



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:56 PM GMT

PDB ID : 2D7F  
Title : Crystal structure of A lectin from canavalia gladiata seeds complexed with al  
pha-methyl-mannosideand 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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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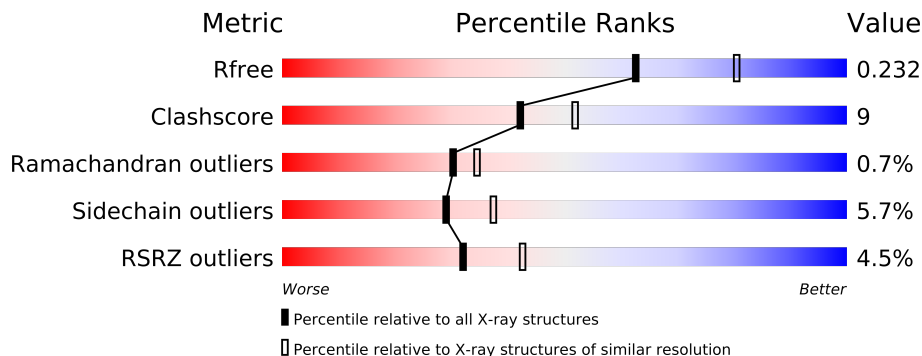
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 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))
$R_{free}$	66092	3293 (2.34-2.30)
Clashscore	79885	4097 (2.34-2.30)
Ramachandran outliers	78287	4055 (2.34-2.30)
Sidechain outliers	78261	4054 (2.34-2.30)
RSRZ outliers	66119	3294 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	237	
1	F	237	
1	L	237	
1	S	237	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MMA	A	238	-	X
2	MMA	L	2238	-	X
2	MMA	S	3238	-	X
5	DBB	F	901	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	DBB	L	902	-	X
5	DBB	S	904	-	X

## 2 Entry composition i

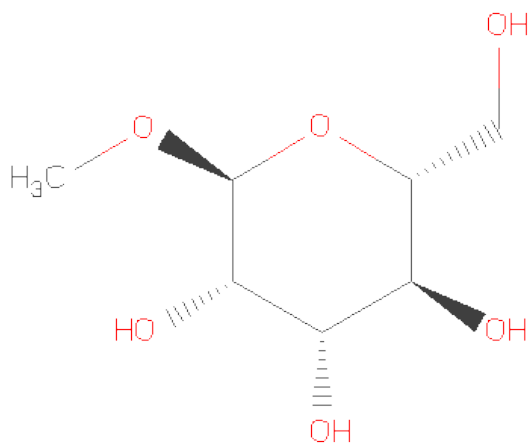
There are 6 unique types of molecules in this entry. The entry contains 7492 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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 SUGAR (O1-METHYL-MANNOSE) (three-letter code: MMA) (formula:  $C_7H_{14}O_6$ ).



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		

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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		

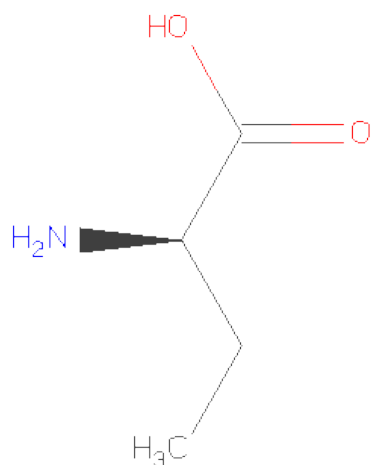
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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

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

- Molecule 5 is D-ALPHA-AMINOBUTYRIC ACID (three-letter code: DBB) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>).



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

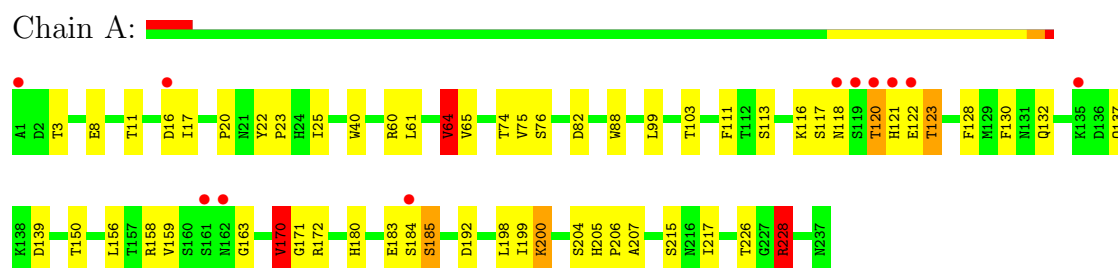
- Molecule 6 is water.

