Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2024 – 09:27 PM EST

PDB ID	:	3LP9
Title	:	Crystal structure of LS24, A Seed Albumin from Lathyrus sativus
Authors	:	Gaur, V.; Qureshi, I.A.; Singh, A.; Chanana, V.; Salunke, D.M.
Deposited on	:	2010-02-05
Resolution	:	2.20 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 (1)) were used in the production of this report:

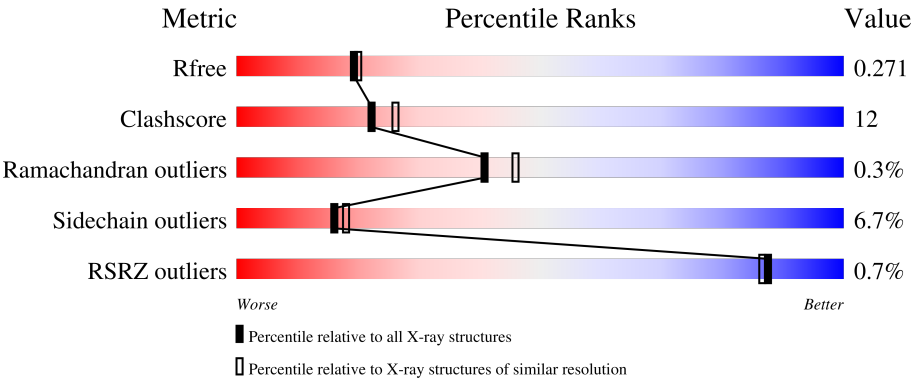
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	227	78% 19%
1	B	227	74% 22%
1	C	227	69% 29%
1	D	227	77% 20%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7811 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 LS-24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1805	1167	290	343	5			
1	B	227	Total	C	N	O	S	0	0	0
			1805	1167	290	343	5			
1	C	227	Total	C	N	O	S	0	0	0
			1805	1167	290	343	5			
1	D	227	Total	C	N	O	S	0	0	0
			1805	1167	290	343	5			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

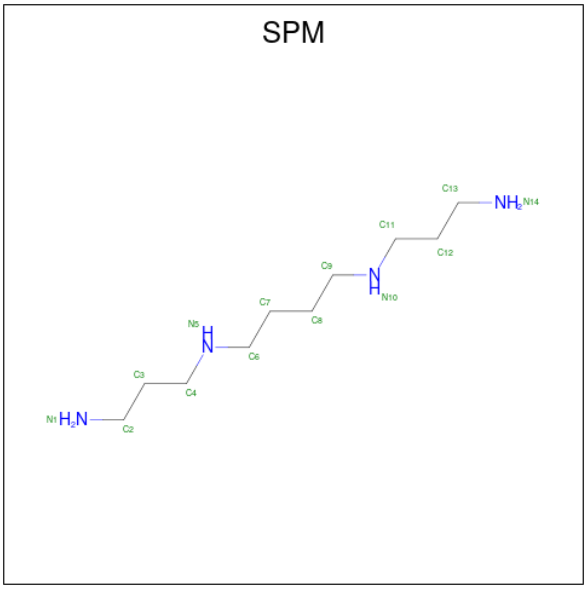
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Na 1 1	0	0
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0

- Molecule 5 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C N 14 10 4	0	0

- Molecule 6 is water.

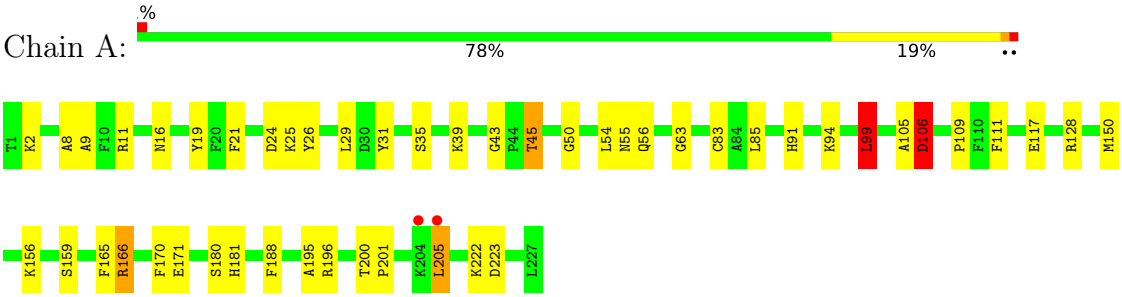
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	156	Total O 156 156	0	0
6	B	141	Total O 141 141	0	0
6	C	129	Total O 129 129	0	0
6	D	139	Total O 139 139	0	0

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.

