Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 10:24 PM EST

PDB ID	:	2D7F
Title	:	Crystal structure of A lectin from canavalia gladiata seeds complexed with alpha-methyl-mannoside and alpha-aminobutyric acid
Authors	:	Delatorre, P.; Rocha, B.A.M.; Souza, E.P.; Freitas, B.T.; Moreno, F.B.B.M.; Sampaio, A.H.; Azevedo Jr., W.F.; Cavada, B.S.
Deposited on	:	2005-11-19
Resolution	:	2.31 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 (i) 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 (i)) were used in the production of this report:

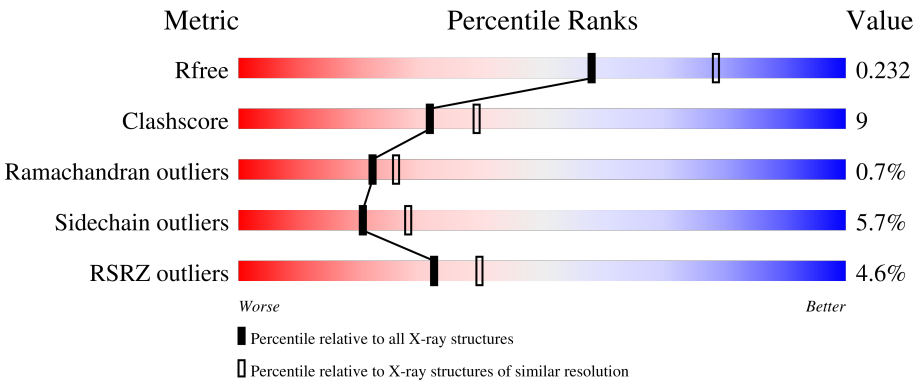
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 <=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	237	4% 75% 22% • •
1	F	237	5% 73% 20% 5% •
1	L	237	4% 73% 23% • •
1	S	237	5% 73% 22% • •

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
2	MMA	A	238	X	-	-	-
2	MMA	F	1238	X	-	-	-
2	MMA	L	2238	X	-	-	-
2	MMA	S	3238	X	-	-	-
5	DBB	F	901	-	-	X	-

2 Entry composition (i)

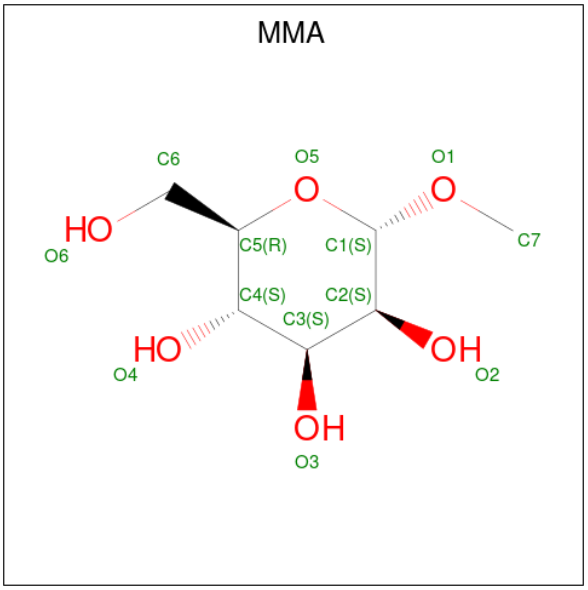
There are 6 unique types of molecules in this entry. The entry contains 7492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Concanavalin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	237	1805	1138	303	362	2	0	0	0
1	F	237	1805	1138	303	362	2	0	0	0
1	L	237	1805	1138	303	362	2	0	0	0
1	S	237	1805	1138	303	362	2	0	0	0

- Molecule 2 is methyl alpha-D-mannopyranoside (three-letter code: MMA) (formula: $C_7H_{14}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	7	6	0	0
2	F	1	13	7	6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	L	1	13	7	6	0	0
			Total	C	O		
2	S	1	13	7	6	0	0

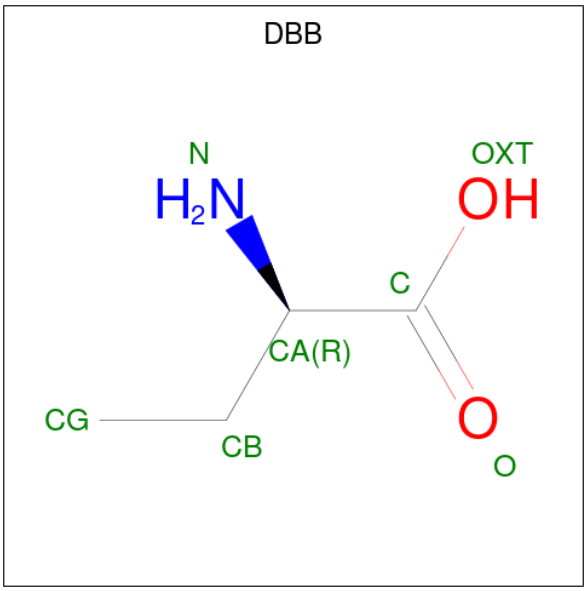
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	1	1	1	0	0
			Total	Mn		
3	F	1	1	1	0	0
			Total	Mn		
3	L	1	1	1	0	0
			Total	Mn		
3	S	1	1	1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
			Total	Ca		
4	F	1	1	1	0	0
			Total	Ca		
4	L	1	1	1	0	0
			Total	Ca		
4	S	1	1	1	0	0

- Molecule 5 is D-ALPHA-AMINOBUTYRIC ACID (three-letter code: DBB) (formula: $C_4H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	7	4	1	2	0	0
5	F	1	7	4	1	2	0	0
5	L	1	7	4	1	2	0	0
5	S	1	7	4	1	2	0	0

- Molecule 6 is water.

