



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2017 – 10:55 AM EST

PDB ID : 5MVZ
Title : Fab 4AB007 bound to Interleukin-1-beta
Authors : Stark, W.; Seibert, V.
Deposited on : 2017-01-17
Resolution : 2.15 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

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

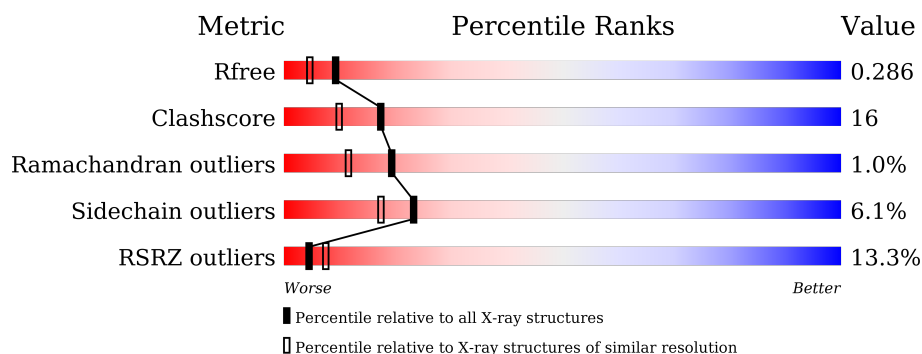
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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. 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	240	<div> <div>3%</div> <div>82%</div> <div>9%</div> <div>8%</div> </div>
1	H	240	<div> <div>2%</div> <div>77%</div> <div>12%</div> <div>8%</div> </div>
2	B	249	<div> <div>4%</div> <div>75%</div> <div>11%</div> <div>14%</div> </div>
2	L	249	<div> <div>2%</div> <div>71%</div> <div>14%</div> <div>14%</div> </div>
3	U	177	<div> <div>28%</div> <div>52%</div> <div>23%</div> <div>23%</div> </div>
3	V	177	<div> <div>44%</div> <div>34%</div> <div>32%</div> <div>14%</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	301	-	-	X	X
4	GOL	B	302	-	-	-	X
4	GOL	H	301	-	-	-	X
4	GOL	L	301	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9536 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 Fab 4AB007 H-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	221	Total	C	N	O	S	0	0	0
			1659	1053	269	328	9			
1	A	221	Total	C	N	O	S	0	0	0
			1659	1053	269	328	9			

- Molecule 2 is a protein called Fab 4AB007 L-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1662	1040	282	335	5			
2	B	214	Total	C	N	O	S	0	0	0
			1653	1035	281	332	5			

- Molecule 3 is a protein called Interleukin-1 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	U	136	Total	C	N	O	S	0	0	0
			1084	694	175	208	7			
3	V	144	Total	C	N	O	S	0	0	0
			1137	727	187	215	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	-23	MET	-	initiating methionine	UNP B5BUQ8
U	-22	ALA	-	expression tag	UNP B5BUQ8
U	-21	HIS	-	expression tag	UNP B5BUQ8
U	-20	HIS	-	expression tag	UNP B5BUQ8
U	-19	HIS	-	expression tag	UNP B5BUQ8
U	-18	HIS	-	expression tag	UNP B5BUQ8
U	-17	HIS	-	expression tag	UNP B5BUQ8
U	-16	HIS	-	expression tag	UNP B5BUQ8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
U	-15	HIS	-	expression tag	UNP B5BUQ8
U	-14	HIS	-	expression tag	UNP B5BUQ8
U	-13	HIS	-	expression tag	UNP B5BUQ8
U	-12	HIS	-	expression tag	UNP B5BUQ8
U	-11	HIS	-	expression tag	UNP B5BUQ8
U	-10	HIS	-	expression tag	UNP B5BUQ8
U	-9	PRO	-	expression tag	UNP B5BUQ8
U	-8	ALA	-	expression tag	UNP B5BUQ8
U	-7	GLY	-	expression tag	UNP B5BUQ8
U	-6	GLU	-	expression tag	UNP B5BUQ8
U	-5	ASN	-	expression tag	UNP B5BUQ8
U	-4	LEU	-	expression tag	UNP B5BUQ8
U	-3	TYR	-	expression tag	UNP B5BUQ8
U	-2	PHE	-	expression tag	UNP B5BUQ8
U	-1	GLN	-	expression tag	UNP B5BUQ8
U	0	GLY	-	expression tag	UNP B5BUQ8
V	-23	MET	-	initiating methionine	UNP B5BUQ8
V	-22	ALA	-	expression tag	UNP B5BUQ8
V	-21	HIS	-	expression tag	UNP B5BUQ8
V	-20	HIS	-	expression tag	UNP B5BUQ8
V	-19	HIS	-	expression tag	UNP B5BUQ8
V	-18	HIS	-	expression tag	UNP B5BUQ8
V	-17	HIS	-	expression tag	UNP B5BUQ8
V	-16	HIS	-	expression tag	UNP B5BUQ8
V	-15	HIS	-	expression tag	UNP B5BUQ8
V	-14	HIS	-	expression tag	UNP B5BUQ8
V	-13	HIS	-	expression tag	UNP B5BUQ8
V	-12	HIS	-	expression tag	UNP B5BUQ8
V	-11	HIS	-	expression tag	UNP B5BUQ8
V	-10	HIS	-	expression tag	UNP B5BUQ8
V	-9	PRO	-	expression tag	UNP B5BUQ8
V	-8	ALA	-	expression tag	UNP B5BUQ8
V	-7	GLY	-	expression tag	UNP B5BUQ8
V	-6	GLU	-	expression tag	UNP B5BUQ8
V	-5	ASN	-	expression tag	UNP B5BUQ8
V	-4	LEU	-	expression tag	UNP B5BUQ8
V	-3	TYR	-	expression tag	UNP B5BUQ8
V	-2	PHE	-	expression tag	UNP B5BUQ8
V	-1	GLN	-	expression tag	UNP B5BUQ8
V	0	GLY	-	expression tag	UNP B5BUQ8

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	136	Total	O	0	0
			136	136		
5	L	152	Total	O	0	0
			152	152		
5	U	28	Total	O	0	0
			28	28		
5	A	130	Total	O	0	0
			130	130		

Continued on next page...