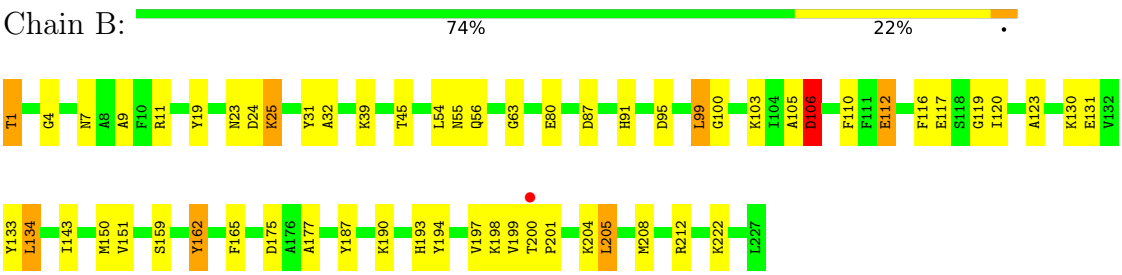
• Molecule 1: LS-24

Chain A:



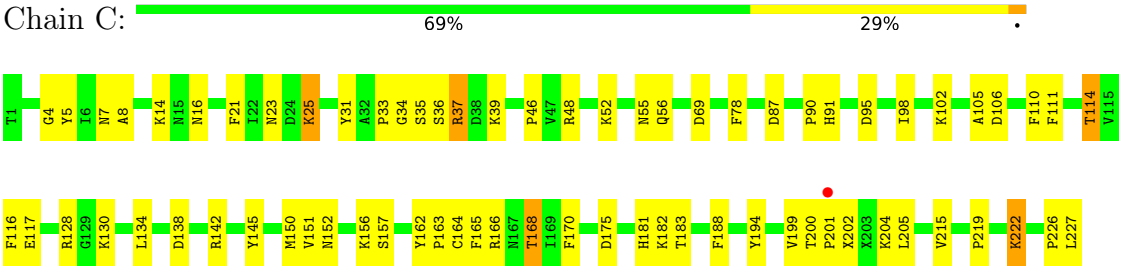
• Molecule 1: LS-24

Chain B:



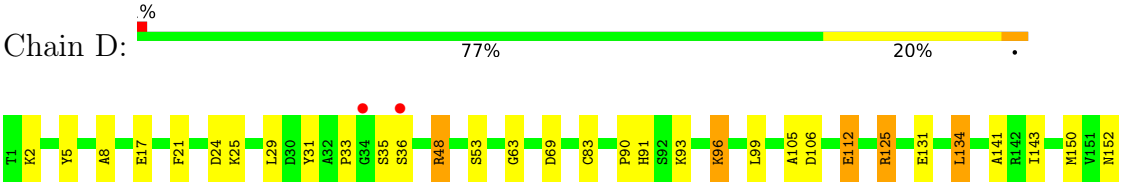
• Molecule 1: LS-24

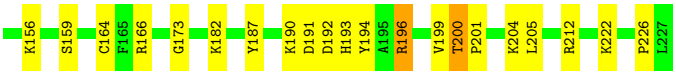
Chain C:



• Molecule 1: LS-24

Chain D:




K156
S159
C164
F165
R166
G173
K182
Y187
K190
D191
D192
H193
Y194
A195
R196
V199
T200
P201
K204
L205
R212
K222
P226
L227

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.17Å 88.14Å 154.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.63 – 2.20 47.63 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.5 (47.63-2.20) 93.4 (47.63-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.266 0.250 , 0.271	Depositor DCC
R_{free} test set	5549 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.937	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7811	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1908e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, SPM, 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	1.01	1/1840 (0.1%)	0.96	4/2485 (0.2%)
1	B	1.00	0/1840	0.88	2/2485 (0.1%)
1	C	0.97	0/1840	0.91	1/2485 (0.0%)
1	D	0.99	1/1840 (0.1%)	0.92	2/2485 (0.1%)
All	All	0.99	2/7360 (0.0%)	0.92	9/9940 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	CYS	CB-SG	-6.00	1.72	1.81
1	D	83	CYS	CB-SG	-5.17	1.73	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	LEU	CA-CB-CG	8.13	134.00	115.30
1	A	106	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	106	ASP	CB-CG-OD2	6.70	124.33	118.30
1	D	134	LEU	CA-CB-CG	6.16	129.46	115.30
1	A	205	LEU	CA-CB-CG	-5.99	101.52	115.30
1	D	204	LYS	N-CA-C	-5.62	95.81	111.00
1	B	134	LEU	CA-CB-CG	5.55	128.07	115.30
1	A	106	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	C	175	ASP	CB-CG-OD1	5.31	123.08	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1720	28	0
1	B	1805	0	1720	41	0
1	C	1805	0	1722	59	0
1	D	1805	0	1719	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	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	D	14	0	26	4	0
6	A	156	0	0	5	1
6	B	141	0	0	8	0
6	C	129	0	0	8	1
6	D	139	0	0	11	0
All	All	7811	0	6907	166	1

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 12.

