



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:32 AM UTC

PDB ID : 2D7F / pdb_00002d7f
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

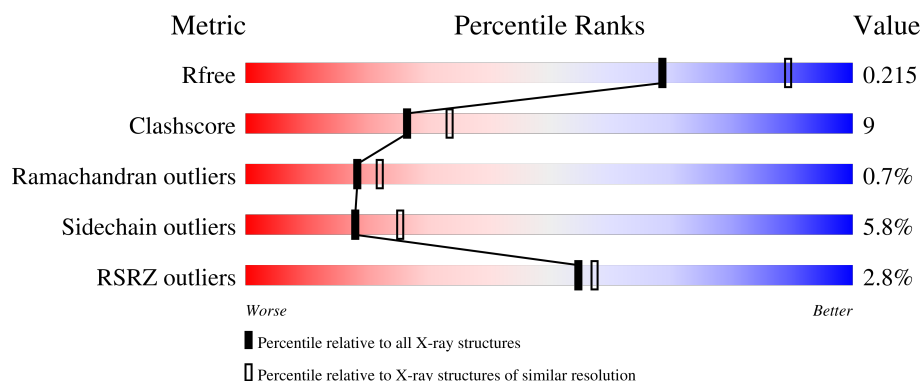
1 Overall quality at a glance

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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (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 $\leq 5\%$. 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	237	3% 70% 24% ..
1	F	237	3% 67% 28% ..
1	L	237	2% 72% 25% ..
1	S	237	4% 70% 25% ..

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](#)

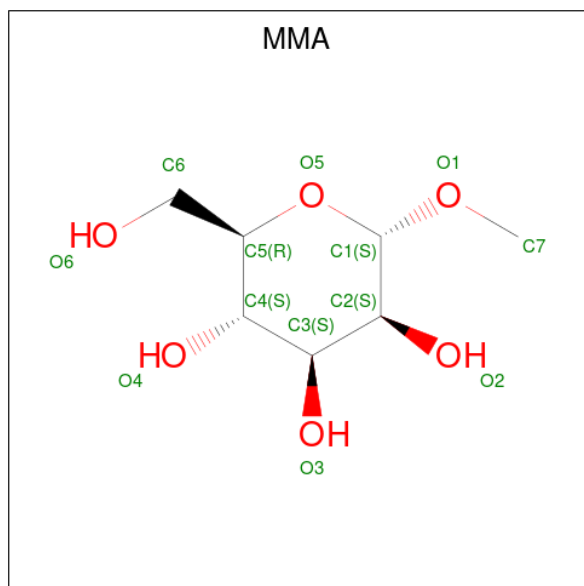
There are 6 unique types of molecules in this entry. The entry contains 7492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	237	Total	C	N	O	S	0	0	0
			1805	1138	303	362	2			
1	F	237	Total	C	N	O	S	0	0	0
			1805	1138	303	362	2			
1	L	237	Total	C	N	O	S	0	0	0
			1805	1138	303	362	2			
1	S	237	Total	C	N	O	S	0	0	0
			1805	1138	303	362	2			

- Molecule 2 is methyl alpha-D-mannopyranoside (CCD ID: MMA) (formula: C₇H₁₄O₆).



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

Continued on next page...

Continued from previous page...

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

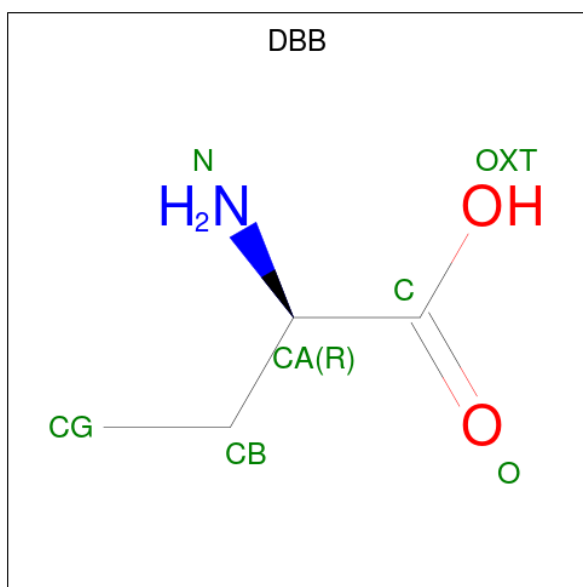
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is D-ALPHA-AMINOBUTYRIC ACID (CCD ID: DBB) (formula: C₄H₉NO₂).