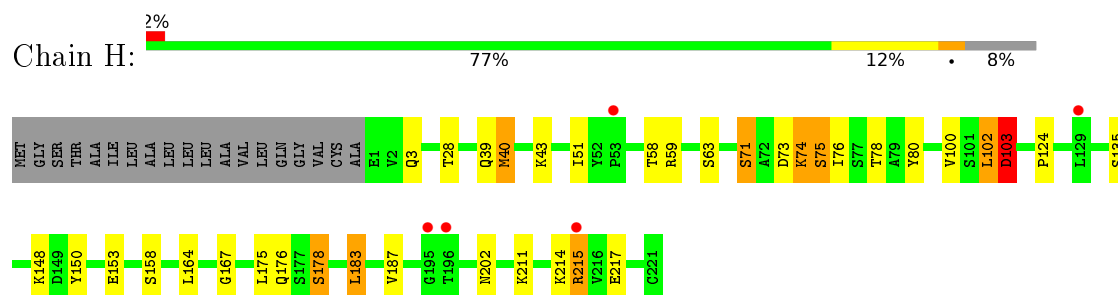
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	156	Total 156	O 156	0	0
5	V	32	Total 32	O 32	0	0

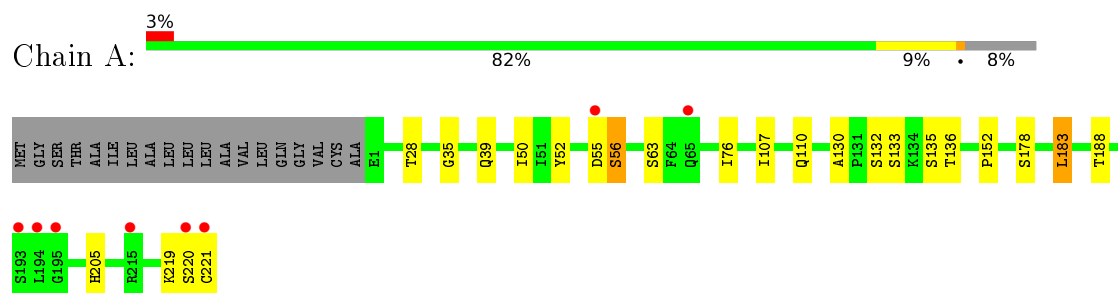
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

