



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:00 am BST

PDB ID : 3IPV  
Title : Crystal structure of Spatholobus parviflorus seed lectin  
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Deposited on : 2009-08-18  
Resolution : 2.04 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](mailto: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.

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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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

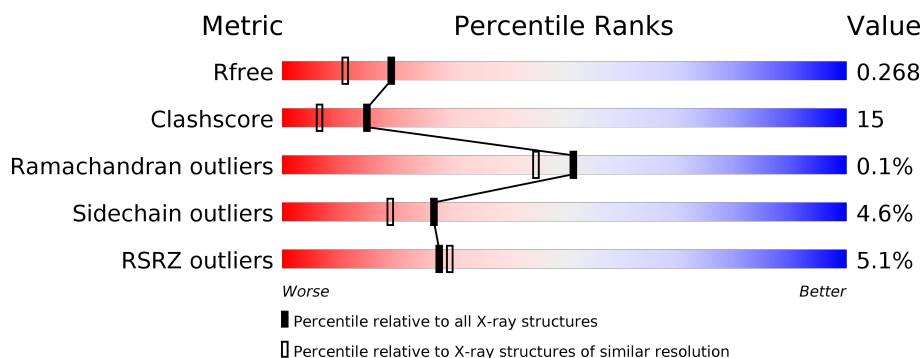
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 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	251	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>..</div> </div> </div>
1	C	251	<div> <div>8%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
2	B	239	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>5%</div> </div> </div>
2	D	239	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7987 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 Lectin alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	0	0	0
			1853	1199	289	365			
1	C	249	Total	C	N	O	0	0	0
			1853	1199	289	365			

- Molecule 2 is a protein called Lectin beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	0	0	0
			1790	1162	277	351			
2	D	239	Total	C	N	O	0	0	0
			1790	1162	277	351			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		

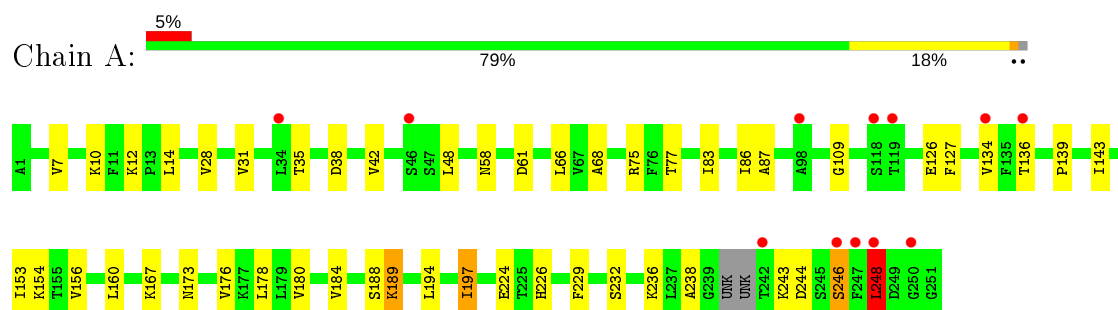
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	173	Total	O	0	0
			173	173		
5	B	172	Total	O	0	0
			172	172		
5	C	169	Total	O	0	0
			169	169		
5	D	179	Total	O	0	0
			179	179		

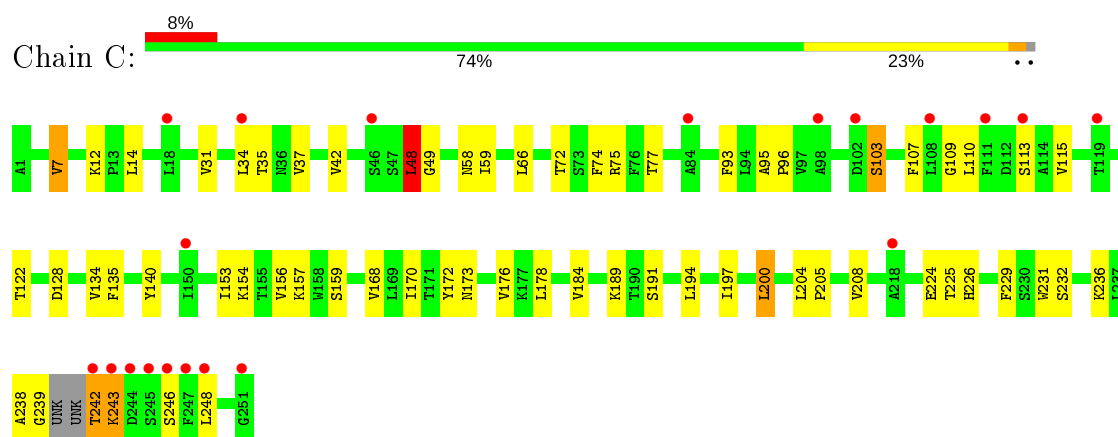
### 3 Residue-property plots [i](#)