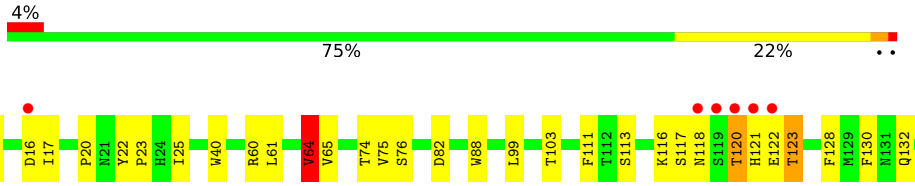
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	56	56	56	0	0
6	F	43	43	43	0	0
6	L	41	41	41	0	0
6	S	44	44	44	0	0

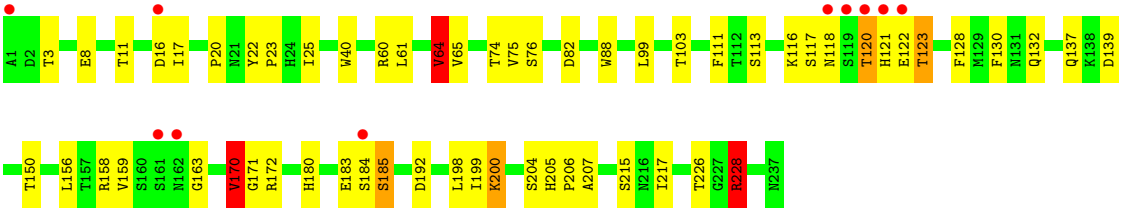
3 Residue-property plots (i)

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: Concanavalin A

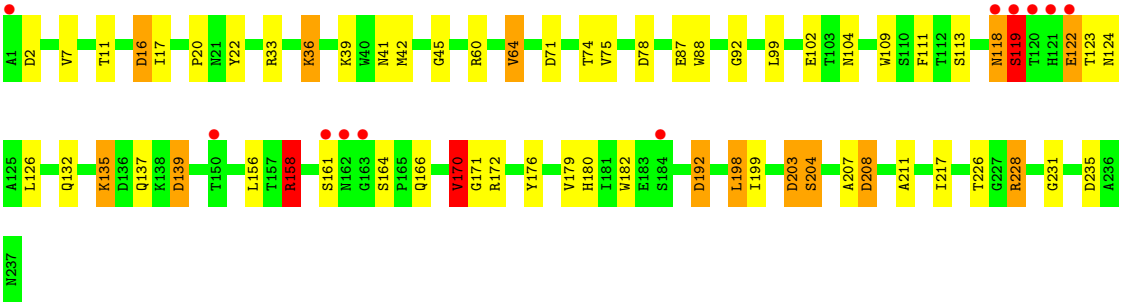
Chain A:





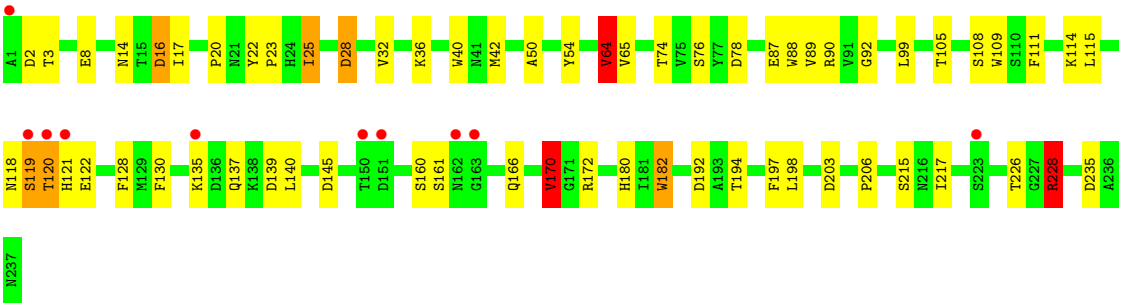
• Molecule 1: Concanavalin A

Chain F:



• Molecule 1: Concanavalin A

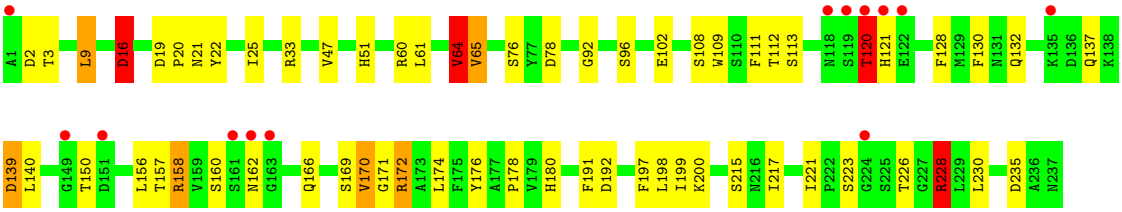
Chain L:



• Molecule 1: Concanavalin A

Chain S:

5%
73%
22%


A1 D2 T3 L9 D16 D19 P20 N21 Y22 I25 R33 V47 H51 R60 L61 V64 V65 S76 Y77 D78 G92 S96 E102 S108 W109 S110 F111 T112 S113 N118 S119 T120 H121 E122 F128 M129 F130 N131 Q132 K135 D136 Q137 K138
D139 L140 G149 T150 D151 L156 T157 R158 V159 S160 S161 N162 G163 Q166 S169 V170 G171 R172 A173 L174 F175 Y176 A177 P178 V179 H180 F191 D192 F197 L198 I199 K200 S215 N216 I217 I221 P222 S223 G224 S225 T226 G227 R228 L229 L230 D235 A236 N237

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	100.92Å 115.75Å 241.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.99 – 2.31 9.99 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.2 (9.99-2.31) 99.2 (9.99-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.180 , 0.227 0.190 , 0.232	Depositor DCC
R_{free} test set	3097 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7492	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, DBB, MMA, CA

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	1.34	7/1847 (0.4%)	1.23	11/2516 (0.4%)
1	F	1.39	9/1847 (0.5%)	1.28	21/2516 (0.8%)
1	L	1.22	5/1847 (0.3%)	1.18	15/2516 (0.6%)
1	S	1.25	4/1847 (0.2%)	1.29	16/2516 (0.6%)
All	All	1.30	25/7388 (0.3%)	1.25	63/10064 (0.6%)

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
1	F	0	4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	LYS	CD-CE	9.51	1.75	1.51
1	S	200	LYS	CD-CE	8.49	1.72	1.51
1	F	16	ASP	CB-CG	-7.47	1.36	1.51
1	A	192	ASP	CB-CG	-6.93	1.37	1.51
1	F	39	LYS	CE-NZ	6.82	1.66	1.49
1	A	204	SER	CB-OG	-6.69	1.33	1.42
1	F	39	LYS	CD-CE	6.59	1.67	1.51
1	F	176	TYR	CD1-CE1	-6.59	1.29	1.39
1	A	137	GLN	CG-CD	-6.37	1.36	1.51
1	F	172	ARG	CD-NE	-6.21	1.35	1.46
1	A	172	ARG	CD-NE	-6.02	1.36	1.46
1	F	36	LYS	CD-CE	6.02	1.66	1.51
1	A	200	LYS	CE-NZ	5.89	1.63	1.49
1	F	192	ASP	CB-CG	-5.78	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	176	TYR	CG-CD2	-5.65	1.31	1.39
1	S	65	VAL	CB-CG2	-5.62	1.41	1.52
1	L	182	TRP	CE3-CZ3	5.60	1.48	1.38
1	F	41	ASN	CB-CG	5.60	1.64	1.51
1	L	172	ARG	NE-CZ	-5.48	1.25	1.33
1	L	172	ARG	CD-NE	-5.33	1.37	1.46
1	L	89	VAL	CB-CG1	-5.26	1.41	1.52
1	L	54	TYR	CD2-CE2	5.24	1.47	1.39
1	A	185	SER	CB-OG	5.17	1.49	1.42
1	F	228	ARG	CZ-NH1	-5.09	1.26	1.33
1	S	158	ARG	NE-CZ	5.03	1.39	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	16	ASP	CB-CG-OD2	14.89	131.70	118.30
1	S	228	ARG	NE-CZ-NH1	12.53	126.56	120.30
1	A	172	ARG	NE-CZ-NH2	-12.47	114.07	120.30
1	L	172	ARG	NE-CZ-NH2	-10.89	114.86	120.30
1	S	228	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	F	228	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	F	172	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	F	208	ASP	CB-CG-OD2	8.94	126.35	118.30
1	A	172	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	A	228	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	16	ASP	CB-CG-OD2	8.73	126.16	118.30
1	F	16	ASP	N-CA-CB	-8.15	95.94	110.60
1	S	78	ASP	CB-CG-OD2	7.96	125.47	118.30
1	L	78	ASP	CB-CG-OD2	7.92	125.43	118.30
1	L	28	ASP	CB-CG-OD2	7.83	125.35	118.30
1	A	64	VAL	CB-CA-C	-7.68	96.82	111.40
1	L	16	ASP	CB-CG-OD2	7.50	125.05	118.30
1	S	16	ASP	CB-CG-OD1	-7.50	111.55	118.30
1	S	19	ASP	CB-CG-OD2	7.46	125.01	118.30
1	F	235	ASP	CB-CG-OD1	7.45	125.01	118.30
1	S	16	ASP	N-CA-CB	-7.44	97.21	110.60
1	A	170	VAL	CB-CA-C	-7.36	97.42	111.40
1	F	2	ASP	CB-CG-OD2	7.29	124.86	118.30
1	F	60	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	F	119	SER	N-CA-C	7.22	130.50	111.00
1	F	172	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	L	64	VAL	CB-CA-C	-7.13	97.85	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	170	VAL	CB-CA-C	-7.10	97.90	111.40
1	S	172	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	F	158	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	82	ASP	CB-CG-OD1	6.92	124.53	118.30
1	S	2	ASP	CB-CG-OD2	6.83	124.45	118.30
1	F	208	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	F	64	VAL	CB-CA-C	-6.67	98.73	111.40
1	A	228	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	F	33	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	L	170	VAL	CB-CA-C	-6.44	99.16	111.40
1	A	170	VAL	CG1-CB-CG2	6.33	121.02	110.90
1	F	39	LYS	CD-CE-NZ	6.32	126.23	111.70
1	L	2	ASP	CB-CG-OD1	6.28	123.95	118.30
1	S	64	VAL	CB-CA-C	-6.18	99.65	111.40
1	F	71	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	F	139	ASP	CB-CG-OD2	5.98	123.69	118.30
1	A	158	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	S	33	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	L	228	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	S	192	ASP	CB-CG-OD2	5.83	123.55	118.30
1	F	78	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	170	VAL	CA-CB-CG2	5.65	119.37	110.90
1	L	235	ASP	CB-CG-OD2	5.51	123.26	118.30
1	L	203	ASP	CB-CG-OD2	5.37	123.13	118.30
1	L	25	ILE	CG1-CB-CG2	-5.30	99.73	111.40
1	S	9	LEU	CB-CG-CD2	-5.29	102.02	111.00
1	S	235	ASP	CB-CG-OD1	5.28	123.05	118.30
1	L	139	ASP	CB-CG-OD2	5.27	123.04	118.30
1	F	170	VAL	CG1-CB-CG2	5.26	119.31	110.90
1	F	203	ASP	CB-CG-OD2	5.24	123.01	118.30
1	F	228	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	L	172	ARG	CB-CG-CD	-5.23	98.00	111.60
1	L	228	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	L	145	ASP	CB-CG-OD2	5.17	122.95	118.30
1	S	139	ASP	CB-CG-OD2	5.13	122.91	118.30
1	S	120	THR	N-CA-CB	5.03	119.85	110.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	118	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	F	119	SER	Peptide
1	F	123	THR	Peptide
1	F	203	ASP	Peptide