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		

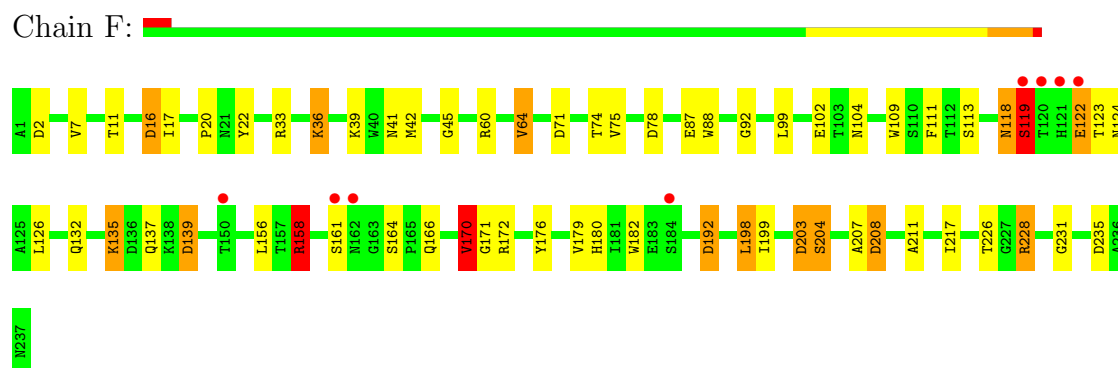
### 3 Residue-property plots

These plots are drawn for all protein, RNA 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.

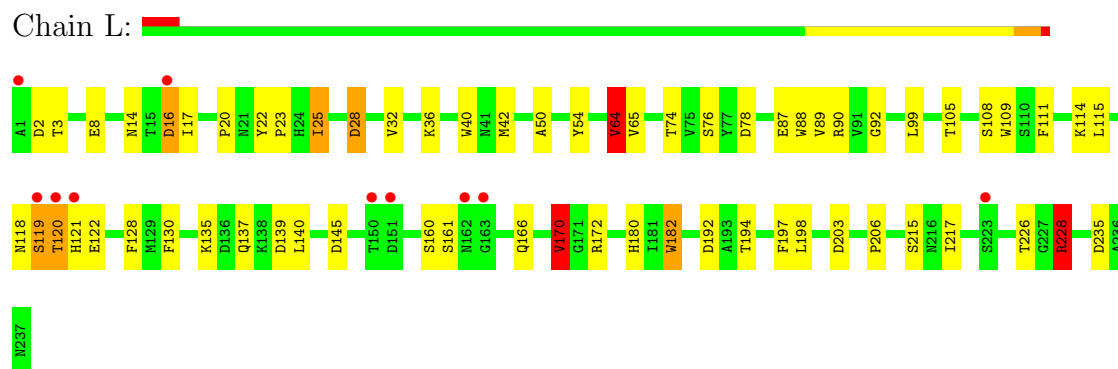
- Molecule 1: Concanavalin A



- Molecule 1: Concanavalin A

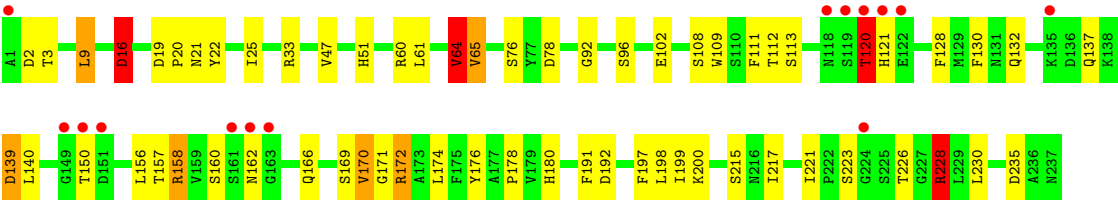


- Molecule 1: Concanavalin A



- Molecule 1: Concanavalin A







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.180 , 0.227 0.191 , 0.232	Depositor DCC
$R_{free}$ test set	3097 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 17.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 60923 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7492	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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, MMA, MN