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

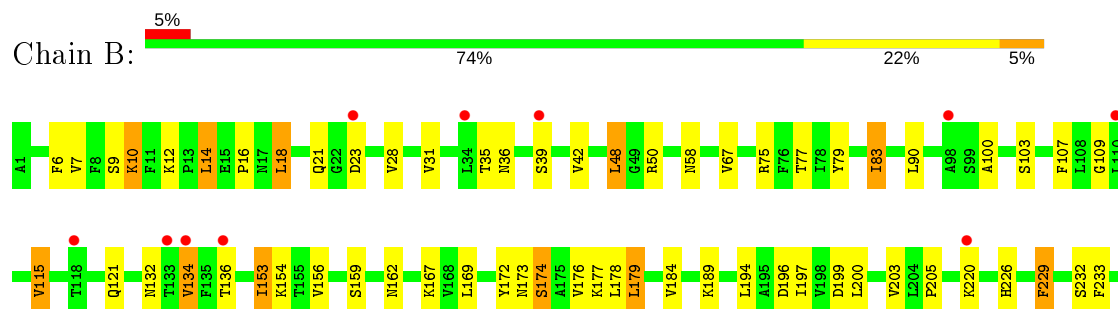
#### • Molecule 1: Lectin alpha chain



#### • Molecule 1: Lectin alpha chain

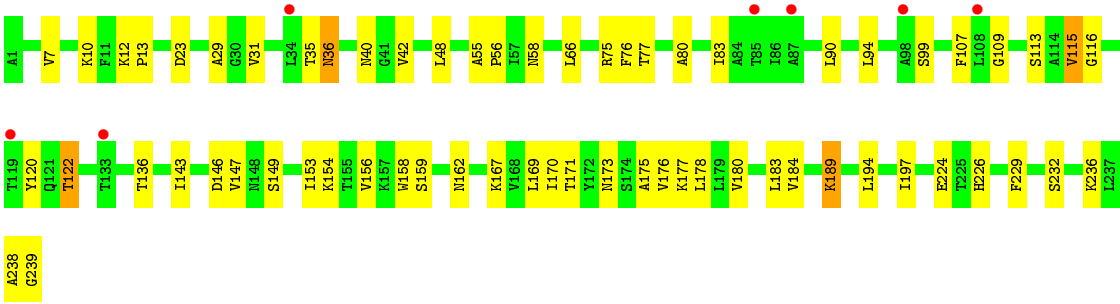


#### • Molecule 2: Lectin beta chain





● Molecule 2: Lectin beta chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.00Å 60.79Å 78.18Å 101.32° 91.38° 104.32°	Depositor
Resolution (Å)	19.82 – 2.04 19.82 – 2.04	Depositor EDS
% Data completeness (in resolution range)	92.4 (19.82-2.04) 92.4 (19.82-2.04)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.85 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.199 , 0.264 0.202 , 0.268	Depositor DCC
$R_{free}$ test set	3179 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	1.09	3/1898 (0.2%)	0.94	2/2593 (0.1%)
1	C	1.09	3/1898 (0.2%)	0.93	2/2593 (0.1%)
2	B	1.08	4/1836 (0.2%)	0.91	3/2515 (0.1%)
2	D	1.12	1/1836 (0.1%)	0.91	0/2515
All	All	1.09	11/7468 (0.1%)	0.92	7/10216 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	159	SER	CB-OG	6.55	1.50	1.42
2	B	159	SER	CB-OG	5.96	1.50	1.42
1	C	231	TRP	CB-CG	5.94	1.60	1.50
2	D	159	SER	CB-OG	5.83	1.49	1.42
2	B	229	PHE	CD2-CE2	-5.69	1.27	1.39
2	B	79	TYR	CD1-CE1	5.60	1.47	1.39
1	A	127	PHE	CE1-CZ	5.47	1.47	1.37
2	B	100	ALA	CA-CB	5.38	1.63	1.52
1	A	180	VAL	CB-CG2	5.38	1.64	1.52
1	C	7	VAL	CB-CG2	-5.28	1.41	1.52
1	A	68	ALA	CA-CB	5.04	1.63	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	179	LEU	CA-CB-CG	5.80	128.64	115.30
2	B	10	LYS	CD-CE-NZ	5.77	124.98	111.70
1	C	128	ASP	CB-CG-OD1	5.44	123.19	118.30
1	C	48	LEU	CB-CG-CD2	5.41	120.20	111.00
1	A	197	ILE	CG1-CB-CG2	-5.24	99.88	111.40
1	A	248	LEU	CA-CB-CG	5.13	127.10	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1853	0	1821	53	0
1	C	1853	0	1821	65	0
2	B	1790	0	1757	59	0
2	D	1790	0	1757	64	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	173	0	0	17	0
5	B	172	0	0	25	0
5	C	169	0	0	16	0
5	D	179	0	0	18	0
All	All	7987	0	7156	218	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 15.