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	1805	0	1751	31	0
1	F	1805	0	1751	37	0
1	L	1805	0	1751	27	0
1	S	1805	0	1751	34	0
2	A	13	0	14	3	0
2	F	13	0	14	1	0
2	L	13	0	14	1	0
2	S	13	0	14	1	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
3	L	1	0	0	0	0
3	S	1	0	0	0	0
4	A	1	0	0	0	0
4	F	1	0	0	0	0
4	L	1	0	0	0	0
4	S	1	0	0	0	0
5	A	7	0	8	1	0
5	F	7	0	8	10	0
5	L	7	0	8	3	0
5	S	7	0	8	2	0
6	A	56	0	0	0	0
6	F	43	0	0	0	0
6	L	41	0	0	0	0
6	S	44	0	0	1	0
All	All	7492	0	7092	129	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 9.

All (129) 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:A:200:LYS:CD	1:A:200:LYS:CE	1.75	1.60
1:F:170:VAL:HG22	1:F:226:THR:HG22	1.52	0.92
1:A:25:ILE:HD12	1:A:65:VAL:HG23	1.50	0.91
1:A:170:VAL:HG22	1:A:226:THR:HG22	1.54	0.89
1:F:179:VAL:HA	5:F:901:DBB:HG1	1.51	0.89
1:L:180:HIS:O	5:L:902:DBB:HG2	1.75	0.86
1:F:179:VAL:HG13	5:F:901:DBB:CG	2.08	0.84
1:S:16:ASP:OD1	1:S:228:ARG:NH2	2.10	0.83
1:A:17:ILE:HD13	1:A:228:ARG:HD3	1.61	0.83
1:F:88:TRP:HB3	1:F:217:ILE:HD11	1.68	0.76
1:S:170:VAL:HG22	1:S:226:THR:HG22	1.68	0.74
1:F:179:VAL:HG13	5:F:901:DBB:HG3	1.70	0.73
1:A:25:ILE:HD12	1:A:65:VAL:CG2	2.20	0.71
1:L:170:VAL:HG22	1:L:226:THR:HG22	1.71	0.71
1:F:228:ARG:HG2	2:F:1238:MMA:O3	1.92	0.70
1:A:183:GLU:HG2	1:A:185:SER:OG	1.93	0.69
1:A:88:TRP:HB3	1:A:217:ILE:HD11	1.75	0.67
1:A:180:HIS:O	5:A:903:DBB:HG2	1.95	0.66
1:A:120:THR:HG22	1:A:121:HIS:CD2	2.32	0.64
1:F:135:LYS:NZ	1:F:135:LYS:HB3	2.13	0.63
1:F:170:VAL:HG22	1:F:226:THR:CG2	2.27	0.63
1:L:137:GLN:HG2	1:L:140:LEU:HD12	1.81	0.62
1:F:156:LEU:O	1:F:171:GLY:HA3	2.01	0.61
1:F:124:ASN:HB3	5:F:901:DBB:O	2.02	0.59
1:A:170:VAL:HG22	1:A:226:THR:CG2	2.29	0.59
1:F:158:ARG:HH11	1:F:158:ARG:HG3	1.67	0.58
1:L:88:TRP:HB3	1:L:217:ILE:HD11	1.87	0.57
1:S:25:ILE:CD1	1:S:65:VAL:HG21	2.35	0.57
1:L:180:HIS:O	5:L:902:DBB:CG	2.52	0.57
1:S:51:HIS:HB2	1:S:64:VAL:HG23	1.86	0.56
1:F:17:ILE:HD13	1:F:228:ARG:HD3	1.86	0.56
1:S:228:ARG:HG2	2:S:3238:MMA:O3	2.06	0.56
1:S:172:ARG:HD2	1:S:221:ILE:HG13	1.87	0.56
1:A:116:LYS:HG2	1:A:123:THR:HG23	1.88	0.55
1:F:16:ASP:OD1	1:F:228:ARG:NH2	2.39	0.55
1:S:102:GLU:HB2	1:S:199:ILE:HG23	1.88	0.55
1:S:156:LEU:O	1:S:171:GLY:HA3	2.07	0.55
1:A:11:THR:O	1:A:205:HIS:HE1	1.90	0.54
1:S:160:SER:HB3	1:S:166:GLN:NE2	2.23	0.54
1:F:179:VAL:CA	5:F:901:DBB:HG1	2.32	0.53
1:S:178:PRO:HB3	1:S:217:ILE:HD11	1.90	0.53
1:S:3:THR:O	1:S:215:SER:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:GLU:OE2	1:F:104:ASN:ND2	2.39	0.52
1:F:158:ARG:HG2	1:F:166:GLN:HG3	1.92	0.52
1:F:180:HIS:H	5:F:901:DBB:HB2	1.75	0.52
1:A:60:ARG:HD3	1:A:76:SER:HB3	1.92	0.51
1:F:119:SER:HB2	1:F:122:GLU:HG3	1.91	0.51
1:A:20:PRO:HB2	1:A:22:TYR:CZ	2.46	0.51
1:F:119:SER:HB2	1:F:122:GLU:CG	2.39	0.51
1:L:120:THR:HG22	1:L:121:HIS:CD2	2.46	0.50
1:L:36:LYS:HG2	1:L:76:SER:O	2.11	0.50
1:A:159:VAL:CG1	1:A:163:GLY:HA2	2.41	0.49
1:S:111:PHE:HB3	1:S:128:PHE:CZ	2.48	0.49
1:S:92:GLY:HA2	1:S:109:TRP:CH2	2.47	0.49
1:S:120:THR:HG22	1:S:121:HIS:CD2	2.48	0.48
1:A:61:LEU:O	1:A:76:SER:HA	2.14	0.48
1:L:87:GLU:HG3	1:L:182:TRP:O	2.13	0.48
1:L:25:ILE:HD12	1:L:65:VAL:HG21	1.94	0.48
1:L:92:GLY:HA2	1:L:109:TRP:CH2	2.49	0.47
1:L:42:MET:CE	1:L:206:PRO:HG2	2.45	0.47
1:S:180:HIS:O	5:S:904:DBB:HG2	2.15	0.47
1:F:102:GLU:HB2	1:F:199:ILE:HG23	1.96	0.47