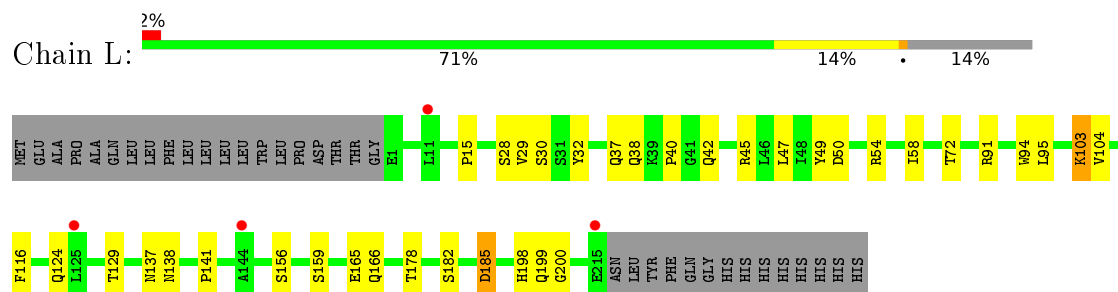
• Molecule 1: Fab 4AB007 H-chain



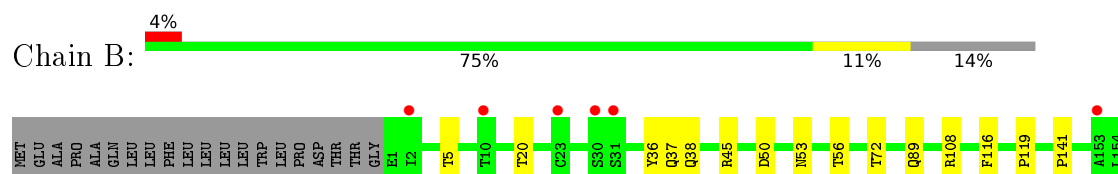
• Molecule 1: Fab 4AB007 H-chain

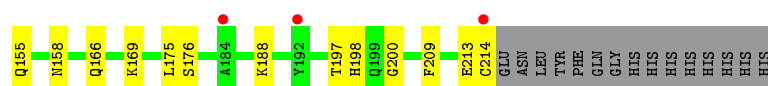


• Molecule 2: Fab 4AB007 L-chain

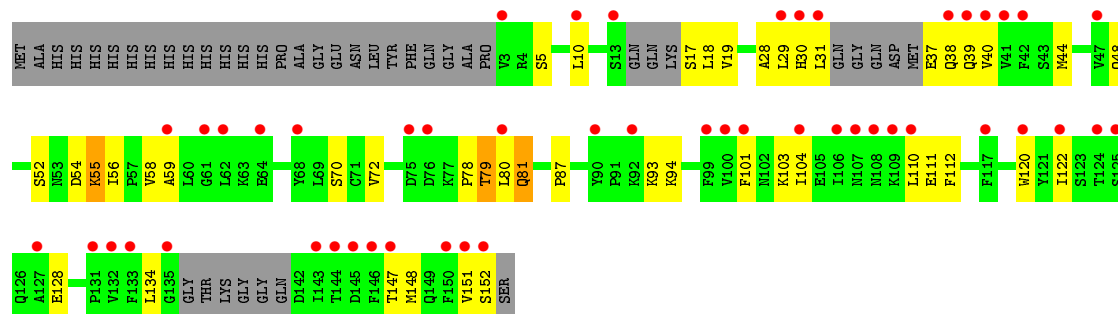


• Molecule 2: Fab 4AB007 L-chain

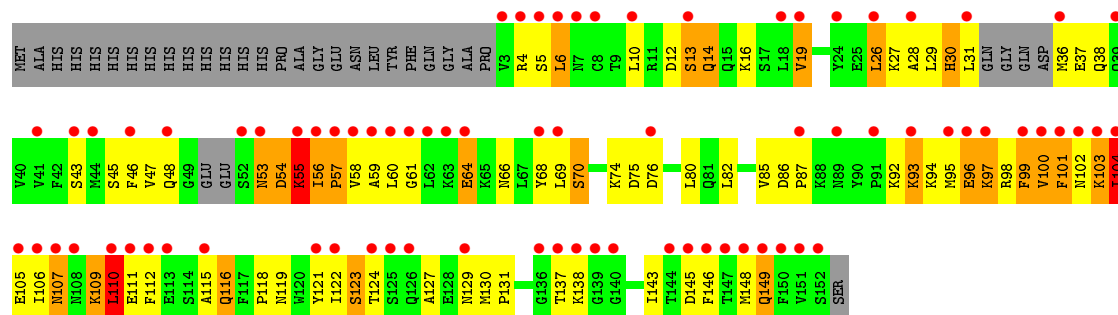




• Molecule 3: Interleukin-1 beta



• Molecule 3: Interleukin-1 beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	111.04Å 158.38Å 153.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.68 – 2.15 45.53 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.68-2.15) 99.6 (45.53-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.219 , 0.281 0.232 , 0.286	Depositor DCC
R_{free} test set	3665 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	40.1	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 73.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9536	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.2605e-03.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.71	0/1702	0.76	1/2316 (0.0%)
1	H	0.71	0/1702	0.75	1/2316 (0.0%)
2	B	0.75	0/1690	0.85	1/2297 (0.0%)
2	L	0.77	0/1699	0.84	0/2309
3	U	0.48	0/1103	0.65	0/1484
3	V	0.64	0/1157	0.90	2/1556 (0.1%)
All	All	0.70	0/9053	0.80	5/12278 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	V	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	104	ILE	CG1-CB-CG2	8.56	130.24	111.40
3	V	110	LEU	CA-CB-CG	6.87	131.10	115.30
2	B	108	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	H	103	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	183	LEU	CA-CB-CG	5.55	128.06	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	V	137	THR	Peptide
3	V	57	PRO	Peptide

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	1659	0	1626	21	8
1	H	1659	0	1625	28	0
2	B	1653	0	1603	17	0
2	L	1662	0	1608	36	0
3	U	1084	0	1066	38	0
3	V	1137	0	1124	155	9
4	A	6	0	8	4	0
4	B	18	0	24	1	0
4	H	6	0	8	3	0
4	L	18	0	24	9	0
5	A	130	0	0	0	0
5	B	156	0	0	3	1
5	H	136	0	0	7	0
5	L	152	0	0	10	1
5	U	28	0	0	2	1
5	V	32	0	0	11	0
All	All	9536	0	8716	284	11

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 16.