All (218) 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)
2:D:29:ALA:HB3	5:D:733:HOH:O	1.41	1.21
1:C:248:LEU:HD11	2:D:169:LEU:HD21	1.23	1.17
1:A:197:ILE:HD13	2:B:189:LYS:HE2	1.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:VAL:HG22	5:C:669:HOH:O	1.54	1.07
2:B:176:VAL:HG21	5:B:731:HOH:O	1.55	1.06
2:B:153:ILE:HB	5:B:311:HOH:O	1.57	1.02
2:B:167:LYS:HE2	5:B:756:HOH:O	1.66	0.94
1:C:140:TYR:HB2	5:C:478:HOH:O	1.69	0.92
1:C:248:LEU:CD1	2:D:169:LEU:HD21	1.98	0.92
2:D:176:VAL:HG21	5:D:749:HOH:O	1.70	0.92
2:B:156:VAL:HG22	5:B:284:HOH:O	1.70	0.91
1:A:31:VAL:HG22	5:A:671:HOH:O	1.69	0.90
1:A:176:VAL:HG21	5:B:756:HOH:O	1.75	0.85
1:C:75:ARG:HD3	5:C:293:HOH:O	1.77	0.85
2:D:177:LYS:HE3	5:D:770:HOH:O	1.80	0.82
1:A:154:LYS:HG2	1:A:194:LEU:HD11	1.62	0.81
2:B:42:VAL:HG21	5:B:304:HOH:O	1.81	0.80
2:D:122:THR:HG21	5:D:245:HOH:O	1.81	0.80
1:C:157:LYS:HE3	5:C:478:HOH:O	1.80	0.80
1:C:176:VAL:HG21	5:C:680:HOH:O	1.83	0.78
2:B:83:ILE:HD12	2:B:162:ASN:HB2	1.65	0.78
2:D:66:LEU:CD2	5:D:799:HOH:O	2.31	0.76
2:D:7:VAL:HG23	5:D:433:HOH:O	1.84	0.76
1:C:115:VAL:HG23	5:C:491:HOH:O	1.85	0.76
2:D:31:VAL:HG22	5:D:668:HOH:O	1.86	0.76
1:A:35:THR:OG1	1:A:226:HIS:HD2	1.68	0.75
1:C:66:LEU:HD23	5:C:464:HOH:O	1.84	0.75
1:A:156:VAL:HG22	5:A:260:HOH:O	1.87	0.74
2:D:178:LEU:HD12	2:D:197:ILE:HD13	1.70	0.74
1:A:246:SER:HB3	5:A:488:HOH:O	1.87	0.73
2:D:239:GLY:HA3	5:D:356:HOH:O	1.87	0.73
2:D:7:VAL:HG22	2:D:232:SER:HB2	1.69	0.73
2:B:7:VAL:HG23	5:C:366:HOH:O	1.88	0.72
1:C:239:GLY:HA3	5:C:764:HOH:O	1.90	0.71
2:D:115:VAL:HG12	5:D:268:HOH:O	1.90	0.71
2:D:156:VAL:HG22	5:D:315:HOH:O	1.91	0.70
1:A:229:PHE:HD1	5:A:671:HOH:O	1.73	0.70
1:A:75:ARG:HD3	5:A:318:HOH:O	1.92	0.70
1:A:42:VAL:HG22	5:A:311:HOH:O	1.91	0.70
1:C:178:LEU:HD21	2:D:184:VAL:HG11	1.73	0.69
1:C:35:THR:OG1	1:C:226:HIS:HD2	1.76	0.68
2:B:31:VAL:HG12	5:B:681:HOH:O	1.92	0.68
2:B:75:ARG:HD3	5:B:734:HOH:O	1.93	0.68
2:B:58:ASN:HD21	1:C:12:LYS:NZ	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:LEU:HD23	5:D:799:HOH:O	1.92	0.68