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

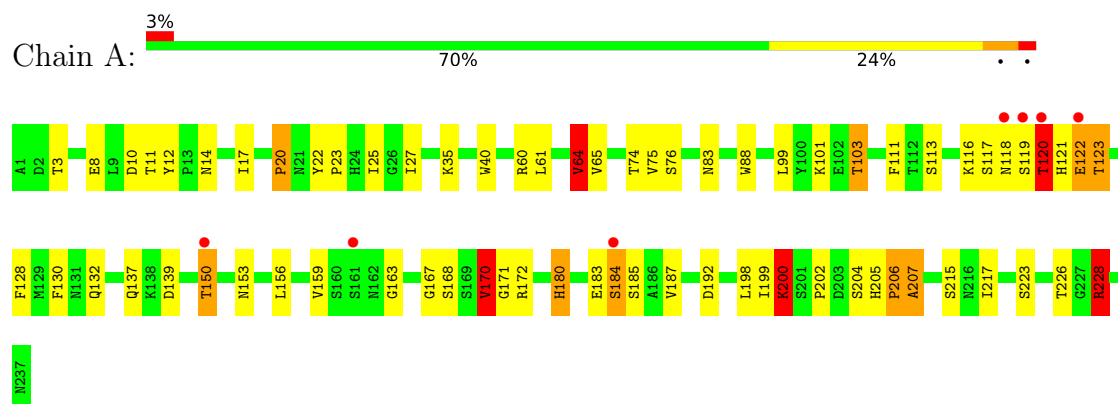
- Molecule 6 is water.

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

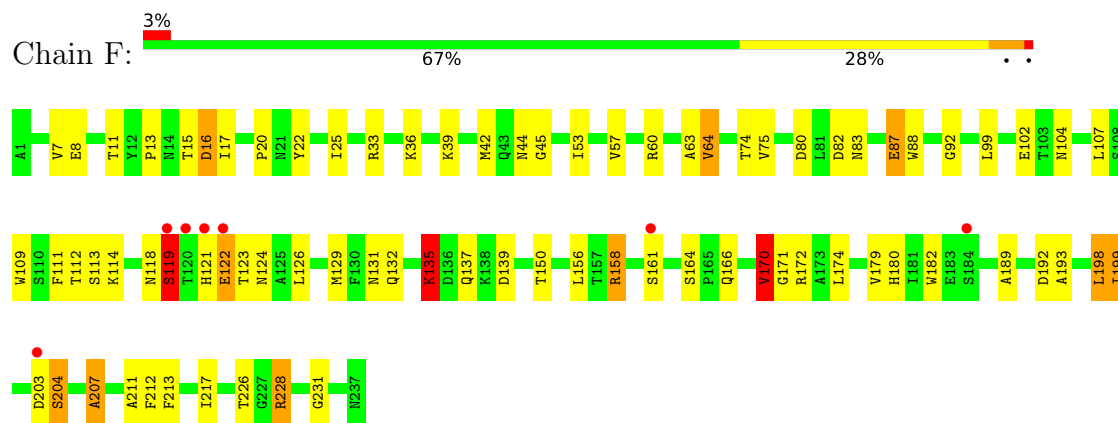
3 Residue-property plots

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.