All (284) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:4:ARG:CZ	5:V:201:HOH:O	1.75	1.26
3:V:45:SER:O	3:V:59:ALA:HB3	1.31	1.24
3:V:104:ILE:HD12	3:V:110:LEU:CA	1.72	1.17
3:V:104:ILE:CD1	3:V:109:LYS:O	1.93	1.16
3:V:47:VAL:HG22	3:V:58:VAL:CG1	1.77	1.14
3:V:104:ILE:HD12	3:V:110:LEU:HA	1.21	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:104:ILE:HG21	3:V:110:LEU:HG	1.27	1.11
3:V:127:ALA:HB1	5:V:208:HOH:O	1.49	1.08
3:V:4:ARG:NH1	5:V:201:HOH:O	1.75	1.07
3:V:4:ARG:NH2	5:V:202:HOH:O	1.87	1.06
3:V:104:ILE:HD12	3:V:109:LYS:C	1.77	1.04
3:V:104:ILE:HD12	3:V:109:LYS:O	1.54	1.04
3:V:104:ILE:HG21	3:V:110:LEU:CG	1.87	1.03
3:V:47:VAL:HG22	3:V:58:VAL:HG11	1.36	1.02
3:V:57:PRO:HA	3:V:103:LYS:HB3	1.02	1.01
3:V:57:PRO:CA	3:V:103:LYS:HB3	1.91	0.99
3:V:104:ILE:CD1	3:V:110:LEU:CA	2.35	0.99
3:V:6:LEU:HD21	3:V:46:PHE:CE1	1.97	0.99
3:V:56:ILE:O	3:V:103:LYS:HB2	1.63	0.98
3:V:57:PRO:HA	3:V:103:LYS:CB	1.94	0.97
1:H:100:VAL:HG23	1:H:102:LEU:HD22	1.47	0.97
3:V:56:ILE:O	3:V:103:LYS:CB	2.12	0.96
3:V:104:ILE:CD1	3:V:110:LEU:HA	1.64	0.96
3:V:104:ILE:HD12	3:V:110:LEU:N	1.79	0.96
3:V:104:ILE:CG2	3:V:110:LEU:HG	1.96	0.95
3:V:104:ILE:HG21	3:V:110:LEU:CB	1.97	0.94
3:V:121:TYR:O	3:V:123:SER:OG	1.86	0.93
3:V:45:SER:O	3:V:59:ALA:CB	2.17	0.92
3:V:47:VAL:CG2	3:V:58:VAL:HG11	2.03	0.89
3:V:104:ILE:CG2	3:V:110:LEU:CB	2.50	0.88
3:V:61:GLY:HA3	5:V:219:HOH:O	1.72	0.88
1:H:153:GLU:OE2	5:H:401:HOH:O	1.92	0.87
1:A:188:THR:HG21	5:B:442:HOH:O	1.73	0.87
3:V:104:ILE:CG2	3:V:110:LEU:CG	2.55	0.85
3:V:6:LEU:HD21	3:V:46:PHE:CZ	2.13	0.83
3:V:6:LEU:HD23	3:V:6:LEU:N	1.93	0.83
3:V:104:ILE:HD13	3:V:105:GLU:CA	2.09	0.83
1:A:55:ASP:OD1	1:A:56:SER:N	2.12	0.82
3:U:52:SER:C	3:U:55:LYS:NZ	2.29	0.82
3:V:104:ILE:CG2	3:V:110:LEU:CA	2.58	0.81
1:H:39:GLN:HE22	2:L:38:GLN:HE22	1.30	0.80
1:H:215:ARG:NH2	1:H:217:GLU:OE2	2.14	0.80
3:V:104:ILE:CD1	3:V:109:LYS:C	2.45	0.79
2:L:166:GLN:HB2	4:L:301:GOL:H32	1.67	0.77
2:B:36:TYR:HE2	2:B:89:GLN:HG2	1.51	0.76
3:V:104:ILE:HD13	3:V:105:GLU:N	2.03	0.74
3:V:104:ILE:CB	3:V:110:LEU:HA	2.03	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:104:ILE:HG21	3:V:110:LEU:CA	2.17	0.74
3:U:112:PHE:HB2	3:U:122:ILE:HD12	1.69	0.73
1:A:152:PRO:O	1:A:205:HIS:HE1	1.71	0.73
3:U:30:HIS:N	3:U:128:GLU:OE2	2.22	0.72
3:V:104:ILE:CB	3:V:110:LEU:CA	2.65	0.71
3:V:104:ILE:HD13	3:V:105:GLU:HA	1.72	0.71
3:V:101:PHE:CE2	3:V:103:LYS:HA	2.26	0.70
1:A:110:GLN:HE21	4:A:301:GOL:C1	2.05	0.70
1:A:220:SER:HA	1:A:221:CYS:OXT	1.90	0.70
1:A:55:ASP:C	1:A:55:ASP:OD1	2.29	0.69
3:V:149:GLN:OE1	5:V:203:HOH:O	2.09	0.69
3:V:47:VAL:HG21	3:V:100:VAL:HG11	1.74	0.69
3:V:104:ILE:HD11	3:V:109:LYS:O	1.89	0.69
3:U:19:VAL:HA	3:U:40:VAL:HG23	1.73	0.68
3:V:56:ILE:O	3:V:103:LYS:HB3	1.92	0.68
3:V:58:VAL:HG13	3:V:100:VAL:HB	1.76	0.68
2:B:36:TYR:CE2	2:B:89:GLN:HG2	2.28	0.68
3:V:97:LYS:HD2	3:V:116:GLN:HB2	1.76	0.68
1:A:132:SER:HB2	1:A:221:CYS:HB3	1.74	0.68
1:H:71:SER:OG	5:H:402:HOH:O	2.11	0.68
2:B:36:TYR:HE2	2:B:89:GLN:CG	2.07	0.67
3:V:104:ILE:HG21	3:V:110:LEU:C	2.15	0.67
2:B:20:THR:HG23	2:B:72:THR:HG23	1.75	0.67
3:U:112:PHE:CB	3:U:122:ILE:HD12	2.24	0.66
3:V:97:LYS:HB2	3:V:100:VAL:N	2.11	0.66
3:U:52:SER:N	3:U:55:LYS:NZ	2.37	0.66
2:B:166:GLN:HB2	4:B:302:GOL:H2	1.78	0.65
1:H:73:ASP:OD2	5:H:403:HOH:O	2.14	0.65
3:V:101:PHE:CE2	3:V:112:PHE:HD1	2.15	0.65
3:V:29:LEU:HD13	3:V:129:ASN:OD1	1.95	0.65
3:V:16:LYS:HD2	3:V:29:LEU:HA	1.76	0.65
3:V:6:LEU:HD21	3:V:46:PHE:HE1	1.59	0.64
1:H:51:ILE:HD12	1:H:58:THR:OG1	1.97	0.64
3:U:44:MET:HE3	3:U:148:MET:SD	2.38	0.64
3:V:102:ASN:O	3:V:103:LYS:HG2	1.98	0.64
3:V:104:ILE:CD1	3:V:110:LEU:N	2.55	0.63
1:H:28:THR:HG21	3:U:87:PRO:HD2	1.79	0.63
3:V:104:ILE:HG23	3:V:110:LEU:CB	2.27	0.63
3:U:19:VAL:HA	3:U:40:VAL:CG2	2.28	0.63
3:V:112:PHE:CB	3:V:122:ILE:HD12	2.29	0.62
2:L:124:GLN:HG2	2:L:129:THR:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:104:ILE:HB	3:V:111:GLU:O	2.00	0.62
1:H:100:VAL:HG23	1:H:102:LEU:CD2	2.28	0.61
1:A:110:GLN:HE21	4:A:301:GOL:H11	1.66	0.61
3:V:54:ASP:HB2	3:V:103:LYS:HE2	1.82	0.61
1:A:52:TYR:O	1:A:55:ASP:O	2.19	0.61
2:L:40:PRO:HB2	5:L:516:HOH:O	1.99	0.60
3:V:12:ASP:OD2	3:V:16:LYS:NZ	2.30	0.60
3:V:104:ILE:CG2	3:V:110:LEU:HA	2.29	0.60
1:H:102:LEU:C	1:H:102:LEU:HD23	2.23	0.59
3:U:78:PRO:HD2	3:U:120:TRP:CH2	2.37	0.59
3:V:6:LEU:CD2	3:V:46:PHE:CE1	2.79	0.59
3:V:102:ASN:O	3:V:103:LYS:CG	2.49	0.59
2:L:166:GLN:H	4:L:301:GOL:C3	2.15	0.59
3:V:47:VAL:HG22	3:V:58:VAL:HG12	1.80	0.59
2:L:166:GLN:H	4:L:301:GOL:H32	1.67	0.59
3:V:47:VAL:CG2	3:V:100:VAL:HG11	2.33	0.58
3:V:16:LYS:HG2	3:V:30:HIS:ND1	2.17	0.58
3:U:44:MET:SD	3:U:58:VAL:HG21	2.43	0.58
3:V:110:LEU:HD23	3:V:146:PHE:HB2	1.85	0.58
1:H:135:SER:HA	2:L:116:PHE:CD1	2.39	0.58
3:V:14:GLN:NE2	3:V:30:HIS:CE1	2.72	0.58
2:B:198:HIS:CD2	2:B:200:GLY:H	2.22	0.57
2:L:103:LYS:HE3	5:L:422:HOH:O	2.04	0.57
1:H:28:THR:HG21	3:U:87:PRO:CD	2.36	0.56
3:V:112:PHE:HB3	3:V:122:ILE:HD12	1.87	0.56
3:U:44:MET:CG	3:U:58:VAL:HG21	2.36	0.56
3:V:6:LEU:CD2	3:V:46:PHE:HE1	2.17	0.56
1:H:175:LEU:HB3	5:H:498:HOH:O	2.05	0.56
2:B:155:GLN:HE21	2:B:158:ASN:HD21	1.54	0.56
2:L:15:PRO:HB2	4:L:302:GOL:H31	1.86	0.56
3:V:101:PHE:CE2	3:V:112:PHE:CD1	2.94	0.55
3:V:54:ASP:OD2	3:V:54:ASP:N	2.40	0.55
2:L:199:GLN:HG2	5:L:536:HOH:O	2.06	0.55
3:V:56:ILE:HG12	3:V:56:ILE:O	2.06	0.55
3:U:18:LEU:O	3:U:39:GLN:HG2	2.05	0.55
3:V:97:LYS:HD3	3:V:116:GLN:N	2.22	0.55
3:V:104:ILE:HG23	3:V:110:LEU:HB2	1.89	0.55
2:L:198:HIS:CD2	2:L:200:GLY:H	2.24	0.55
3:V:104:ILE:HG23	3:V:104:ILE:O	2.07	0.55
3:V:101:PHE:CD2	3:V:103:LYS:HA	2.42	0.55
3:V:112:PHE:HB2	3:V:122:ILE:HD12	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:HA	2:B:116:PHE:CD1	2.42	0.54
2:L:166:GLN:CB	4:L:301:GOL:H32	2.37	0.54
2:L:40:PRO:CB	5:L:516:HOH:O	2.55	0.54
3:V:112:PHE:HB2	3:V:122:ILE:HB	1.88	0.54
3:V:57:PRO:O	3:V:101:PHE:O	2.25	0.54
3:V:16:LYS:HG3	3:V:30:HIS:CE1	2.43	0.54
1:H:76:ILE:O	1:H:76:ILE:HG22	2.08	0.53
3:V:12:ASP:HB2	3:V:16:LYS:H	1.74	0.53
3:V:27:LYS:HG2	3:V:131:PRO:HA	1.91	0.53
1:H:76:ILE:HG22	1:H:78:THR:OG1	2.09	0.53
1:A:220:SER:HA	1:A:221:CYS:C	2.26	0.52
3:V:64:GLU:CB	5:V:210:HOH:O	2.56	0.52
1:H:211:LYS:NZ	5:H:404:HOH:O	2.14	0.52
2:L:42:GLN:NE2	5:L:407:HOH:O	2.40	0.52
3:V:104:ILE:HB	3:V:111:GLU:C	2.23	0.52
3:V:97:LYS:CD	3:V:116:GLN:N	2.73	0.52
1:H:183:LEU:HD12	1:H:183:LEU:C	2.30	0.52
1:H:74:LYS:HG2	5:H:454:HOH:O	2.10	0.52