2:D:75:ARG:HG2	2:D:229:PHE:HD2	1.58	0.67
2:D:120:TYR:O	2:D:122:THR:HG23	1.93	0.67
2:D:23:ASP:HB3	2:D:36:ASN:ND2	2.10	0.67
2:D:35:THR:OG1	2:D:226:HIS:HD2	1.78	0.67
1:A:176:VAL:HG23	1:A:178:LEU:H	1.59	0.67
1:A:42:VAL:HG21	5:A:303:HOH:O	1.95	0.67
1:C:7:VAL:HG22	1:C:232:SER:HB2	1.76	0.66
2:D:154:LYS:HG2	2:D:194:LEU:HD11	1.77	0.66
1:A:77:THR:OG1	1:A:229:PHE:HE2	1.79	0.66
2:B:35:THR:OG1	2:B:226:HIS:HD2	1.79	0.66
1:A:77:THR:OG1	1:A:229:PHE:CE2	2.49	0.65
1:A:7:VAL:HG22	1:A:232:SER:HB2	1.78	0.65
1:C:172:TYR:CZ	1:C:200:LEU:HD22	2.32	0.65
1:A:178:LEU:HD21	2:B:184:VAL:HG11	1.77	0.65
1:C:197:ILE:HG12	2:D:189:LYS:HE3	1.78	0.65
2:B:153:ILE:CG1	5:B:256:HOH:O	2.45	0.65
1:C:48:LEU:HD21	1:C:109:GLY:HA3	1.79	0.65
2:B:154:LYS:HG2	2:B:194:LEU:HD11	1.80	0.64
2:B:58:ASN:HD21	1:C:12:LYS:HZ2	1.45	0.64
2:D:229:PHE:HD1	5:D:668:HOH:O	1.80	0.64
1:C:42:VAL:HG21	5:C:305:HOH:O	1.98	0.64
2:D:42:VAL:HG22	5:D:276:HOH:O	1.97	0.64
1:C:172:TYR:CE2	1:C:200:LEU:HD22	2.33	0.63
1:A:134:VAL:HB	5:A:354:HOH:O	1.97	0.63
1:A:28:VAL:HG13	5:A:292:HOH:O	1.98	0.63
2:B:153:ILE:HG13	5:B:256:HOH:O	1.98	0.63
1:C:236:LYS:HE3	1:C:242:THR:N	2.14	0.63
1:C:243:LYS:HA	1:C:243:LYS:HE3	1.79	0.63
1:C:66:LEU:CD2	5:C:464:HOH:O	2.44	0.62
2:B:115:VAL:HG22	5:B:442:HOH:O	1.99	0.62
1:A:153:ILE:HD13	5:A:316:HOH:O	1.99	0.61
2:B:42:VAL:CG2	5:B:304:HOH:O	2.45	0.61
2:D:107:PHE:CE1	2:D:113:SER:HA	2.35	0.61
2:B:12:LYS:NZ	1:C:58:ASN:HD21	1.99	0.60
1:C:242:THR:HG22	5:C:628:HOH:O	2.02	0.60
1:C:75:ARG:HG2	1:C:229:PHE:HD2	1.67	0.60
2:D:120:TYR:O	2:D:122:THR:CG2	2.50	0.59
1:C:229:PHE:HD1	5:C:669:HOH:O	1.84	0.59
1:A:178:LEU:HD21	2:B:184:VAL:CG1	2.33	0.58
1:C:243:LYS:HG3	1:C:246:SER:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:PHE:HE1	2:D:113:SER:HA	1.68	0.58
2:B:67:VAL:O	2:B:174:SER:OG	2.22	0.58
1:C:178:LEU:HD12	1:C:197:ILE:HD13	1.85	0.57
2:D:115:VAL:HG22	5:D:244:HOH:O	2.03	0.57
1:C:107:PHE:HE2	1:C:113:SER:HA	1.69	0.57
1:C:205:PRO:HD2	1:C:208:VAL:HG12	1.87	0.57