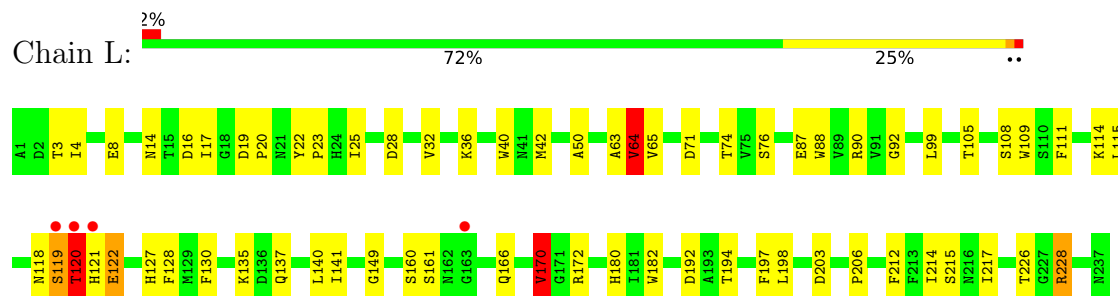
• Molecule 1: Concanavalin A



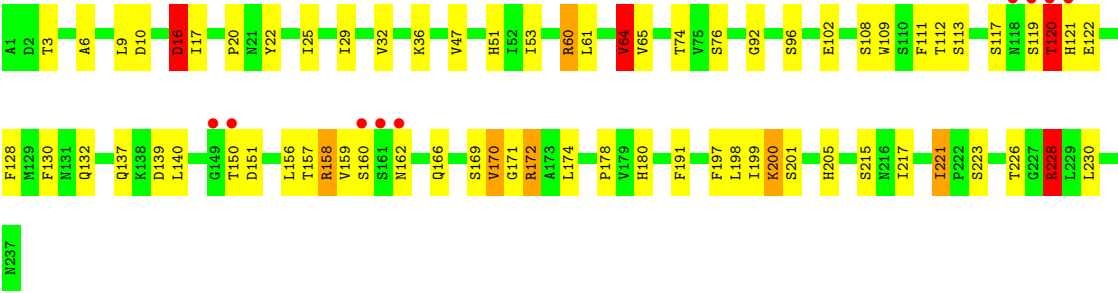
• Molecule 1: Concanavalin A



• Molecule 1: Concanavalin A



• Molecule 1: Concanavalin A



4 Data and refinement statistics

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) 97.8 (9.99-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.180 , 0.227 (Not available) , 0.215	Depositor DCC
R_{free} test set	3097 reflections (5.04%)	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 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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: CA, DBB, MN, MMA

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	1.67	21/1847 (1.1%)	1.31	9/2516 (0.4%)
1	F	1.77	32/1847 (1.7%)	1.38	17/2516 (0.7%)
1	L	1.56	11/1847 (0.6%)	1.24	6/2516 (0.2%)
1	S	1.57	17/1847 (0.9%)	1.33	10/2516 (0.4%)
All	All	1.64	81/7388 (1.1%)	1.31	42/10064 (0.4%)