1:L:119:SER:CB	1:L:122:GLU:HG3	2.44	0.47
1:A:207:ALA:HB1	2:A:238:MMA:H61	1.98	0.47
1:F:20:PRO:HB2	1:F:22:TYR:CZ	2.50	0.47
1:S:60:ARG:HD3	1:S:76:SER:HB3	1.97	0.47
1:S:137:GLN:HG2	1:S:140:LEU:HD12	1.97	0.47
1:F:137:GLN:NE2	1:F:139:ASP:OD1	2.48	0.46
1:F:87:GLU:HG3	1:F:182:TRP:O	2.14	0.46
1:L:160:SER:HB3	1:L:166:GLN:NE2	2.29	0.46
1:F:179:VAL:CG1	5:F:901:DBB:HG3	2.44	0.46
1:L:105:THR:O	1:L:197:PHE:HA	2.15	0.46
1:A:64:VAL:HG13	1:A:74:THR:OG1	2.15	0.46
1:L:111:PHE:HB3	1:L:128:PHE:CZ	2.51	0.46
1:A:207:ALA:CB	2:A:238:MMA:H61	2.46	0.46
1:S:9:LEU:HD12	1:S:25:ILE:HD12	1.98	0.46
1:S:108:SER:HA	1:S:130:PHE:O	2.16	0.46
1:A:117:SER:OG	1:A:122:GLU:HB2	2.16	0.46
1:F:102:GLU:HG2	1:F:207:ALA:O	2.15	0.46
1:F:170:VAL:HG11	1:F:231:GLY:HA2	1.97	0.46
1:L:17:ILE:HD13	1:L:228:ARG:HD3	1.98	0.46
1:S:172:ARG:HD2	1:S:221:ILE:CG1	2.44	0.46
1:F:74:THR:HG22	1:F:75:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:61:LEU:O	1:S:76:SER:HA	2.16	0.45
1:L:20:PRO:HB2	1:L:22:TYR:CZ	2.52	0.45
1:A:23:PRO:HB2	1:A:40:TRP:O	2.17	0.45
1:A:205:HIS:ND1	1:A:206:PRO:HD2	2.31	0.45
1:S:170:VAL:HG22	1:S:226:THR:CG2	2.43	0.45
1:F:92:GLY:HA2	1:F:109:TRP:CH2	2.52	0.45
1:L:64:VAL:HG13	1:L:74:THR:OG1	2.16	0.45
1:A:156:LEU:O	1:A:171:GLY:HA3	2.17	0.45
1:L:90:ARG:NH1	1:L:217:ILE:HG23	2.32	0.44
1:F:11:THR:HG22	1:F:42:MET:HG3	2.00	0.44
1:L:180:HIS:HB3	5:L:902:DBB:HA	2.00	0.44
1:S:25:ILE:HD11	1:S:65:VAL:HG21	2.00	0.44
1:S:111:PHE:CE2	1:S:113:SER:HB2	2.53	0.44
1:A:3:THR:O	1:A:215:SER:HA	2.17	0.43
1:S:157:THR:HB	1:S:169:SER:HB3	2.00	0.43
1:S:174:LEU:HD12	1:S:174:LEU:N	2.33	0.43
1:S:96:SER:OG	1:S:230:LEU:HA	2.18	0.43
1:S:137:GLN:NE2	1:S:139:ASP:OD1	2.45	0.43
1:A:139:ASP:OD2	5:S:904:DBB:OXT	2.37	0.42
1:L:8:GLU:OE1	1:L:28:ASP:OD2	2.37	0.42
1:F:88:TRP:HB3	1:F:217:ILE:CD1	2.44	0.42
1:S:172:ARG:NH2	6:S:982:HOH:O	2.45	0.42
1:L:3:THR:O	1:L:215:SER:HA	2.20	0.42
1:F:179:VAL:CG1	5:F:901:DBB:CG	2.91	0.42
1:F:45:GLY:HA2	1:F:198:LEU:HD11	2.01	0.41
1:F:180:HIS:H	5:F:901:DBB:CG	2.33	0.41
1:S:47:VAL:HA	1:S:197:PHE:O	2.20	0.41
1:S:20:PRO:HB2	1:S:22:TYR:CZ	2.55	0.41
1:A:74:THR:HG22	1:A:75:VAL:N	2.34	0.41
1:A:111:PHE:CE2	1:A:113:SER:HB2	2.56	0.41
1:F:87:GLU:CG	1:F:180:HIS:HE2	2.33	0.41
1:L:14:ASN:ND2	2:L:2238:MMA:O4	2.42	0.41
1:L:25:ILE:HD12	1:L:25:ILE:HG23	1.61	0.41
1:L:50:ALA:O	1:L:194:THR:HA	2.20	0.41
1:S:112:THR:O	1:S:191:PHE:HA	2.21	0.41
1:A:128:PHE:CD1	1:A:130:PHE:CE2	3.09	0.40
1:L:23:PRO:HB2	1:L:40:TRP:O	2.20	0.40
1:A:8:GLU:O	1:A:25:ILE:HA	2.20	0.40
1:A:103:THR:O	1:A:199:ILE:HA	2.21	0.40
1:F:7:VAL:O	1:F:211:ALA:HA	2.21	0.40
1:F:111:PHE:CE2	1:F:113:SER:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:SER:HA	1:L:130:PHE:O	2.22	0.40
1:A:228:ARG:HG2	2:A:238:MMA:O3	2.21	0.40
1:F:126:LEU:CB	5:F:901:DBB:HG2	2.51	0.40
1:S:160:SER:OG	1:S:162:ASN:ND2	2.54	0.40
1:S:178:PRO:HB3	1:S:217:ILE:CD1	2.51	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	235/237 (99%)	223 (95%)	10 (4%)	2 (1%)	17	19
1	F	235/237 (99%)	223 (95%)	11 (5%)	1 (0%)	34	41
1	L	235/237 (99%)	228 (97%)	5 (2%)	2 (1%)	17	19
1	S	235/237 (99%)	223 (95%)	10 (4%)	2 (1%)	17	19
All	All	940/948 (99%)	897 (95%)	36 (4%)	7 (1%)	22	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	204	SER
1	S	16	ASP
1	S	120	THR
1	A	120	THR
1	A	184	SER
1	L	119	SER
1	L	120	THR