1:A:75:ARG:HD2	1:A:167:LYS:HZ2	1.69	0.57
2:B:14:LEU:HD22	2:B:16:PRO:HD3	1.86	0.57
2:B:7:VAL:HG22	2:B:232:SER:HB2	1.85	0.57
2:B:12:LYS:HZ2	1:C:58:ASN:HD21	1.53	0.57
2:B:136:THR:HG22	2:B:136:THR:O	2.05	0.56
2:B:28:VAL:HG13	5:B:636:HOH:O	2.06	0.56
2:D:178:LEU:CD1	2:D:197:ILE:HD13	2.37	0.55
1:A:244:ASP:HB2	5:A:474:HOH:O	2.06	0.55
1:C:184:VAL:HG11	2:D:178:LEU:HD21	1.89	0.55
1:A:66:LEU:HD12	1:A:238:ALA:O	2.07	0.55
2:B:229:PHE:HD1	5:B:681:HOH:O	1.90	0.55
1:C:178:LEU:HD21	2:D:184:VAL:CG1	2.36	0.55
2:D:42:VAL:HG21	5:D:652:HOH:O	2.05	0.55
2:D:77:THR:HG1	2:D:229:PHE:HE2	1.46	0.55
2:D:40:ASN:ND2	5:D:310:HOH:O	2.40	0.54
1:A:12:LYS:NZ	2:D:58:ASN:HD21	2.04	0.54
1:C:153:ILE:HG21	5:C:277:HOH:O	2.07	0.54
1:C:242:THR:CG2	5:C:628:HOH:O	2.54	0.54
1:C:154:LYS:HG2	1:C:194:LEU:HD11	1.90	0.54
1:A:173:ASN:HB3	1:A:176:VAL:HG22	1.90	0.54
1:A:75:ARG:HD2	1:A:167:LYS:NZ	2.24	0.53
1:A:248:LEU:HD21	2:B:169:LEU:HD21	1.90	0.53
2:D:116:GLY:HA3	5:D:797:HOH:O	2.08	0.52
2:D:75:ARG:HD2	2:D:167:LYS:NZ	2.24	0.52
1:C:134:VAL:HG12	1:C:135:PHE:CD1	2.45	0.52
5:B:477:HOH:O	1:C:14:LEU:HD21	2.09	0.52
1:C:48:LEU:HD21	1:C:109:GLY:CA	2.38	0.52
1:C:77:THR:HG1	1:C:229:PHE:HE2	1.47	0.52
2:D:176:VAL:HG23	2:D:178:LEU:H	1.73	0.52
2:D:76:PHE:CD2	2:D:90:LEU:HD21	2.45	0.52
1:A:38:ASP:OD1	1:A:38:ASP:C	2.48	0.52
1:C:156:VAL:HG22	5:C:309:HOH:O	2.09	0.52
1:A:167:LYS:HD2	5:B:434:HOH:O	2.09	0.52
2:D:77:THR:OG1	2:D:229:PHE:CZ	2.63	0.51
2:B:176:VAL:HG23	2:B:178:LEU:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:VAL:HG22	1:C:232:SER:CB	2.41	0.51
2:D:75:ARG:HD2	2:D:167:LYS:HZ2	1.76	0.51
2:B:156:VAL:CG2	5:B:284:HOH:O	2.42	0.51
1:C:200:LEU:HG	1:C:204:LEU:HD12	1.91	0.51
1:C:34:LEU:O	1:C:49:GLY:HA3	2.11	0.51
1:A:229:PHE:CD1	5:A:671:HOH:O	2.52	0.50
2:B:77:THR:HG1	2:B:229:PHE:HZ	1.54	0.50
2:D:83:ILE:HD13	2:D:162:ASN:HB2	1.92	0.50
1:C:66:LEU:HD12	1:C:238:ALA:O	2.11	0.50
2:B:103:SER:O	2:B:107:PHE:HB2	2.12	0.50
1:A:12:LYS:HZ2	2:D:58:ASN:HD21	1.60	0.50