All (166) 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:D:199:VAL:HA	1:D:205:LEU:HD22	1.44	0.95
6:B:244:HOH:O	5:D:230:SPM:H91	1.69	0.93
1:C:114:THR:HG22	1:C:116:PHE:H	1.37	0.90
1:A:43:GLY:HA2	1:A:45:THR:HG22	1.56	0.88
1:B:4:GLY:H	1:B:23:ASN:HD21	1.19	0.86
1:B:204:LYS:C	1:B:205:LEU:HG	1.96	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HB3	1:A:99:LEU:HB2	1.59	0.83
1:C:199:VAL:HA	1:C:205:LEU:HD23	1.66	0.77
1:B:199:VAL:HA	1:B:205:LEU:HD23	1.67	0.76
1:C:168:THR:HG22	1:C:170:PHE:H	1.50	0.76
1:C:111:PHE:O	1:C:114:THR:HB	1.90	0.71
1:C:128:ARG:NH1	1:C:142:ARG:NH2	2.39	0.71
1:D:33:PRO:HB2	1:D:182:LYS:HD2	1.73	0.70
1:C:199:VAL:O	1:C:200:THR:HG23	1.92	0.69
1:A:105:ALA:HB2	1:A:117:GLU:HG3	1.74	0.68
1:D:164:CYS:HB3	1:D:205:LEU:O	1.96	0.67
1:A:31:TYR:OH	1:A:181:HIS:HD2	1.77	0.66
1:C:128:ARG:NH1	1:C:142:ARG:HH22	1.93	0.66
1:B:4:GLY:H	1:B:23:ASN:ND2	1.93	0.66
1:A:171:GLU:HB3	6:A:374:HOH:O	1.94	0.66
1:C:105:ALA:HB2	1:C:117:GLU:HG3	1.78	0.66
1:C:165:PHE:O	1:C:168:THR:HB	1.98	0.63
1:C:199:VAL:HG12	1:C:205:LEU:HD23	1.81	0.63
1:C:39:LYS:HB3	6:C:231:HOH:O	1.99	0.63
1:C:222:LYS:HG3	6:C:305:HOH:O	1.99	0.63
1:D:156:LYS:HD3	6:D:552:HOH:O	2.00	0.62
5:D:230:SPM:H112	6:D:435:HOH:O	2.00	0.62
1:C:91:HIS:H	1:C:91:HIS:CD2	2.18	0.61
1:D:141:ALA:HB1	1:D:150:MET:HE3	1.82	0.61
1:C:87:ASP:O	1:C:95:ASP:HA	2.01	0.61
1:C:128:ARG:HH12	1:C:142:ARG:HH22	1.48	0.61
1:C:199:VAL:HG12	1:C:205:LEU:CD2	2.31	0.60
1:A:55:ASN:ND2	1:A:56:GLN:HG3	2.16	0.60
1:C:130:LYS:HD3	1:C:145:TYR:CE2	2.36	0.60
1:C:31:TYR:OH	1:C:181:HIS:HD2	1.85	0.59
1:D:201:PRO:HG2	6:D:434:HOH:O	2.03	0.58
1:A:91:HIS:HE1	6:A:233:HOH:O	1.86	0.58
1:C:4:GLY:H	1:C:23:ASN:HD21	1.50	0.58
5:D:230:SPM:N1	6:D:282:HOH:O	2.32	0.58
1:A:31:TYR:OH	1:A:181:HIS:CD2	2.57	0.57
1:D:8:ALA:HB3	1:D:21:PHE:HB2	1.86	0.57
1:B:9:ALA:HA	1:B:19:TYR:O	2.05	0.56
1:C:14:LYS:HD2	1:C:90:PRO:HB2	1.87	0.56
1:C:55:ASN:HD22	1:C:56:GLN:HG3	1.71	0.56
1:D:105:ALA:HB1	1:D:112:GLU:HB2	1.86	0.56
1:D:199:VAL:O	1:D:200:THR:HG23	2.05	0.56
1:B:131:GLU:HG2	1:B:151:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:TYR:HA	1:C:205:LEU:HD13	1.87	0.55
1:B:105:ALA:HB2	1:B:117:GLU:HG3	1.88	0.55
1:C:31:TYR:OH	1:C:181:HIS:CD2	2.60	0.55
1:C:163:PRO:HD2	1:C:205:LEU:HD12	1.89	0.55
1:C:200:THR:O	1:C:202:UNK:N	2.40	0.55
1:D:212:ARG:HD3	6:D:453:HOH:O	2.07	0.55
1:A:8:ALA:HB3	1:A:21:PHE:HB2	1.87	0.55