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 (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	THR	CA-CB	8.38	1.65	1.52
1	A	200	LYS	CD-CE	7.52	1.75	1.52
1	A	153	ASN	C-O	-7.50	1.14	1.23
1	F	172	ARG	CD-NE	-7.40	1.35	1.46
1	F	121	HIS	N-CA	7.33	1.55	1.46
1	F	63	ALA	C-O	-7.29	1.15	1.23
1	F	53	ILE	C-O	-7.21	1.17	1.24
1	A	172	ARG	CD-NE	-7.17	1.36	1.46
1	F	83	ASN	C-O	-7.03	1.14	1.24
1	A	120	THR	CA-CB	6.74	1.64	1.53
1	S	120	THR	CA-CB	6.72	1.64	1.53
1	S	200	LYS	CD-CE	6.67	1.72	1.52
1	L	120	THR	CA-CB	6.64	1.64	1.53
1	L	212	PHE	C-O	-6.52	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	172	ARG	NE-CZ	-6.48	1.25	1.33
1	A	206	PRO	C-O	-6.43	1.16	1.23
1	F	16	ASP	CB-CG	-6.39	1.36	1.52
1	L	172	ARG	CD-NE	-6.33	1.37	1.46
1	A	137	GLN	CG-CD	-6.26	1.36	1.52
1	L	71	ASP	CA-C	6.25	1.60	1.52
1	F	193	ALA	C-O	-6.24	1.16	1.23
1	F	150	THR	CA-CB	6.06	1.61	1.53
1	S	60	ARG	C-O	-5.97	1.17	1.24
1	S	158	ARG	NE-CZ	5.94	1.39	1.33
1	A	192	ASP	CB-CG	-5.94	1.37	1.52
1	A	207	ALA	CA-CB	-5.86	1.44	1.53
1	A	83	ASN	C-O	-5.84	1.15	1.23
1	A	202	PRO	C-O	-5.84	1.17	1.24
1	F	119	SER	CA-C	5.80	1.60	1.52
1	F	228	ARG	CD-NE	-5.72	1.38	1.46
1	F	172	ARG	C-O	-5.71	1.16	1.23
1	F	199	ILE	CA-C	5.66	1.59	1.52
1	L	63	ALA	C-O	-5.65	1.17	1.23
1	S	53	ILE	C-O	-5.62	1.18	1.24
1	F	212	PHE	C-O	-5.61	1.17	1.24
1	A	35	LYS	C-O	-5.61	1.16	1.24
1	F	39	LYS	CE-NZ	5.58	1.66	1.49
1	F	57	VAL	CA-CB	5.58	1.62	1.54
1	L	127	HIS	N-CA	-5.56	1.39	1.46
1	A	27	ILE	C-O	-5.56	1.18	1.24
1	L	214	ILE	C-O	-5.55	1.18	1.24
1	S	172	ARG	CD-NE	-5.52	1.38	1.46
1	F	64	VAL	CA-CB	5.51	1.62	1.54
1	A	101	LYS	N-CA	-5.47	1.39	1.45
1	A	20	PRO	CA-C	5.47	1.59	1.52
1	F	131	ASN	C-O	-5.47	1.16	1.24
1	S	6	ALA	CA-CB	-5.44	1.44	1.53
1	S	122	GLU	CA-C	5.42	1.59	1.53
1	L	122	GLU	N-CA	5.41	1.52	1.46
1	A	122	GLU	C-O	5.40	1.31	1.23
1	F	8	GLU	CA-C	-5.39	1.46	1.52
1	L	141	ILE	C-O	-5.38	1.17	1.23
1	S	32	VAL	N-CA	5.36	1.53	1.46
1	S	221	ILE	CA-CB	-5.35	1.47	1.54
1	F	213	PHE	N-CA	-5.34	1.39	1.45
1	L	4	ILE	CA-CB	5.33	1.61	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	HIS	C-O	-5.32	1.17	1.23
1	F	87	GLU	C-O	-5.31	1.18	1.24
1	A	12	TYR	N-CA	-5.29	1.38	1.46
1	S	60	ARG	N-CA	-5.29	1.40	1.46
1	F	60	ARG	NE-CZ	-5.26	1.27	1.33
1	S	17	ILE	CA-CB	5.25	1.61	1.54
1	F	13	PRO	C-O	-5.24	1.17	1.24
1	F	33	ARG	N-CA	-5.23	1.40	1.46
1	A	150	THR	CB-OG1	5.19	1.52	1.43
1	F	15	THR	C-O	-5.18	1.17	1.24
1	A	228	ARG	CD-NE	-5.16	1.39	1.46
1	A	207	ALA	C-O	-5.15	1.17	1.23
1	F	112	THR	CA-C	-5.15	1.46	1.52
1	F	207	ALA	CA-CB	-5.11	1.45	1.53
1	S	10	ASP	CA-CB	-5.11	1.46	1.53
1	S	74	THR	CA-C	-5.10	1.46	1.52
1	F	39	LYS	CD-CE	5.09	1.67	1.52
1	F	107	LEU	CA-C	5.08	1.59	1.52
1	S	201	SER	C-O	-5.07	1.19	1.24
1	F	114	LYS	C-O	-5.06	1.17	1.23
1	S	205	HIS	C-O	-5.06	1.18	1.24
1	F	174	LEU	CA-C	-5.04	1.46	1.52
1	F	80	ASP	N-CA	-5.04	1.40	1.46
1	F	129	MET	C-O	-5.01	1.18	1.23
1	S	29	ILE	CA-CB	5.01	1.59	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	119	SER	N-CA-C	15.29	130.50	111.69
1	A	64	VAL	CB-CA-C	-8.89	96.82	110.50
1	F	16	ASP	N-CA-CB	-8.61	95.94	110.49
1	L	64	VAL	CB-CA-C	-8.53	97.85	110.81
1	S	16	ASP	N-CA-CB	-7.86	97.21	110.49
1	F	64	VAL	CB-CA-C	-7.64	98.73	110.50
1	A	187	VAL	N-CA-C	-7.50	104.47	111.45
1	A	170	VAL	CB-CA-C	-7.42	97.42	110.71
1	F	170	VAL	CB-CA-C	-7.24	97.90	111.30
1	S	64	VAL	CB-CA-C	-7.04	99.65	110.50
1	S	117	SER	CA-C-N	7.00	129.67	120.28
1	S	117	SER	C-N-CA	7.00	129.67	120.28
1	A	119	SER	N-CA-C	6.70	120.91	112.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	170	VAL	CB-CA-C	-6.67	99.16	110.71
1	F	119	SER	CA-C-N	6.32	133.08	121.70
1	F	119	SER	C-N-CA	6.32	133.08	121.70
1	F	135	LYS	CA-C-N	-6.15	114.71	123.20
1	F	135	LYS	C-N-CA	-6.15	114.71	123.20
1	S	119	SER	N-CA-C	5.84	119.51	112.38
1	S	16	ASP	CB-CG-OD2	5.78	131.70	118.40
1	L	172	ARG	CB-CG-CD	-5.78	98.00	111.30
1	F	15	THR	CA-C-N	5.77	132.56	121.54
1	F	15	THR	C-N-CA	5.77	132.56	121.54
1	A	172	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	L	203	ASP	CA-C-N	5.57	128.00	120.38
1	L	203	ASP	C-N-CA	5.57	128.00	120.38
1	A	204	SER	CB-CA-C	-5.55	101.24	110.68
1	F	189	ALA	N-CA-C	-5.55	99.85	108.90
1	S	120	THR	N-CA-CB	5.54	119.85	110.49
1	S	159	VAL	N-CA-C	-5.53	100.16	108.12
1	F	25	ILE	N-CA-C	-5.46	100.57	108.71
1	A	228	ARG	CB-CG-CD	5.45	123.83	111.30
1	A	170	VAL	CA-CB-CG2	5.28	119.37	110.40
1	F	228	ARG	CB-CG-CD	5.28	123.44	111.30
1	F	170	VAL	N-CA-CB	5.26	119.99	111.36
1	F	172	ARG	CB-CG-CD	-5.18	99.39	111.30
1	A	103	THR	N-CA-C	-5.15	103.23	110.50
1	F	44	ASN	N-CA-C	5.12	117.73	110.10
1	F	82	ASP	CB-CA-C	-5.08	102.05	110.68
1	L	149	GLY	N-CA-C	5.07	119.72	113.79
1	S	228	ARG	NE-CZ-NH1	5.07	126.56	121.50
1	S	151	ASP	N-CA-C	5.01	118.68	112.47