3:U:103:LYS:HG2	3:U:110:LEU:HD22	1.92	0.52
3:V:97:LYS:HA	3:V:99:PHE:N	2.24	0.52
3:V:66:ASN:HB3	3:V:85:VAL:O	2.10	0.52
3:U:44:MET:CG	3:U:58:VAL:CG2	2.88	0.52
3:V:100:VAL:HG23	3:V:100:VAL:O	2.10	0.51
1:A:110:GLN:NE2	4:A:301:GOL:H11	2.26	0.51
3:V:97:LYS:HA	3:V:99:PHE:H	1.76	0.51
3:V:56:ILE:C	3:V:103:LYS:HD3	2.31	0.51
3:U:55:LYS:HA	3:U:103:LYS:O	2.11	0.50
3:V:61:GLY:CA	5:V:219:HOH:O	2.43	0.50
3:V:96:GLU:O	3:V:99:PHE:CD1	2.65	0.49
3:V:96:GLU:HA	3:V:96:GLU:OE1	2.12	0.49
3:V:36:MET:CB	3:V:38:GLN:OE1	2.61	0.49
3:V:55:LYS:O	3:V:57:PRO:HD3	2.13	0.49
3:V:69:LEU:O	3:V:99:PHE:HA	2.13	0.49
3:V:47:VAL:HB	3:V:93:LYS:O	2.13	0.49
2:L:54:ARG:NE	5:L:408:HOH:O	2.44	0.49
3:V:103:LYS:CG	3:V:104:ILE:N	2.74	0.49
3:V:57:PRO:CG	3:V:58:VAL:HG23	2.43	0.49
1:A:76:ILE:HG22	1:A:76:ILE:O	2.13	0.49
1:H:80:TYR:OH	5:H:405:HOH:O	2.19	0.49
1:H:102:LEU:HG	2:L:49:TYR:CD2	2.48	0.49
3:V:53:ASN:OD1	3:V:53:ASN:C	2.51	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ALA:HB1	1:A:219:LYS:HB2	1.94	0.48
2:L:42:GLN:NE2	5:L:411:HOH:O	2.46	0.48
3:U:5:SER:HA	3:U:44:MET:O	2.13	0.48
1:A:110:GLN:HE21	4:A:301:GOL:H12	1.78	0.48
3:V:97:LYS:HD2	3:V:116:GLN:CB	2.42	0.48
3:V:56:ILE:O	3:V:103:LYS:HD3	2.14	0.48
2:L:15:PRO:CB	4:L:302:GOL:H31	2.44	0.48
3:V:4:ARG:HD3	3:V:46:PHE:CD1	2.49	0.48
1:A:39:GLN:HE22	2:B:38:GLN:HE22	1.62	0.48
3:U:87:PRO:HG3	5:U:212:HOH:O	2.13	0.48
3:V:19:VAL:HG11	3:V:29:LEU:HD21	1.94	0.48
3:V:70:SER:HA	3:V:98:ARG:O	2.13	0.48
4:H:301:GOL:O3	2:L:137:ASN:ND2	2.47	0.47
3:V:37:GLU:N	3:V:38:GLN:HB3	2.29	0.47
3:U:151:VAL:O	3:U:152:SER:C	2.51	0.47
3:U:37:GLU:O	3:U:37:GLU:CG	2.62	0.47
3:U:55:LYS:O	3:U:55:LYS:HG2	2.14	0.47
3:V:30:HIS:O	3:V:31:LEU:HD23	2.14	0.47
3:V:68:TYR:HB3	3:V:99:PHE:HD2	1.80	0.47
3:V:10:LEU:HD21	3:V:148:MET:CE	2.44	0.47
1:A:28:THR:HG21	3:V:86:ASP:HA	1.96	0.47
3:V:104:ILE:HD13	3:V:104:ILE:C	2.35	0.47
2:L:166:GLN:N	4:L:301:GOL:H32	2.29	0.46
3:V:14:GLN:O	3:V:30:HIS:NE2	2.47	0.46
3:U:17:SER:O	3:U:28:ALA:HA	2.14	0.46
3:V:104:ILE:CB	3:V:111:GLU:O	2.62	0.46
1:H:40:MET:HB3	1:H:43:LYS:HD2	1.96	0.46
2:B:37:GLN:HE22	2:B:45:ARG:HH21	1.62	0.46
3:V:5:SER:C	3:V:6:LEU:HD23	2.35	0.46
3:V:37:GLU:HA	3:V:38:GLN:HB3	1.97	0.46
2:L:91:ARG:HA	2:L:95:LEU:O	2.16	0.46
1:H:73:ASP:OD1	1:H:75:SER:OG	2.25	0.45
3:U:101:PHE:CE1	3:U:122:ILE:HD11	2.51	0.45
3:V:10:LEU:HD21	3:V:148:MET:HE2	1.97	0.45
3:V:37:GLU:CA	3:V:38:GLN:HB3	2.46	0.45
1:H:164:LEU:HD21	1:H:187:VAL:HG21	1.98	0.45
3:V:36:MET:HB3	3:V:38:GLN:OE1	2.17	0.45
3:V:112:PHE:O	3:V:122:ILE:N	2.46	0.45
2:B:141:PRO:O	2:B:198:HIS:HE1	1.98	0.45
3:V:47:VAL:CG2	3:V:58:VAL:CG1	2.66	0.45
3:V:54:ASP:CB	3:V:103:LYS:HE2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:19:VAL:CA	3:U:40:VAL:CG2	2.93	0.45
3:V:57:PRO:CB	3:V:58:VAL:HG23	2.47	0.45
1:H:124:PRO:HB3	1:H:150:TYR:HB3	1.99	0.45
3:U:19:VAL:CA	3:U:40:VAL:HG23	2.43	0.45
2:B:175:LEU:HD23	2:B:176:SER:N	2.32	0.45
2:L:72:THR:HG23	5:L:529:HOH:O	2.16	0.44
3:V:64:GLU:HB2	5:V:210:HOH:O	2.14	0.44
3:V:74:LYS:NZ	5:V:205:HOH:O	2.41	0.44
2:L:199:GLN:CG	5:L:536:HOH:O	2.65	0.44
3:U:30:HIS:HB2	3:U:128:GLU:OE2	2.17	0.44
3:V:16:LYS:CG	3:V:30:HIS:CE1	3.00	0.44
3:V:43:SER:HB3	5:V:219:HOH:O	2.17	0.44
3:V:28:ALA:HB3	3:V:124:THR:CG2	2.48	0.44
1:H:59:ARG:HG3	2:L:94:TRP:CE3	2.52	0.44
3:V:26:LEU:HA	3:V:26:LEU:HD22	1.90	0.44
3:V:102:ASN:O	3:V:103:LYS:CB	2.66	0.43
3:V:61:GLY:HA2	3:V:68:TYR:HA	2.00	0.43
3:V:4:ARG:HD3	3:V:46:PHE:CE1	2.53	0.43
3:U:44:MET:HG3	3:U:58:VAL:CG2	2.48	0.43
3:U:72:VAL:O	3:U:79:THR:N	2.52	0.43
2:L:37:GLN:HE22	2:L:45:ARG:HH21	1.67	0.43
2:L:141:PRO:O	2:L:198:HIS:HE1	2.02	0.43
3:V:118:PRO:O	3:V:119:ASN:HB2	2.19	0.43
2:L:32:TYR:HA	2:L:50:ASP:HA	2.01	0.43
3:U:94:LYS:O	3:U:94:LYS:NZ	2.31	0.43
2:L:199:GLN:CB	5:L:536:HOH:O	2.67	0.42
3:U:58:VAL:HG22	3:U:59:ALA:N	2.34	0.42
3:V:57:PRO:HG2	3:V:58:VAL:HG23	2.00	0.42
2:L:182:SER:OG	2:L:185:ASP:OD1	2.36	0.42
3:V:111:GLU:HG2	3:V:145:ASP:HA	2.01	0.42
1:A:188:THR:CG2	5:B:442:HOH:O	2.49	0.42
2:L:29:VAL:HG12	2:L:30:SER:N	2.35	0.42
3:V:92:LYS:HB3	3:V:95:MET:SD	2.59	0.42
2:B:119:PRO:HB3	2:B:209:PHE:CZ	2.54	0.42
3:V:103:LYS:O	3:V:112:PHE:HA	2.19	0.42
3:V:47:VAL:H	3:V:58:VAL:HG11	1.85	0.42
3:V:13:SER:OG	3:V:143:ILE:CG2	2.67	0.42
1:A:221:CYS:SG	2:B:214:CYS:HB2	2.59	0.42
1:H:158:SER:OG	1:H:202:ASN:OD1	2.38	0.42
3:V:57:PRO:HB2	3:V:58:VAL:HG23	2.01	0.42
2:L:165:GLU:HB3	4:L:301:GOL:H31	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:103:LYS:HE2	2:L:104:VAL:O	2.20	0.42
3:U:52:SER:HB3	5:U:219:HOH:O	2.18	0.42
1:A:28:THR:HG21	3:V:87:PRO:HD2	2.02	0.41
2:B:50:ASP:HB3	2:B:53:ASN:ND2	2.35	0.41
1:H:167:GLY:HA2	4:H:301:GOL:H11	2.01	0.41
3:V:86:ASP:OD1	3:V:87:PRO:HD2	2.20	0.41
3:U:70:SER:OG	3:U:81:GLN:NE2	2.53	0.41
3:V:107:ASN:HA	3:V:107:ASN:HD22	1.66	0.41
3:U:30:HIS:O	3:U:31:LEU:C	2.59	0.41
3:V:121:TYR:O	3:V:122:ILE:C	2.57	0.41
3:V:12:ASP:HB2	3:V:16:LYS:N	2.34	0.41
2:B:5:THR:HG23	5:B:402:HOH:O	2.21	0.41
1:H:148:LYS:NZ	1:H:176:GLN:OE1	2.53	0.41
2:L:47:LEU:HD23	2:L:58:ILE:HD12	2.02	0.41
3:V:55:LYS:HG2	3:V:55:LYS:H	1.08	0.41
1:A:35:GLY:CA	1:A:50:ILE:HD12	2.50	0.41
3:U:104:ILE:HB	3:U:111:GLU:HB2	2.03	0.41
3:U:10:LEU:O	3:U:39:GLN:NE2	2.54	0.41
3:U:80:LEU:HB2	3:U:134:LEU:HB2	2.03	0.40
3:V:69:LEU:HD22	3:V:80:LEU:HD11	2.04	0.40
3:V:96:GLU:O	3:V:99:PHE:HD1	2.04	0.40
3:V:26:LEU:HD23	3:V:82:LEU:HD11	2.03	0.40
3:V:36:MET:HB2	3:V:38:GLN:OE1	2.21	0.40
3:V:47:VAL:H	3:V:58:VAL:CG1	2.34	0.40
3:V:6:LEU:N	3:V:6:LEU:CD2	2.69	0.40
3:V:97:LYS:NZ	3:V:115:ALA:HB3	2.36	0.40
2:B:213:GLU:O	2:B:214:CYS:HB3	2.21	0.40
4:H:301:GOL:H2	2:L:138:ASN:HD21	1.86	0.40
3:V:16:LYS:CG	3:V:30:HIS:ND1	2.85	0.40
2:L:103:LYS:NZ	4:L:301:GOL:H2	2.37	0.40
2:L:159:SER:HA	2:L:178:THR:O	2.22	0.40
3:U:18:LEU:O	3:U:40:VAL:HG23	2.22	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:SER:O	3:V:55:LYS:NZ[5_555]	1.12	1.08
1:A:133:SER:N	3:V:55:LYS:CE[5_555]	1.61	0.59
1:A:133:SER:CA	3:V:55:LYS:CD[5_555]	1.67	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:OG1	3:V:55:LYS:NZ[5_555]	1.90	0.30
1:A:132:SER:C	3:V:55:LYS:CE[5_555]	1.92	0.28
1:A:132:SER:O	3:V:55:LYS:CE[5_555]	1.93	0.27
1:A:132:SER:C	3:V:55:LYS:NZ[5_555]	2.09	0.11
5:L:477:HOH:O	5:B:535:HOH:O[8_445]	2.11	0.09
1:A:133:SER:C	3:V:55:LYS:CE[5_555]	2.13	0.07
5:U:211:HOH:O	5:U:211:HOH:O[3_654]	2.17	0.03
3:V:14:GLN:NE2	3:V:14:GLN:NE2[3_555]	2.17	0.03