2:B:48:LEU:HD21	2:B:109:GLY:HA3	1.94	0.50
1:A:178:LEU:CD2	2:B:184:VAL:HG11	2.40	0.49
1:C:224:GLU:OE2	1:C:226:HIS:HE1	1.95	0.49
1:C:184:VAL:CG1	2:D:178:LEU:HD21	2.42	0.49
1:C:103:SER:HB3	1:C:107:PHE:CG	2.48	0.48
2:B:132:ASN:HB3	2:B:134:VAL:HG13	1.96	0.48
2:D:173:ASN:OD1	2:D:175:ALA:N	2.47	0.48
2:D:48:LEU:HD11	2:D:109:GLY:HA3	1.94	0.48
2:B:21:GLN:HB2	2:B:50:ARG:HB2	1.96	0.48
2:B:9:SER:HB2	5:B:276:HOH:O	2.13	0.48
2:D:66:LEU:HD12	2:D:238:ALA:O	2.14	0.48
2:D:136:THR:O	2:D:136:THR:HG22	2.14	0.48
1:C:95:ALA:HB1	1:C:96:PRO:CD	2.45	0.47
5:B:763:HOH:O	1:C:7:VAL:HG23	2.15	0.47
2:B:31:VAL:CG1	5:B:681:HOH:O	2.56	0.47
1:C:77:THR:OG1	1:C:229:PHE:CZ	2.65	0.47
2:D:23:ASP:HB3	2:D:36:ASN:HD22	1.78	0.47
2:B:153:ILE:HG12	5:B:256:HOH:O	2.12	0.46
1:A:83:ILE:HD11	1:A:160:LEU:HD23	1.96	0.46
1:A:61:ASP:OD1	2:D:12:LYS:NZ	2.48	0.46
1:A:126:GLU:O	1:A:143:ILE:HA	2.16	0.45
2:B:28:VAL:HG22	5:B:781:HOH:O	2.16	0.45
1:C:110:LEU:HD22	1:C:122:THR:HG21	1.98	0.45
1:A:243:LYS:HE2	2:B:7:VAL:HG21	1.98	0.45
2:B:75:ARG:HG2	2:B:229:PHE:HD2	1.80	0.45
2:D:143:ILE:HG13	2:D:158:TRP:HB2	1.99	0.45
1:A:7:VAL:HG23	5:A:304:HOH:O	2.17	0.45
2:B:220:LYS:HD3	2:B:220:LYS:HA	1.81	0.44
2:B:103:SER:HB2	2:B:107:PHE:CG	2.52	0.44
2:B:173:ASN:O	2:B:177:LYS:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:PHE:CE2	1:C:113:SER:HA	2.51	0.44
1:C:243:LYS:HE3	1:C:243:LYS:CA	2.46	0.44
2:B:173:ASN:HB3	2:B:176:VAL:HG22	1.99	0.44
1:C:107:PHE:HE2	1:C:113:SER:CA	2.31	0.44
1:C:74:PHE:CZ	1:C:168:VAL:HG11	2.52	0.44
1:A:188:SER:C	1:A:189:LYS:HG2	2.37	0.43
1:A:7:VAL:HG22	1:A:232:SER:CB	2.48	0.43
1:A:188:SER:C	1:A:189:LYS:CG	2.86	0.43
1:A:136:THR:HG22	1:A:136:THR:O	2.18	0.43
2:B:23:ASP:HB3	2:B:36:ASN:ND2	2.33	0.43
1:C:72:THR:HG22	1:C:170:ILE:HB	2.01	0.43
2:D:153:ILE:HD12	5:D:705:HOH:O	2.18	0.43
1:A:189:LYS:HE2	5:A:443:HOH:O	2.19	0.43
2:B:199:ASP:O	2:B:203:VAL:HG22	2.18	0.43
1:A:83:ILE:HD11	1:A:160:LEU:CD2	2.49	0.43
1:A:224:GLU:OE2	1:A:226:HIS:HE1	2.02	0.43
2:B:173:ASN:OD1	2:B:173:ASN:C	2.57	0.42