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	118	ASN	Peptide
1	F	119	SER	Peptide
1	F	123	THR	Peptide
1	F	203	ASP	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	1805	0	1751	35	0
1	F	1805	0	1751	37	0
1	L	1805	0	1751	28	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	134	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 (134) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:10:ASP:OD1	1:A:10:ASP:C	2.58	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:183:GLU:O	1:A:184:SER:C	2.62	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:A:167:GLY:O	1:A:168:SER:C	2.62	0.42
1:F:179:VAL:CG1	5:F:901:DBB:CG	2.91	0.42
1:L:14:ASN:C	1:L:19:ASP:HB2	2.45	0.41
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:14:ASN:CG	1:A:228:ARG:HB3	2.46	0.40
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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	235/237 (99%)	223 (95%)	10 (4%)	2 (1%)	14	16
1	F	235/237 (99%)	223 (95%)	11 (5%)	1 (0%)	30	37
1	L	235/237 (99%)	228 (97%)	5 (2%)	2 (1%)	14	16
1	S	235/237 (99%)	223 (95%)	10 (4%)	2 (1%)	14	16
All	All	940/948 (99%)	897 (95%)	36 (4%)	7 (1%)	18	22

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 ⓘ

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%)	191 (95%)	11 (5%)	20	28
1	F	202/202 (100%)	189 (94%)	13 (6%)	16	22
1	L	202/202 (100%)	189 (94%)	13 (6%)	16	22
1	S	202/202 (100%)	192 (95%)	10 (5%)	22	32
All	All	808/808 (100%)	761 (94%)	47 (6%)	18	25

All (47) 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	200	LYS
1	A	223	SER
1	A	228	ARG
1	F	36	LYS
1	F	64	VAL
1	F	99	LEU
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

Continued on next page...

Continued from previous page...