1:B:1:THR:HG21	1:B:7:ASN:OD1	2.07	0.54
1:A:35:SER:HB2	6:A:362:HOH:O	2.07	0.54
1:D:29:LEU:HD23	1:D:31:TYR:HB3	1.90	0.53
1:B:99:LEU:C	1:B:99:LEU:HD23	2.30	0.52
1:B:123:ALA:HA	1:B:133:TYR:O	2.10	0.52
1:B:199:VAL:HA	1:B:205:LEU:CD2	2.37	0.52
1:B:87:ASP:O	1:B:95:ASP:HA	2.09	0.52
1:A:171:GLU:HG2	1:D:91:HIS:HB2	1.92	0.52
1:C:39:LYS:HD3	6:C:231:HOH:O	2.10	0.52
1:C:164:CYS:SG	1:C:205:LEU:HB2	2.50	0.52
1:A:26:TYR:HE1	1:A:50:GLY:HA3	1.75	0.51
1:B:198:LYS:NZ	6:B:299:HOH:O	2.42	0.51
1:B:25:LYS:HB3	1:B:45:THR:O	2.11	0.51
1:C:168:THR:CG2	1:C:170:PHE:H	2.22	0.51
1:A:29:LEU:HD23	1:A:31:TYR:HB3	1.93	0.50
1:A:159:SER:O	1:A:166:ARG:NH2	2.37	0.50
1:D:199:VAL:HG12	1:D:205:LEU:HD13	1.92	0.50
1:B:55:ASN:ND2	1:B:56:GLN:HG3	2.26	0.50
6:B:418:HOH:O	1:C:157:SER:HB3	2.11	0.50
1:C:128:ARG:HH11	1:C:142:ARG:NH2	2.10	0.50
1:D:48:ARG:HB3	6:D:460:HOH:O	2.11	0.50
1:B:200:THR:H	1:B:205:LEU:HD23	1.76	0.49
1:D:69:ASP:O	1:D:125:ARG:HG2	2.12	0.49
1:A:106:ASP:HB2	6:C:228:HOH:O	2.12	0.49
1:A:165:PHE:HZ	1:A:188:PHE:CD2	2.31	0.49
1:D:5:TYR:CZ	1:D:226:PRO:HB3	2.47	0.49
1:B:91:HIS:HE1	6:B:309:HOH:O	1.94	0.48
1:B:162:TYR:N	1:B:162:TYR:CD2	2.81	0.48
1:D:152:ASN:HB2	6:D:525:HOH:O	2.14	0.48
1:B:165:PHE:CZ	1:B:197:VAL:HG21	2.48	0.48
1:B:105:ALA:HB1	1:B:112:GLU:HB2	1.94	0.48
1:D:53:SER:CB	1:D:96:LYS:HA	2.44	0.48
1:D:90:PRO:O	1:D:93:LYS:CE	2.62	0.48
1:B:199:VAL:CA	1:B:205:LEU:HD23	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:PHE:HD1	1:B:120:ILE:HG12	1.79	0.47
1:B:119:GLY:C	1:B:120:ILE:HG13	2.33	0.47
1:B:193:HIS:HD2	6:B:302:HOH:O	1.98	0.47
1:D:194:TYR:CE1	1:D:212:ARG:HB2	2.50	0.47
1:B:1:THR:HB	1:B:175:ASP:CG	2.35	0.47
1:C:8:ALA:HB3	1:C:21:PHE:HB2	1.96	0.47
1:C:219:PRO:O	1:C:222:LYS:HB2	2.15	0.47
1:C:33:PRO:C	1:C:35:SER:H	2.17	0.47
1:B:110:PHE:CD2	1:B:150:MET:HG3	2.50	0.46
1:A:170:PHE:CE2	1:A:195:ALA:HB2	2.51	0.46
1:D:191:ASP:HB2	6:D:498:HOH:O	2.15	0.46
1:C:16:ASN:HA	1:C:181:HIS:CD2	2.51	0.46
1:C:25:LYS:HE2	1:C:227:LEU:HD21	1.98	0.46
1:B:130:LYS:NZ	6:B:298:HOH:O	2.43	0.46
1:D:25:LYS:HE3	6:D:520:HOH:O	2.15	0.46
1:C:36:SER:O	1:C:37:ARG:CB	2.64	0.45
1:C:91:HIS:CD2	1:C:91:HIS:N	2.83	0.45
1:C:114:THR:HG22	1:C:116:PHE:N	2.18	0.45
1:C:114:THR:CG2	1:C:116:PHE:H	2.19	0.45
1:B:103:LYS:O	1:B:106:ASP:HB2	2.17	0.44
1:B:177:ALA:HA	1:B:187:TYR:O	2.17	0.44
1:B:194:TYR:CE1	1:B:212:ARG:HB2	2.52	0.44
1:D:222:LYS:HE2	6:D:549:HOH:O	2.17	0.44