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(°)	Ideal(°)
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(°)	Ideal(°)
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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (129) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:170:VAL:HG22	1:F:226:THR:CG2	2.27	0.63
1:F:135:LYS:NZ	1:F:135:LYS:HB3	2.13	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:HG3	1:F:158:ARG:HH11	1.67	0.58
1:S:25:ILE:CD1	1:S:65:VAL:HG21	2.35	0.57
1:L:88:TRP:HB3	1:L:217:ILE:HD11	1.87	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:156:LEU:O	1:S:171:GLY:HA3	2.07	0.55
1:S:102:GLU:HB2	1:S:199:ILE:HG23	1.88	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	Distance(Å)	Clash(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:F:119:SER:HB2	1:F:122:GLU:CG	2.39	0.51
1:A:20:PRO:HB2	1:A:22:TYR:CZ	2.46	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:S:180:HIS:O	5:S:904:DBB:HG2	2.15	0.47
1:L:42:MET:CE	1:L:206:PRO:HG2	2.45	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:S:137:GLN:HG2	1:S:140:LEU:HD12	1.97	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: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:F:170:VAL:HG11	1:F:231:GLY:HA2	1.97	0.46
1:F:102:GLU:HG2	1:F:207:ALA:O	2.15	0.46
1:A:117:SER:OG	1:A:122:GLU:HB2	2.16	0.46
1:S:172:ARG:HD2	1:S:221:ILE:CG1	2.44	0.46
1:L:17:ILE:HD13	1:L:228:ARG:HD3	1.98	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:20:PRO:HB2	1:L:22:TYR:CZ	2.52	0.45
1:A:205:HIS:ND1	1:A:206:PRO:HD2	2.31	0.45
1:A:23:PRO:HB2	1:A:40:TRP:O	2.17	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:N	1:S:174:LEU:HD12	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:180:HIS:H	5:F:901:DBB:CG	2.33	0.41
1:F:45:GLY:HA2	1:F:198:LEU:HD11	2.01	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:F:87:GLU:CG	1:F:180:HIS:HE2	2.33	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:L:14:ASN:ND2	2:L:2238:MMA:O4	2.42	0.41
1:S:112:THR:O	1:S:191:PHE:HA	2.21	0.41
1:A:111:PHE:CE2	1:A:113:SER:HB2	2.56	0.41
1:L:23:PRO:HB2	1:L:40:TRP:O	2.20	0.40
1:A:128:PHE:CD1	1:A:130:PHE:CE2	3.09	0.40
1:A:8:GLU:O	1:A:25:ILE:HA	2.20	0.40
1:L:108:SER:HA	1:L:130:PHE:O	2.22	0.40
1:F:111:PHE:CE2	1:F:113:SER:HB2	2.56	0.40
1:F:7:VAL:O	1:F:211:ALA:HA	2.21	0.40
1:A:103:THR:O	1:A:199:ILE:HA	2.21	0.40
1:A:228:ARG:HG2	2:A:238:MMA:O3	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	25	26
1	F	235/237 (99%)	223 (95%)	11 (5%)	1 (0%)	43	52
1	L	235/237 (99%)	228 (97%)	5 (2%)	2 (1%)	25	26
1	S	235/237 (99%)	223 (95%)	10 (4%)	2 (1%)	25	26
All	All	940/948 (99%)	897 (95%)	36 (4%)	7 (1%)	30	34

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%)	193 (96%)	9 (4%)	38	50
1	F	202/202 (100%)	187 (93%)	15 (7%)	20	23
1	L	202/202 (100%)	189 (94%)	13 (6%)	25	31
1	S	202/202 (100%)	193 (96%)	9 (4%)	38	50
All	All	808/808 (100%)	762 (94%)	46 (6%)	29	37

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
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

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Mol	Chain	Res	Type
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

Some 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 ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	A	238	-	13,13,13	1.64	3 (23%)	18,18,18	4.87	9 (50%)
5	DBB	A	903	-	6,6,6	0.69	0	7,7,7	1.69	3 (42%)
2	MMA	F	1238	-	13,13,13	1.33	2 (15%)	18,18,18	4.53	8 (44%)
5	DBB	F	901	-	6,6,6	1.30	1 (16%)	7,7,7	5.62	4 (57%)
2	MMA	L	2238	-	13,13,13	1.54	2 (15%)	18,18,18	4.04	9 (50%)
5	DBB	L	902	-	6,6,6	1.56	1 (16%)	7,7,7	1.85	2 (28%)
2	MMA	S	3238	-	13,13,13	1.24	3 (23%)	18,18,18	3.90	9 (50%)
5	DBB	S	904	-	6,6,6	0.57	0	7,7,7	1.99	3 (42%)

