



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:24 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

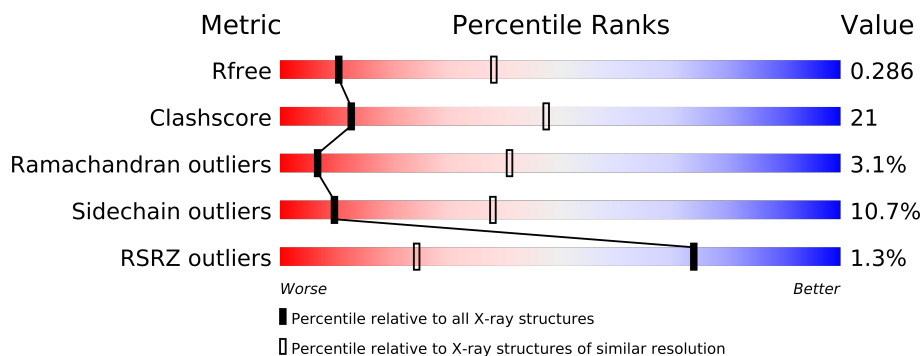
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

2 Entry composition

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

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.

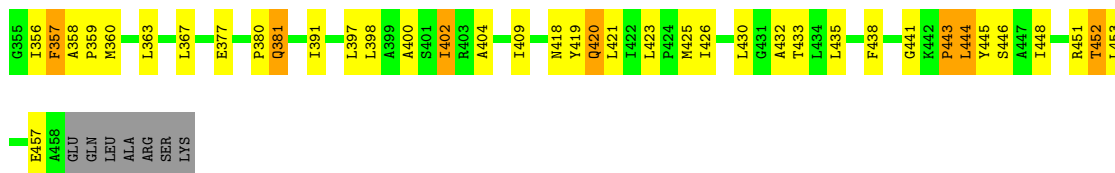
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3333	2190	560	563	20			
1	B	441	Total	C	N	O	S	0	0	0
			3304	2174	553	557	20			

- 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			

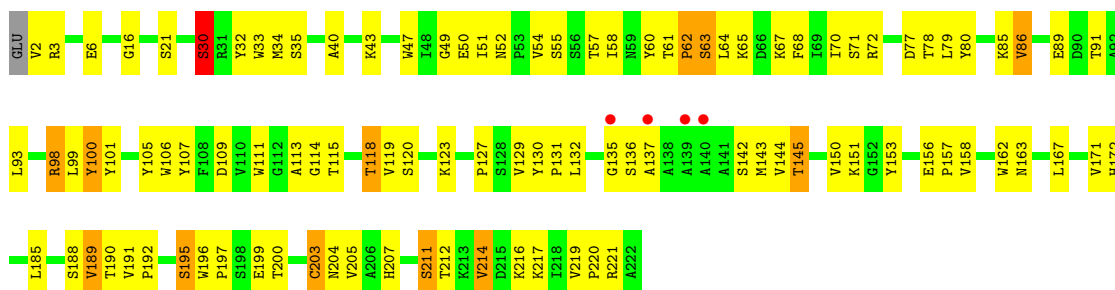
- Molecule 3 is a protein called Fab fragment, light chain.

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			



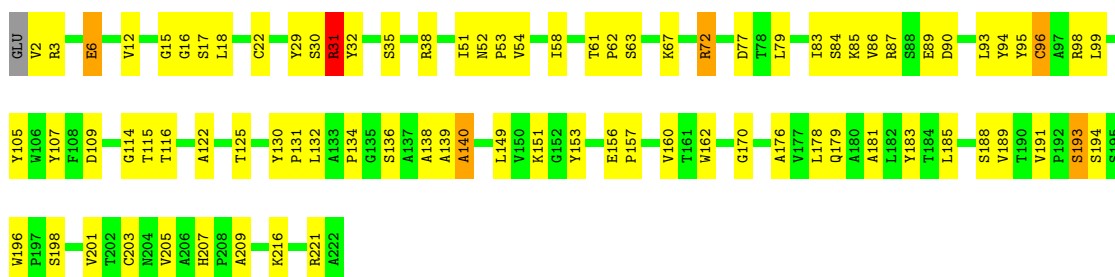
- Molecule 2: Fab fragment, heavy chain

Chain J:



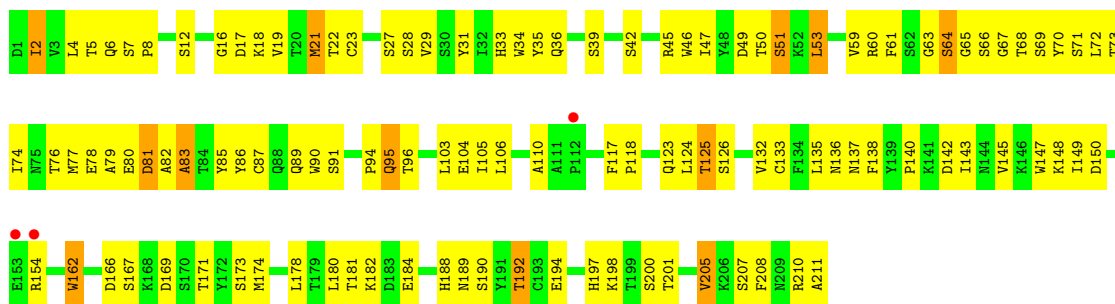
- Molecule 2: Fab fragment, heavy chain

Chain I:



- Molecule 3: Fab fragment, light chain

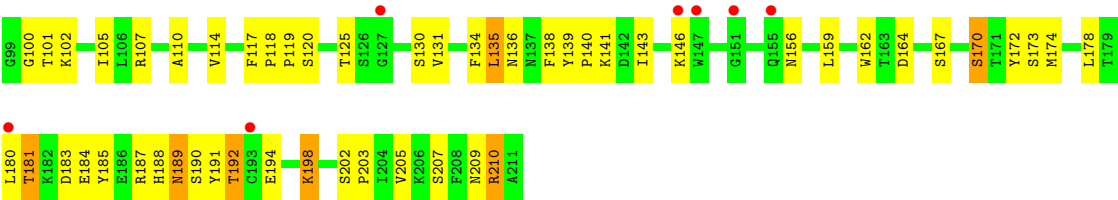
Chain O:



- Molecule 3: Fab fragment, light chain

Chain L:





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 0.250 , 0.286	Depositor DCC
R_{free} test set	2341 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	109.4	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 100.0	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 46298 reflections	Xtriage
F_o, F_c correlation	0.91	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (556) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:200:ILE:HA	1:A:204:MET:HB2	1.59	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:O:31:TYR:HB3	3:O:49:ASP:HA	1.64	0.79
1:A:86:SER:HB3	1:A:299:GLY:O	1.82	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
2:I:31:ARG:HA	2:I:31:ARG:HH11	1.54	0.71
1:B:98:ARG:NH2	1:B:102:PRO:HB3	2.06	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:B:148:GLU:CD	1:B:148:GLU:H	1.93	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:L:7:SER:HB2	3:L:22:THR:CB	2.22	0.63
1:B:125:TRP:CD1	1:B:126:ARG:HG3	2.32	0.63
1:A:98:ARG:HD2	1:A:291:TRP:CE3	2.33	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:O:22:THR:HG22	3:O:23:CYS:H	1.64	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: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
2:J:171:VAL:HG22	2:J:189:VAL:HG23	1.81	0.61
1:A:262:PHE:CE2	1:A:367:LEU:HD23	2.35	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:243:LYS:HG2	2:I:31:ARG:HH21	1.65	0.60
1:B:202:GLU:OE1	1:B:404:ALA:HB1	2.02	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
3:L:136:ASN:HD22	3:L:173:SER:HB3	1.67	0.59
2:J:61:THR:HG23	2:J:63:SER:HB2	1.83	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
3:L:1:ASP:HB3	3:L:94:PRO:HD2	1.85	0.58
1:A:144:VAL:O	1:A:144:VAL:HG12	2.03	0.58
2:I:52:ASN:HB2	2:I:53:PRO:CD	2.33	0.58
1:A:154:ILE:O	1:A:158:ILE:HG12	2.04	0.58
3:O:194:GLU:HG2	3:O:205:VAL:CG1	2.32	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:287:ASN:ND2	1:A:290:LYS:HG3	2.17	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
3:O:19:VAL:HB	3:O:74:ILE:HD12	1.87	0.57
1:A:198:LEU:HD12	1:A:406:LEU:HG	1.84	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:HG12	1.87	0.56
1:A:270:ASN:HA	1:A:273:VAL:CG1	2.35	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:274:LEU:HA	1:A:277:GLN:NE2	2.20	0.56
3:O:162:TRP:N	3:O:162:TRP:CE3	2.73	0.56
1:B:187:ALA:CB	1:B:222:VAL:HG13	2.36	0.56
2:J:30:SER:C	2:J:32:TYR:H	2.09	0.56
3:O:47:ILE:HD12	3:O:72:LEU:HG	1.88	0.56
1:B:264:ILE:O	1:B:267:PRO:HD2	2.06	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
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
1:B:122:VAL:HB	1:B:160:ARG:HG2	1.89	0.55
1:A:235:GLU:O	1:A:236:VAL:HG22	2.06	0.55
2:J:135:GLY:CA	2:J:221:ARG:HD3	2.21	0.55
2:J:129:VAL:CG2	2:J:214:VAL:HG11	2.37	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:95:GLN:OE1	3:L:95:GLN:N	2.38	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:O:6:GLN:NE2	3:O:86:TYR:HA	2.18	0.54
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.22	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
3:O:2:ILE:HD13	3:O:2:ILE:N	2.23	0.54
1:A:258:LEU:HA	1:A:261:ILE:HD12	1.88	0.54
1:A:430:LEU:CD1	1:B:219:PHE:HB3	2.38	0.54
1:A:77:LEU:O	1:A:80:THR:HB	2.07	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
3:O:50:THR:O	3:O:51:SER:HB3	2.09	0.53
1:A:148:GLU:OE1	1:A:357:PHE:HB2	2.06	0.53
1:B:68:LEU:HD21	1:B:82:ALA:HB2	1.91	0.53
1:A:241:VAL:HG11	1:A:391:ILE:HD11	1.91	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
1:A:42:VAL:O	1:A:46:VAL:HG23	2.07	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
3:L:194:GLU:CG	3:L:205:VAL:HG12	2.26	0.52
2:J:63:SER:HG	2:J:68:PHE:HE1	1.57	0.52
3:O:133:CYS:HB2	3:O:147:TRP:CH2	2.45	0.52
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:138:THR:HG21	1:A:353:PRO:HD2	1.92	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:421:LEU:O	1:B:425:MET:HG3	2.10	0.51
1:B:116:LEU:HB3	1:B:206:PRO:HD3	1.93	0.51
3:L:6:GLN:NE2	3:L:100:GLY:H	2.08	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
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.26	0.51
1:A:78:LEU:HD11	1:A:307:PHE:CZ	2.46	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
3:O:17:ASP:OD1	3:O:18:LYS:N	2.44	0.50
1:B:305:LEU:C	1:B:307:PHE:H	2.15	0.50
1:A:423:LEU:HD11	1:B:226:THR:HG21	1.92	0.50
1:A:211:THR:HG22	1:A:212:LEU:H	1.76	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: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:A:116:LEU:HB3	1:A:206:PRO:HD3	1.94	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
3:L:6:GLN:HA	3:L:22:THR:O	2.13	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: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: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