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	36	LYS
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	200	LYS
1	S	223	SER
1	S	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	121	HIS
1	F	21	ASN
1	F	41	ASN
1	F	43	GLN
1	F	132	GLN
1	L	43	GLN
1	L	121	HIS
1	L	132	GLN
1	S	21	ASN
1	S	43	GLN
1	S	118	ASN
1	S	121	HIS
1	S	132	GLN
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 oligosaccharides 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$
5	DBB	F	901	-	5,6,6	1.02	0	4,7,7	3.02	2 (50%)
5	DBB	A	903	-	5,6,6	0.62	0	4,7,7	1.29	1 (25%)
2	MMA	F	1238	-	13,13,13	1.37	2 (15%)	18,18,18	4.56	8 (44%)
5	DBB	L	902	-	5,6,6	1.21	0	4,7,7	1.98	1 (25%)
2	MMA	A	238	-	13,13,13	1.65	3 (23%)	18,18,18	4.82	10 (55%)
2	MMA	L	2238	-	13,13,13	1.58	2 (15%)	18,18,18	4.15	9 (50%)
2	MMA	S	3238	-	13,13,13	1.27	3 (23%)	18,18,18	3.87	9 (50%)
5	DBB	S	904	-	5,6,6	0.77	0	4,7,7	1.50	1 (25%)

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
5	DBB	F	901	-	-	4/6/6/6	-
5	DBB	A	903	-	-	4/6/6/6	-
2	MMA	F	1238	-	1/1/5/5	0/4/24/24	0/1/1/1
5	DBB	L	902	-	-	4/6/6/6	-
2	MMA	A	238	-	1/1/5/5	0/4/24/24	0/1/1/1
2	MMA	L	2238	-	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	S	904	-	-	4/6/6/6	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1238	MMA	C4-C3	3.14	1.60	1.52
2	L	2238	MMA	C3-C2	3.05	1.60	1.52
2	S	3238	MMA	C4-C3	3.01	1.60	1.52
2	A	238	MMA	C4-C3	2.86	1.59	1.52
2	L	2238	MMA	C4-C3	2.81	1.59	1.52
2	A	238	MMA	O2-C2	2.54	1.49	1.43
2	F	1238	MMA	C4-C5	2.43	1.58	1.53
2	S	3238	MMA	C3-C2	2.27	1.58	1.52
2	S	3238	MMA	C4-C5	2.17	1.57	1.53
2	A	238	MMA	O3-C3	-2.05	1.37	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1238	MMA	O1-C1-C2	14.21	124.53	108.14
2	L	2238	MMA	O1-C1-C2	13.48	123.69	108.14
2	A	238	MMA	O1-C1-C2	11.87	121.83	108.14
2	S	3238	MMA	O1-C1-C2	10.16	119.86	108.14
2	A	238	MMA	C1-C2-C3	-9.85	89.28	110.01
2	F	1238	MMA	C1-C2-C3	-8.58	91.96	110.01
2	A	238	MMA	O2-C2-C1	7.55	128.06	110.08
2	S	3238	MMA	C1-C2-C3	-7.15	94.97	110.01
2	S	3238	MMA	O3-C3-C4	6.26	125.14	110.38
2	L	2238	MMA	C1-O5-C5	-6.09	101.83	113.72
2	A	238	MMA	C1-O5-C5	-5.62	102.75	113.72
2	A	238	MMA	O4-C4-C5	-5.54	95.67	109.32
2	F	1238	MMA	O3-C3-C4	5.06	122.31	110.38
2	F	1238	MMA	C1-O5-C5	-4.89	104.17	113.72
2	S	3238	MMA	C1-O5-C5	-4.88	104.19	113.72
5	F	901	DBB	CB-CA-C	-4.70	94.30	111.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	238	MMA	O3-C3-C4	4.24	120.38	110.38
2	L	2238	MMA	O5-C1-C2	-4.11	101.93	110.37
2	L	2238	MMA	C1-C2-C3	-4.10	101.39	110.01
2	F	1238	MMA	O2-C2-C1	4.01	119.63	110.08
2	L	2238	MMA	C7-O1-C1	3.92	119.21	113.26
2	F	1238	MMA	C6-C5-C4	3.70	122.10	113.02
2	A	238	MMA	O6-C6-C5	-3.54	99.28	111.33
2	A	238	MMA	C3-C4-C5	3.53	116.62	110.23
2	S	3238	MMA	O2-C2-C1	3.47	118.35	110.08
5	L	902	DBB	CB-CA-N	3.35	123.70	110.57
2	L	2238	MMA	C6-C5-C4	3.27	121.05	113.02
2	L	2238	MMA	C3-C4-C5	3.16	115.96	110.23
5	F	901	DBB	CG-CB-CA	-3.16	105.44	113.34
2	L	2238	MMA	O3-C3-C4	3.07	117.61	110.38
2	S	3238	MMA	C7-O1-C1	3.01	117.83	113.26
2	S	3238	MMA	C6-C5-C4	2.86	120.04	113.02
2	S	3238	MMA	O5-C1-O1	2.81	117.48	110.94
2	A	238	MMA	O5-C5-C6	-2.73	99.67	106.44
2	F	1238	MMA	C3-C4-C5	2.50	114.76	110.23
5	S	904	DBB	CB-CA-N	2.45	120.17	110.57
2	L	2238	MMA	O3-C3-C2	2.32	115.83	110.38
5	A	903	DBB	CB-CA-N	2.23	119.31	110.57
2	S	3238	MMA	C3-C4-C5	2.14	114.11	110.23
2	F	1238	MMA	O5-C1-C2	-2.13	105.98	110.37
2	A	238	MMA	C7-O1-C1	2.01	116.31	113.26