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	219/240 (91%)	214 (98%)	3 (1%)	2 (1%)	21	13
1	H	219/240 (91%)	209 (95%)	8 (4%)	2 (1%)	21	13
2	B	212/249 (85%)	203 (96%)	9 (4%)	0	100	100
2	L	213/249 (86%)	204 (96%)	9 (4%)	0	100	100
3	U	128/177 (72%)	123 (96%)	5 (4%)	0	100	100
3	V	138/177 (78%)	114 (83%)	17 (12%)	7 (5%)	2	0
All	All	1129/1332 (85%)	1067 (94%)	51 (4%)	11 (1%)	19	11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	V	103	LYS
1	H	178	SER
3	V	101	PHE
3	V	138	LYS
1	A	56	SER
1	A	178	SER
3	V	30	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	V	55	LYS
1	H	103	ASP
3	V	100	VAL
3	V	106	ILE

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	188/201 (94%)	185 (98%)	3 (2%)	70	76
1	H	188/201 (94%)	176 (94%)	12 (6%)	22	15
2	B	186/217 (86%)	182 (98%)	4 (2%)	60	63
2	L	187/217 (86%)	183 (98%)	4 (2%)	61	65
3	U	125/160 (78%)	115 (92%)	10 (8%)	15	9
3	V	128/160 (80%)	100 (78%)	28 (22%)	1	0
All	All	1002/1156 (87%)	941 (94%)	61 (6%)	23	17