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:22:THR:CG2	3:O:23:CYS:H	2.25	0.49
3:O:124:LEU:C	3:O:126:SER:N	2.65	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
3:O:47:ILE:HG23	3:O:51:SER:HA	1.94	0.48
1:B:212:LEU:HD12	1:B:212:LEU:N	2.28	0.48
1:B:163:LEU:HD12	1:B:168:LEU:HB2	1.95	0.48
1:A:305:LEU:C	1:A:307:PHE:H	2.16	0.48
1:B:356:ILE:HG23	1:B:360:MET:CE	2.43	0.48
3:O:34:TRP:HB2	3:O:47:ILE:HB	1.95	0.48
2:J:43:LYS:HB3	2:J:43:LYS:HZ2	1.79	0.48
1:A:269:PHE:O	1:A:273:VAL:HG12	2.13	0.48
3:L:90:TRP:CE2	3:L:95:GLN:NE2	2.81	0.48
2:J:127:PRO:HD2	2:J:212:THR:HG21	1.94	0.48
1:A:98:ARG:HA	1:A:98:ARG:NE	2.29	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:93:HIS:CG	3:L:94:PRO:HA	2.48	0.48
2:I:193:SER:O	2:I:196:TRP:O	2.32	0.48
1:B:128:LEU:HB2	1:B:129:PRO:HD3	1.96	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
1:A:377:GLU:HG3	1:A:378:LEU:N	2.29	0.48
3:L:114:VAL:HG13	3:L:135:LEU:HD23	1.96	0.48
3:L:8:PRO:O	3:L:101:THR:HG23	2.14	0.48
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.49	0.48
1:A:281:HIS:O	1:A:285:GLY:N	2.44	0.48
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:B:243:LYS:CG	2:I:31:ARG:HH21	2.27	0.47
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
3:L:65:GLY:HA3	3:L:70:TYR:HA	1.95	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:139:TYR:CD2	3:L:140:PRO:HA	2.49	0.47
3:O:162:TRP:CG	3:O:174:MET:HG3	2.49	0.47
1:A:265:PHE:HA	1:A:268:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:I:131:PRO:HD3	2:I:216:LYS:HG2	1.95	0.47
1:A:239:ILE:HD13	1:A:394:MET:HE3	1.96	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:271:LYS:CE	1:B:271:LYS:HG3	2.44	0.47
1:B:171:ASP:HA	1:B:174:ARG:HH12	1.80	0.47
3:O:150:ASP:N	3:O:190:SER:O	2.45	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:139:LEU:HD11	1:A:145:LEU:O	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: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:B:98:ARG:HB3	1:B:288:ILE:CG1	2.45	0.46
1:A:449:LEU:HD23	1:B:25:LEU:HD11	1.96	0.46
2:J:167:LEU:HD21	2:J:191:VAL:HG11	1.97	0.46
3:O:125:THR:CG2	3:O:125:THR:O	2.63	0.46
3:L:189:ASN:C	3:L:189:ASN:HD22	2.17	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: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
1:A:119:GLN:O	1:A:120:ARG:HD2	2.15	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: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:358:ALA:HB3	1:B:359:PRO:CD	2.36	0.46
1:B:171:ASP:HB3	1:B:212:LEU:HD13	1.97	0.46
1:B:42:VAL:O	1:B:46:VAL:HG23	2.16	0.46
2:J:189:VAL:CG1	2:J:189:VAL:O	2.54	0.46
1:B:84:LEU:O	1:B:88:VAL:HG23	2.14	0.46
2:J:145:THR:HG22	3:O:117:PHE:HZ	1.81	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
3:O:189:ASN:HD22	3:O:210:ARG:HB2	1.81	0.46
1:A:263:GLY:HA3	1:A:435:LEU:CB	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:83:PHE:C	1:B:83:PHE:CD1	2.90	0.45
2:J:52:ASN:HD22	2:J:57:THR:HB	1.80	0.45
1:B:138:THR:O	1:B:143:MET:HB2	2.16	0.45
1:A:122:VAL:HB	1:A:160:ARG:HG2	1.99	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
1:B:110:PRO:HG3	1:B:448:ILE:HG21	1.99	0.45
3:O:138:PHE:CE1	3:O:143:ILE:HB	2.51	0.45
2:J:131:PRO:HD3	2:J:216:LYS:HG2	1.99	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: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: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
1:A:345:LEU:O	1:A:349:SER:HB2	2.17	0.45
2:J:67:LYS:NZ	2:J:85:LYS:O	2.50	0.45
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.82	0.45
3:O:63:GLY:O	3:O:64:SER:HB3	2.17	0.45
2:J:47:TRP:CZ2	2:J:49:GLY:HA2	2.52	0.45
2:I:52:ASN:HB2	2:I:53:PRO:HD3	1.99	0.45
1:B:132:PHE:O	1:B:136:LEU:HD13	2.17	0.45
1:A:414:GLU:HG2	1:B:419:TYR:CE1	2.52	0.45
1:B:281:HIS:O	1:B:285:GLY:N	2.43	0.45
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.99	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
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
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: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
2:I:15:GLY:O	2:I:85:LYS:HA	2.18	0.44
1:B:235:GLU:O	1:B:236:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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
1:B:171:ASP:HA	1:B:174:ARG:NH1	2.32	0.44
3:O:82:ALA:O	3:O:83:ALA:HB2	2.18	0.44
1:B:183:ALA:C	1:B:185:GLY:N	2.72	0.44
1:A:421:LEU:HA	1:A:421:LEU:HD23	1.78	0.44
1:B:125:TRP:HD1	1:B:126:ARG:HG3	1.82	0.44
1:A:123:ARG:NE	1:A:126:ARG:HD2	2.27	0.44
3:L:88:GLN:HB2	3:L:97:PHE:CD1	2.52	0.44
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.83	0.43
3:O:188:HIS:O	3:O:210:ARG:NE	2.51	0.43
1:A:124:TRP:O	1:A:126:ARG:N	2.50	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
1:B:53:PHE:CE1	1:B:136:LEU:HD12	2.53	0.43