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	903	DBB	OXT-C-CA-N
5	L	902	DBB	OXT-C-CA-N
5	S	904	DBB	OXT-C-CA-N
5	S	904	DBB	OXT-C-CA-CB
5	F	901	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
5	F	901	DBB	10	0
5	A	903	DBB	1	0
2	F	1238	MMA	1	0
5	L	902	DBB	3	0
2	A	238	MMA	3	0
2	L	2238	MMA	1	0
2	S	3238	MMA	1	0
5	S	904	DBB	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	237/237 (100%)	-0.57	7 (2%) 52 55	12, 18, 39, 62	0
1	F	237/237 (100%)	-0.53	7 (2%) 52 55	12, 18, 38, 60	0
1	L	237/237 (100%)	-0.45	4 (1%) 69 71	13, 23, 39, 58	0
1	S	237/237 (100%)	-0.42	9 (3%) 44 47	14, 21, 40, 59	0
All	All	948/948 (100%)	-0.49	27 (2%) 55 57	12, 20, 39, 62	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	120	THR	3.9
1	L	119	SER	3.8
1	S	118	ASN	3.6
1	A	119	SER	3.5
1	F	121	HIS	3.2
1	A	122	GLU	3.0
1	A	118	ASN	2.9
1	L	120	THR	2.9
1	F	119	SER	2.9
1	S	161	SER	2.7
1	A	120	THR	2.6
1	S	149	GLY	2.5
1	L	163	GLY	2.5
1	A	161	SER	2.5
1	S	121	HIS	2.5
1	F	161	SER	2.4
1	A	184	SER	2.4
1	F	203	ASP	2.3
1	S	150	THR	2.3
1	F	122	GLU	2.3
1	F	184	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	S	119	SER	2.3
1	S	162	ASN	2.2
1	A	150	THR	2.2
1	S	120	THR	2.2
1	L	121	HIS	2.1
1	S	160	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MN	A	239	1/1	0.44	0.03	17,17,17,17	0
5	DBB	L	902	7/7	0.77	0.13	15,20,23,24	1
5	DBB	F	901	7/7	0.82	0.14	29,31,32,33	1
5	DBB	S	904	7/7	0.87	0.11	25,26,28,28	1
5	DBB	A	903	7/7	0.89	0.09	14,20,23,23	1
2	MMA	L	2238	13/13	0.89	0.14	25,37,52,53	0
2	MMA	S	3238	13/13	0.89	0.09	20,30,40,41	0
2	MMA	A	238	13/13	0.89	0.12	20,27,44,46	0
4	CA	A	240	1/1	0.92	0.03	18,18,18,18	0
2	MMA	F	1238	13/13	0.94	0.07	15,20,31,31	0
4	CA	S	240	1/1	0.95	0.02	20,20,20,20	0
3	MN	S	239	1/1	0.96	0.05	21,21,21,21	0
3	MN	F	239	1/1	0.97	0.05	20,20,20,20	0
4	CA	L	240	1/1	0.98	0.02	19,19,19,19	0
4	CA	F	240	1/1	0.98	0.02	19,19,19,19	0
3	MN	L	239	1/1	0.99	0.02	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.