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	40	MET
1	H	63	SER
1	H	71	SER
1	H	74	LYS
1	H	75	SER
1	H	102	LEU
1	H	103	ASP
1	H	178	SER
1	H	183	LEU
1	H	214	LYS
1	H	215	ARG
2	L	28	SER
2	L	103	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	156	SER
2	L	185	ASP
3	U	29	LEU
3	U	38	GLN
3	U	48	GLN
3	U	54	ASP
3	U	55	LYS
3	U	56	ILE
3	U	79	THR
3	U	81	GLN
3	U	93	LYS
3	U	147	THR
1	A	63	SER
1	A	107	ILE
1	A	183	LEU
2	B	56	THR
2	B	169	LYS
2	B	188	LYS
2	B	197	THR
3	V	6	LEU
3	V	13	SER
3	V	14	GLN
3	V	19	VAL
3	V	26	LEU
3	V	48	GLN
3	V	53	ASN
3	V	54	ASP
3	V	55	LYS
3	V	56	ILE
3	V	60	LEU
3	V	64	GLU
3	V	70	SER
3	V	75	ASP
3	V	76	ASP
3	V	93	LYS
3	V	94	LYS
3	V	96	GLU
3	V	97	LYS
3	V	99	PHE
3	V	104	ILE
3	V	107	ASN
3	V	109	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	V	110	LEU
3	V	116	GLN
3	V	123	SER
3	V	130	MET
3	V	149	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	37	GLN
2	L	38	GLN
2	L	89	GLN
2	L	138	ASN
2	L	155	GLN
2	L	160	GLN
2	L	198	HIS
3	U	81	GLN
3	U	102	ASN
1	A	169	HIS
1	A	176	GLN
1	A	205	HIS
2	B	37	GLN
2	B	38	GLN
2	B	53	ASN
2	B	89	GLN
2	B	155	GLN
2	B	160	GLN
2	B	198	HIS
3	V	14	GLN
3	V	107	ASN
3	V	116	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

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	A	301	-	5,5,5	0.70	0	5,5,5	1.35	0
4	GOL	B	301	-	5,5,5	0.64	0	5,5,5	0.87	0
4	GOL	B	302	-	5,5,5	0.67	0	5,5,5	0.61	0
4	GOL	B	303	-	5,5,5	0.25	0	5,5,5	0.52	0
4	GOL	H	301	-	5,5,5	0.23	0	5,5,5	0.40	0
4	GOL	L	301	-	5,5,5	0.55	0	5,5,5	1.19	0
4	GOL	L	302	-	5,5,5	0.59	0	5,5,5	0.94	0
4	GOL	L	303	-	5,5,5	0.40	0	5,5,5	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	301	-	-	0/4/4/4	0/0/0/0
4	GOL	B	301	-	-	0/4/4/4	0/0/0/0
4	GOL	B	302	-	-	0/4/4/4	0/0/0/0
4	GOL	B	303	-	-	0/4/4/4	0/0/0/0
4	GOL	H	301	-	-	0/4/4/4	0/0/0/0
4	GOL	L	301	-	-	0/4/4/4	0/0/0/0
4	GOL	L	302	-	-	0/4/4/4	0/0/0/0
4	GOL	L	303	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GOL	4	0
4	B	302	GOL	1	0
4	H	301	GOL	3	0
4	L	301	GOL	7	0
4	L	302	GOL	2	0