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	202/202 (100%)	193 (96%)	9 (4%)	27	38
1	F	202/202 (100%)	187 (93%)	15 (7%)	13	17
1	L	202/202 (100%)	189 (94%)	13 (6%)	17	23
1	S	202/202 (100%)	193 (96%)	9 (4%)	27	38
All	All	808/808 (100%)	762 (94%)	46 (6%)	20	28

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	VAL
1	A	99	LEU
1	A	118	ASN
1	A	123	THR
1	A	132	GLN
1	A	150	THR
1	A	170	VAL
1	A	198	LEU
1	A	228	ARG
1	F	36	LYS
1	F	64	VAL
1	F	99	LEU
1	F	118	ASN
1	F	122	GLU
1	F	132	GLN
1	F	135	LYS
1	F	158	ARG
1	F	161	SER
1	F	164	SER
1	F	170	VAL
1	F	192	ASP
1	F	198	LEU
1	F	204	SER
1	F	208	ASP

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Mol	Chain	Res	Type
1	L	16	ASP
1	L	32	VAL
1	L	64	VAL
1	L	99	LEU
1	L	114	LYS
1	L	115	LEU
1	L	118	ASN
1	L	135	LYS
1	L	161	SER
1	L	170	VAL
1	L	192	ASP
1	L	198	LEU
1	L	228	ARG
1	S	21	ASN
1	S	64	VAL
1	S	132	GLN
1	S	150	THR
1	S	158	ARG
1	S	170	VAL
1	S	198	LEU
1	S	223	SER
1	S	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	43	GLN
1	A	121	HIS
1	F	21	ASN
1	F	43	GLN
1	F	132	GLN
1	L	43	GLN
1	L	121	HIS
1	L	132	GLN
1	L	162	ASN
1	S	21	ASN
1	S	118	ASN
1	S	121	HIS
1	S	162	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
2	MMA	L	2238	-	13,13,13	1.61	2 (15%)	18,18,18	4.11	9 (50%)
2	MMA	A	238	-	13,13,13	1.70	3 (23%)	18,18,18	4.79	9 (50%)
2	MMA	S	3238	-	13,13,13	1.30	3 (23%)	18,18,18	3.87	9 (50%)
5	DBB	F	901	-	5,6,6	0.99	0	4,7,7	2.62	2 (50%)
5	DBB	S	904	-	5,6,6	0.73	0	4,7,7	0.94	0
5	DBB	A	903	-	5,6,6	0.61	0	4,7,7	0.68	0
5	DBB	L	902	-	5,6,6	1.19	0	4,7,7	1.47	0
2	MMA	F	1238	-	13,13,13	1.39	3 (23%)	18,18,18	4.54	8 (44%)

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
2	MMA	L	2238	-	1/1/5/5	0/4/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MMA	A	238	-	1/1/5/5	0/4/24/24	0/1/1/1
2	MMA	S	3238	-	1/1/5/5	0/4/24/24	0/1/1/1
5	DBB	F	901	-	-	4/6/6/6	-
5	DBB	S	904	-	-	4/6/6/6	-
5	DBB	A	903	-	-	4/6/6/6	-
5	DBB	L	902	-	-	4/6/6/6	-
2	MMA	F	1238	-	1/1/5/5	0/4/24/24	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1238	MMA	C4-C3	3.20	1.60	1.52
2	L	2238	MMA	C3-C2	3.11	1.60	1.52
2	S	3238	MMA	C4-C3	3.08	1.60	1.52
2	A	238	MMA	C4-C3	2.92	1.59	1.52
2	L	2238	MMA	C4-C3	2.87	1.59	1.52