3:L:6:GLN:HE22	3:L:86:TYR:HA	1.83	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
2:I:38:ARG:NH1	2:I:90:ASP:HA	2.34	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
3:O:29:VAL:HG23	3:O:70:TYR:CE1	2.53	0.43
1:B:402:ILE:HD12	1:B:445:TYR:CD1	2.54	0.43
3:O:6:GLN:NE2	3:O:87:CYS:H	2.15	0.43
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.54	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
3:L:190:SER:HA	3:L:209:ASN:OD1	2.18	0.43
2:I:153:TYR:CE1	2:I:183:TYR:HB2	2.54	0.43
1:A:356:ILE:CG2	1:A:360:MET:CE	2.85	0.43
1:B:216:LYS:O	1:B:220:ILE:HG13	2.19	0.43
1:A:163:LEU:HD12	1:A:168:LEU:HB2	2.00	0.43
1:A:78:LEU:HD11	1:A:307:PHE:CE1	2.54	0.43
1:A:31:THR:HA	1:A:32:PRO:HD2	1.89	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
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:O:4:LEU:HD21	3:O:89:GLN:HG2	2.00	0.42
1:A:449:LEU:O	1:A:453:LEU:HB2	2.19	0.42
1:A:199:PHE:HA	1:A:407:THR:OG1	2.19	0.42
2:I:94:TYR:O	2:I:114:GLY:HA2	2.18	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:B:150:PRO:HD3	1:B:354:GLY:CA	2.39	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: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
3:O:90:TRP:CG	3:O:95:GLN:HB3	2.55	0.42
1:B:124:TRP:O	1:B:126:ARG:N	2.52	0.42
3:L:80:GLU:HA	3:L:167:SER:O	2.19	0.42
2:J:6:GLU:HA	2:J:21:SER:O	2.19	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
1:A:251:THR:HG22	1:A:255:TYR:HE1	1.83	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
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
1:B:37:PHE:O	1:B:41:VAL:HG12	2.19	0.42
3:L:15:PRO:HD3	3:L:105:ILE:HG23	2.01	0.42
1:A:383:HIS:ND1	2:J:106:TRP:CD1	2.86	0.42
1:A:219:PHE:HD2	1:B:430:LEU:HD13	1.84	0.42
1:B:212:LEU:H	1:B:212:LEU:HD12	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:426:ILE:HG22	1:B:223:ILE:HD11	2.03	0.41
1:A:150:PRO:O	1:A:154:ILE:HG13	2.20	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:73:ASP:O	1:A:74:ASN:C	2.59	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
1:B:198:LEU:HA	1:B:198:LEU:HD13	1.94	0.41
3:L:162:TRP:CD1	3:L:174:MET:HG3	2.54	0.41
1:B:135:GLY:C	1:B:137:GLY:N	2.74	0.41
1:B:163:LEU:HD13	1:B:173:ALA:O	2.20	0.41
1:A:148:GLU:O	1:A:149:GLY:C	2.59	0.41
3:L:90:TRP:CE3	3:L:95:GLN:HG3	2.56	0.41
1:A:274:LEU:HD23	1:A:277:GLN:HE22	1.86	0.41
2:J:196:TRP:CD1	2:J:197:PRO:HA	2.55	0.41
3:O:19:VAL:HG11	3:O:103:LEU:CD1	2.48	0.41
2:J:217:LYS:HE2	2:J:219:VAL:CG1	2.50	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: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
1:A:284:HIS:HA	1:A:290:LYS:HB3	2.03	0.41
2:I:17:SER:HB3	2:I:84:SER:HA	2.03	0.41
1:A:383:HIS:NE2	2:J:50:GLU:OE1	2.54	0.41
1:B:124:TRP:CE3	1:B:125:TRP:N	2.89	0.41
3:O:60:ARG:CZ	3:O:78:GLU:HG3	2.51	0.41
2:J:30:SER:O	2:J:32:TYR:N	2.51	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
1:A:197:ILE:HG13	1:A:222:VAL:HG21	2.02	0.41
1:A:176:THR:O	1:A:180:THR:HG23	2.20	0.41
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
3:O:65:GLY:O	3:O:66:SER:HB3	2.21	0.41
1:B:31:THR:HA	1:B:32:PRO:HD2	1.87	0.41
1:A:421:LEU:O	1:A:425:MET:HG3	2.21	0.41
3:L:192:THR:HB	3:L:207:SER:HB3	2.03	0.41
1:A:298:ILE:HG12	1:A:346:LEU:HD23	2.03	0.41
1:A:104:ALA:HB2	1:A:127:VAL:HG13	2.02	0.41
2:I:134:PRO:HB2	2:I:138:ALA:HB2	2.03	0.41
1:B:218:VAL:O	1:B:222:VAL:HG23	2.21	0.41
1:A:264:ILE:HG22	1:A:435:LEU:HD12	2.02	0.41
1:B:73:ASP:O	1:B:74:ASN:C	2.59	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:185:TYR:CD1	3:L:191:TYR:CZ	3.09	0.41
1:A:210:TYR:H	1:B:210:TYR:HB2	1.85	0.41
2:I:93:LEU:HD23	2:I:95:TYR:OH	2.20	0.41
1:B:61:GLN:HA	1:B:64:ARG:HE	1.85	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
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: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
1:A:377:GLU:CG	1:A:378:LEU:N	2.84	0.40
3:L:38:LYS:O	3:L:41:THR:HG22	2.22	0.40
2:J:111:TRP:N	2:J:111:TRP:CD1	2.90	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
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: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:L:140:PRO:HD3	3:L:198:LYS:HD3	2.04	0.40
3:O:79:ALA:O	3:O:81:ASP:N	2.55	0.40
3:O:94:PRO:HB2	3:O:95:GLN:OE1	2.21	0.40
1:A:201:ILE:HD13	1:A:201:ILE:HG21	1.91	0.40
2:J:16:GLY:O	2:J:86:VAL:HG23	2.21	0.40
1:B:53:PHE:CE2	1:B:139:LEU:HD12	2.56	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%)	7	43
1	B	439/465 (94%)	369 (84%)	54 (12%)	16 (4%)	5	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	219/222 (99%)	190 (87%)	21 (10%)	8 (4%)	5	34
2	J	219/222 (99%)	186 (85%)	26 (12%)	7 (3%)	6	39
3	L	209/211 (99%)	183 (88%)	24 (12%)	2 (1%)	22	74
3	O	209/211 (99%)	180 (86%)	21 (10%)	8 (4%)	5	34
All	All	1737/1796 (97%)	1485 (86%)	198 (11%)	54 (3%)	7	41