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	221/240 (92%)	0.43	8 (3%)	46	57	45, 59, 77, 94	0
1	H	221/240 (92%)	0.32	5 (2%)	64	72	48, 61, 79, 91	0
2	B	214/249 (85%)	0.59	9 (4%)	40	50	40, 55, 79, 108	0
2	L	215/249 (86%)	0.54	4 (1%)	70	78	41, 54, 76, 125	0
3	U	136/177 (76%)	1.74	49 (36%)	0	1	51, 87, 107, 125	0
3	V	144/177 (81%)	2.89	78 (54%)	0	0	60, 86, 116, 131	0
All	All	1151/1332 (86%)	0.92	153 (13%)	4	7	40, 62, 100, 131	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	V	110	LEU	11.5
3	V	100	VAL	11.0
3	V	3	VAL	9.4
3	V	58	VAL	9.4
3	V	18	LEU	8.7
3	V	139	GLY	8.3
3	U	10	LEU	7.6
3	V	48	GLN	7.1
3	U	108	ASN	7.0
3	V	59	ALA	6.6
3	V	151	VAL	6.6
2	L	215	GLU	6.5
3	V	41	VAL	6.5
3	V	150	PHE	6.4
3	V	137	THR	6.3
3	U	76	ASP	6.2
3	V	56	ILE	6.2
3	V	61	GLY	6.1
3	V	112	PHE	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	V	101	PHE	5.9
3	V	121	TYR	5.9
3	V	6	LEU	5.9
3	V	126	GLN	5.6
3	V	140	GLY	5.6
3	V	10	LEU	5.6
3	U	127	ALA	5.6
3	U	75	ASP	5.5
3	V	5	SER	5.4
3	V	68	TYR	5.3
3	U	120	TRP	5.3
3	V	57	PRO	5.2
3	V	93	LYS	5.1
3	V	4	ARG	5.1
3	V	104	ILE	5.1
3	V	64	GLU	4.9
3	V	28	ALA	4.8
3	U	117	PHE	4.8
3	U	62	LEU	4.8
3	V	53	ASN	4.8
3	V	96	GLU	4.7
3	U	151	VAL	4.7
3	V	63	LYS	4.6
3	V	52	SER	4.5
3	U	122	ILE	4.5
3	V	147	THR	4.4
3	V	144	THR	4.4
3	V	146	PHE	4.4
3	V	97	LYS	4.3
3	V	46	PHE	4.2
3	V	115	ALA	4.2
3	V	55	LYS	4.2
3	V	91	PRO	4.2
2	B	214	CYS	4.2
3	U	146	PHE	4.0
3	U	29	LEU	3.9
3	V	102	ASN	3.9
1	H	196	THR	3.7
3	V	122	ILE	3.6
1	A	195	GLY	3.6
3	U	39	GLN	3.6
1	A	194	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	U	135	GLY	3.6
3	V	129	ASN	3.6
2	B	31	SER	3.6
3	V	107	ASN	3.6
3	U	61	GLY	3.5
3	V	31	LEU	3.5
3	V	62	LEU	3.5
3	V	145	ASP	3.4
3	U	144	THR	3.4
3	U	106	ILE	3.3
3	U	143	ILE	3.3
2	B	2	ILE	3.3
3	V	13	SER	3.3
1	A	193	SER	3.3
3	U	30	HIS	3.3
1	A	215	ARG	3.2
3	V	138	LYS	3.2
2	B	192	TYR	3.2
3	U	107	ASN	3.1
3	V	106	ILE	3.1
3	V	124	THR	3.1
3	V	148	MET	3.1
3	V	44	MET	3.1
3	V	36	MET	3.0
3	V	136	GLY	3.0
3	V	8	CYS	3.0
1	A	221	CYS	2.9
3	U	68	TYR	2.8
1	A	220	SER	2.8
3	V	39	GLN	2.8
3	U	41	VAL	2.8
2	B	153	ALA	2.8
2	B	30	SER	2.8
3	U	40	VAL	2.8
3	V	26	LEU	2.8
3	U	59	ALA	2.8
3	U	150	PHE	2.8
3	U	147	THR	2.7
3	U	125	SER	2.7
3	V	60	LEU	2.7
3	U	13	SER	2.7
3	V	7	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	V	19	VAL	2.6
3	V	76	ASP	2.6
3	U	152	SER	2.6
3	U	31	LEU	2.6
2	L	125	LEU	2.6
3	V	87	PRO	2.5
3	V	105	GLU	2.5
1	A	55	ASP	2.5
3	U	124	THR	2.4
3	U	145	ASP	2.4
1	H	53	PRO	2.4
3	U	38	GLN	2.4
3	V	89	ASN	2.4
2	B	184	ALA	2.4
3	V	43	SER	2.4
3	V	99	PHE	2.4
3	U	64	GLU	2.4
3	V	69	LEU	2.4
3	U	133	PHE	2.3
3	V	103	LYS	2.3
1	H	215	ARG	2.3
3	V	111	GLU	2.3
2	B	23	CYS	2.3
3	V	108	ASN	2.3
3	U	92	LYS	2.2
1	H	195	GLY	2.2
2	B	10	THR	2.2
3	V	152	SER	2.2
3	V	24	TYR	2.1
3	V	125	SER	2.1
3	U	104	ILE	2.1
3	U	42	PHE	2.1
3	U	101	PHE	2.1
3	U	110	LEU	2.1
3	U	47	VAL	2.1
3	U	90	TYR	2.1
3	U	109	LYS	2.1
3	V	113	GLU	2.1
1	H	129	LEU	2.1
3	U	100	VAL	2.1
2	L	144	ALA	2.1
3	U	99	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	U	131	PRO	2.1
1	A	65	GLN	2.1
2	L	11	LEU	2.0
3	U	80	LEU	2.0
3	U	3	VAL	2.0
3	U	132	VAL	2.0
3	V	95	MET	2.0
3	V	149	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	GOL	H	301	6/6	0.67	0.55	38.05	70,75,82,87	0
4	GOL	A	301	6/6	0.81	0.23	4.17	46,59,63,70	0
4	GOL	L	301	6/6	0.75	0.28	3.99	49,56,68,69	0
4	GOL	B	302	6/6	0.85	0.25	3.20	48,57,59,66	0
4	GOL	B	303	6/6	0.90	0.21	1.65	65,74,78,82	0
4	GOL	L	302	6/6	0.84	0.21	1.37	64,65,66,78	0
4	GOL	B	301	6/6	0.94	0.15	0.71	53,54,59,62	0
4	GOL	L	303	6/6	0.82	0.15	-0.16	60,73,76,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.