2	A	238	MMA	O2-C2	2.66	1.49	1.43
2	F	1238	MMA	C4-C5	2.46	1.58	1.53
2	S	3238	MMA	C3-C2	2.32	1.58	1.52
2	S	3238	MMA	C4-C5	2.19	1.57	1.53
2	A	238	MMA	O3-C3	-2.17	1.37	1.43
2	F	1238	MMA	C3-C2	2.03	1.57	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1238	MMA	O1-C1-C2	13.98	124.53	108.15
2	L	2238	MMA	O1-C1-C2	13.26	123.69	108.15
2	A	238	MMA	O1-C1-C2	11.67	121.83	108.15
2	S	3238	MMA	O1-C1-C2	9.99	119.86	108.15
2	A	238	MMA	C1-C2-C3	-9.95	89.28	110.00
2	F	1238	MMA	C1-C2-C3	-8.66	91.96	110.00
2	A	238	MMA	O2-C2-C1	7.42	128.06	110.05
2	S	3238	MMA	C1-C2-C3	-7.22	94.97	110.00
2	S	3238	MMA	O3-C3-C4	6.40	125.14	110.35
2	L	2238	MMA	C1-O5-C5	-6.04	101.83	113.69
2	A	238	MMA	C1-O5-C5	-5.57	102.75	113.69
2	A	238	MMA	O4-C4-C5	-5.49	95.67	109.30
2	F	1238	MMA	O3-C3-C4	5.18	122.31	110.35
2	F	1238	MMA	C1-O5-C5	-4.85	104.17	113.69
2	S	3238	MMA	C1-O5-C5	-4.84	104.19	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	238	MMA	O3-C3-C4	4.34	120.38	110.35
2	L	2238	MMA	C1-C2-C3	-4.13	101.39	110.00
2	L	2238	MMA	O5-C1-C2	-3.98	101.93	110.35
2	F	1238	MMA	O2-C2-C1	3.94	119.63	110.05
2	F	1238	MMA	C6-C5-C4	3.89	122.10	113.00
2	L	2238	MMA	C7-O1-C1	3.85	119.21	113.27
2	A	238	MMA	C3-C4-C5	3.58	116.62	110.24
2	A	238	MMA	O6-C6-C5	-3.50	99.28	111.29
2	L	2238	MMA	C6-C5-C4	3.43	121.05	113.00
2	S	3238	MMA	O2-C2-C1	3.42	118.35	110.05
5	F	901	DBB	CG-CB-CA	-3.39	105.44	113.41
2	L	2238	MMA	C3-C4-C5	3.21	115.96	110.24
2	L	2238	MMA	O3-C3-C4	3.14	117.61	110.35
5	F	901	DBB	OXT-C-CA	3.05	123.78	113.38
2	S	3238	MMA	C6-C5-C4	3.00	120.04	113.00
2	S	3238	MMA	C7-O1-C1	2.95	117.83	113.27
2	S	3238	MMA	O5-C1-O1	2.81	117.48	110.97
2	A	238	MMA	O5-C5-C6	-2.72	99.67	106.44
2	F	1238	MMA	C3-C4-C5	2.53	114.76	110.24
2	L	2238	MMA	O3-C3-C2	2.37	115.83	110.35
2	S	3238	MMA	C3-C4-C5	2.17	114.11	110.24
2	F	1238	MMA	O5-C1-C2	-2.06	105.98	110.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	238	MMA	C1
2	F	1238	MMA	C1
2	L	2238	MMA	C1
2	S	3238	MMA	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	903	DBB	O-C-CA-N
5	F	901	DBB	O-C-CA-N
5	L	902	DBB	O-C-CA-N
5	S	904	DBB	O-C-CA-N
5	F	901	DBB	OXT-C-CA-N
5	A	903	DBB	OXT-C-CA-N
5	L	902	DBB	OXT-C-CA-N
5	S	904	DBB	OXT-C-CA-N