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
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

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Mol	Chain	Res	Type
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%)	9	36
1	B	332/353 (94%)	293 (88%)	39 (12%)	8	34
2	I	181/182 (100%)	166 (92%)	15 (8%)	16	55
2	J	181/182 (100%)	156 (86%)	25 (14%)	5	24
3	L	185/185 (100%)	170 (92%)	15 (8%)	17	56
3	O	185/185 (100%)	166 (90%)	19 (10%)	10	40
All	All	1399/1440 (97%)	1249 (89%)	150 (11%)	10	38

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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%)	0.14	3 (0%) 84 38	94, 117, 145, 163	0
1	B	441/465 (94%)	0.20	6 (1%) 72 22	94, 116, 145, 162	0
2	I	221/222 (99%)	0.17	0 100 100	92, 118, 143, 162	0
2	J	221/222 (99%)	0.24	4 (1%) 65 18	90, 117, 142, 162	0
3	L	211/211 (100%)	0.34	7 (3%) 44 9	82, 112, 145, 154	0
3	O	211/211 (100%)	0.26	3 (1%) 72 22	96, 126, 145, 153	0
All	All	1749/1796 (97%)	0.21	23 (1%) 74 24	82, 118, 145, 163	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	135	GLY	3.9
1	B	73	ASP	3.1
2	J	139	ALA	2.8
3	L	146	LYS	2.8
1	B	165	ILE	2.7
3	L	155	GLN	2.7
2	J	137	ALA	2.6
3	O	154	ARG	2.5
1	B	104	ALA	2.4
3	L	147	TRP	2.4
3	L	180	LEU	2.3
1	A	19	ARG	2.3
1	A	72	ALA	2.2
2	J	140	ALA	2.2
3	O	112	PRO	2.2
3	L	151	GLY	2.2
3	L	127	GLY	2.2
1	B	168	LEU	2.1
3	L	193	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	O	153	GLU	2.1
1	A	447	ALA	2.0
1	B	307	PHE	2.0
1	B	68	LEU	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.