1:A:55:ASN:ND2	6:A:293:HOH:O	2.50	0.44
1:C:168:THR:HG22	1:C:170:PHE:HB2	1.99	0.44
1:C:199:VAL:CA	1:C:205:LEU:HD23	2.44	0.44
1:D:200:THR:HA	1:D:201:PRO:HD2	1.70	0.44
1:A:106:ASP:CB	6:C:228:HOH:O	2.66	0.44
1:A:156:LYS:HE3	1:A:156:LYS:HB2	1.84	0.44
1:C:16:ASN:H	1:C:181:HIS:CD2	2.35	0.43
1:C:151:VAL:HA	6:C:357:HOH:O	2.17	0.43
1:B:31:TYR:O	1:B:32:ALA:C	2.56	0.43
1:D:90:PRO:O	1:D:93:LYS:HE2	2.19	0.43
1:A:171:GLU:CD	1:D:91:HIS:HB2	2.39	0.43
1:C:52:LYS:H	1:C:52:LYS:HG3	1.60	0.43
1:D:17:GLU:HA	1:D:29:LEU:O	2.19	0.43
1:D:141:ALA:HB1	1:D:150:MET:CE	2.47	0.43
1:C:7:ASN:HB2	6:C:339:HOH:O	2.17	0.43
1:C:134:LEU:HD12	1:C:134:LEU:N	2.33	0.43
1:A:105:ALA:O	1:A:109:PRO:HA	2.19	0.43
1:B:99:LEU:HD23	1:B:100:GLY:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ASN:H	1:A:181:HIS:CD2	2.37	0.43
1:C:5:TYR:CZ	1:C:226:PRO:HB3	2.53	0.43
1:B:1:THR:CG2	1:B:7:ASN:OD1	2.66	0.43
1:D:48:ARG:HD2	6:D:478:HOH:O	2.19	0.43
1:D:199:VAL:CA	1:D:205:LEU:HD22	2.32	0.43
1:B:110:PHE:CE2	1:B:143:ILE:HG21	2.53	0.43
1:C:215:VAL:HB	1:C:222:LYS:HG2	2.01	0.42
1:C:163:PRO:HD2	1:C:205:LEU:CD1	2.49	0.42
1:D:187:TYR:CE1	1:D:196:ARG:HD2	2.54	0.42
1:D:2:LYS:HB2	1:D:2:LYS:HE3	1.88	0.42
1:C:34:GLY:HA2	6:C:422:HOH:O	2.18	0.42
1:B:24:ASP:HA	1:B:63:GLY:HA3	2.01	0.42
1:B:7:ASN:HB2	6:B:334:HOH:O	2.20	0.42
1:B:39:LYS:HB3	1:B:39:LYS:HE3	1.89	0.42
1:B:91:HIS:HD2	1:C:138:ASP:OD1	2.02	0.42
1:C:55:ASN:ND2	1:C:56:GLN:HG3	2.35	0.42
1:A:2:LYS:NZ	6:A:309:HOH:O	2.23	0.41
1:D:159:SER:O	1:D:166:ARG:NH2	2.43	0.41
1:C:222:LYS:HB3	1:C:222:LYS:HE2	1.62	0.41
1:D:173:GLY:O	1:D:190:LYS:HD2	2.20	0.41
1:A:9:ALA:HA	1:A:19:TYR:O	2.21	0.41
1:B:190:LYS:HE3	6:B:274:HOH:O	2.20	0.41
1:A:94:LYS:HB2	1:A:94:LYS:HE3	1.27	0.41
1:A:24:ASP:HA	1:A:63:GLY:HA3	2.02	0.41
1:C:46:PRO:HB3	1:C:48:ARG:NH1	2.35	0.41
1:D:192:ASP:OD1	1:D:193:HIS:HD2	2.04	0.41
1:A:11:ARG:NH1	1:A:180:SER:O	2.54	0.41
1:D:131:GLU:HA	1:D:143:ILE:O	2.21	0.41
1:B:4:GLY:N	1:B:23:ASN:HD21	2.01	0.41
1:C:91:HIS:H	1:C:91:HIS:HD2	1.64	0.41
1:C:188:PHE:O	1:C:194:TYR:HA	2.21	0.41
1:B:80:GLU:OE1	5:D:230:SPM:C8	2.70	0.40
1:C:87:ASP:HB2	1:C:98:ILE:HD11	2.04	0.40
1:D:24:ASP:HA	1:D:63:GLY:HA3	2.02	0.40
1:D:35:SER:OG	1:D:36:SER:N	2.54	0.40
1:C:78:PHE:N	1:C:78:PHE:CD2	2.90	0.40
1:C:110:PHE:CD2	1:C:150:MET:HG2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:248:HOH:O	6:C:332:HOH:O[2_765]	2.18	0.02