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	A	238	-	1/1/5/5	0/4/24/24	0/1/1/1
5	DBB	A	903	-	-	0/6/6/6	0/0/0/0
2	MMA	F	1238	-	1/1/5/5	0/4/24/24	0/1/1/1
5	DBB	F	901	-	-	0/6/6/6	0/0/0/0
2	MMA	L	2238	-	1/1/5/5	0/4/24/24	0/1/1/1
5	DBB	L	902	-	-	0/6/6/6	0/0/0/0
2	MMA	S	3238	-	1/1/5/5	0/4/24/24	0/1/1/1
5	DBB	S	904	-	-	0/6/6/6	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1238	MMA	C4-C3	3.04	1.60	1.52
5	L	902	DBB	CB-CA	2.99	1.56	1.53
2	L	2238	MMA	C3-C2	2.95	1.60	1.52
2	S	3238	MMA	C4-C3	2.92	1.60	1.52
2	A	238	MMA	C4-C3	2.77	1.59	1.52
2	L	2238	MMA	C4-C3	2.72	1.59	1.52
5	F	901	DBB	CB-CA	2.62	1.55	1.53
2	A	238	MMA	O2-C2	2.59	1.49	1.43
2	F	1238	MMA	C4-C5	2.35	1.58	1.53
2	S	3238	MMA	C3-C2	2.20	1.58	1.52
2	A	238	MMA	O3-C3	-2.11	1.37	1.43
2	S	3238	MMA	C4-C5	2.10	1.57	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1238	MMA	O1-C1-C2	13.34	124.53	108.18
2	L	2238	MMA	O1-C1-C2	12.65	123.69	108.18
5	F	901	DBB	C-CA-N	11.21	127.93	109.36
2	A	238	MMA	O1-C1-C2	11.14	121.83	108.18
2	A	238	MMA	C1-C2-C3	-10.65	89.28	110.00
2	S	3238	MMA	O1-C1-C2	9.52	119.86	108.18
2	F	1238	MMA	C1-C2-C3	-9.27	91.96	110.00
2	A	238	MMA	O2-C2-C1	8.26	128.06	110.04
2	S	3238	MMA	C1-C2-C3	-7.72	94.97	110.00
5	F	901	DBB	CG-CB-CA	-6.82	105.44	113.15
2	S	3238	MMA	O3-C3-C4	6.59	125.14	110.35
2	L	2238	MMA	C1-O5-C5	-6.12	101.83	113.73
5	F	901	DBB	CB-CA-C	-5.83	94.30	111.08
2	A	238	MMA	C1-O5-C5	-5.65	102.75	113.73
2	F	1238	MMA	O3-C3-C4	5.33	122.31	110.35
2	A	238	MMA	O4-C4-C5	-5.17	95.67	109.28
2	F	1238	MMA	C1-O5-C5	-4.92	104.17	113.73
2	S	3238	MMA	C1-O5-C5	-4.90	104.19	113.73
2	A	238	MMA	O3-C3-C4	4.47	120.38	110.35
2	L	2238	MMA	C1-C2-C3	-4.43	101.39	110.00
2	F	1238	MMA	O2-C2-C1	4.40	119.63	110.04
2	L	2238	MMA	O5-C1-C2	-4.09	101.93	110.31
5	L	902	DBB	CB-CA-N	3.89	123.70	110.87
2	L	2238	MMA	C7-O1-C1	3.87	119.21	113.33
2	S	3238	MMA	O2-C2-C1	3.81	118.35	110.04
2	F	1238	MMA	C6-C5-C4	3.77	122.10	113.00
2	A	238	MMA	C3-C4-C5	3.60	116.62	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	238	MMA	O6-C6-C5	-3.51	99.28	111.36
2	L	2238	MMA	C6-C5-C4	3.33	121.05	113.00
2	L	2238	MMA	O3-C3-C4	3.24	117.61	110.35
2	L	2238	MMA	C3-C4-C5	3.23	115.96	110.20
5	F	901	DBB	OXT-C-CA	3.07	123.78	116.88
5	S	904	DBB	C-CA-N	3.06	114.43	109.36
5	S	904	DBB	CG-CB-CA	-2.98	109.78	113.15
2	S	3238	MMA	C7-O1-C1	2.96	117.83	113.33
2	S	3238	MMA	C6-C5-C4	2.91	120.04	113.00
5	S	904	DBB	CB-CA-N	2.82	120.17	110.87
2	S	3238	MMA	O5-C1-O1	2.77	117.48	110.85
2	A	238	MMA	O5-C5-C6	-2.71	99.67	106.34
5	A	903	DBB	CB-CA-N	2.56	119.31	110.87
2	F	1238	MMA	C3-C4-C5	2.55	114.76	110.20
5	A	903	DBB	C-CA-N	2.46	113.44	109.36
2	L	2238	MMA	O3-C3-C2	2.44	115.83	110.35
5	A	903	DBB	CG-CB-CA	-2.22	110.64	113.15
2	S	3238	MMA	C3-C4-C5	2.19	114.11	110.20
2	F	1238	MMA	O5-C1-C2	-2.11	105.98	110.31
5	L	902	DBB	OXT-C-O	2.00	128.60	124.07

