2.3
1	B	103	GLU	2.2
1	A	393	GLY	2.2
1	B	143	MET	2.1
2	I	59	ASN	2.1
3	L	130	SER	2.1
2	I	2	VAL	2.1
1	A	139	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.