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	222/227 (98%)	203 (91%)	18 (8%)	1 (0%)	29 31
1	B	222/227 (98%)	198 (89%)	24 (11%)	0	100 100
1	C	222/227 (98%)	200 (90%)	20 (9%)	2 (1%)	17 16
1	D	222/227 (98%)	208 (94%)	14 (6%)	0	100 100
All	All	888/908 (98%)	809 (91%)	76 (9%)	3 (0%)	41 46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	201	PRO
1	C	37	ARG
1	A	201	PRO

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	191/193 (99%)	176 (92%)	15 (8%)	12 12
1	B	191/193 (99%)	177 (93%)	14 (7%)	14 15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	191/193 (99%)	178 (93%)	13 (7%)	16 17
1	D	191/193 (99%)	182 (95%)	9 (5%)	26 33
All	All	764/772 (99%)	713 (93%)	51 (7%)	16 18

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	39	LYS
1	A	45	THR
1	A	54	LEU
1	A	99	LEU
1	A	106	ASP
1	A	111	PHE
1	A	128	ARG
1	A	150	MET
1	A	166	ARG
1	A	196	ARG
1	A	200	THR
1	A	205	LEU
1	A	222	LYS
1	A	223	ASP
1	B	1	THR
1	B	11	ARG
1	B	25	LYS
1	B	54	LEU
1	B	99	LEU
1	B	106	ASP
1	B	112	GLU
1	B	134	LEU
1	B	159	SER
1	B	162	TYR
1	B	201	PRO
1	B	205	LEU
1	B	208	MET
1	B	222	LYS
1	C	25	LYS
1	C	69	ASP
1	C	102	LYS
1	C	106	ASP
1	C	114	THR

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Mol	Chain	Res	Type
1	C	152	ASN
1	C	156	LYS
1	C	166	ARG
1	C	168	THR
1	C	182	LYS
1	C	183	THR
1	C	204	LYS
1	C	222	LYS
1	D	48	ARG
1	D	96	LYS
1	D	99	LEU
1	D	106	ASP
1	D	112	GLU
1	D	125	ARG
1	D	134	LEU
1	D	196	ARG
1	D	200	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	91	HIS
1	A	139	GLN
1	A	181	HIS
1	B	23	ASN
1	B	91	HIS
1	B	193	HIS
1	C	23	ASN
1	C	55	ASN
1	C	91	HIS
1	C	181	HIS
1	D	23	ASN
1	D	72	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 13 ligands modelled in this entry, 12 are monoatomic - leaving 1 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	SPM	D	230	-	13,13,13	0.74	0	12,12,12	2.95	7 (58%)

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	SPM	D	230	-	-	1/11/11/11	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	230	SPM	C3-C4-N5	-6.98	93.31	112.14
5	D	230	SPM	C12-C11-N10	3.94	122.78	112.14
5	D	230	SPM	C11-C12-C13	-3.25	102.36	114.28
5	D	230	SPM	C8-C7-C6	-2.80	100.32	113.56
5	D	230	SPM	C7-C6-N5	-2.67	104.94	112.14
5	D	230	SPM	C3-C2-N1	-2.24	96.71	112.78
5	D	230	SPM	C7-C8-C9	-2.23	103.02	113.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	230	SPM	C7-C8-C9-N10

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	230	SPM	4	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, 95^{th} 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	224/227 (98%)	-0.25	2 (0%)	84	83	15, 16, 19, 23	0
1	B	224/227 (98%)	-0.30	1 (0%)	92	91	14, 17, 20, 35	0
1	C	224/227 (98%)	-0.23	1 (0%)	92	91	14, 17, 19, 30	0
1	D	224/227 (98%)	-0.20	2 (0%)	84	83	14, 17, 20, 23	0
All	All	896/908 (98%)	-0.24	6 (0%)	87	86	14, 16, 19, 35	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	LYS	2.8
1	D	36	SER	2.4
1	A	205	LEU	2.4
1	D	34	GLY	2.1
1	B	200	THR	2.0
1	C	201	PRO	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 monosaccharides 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. The B-factors column lists the minimum,

median, 95^{th} 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
5	SPM	D	230	14/14	0.84	0.25	16,19,20,20	0
3	CL	B	315	1/1	0.97	0.10	18,18,18,18	0
2	CA	D	313	1/1	0.97	0.16	15,15,15,15	0
2	CA	C	312	1/1	0.98	0.15	15,15,15,15	0
3	CL	C	316	1/1	0.98	0.06	19,19,19,19	0
3	CL	D	317	1/1	0.98	0.08	19,19,19,19	0
4	NA	B	319	1/1	0.98	0.09	17,17,17,17	0
4	NA	C	320	1/1	0.98	0.10	16,16,16,16	0
4	NA	D	321	1/1	0.98	0.11	16,16,16,16	0
2	CA	B	311	1/1	0.98	0.14	15,15,15,15	0
2	CA	A	310	1/1	0.99	0.17	15,15,15,15	0
4	NA	A	318	1/1	0.99	0.09	17,17,17,17	0
3	CL	A	314	1/1	0.99	0.08	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.