1:C:178:LEU:CD1	1:C:197:ILE:HD13	2.48	0.42
2:D:83:ILE:HD13	2:D:162:ASN:CG	2.39	0.42
1:A:184:VAL:HG11	2:B:178:LEU:HD21	2.00	0.42
1:A:58:ASN:HD21	2:D:12:LYS:NZ	2.17	0.42
2:B:42:VAL:HG22	5:B:264:HOH:O	2.19	0.42
2:B:9:SER:CB	5:B:276:HOH:O	2.68	0.42
1:C:77:THR:HG1	1:C:229:PHE:HZ	1.60	0.42
2:D:66:LEU:N	2:D:66:LEU:HD23	2.34	0.42
1:C:93:PHE:CG	1:C:110:LEU:HD21	2.55	0.42
1:C:173:ASN:C	1:C:173:ASN:OD1	2.58	0.42
2:D:80:ALA:HB3	2:D:83:ILE:HD12	2.01	0.42
1:A:189:LYS:NZ	5:A:287:HOH:O	2.44	0.42
1:A:86:ILE:O	1:A:87:ALA:HB2	2.20	0.42
2:B:121:GLN:HB3	2:B:205:PRO:HD3	2.01	0.42
1:C:184:VAL:HG22	1:C:191:SER:HB3	2.01	0.42
2:B:154:LYS:HD3	2:B:196:ASP:HB2	2.01	0.41
1:A:28:VAL:O	1:A:28:VAL:HG23	2.19	0.41
2:B:172:TYR:CE2	2:B:200:LEU:HD12	2.56	0.41
2:D:146:ASP:HB3	2:D:149:SER:O	2.20	0.41
2:D:147:VAL:CG2	2:D:153:ILE:HD13	2.50	0.41
1:A:48:LEU:HD11	1:A:109:GLY:HA3	2.03	0.41
2:B:77:THR:OG1	2:B:229:PHE:CE2	2.72	0.41
2:D:170:ILE:HA	2:D:180:VAL:O	2.20	0.41
1:A:224:GLU:OE2	1:A:226:HIS:CE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LYS:CE	5:A:443:HOH:O	2.69	0.41
2:D:183:LEU:HD23	2:D:184:VAL:N	2.36	0.41
1:C:37:VAL:HG22	1:C:225:THR:HG22	2.02	0.41
2:B:6:PHE:CZ	2:B:233:PHE:HB3	2.56	0.40
1:C:248:LEU:HD13	2:D:171:THR:HG21	2.01	0.40
2:B:28:VAL:HG23	5:B:454:HOH:O	2.20	0.40
1:A:244:ASP:CB	5:A:474:HOH:O	2.66	0.40
2:D:224:GLU:OE2	2:D:226:HIS:HE1	2.04	0.40
2:D:55:ALA:HA	2:D:56:PRO:HD3	1.88	0.40
2:D:83:ILE:HD13	2:D:162:ASN:CB	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	245/251 (98%)	239 (98%)	5 (2%)	1 (0%)	34	24
1	C	245/251 (98%)	238 (97%)	7 (3%)	0	100	100
2	B	237/239 (99%)	231 (98%)	6 (2%)	0	100	100
2	D	237/239 (99%)	232 (98%)	5 (2%)	0	100	100
All	All	964/980 (98%)	940 (98%)	23 (2%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/201 (100%)	195 (97%)	6 (3%)	41	34
1	C	201/201 (100%)	194 (96%)	7 (4%)	36	29
2	B	194/194 (100%)	180 (93%)	14 (7%)	14	7
2	D	194/194 (100%)	185 (95%)	9 (5%)	27	19
All	All	790/790 (100%)	754 (95%)	36 (5%)	27	19