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Mol	Chain	Res	Type	Atoms
5	F	901	DBB	OXT-C-CA-CB
5	S	904	DBB	OXT-C-CA-CB
5	L	902	DBB	O-C-CA-CB
5	S	904	DBB	O-C-CA-CB
5	A	903	DBB	OXT-C-CA-CB
5	L	902	DBB	OXT-C-CA-CB
5	A	903	DBB	O-C-CA-CB
5	F	901	DBB	O-C-CA-CB

There are no ring outliers.

8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	2238	MMA	1	0
2	A	238	MMA	3	0
2	S	3238	MMA	1	0
5	F	901	DBB	10	0
5	S	904	DBB	2	0
5	A	903	DBB	1	0
5	L	902	DBB	3	0
2	F	1238	MMA	1	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	237/237 (100%)	-0.40	10 (4%)	36	43	12, 18, 39, 62	0
1	F	237/237 (100%)	-0.37	11 (4%)	32	40	12, 18, 38, 60	0
1	L	237/237 (100%)	-0.29	10 (4%)	36	43	13, 23, 39, 58	0
1	S	237/237 (100%)	-0.21	13 (5%)	25	31	14, 21, 40, 59	0
All	All	948/948 (100%)	-0.32	44 (4%)	32	40	12, 20, 39, 62	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	121	HIS	4.7
1	F	120	THR	4.6
1	A	161	SER	4.6
1	S	163	GLY	4.5
1	F	121	HIS	4.3
1	S	161	SER	4.3
1	A	184	SER	4.1
1	S	121	HIS	3.9
1	F	184	SER	3.9
1	L	119	SER	3.7
1	F	161	SER	3.6
1	L	1	ALA	3.6
1	F	150	THR	3.6
1	S	119	SER	3.6
1	S	162	ASN	3.5
1	A	16	ASP	3.4
1	S	1	ALA	3.4
1	A	121	HIS	3.2
1	A	1	ALA	3.2
1	F	162	ASN	3.2
1	L	163	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	118	ASN	3.1
1	A	122	GLU	3.1
1	F	119	SER	3.0
1	S	118	ASN	2.9
1	A	162	ASN	2.8
1	A	120	THR	2.8
1	L	223	SER	2.7
1	L	162	ASN	2.7
1	L	150	THR	2.7
1	S	135	LYS	2.7
1	A	119	SER	2.5
1	F	122	GLU	2.5
1	F	163	GLY	2.5
1	L	120	THR	2.4
1	L	151	ASP	2.4
1	S	122	GLU	2.4
1	S	224	GLY	2.4
1	S	149	GLY	2.3
1	F	1	ALA	2.3
1	S	120	THR	2.2
1	F	118	ASN	2.1
1	S	151	ASP	2.1
1	L	135	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MMA	L	2238	13/13	0.82	0.25	25,37,52,53	0
5	DBB	F	901	7/7	0.84	0.23	29,31,32,33	1
5	DBB	L	902	7/7	0.85	0.18	15,20,23,24	1
2	MMA	A	238	13/13	0.87	0.20	20,27,44,46	0
2	MMA	S	3238	13/13	0.87	0.19	20,30,40,41	0
5	DBB	S	904	7/7	0.88	0.19	25,26,28,28	1
5	DBB	A	903	7/7	0.90	0.15	14,20,23,23	1
2	MMA	F	1238	13/13	0.90	0.15	15,20,31,31	0
4	CA	L	240	1/1	0.95	0.06	19,19,19,19	0
4	CA	S	240	1/1	0.95	0.06	20,20,20,20	0
4	CA	A	240	1/1	0.96	0.06	18,18,18,18	0
3	MN	S	239	1/1	0.97	0.06	21,21,21,21	0
3	MN	F	239	1/1	0.98	0.05	20,20,20,20	0
4	CA	F	240	1/1	0.98	0.05	19,19,19,19	0
3	MN	L	239	1/1	0.98	0.05	22,22,22,22	0
3	MN	A	239	1/1	0.98	0.06	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.