All (4) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	237/237 (100%)	-0.40	11 (4%)	31 41	12, 18, 39, 62	0
1	F	237/237 (100%)	-0.38	8 (3%)	43 53	12, 18, 38, 60	0
1	L	237/237 (100%)	-0.26	10 (4%)	35 45	13, 23, 39, 58	0
1	S	237/237 (100%)	-0.24	14 (5%)	22 31	14, 21, 40, 59	0
All	All	948/948 (100%)	-0.32	43 (4%)	32 42	12, 20, 39, 62	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	161	SER	4.6
1	F	121	HIS	4.3
1	F	120	THR	4.3
1	L	119	SER	4.3
1	S	161	SER	4.2
1	L	121	HIS	4.1
1	F	184	SER	3.9
1	S	119	SER	3.9
1	S	121	HIS	3.8
1	A	16	ASP	3.7
1	A	184	SER	3.6
1	S	163	GLY	3.6
1	L	1	ALA	3.6
1	L	163	GLY	3.5
1	F	119	SER	3.4
1	F	161	SER	3.4
1	F	150	THR	3.2
1	S	162	ASN	3.2
1	S	1	ALA	3.1
1	A	122	GLU	3.1
1	S	118	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	121	HIS	2.9
1	A	119	SER	2.8
1	F	162	ASN	2.8
1	A	162	ASN	2.8
1	A	1	ALA	2.7
1	L	150	THR	2.7
1	L	120	THR	2.7
1	A	120	THR	2.6
1	S	135	LYS	2.6
1	A	118	ASN	2.5
1	S	149	GLY	2.5
1	L	151	ASP	2.4
1	L	162	ASN	2.3
1	L	223	SER	2.3
1	S	150	THR	2.3
1	F	122	GLU	2.2
1	S	151	ASP	2.2
1	S	120	THR	2.1
1	S	224	GLY	2.0
1	L	16	ASP	2.0
1	A	135	LYS	2.0
1	S	122	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MMA	A	238	13/13	0.19	5.84	20,27,44,46	0
2	MMA	L	2238	13/13	0.24	4.57	25,37,52,53	0
5	DBB	F	901	7/7	0.22	3.85	29,31,32,33	1
5	DBB	S	904	7/7	0.18	3.74	25,26,28,28	1
2	MMA	S	3238	13/13	0.18	3.50	20,30,40,41	0
5	DBB	L	902	7/7	0.17	3.27	15,20,23,24	1
2	MMA	F	1238	13/13	0.14	1.63	15,20,31,31	0
5	DBB	A	903	7/7	0.14	1.29	14,20,23,23	1
4	CA	A	240	1/1	0.06	-1.41	18,18,18,18	0
4	CA	L	240	1/1	0.05	-1.45	19,19,19,19	0
4	CA	S	240	1/1	0.06	-1.85	20,20,20,20	0
3	MN	A	239	1/1	0.05	-2.53	17,17,17,17	0
4	CA	F	240	1/1	0.05	-2.67	19,19,19,19	0
3	MN	F	239	1/1	0.05	-3.18	20,20,20,20	0
3	MN	S	239	1/1	0.04	-4.22	21,21,21,21	0
3	MN	L	239	1/1	0.04	-5.41	22,22,22,22	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.