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	14	LEU
1	A	189	LYS
1	A	236	LYS
1	A	246	SER
1	A	248	LEU
2	B	10	LYS
2	B	14	LEU
2	B	18	LEU
2	B	39	SER
2	B	48	LEU
2	B	83	ILE
2	B	90	LEU
2	B	115	VAL
2	B	134	VAL
2	B	153	ILE
2	B	174	SER
2	B	179	LEU
2	B	197	ILE
2	B	236	LYS
1	C	48	LEU
1	C	59	ILE
1	C	103	SER
1	C	189	LYS

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Mol	Chain	Res	Type
1	C	200	LEU
1	C	242	THR
1	C	243	LYS
2	D	10	LYS
2	D	13	PRO
2	D	36	ASN
2	D	94	LEU
2	D	99	SER
2	D	115	VAL
2	D	122	THR
2	D	189	LYS
2	D	236	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	226	HIS
2	B	36	ASN
2	B	58	ASN
2	B	226	HIS
1	C	40	ASN
1	C	58	ASN
1	C	226	HIS
2	D	36	ASN
2	D	40	ASN
2	D	58	ASN
2	D	226	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	249/251 (99%)	0.28	12 (4%) 30 33	9, 14, 22, 45	3 (1%)
1	C	249/251 (99%)	0.32	20 (8%) 12 13	7, 13, 22, 42	3 (1%)
2	B	239/239 (100%)	0.20	11 (4%) 32 35	9, 14, 21, 27	0
2	D	239/239 (100%)	0.19	7 (2%) 51 56	7, 12, 20, 26	0
All	All	976/980 (99%)	0.25	50 (5%) 28 30	7, 13, 21, 45	6 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	119	THR	4.7
2	D	119	THR	4.6
1	C	246	SER	4.3
1	C	248	LEU	4.0
1	A	98	ALA	3.8
2	D	133	THR	3.5
2	B	98	ALA	3.4
2	B	118	THR	3.4
1	A	119	THR	3.3
1	A	136	THR	3.1
1	C	245	SER	3.0
2	B	133	THR	3.0
1	C	111	PHE	3.0
1	A	250	GLY	3.0
1	C	251	GLY	3.0
1	A	134	VAL	3.0
1	C	98	ALA	2.9
1	A	247	PHE	2.9
1	A	246	SER	2.8
1	A	34	LEU	2.8
2	B	39	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	242	THR	2.7
1	C	34	LEU	2.7
2	B	136	THR	2.7
1	C	247	PHE	2.6
1	C	46	SER	2.6
2	B	134	VAL	2.6
2	D	108	LEU	2.6
1	A	118	SER	2.5
1	A	248	LEU	2.5
2	B	239	GLY	2.5
2	D	34	LEU	2.4
1	C	108	LEU	2.4
2	B	110	LEU	2.3
2	D	98	ALA	2.3
1	A	46	SER	2.3
1	C	18	LEU	2.3
1	A	242	THR	2.3
1	C	102	ASP	2.2
1	C	244	ASP	2.2
1	C	113	SER	2.2
1	C	218	ALA	2.2
1	C	84	ALA	2.2
2	D	85	THR	2.2
2	D	87	ALA	2.2
2	B	34	LEU	2.1
1	C	243	LYS	2.1
2	B	220	LYS	2.1
2	B	23	ASP	2.1
1	C	150	ILE	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 [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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CA	C	252	1/1	0.94	0.07	20,20,20,20	0
3	CA	D	240	1/1	0.96	0.06	25,25,25,25	0
3	CA	A	252	1/1	0.97	0.07	22,22,22,22	0
4	MN	B	241	1/1	0.98	0.04	29,29,29,29	0
4	MN	C	253	1/1	0.99	0.04	28,28,28,28	0
3	CA	B	240	1/1	0.99	0.07	25,25,25,25	0
4	MN	D	241	1/1	1.00	0.04	29,29,29,29	0
4	MN	A	253	1/1	1.00	0.03	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.