



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:18 am BST

PDB ID : 1ZGR
Title : Crystal structure of the Parkia platycephala seed lectin
Authors : Gallego del Sol, F.; Cavada, B.S.; Calvete, J.J.
Deposited on : 2005-04-22
Resolution : 2.50 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 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

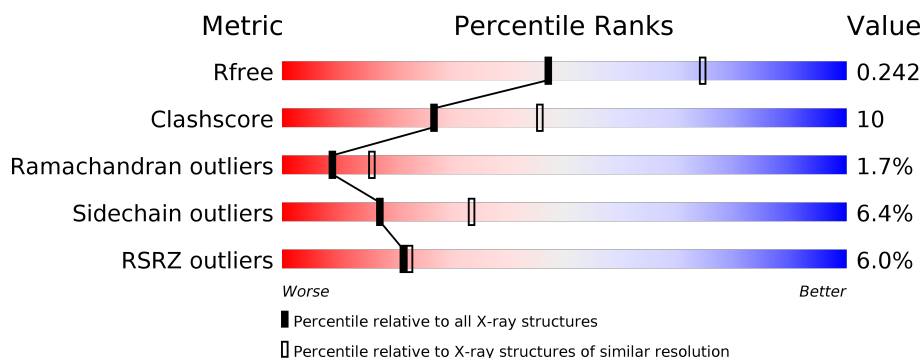
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	447	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	447	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6819 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 Mannose/glucose-specific lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	73	0	0
			3325	2136	541	645	3			
1	B	441	Total	C	N	O	S	206	0	0
			3325	2136	541	645	3			

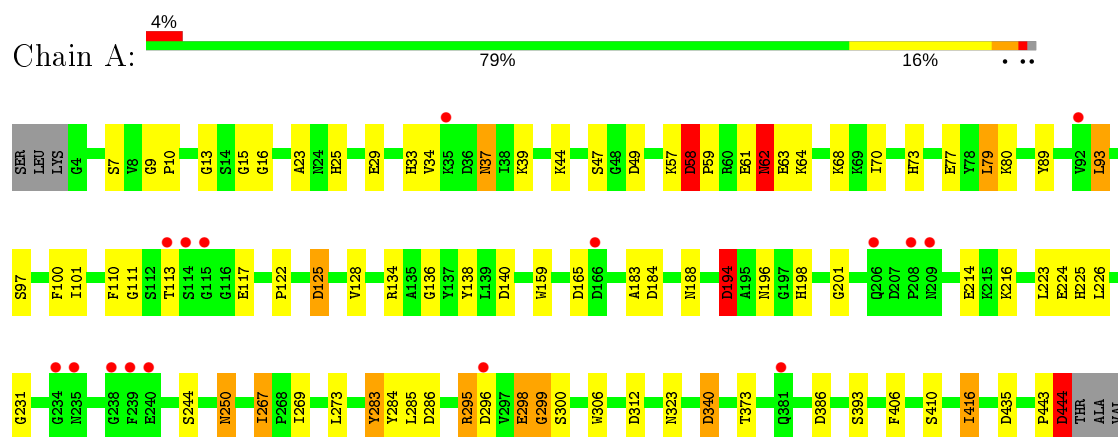
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	97	Total	O	0	0
			97	97		
2	B	72	Total	O	0	0
			72	72		

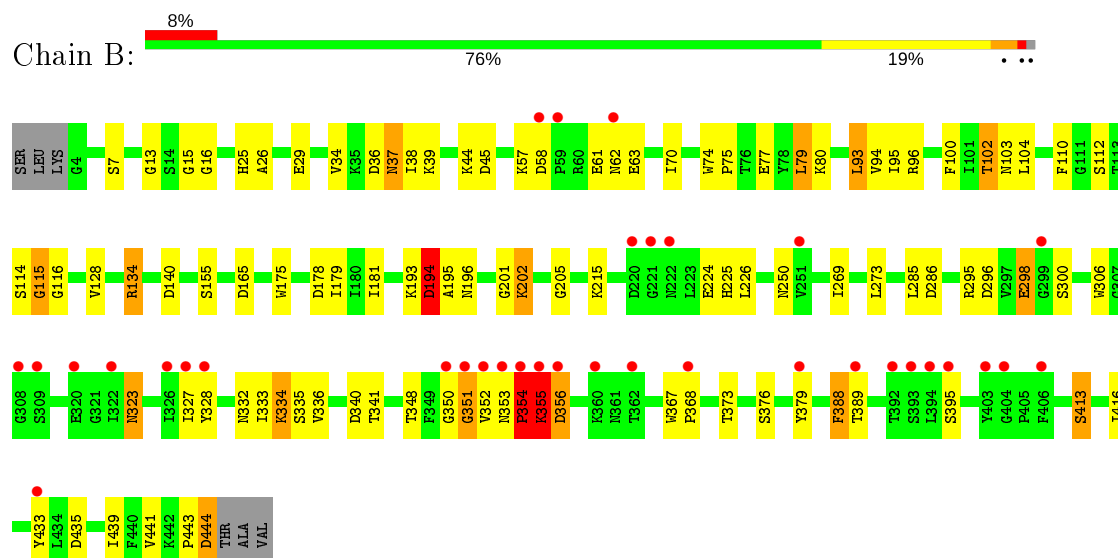
3 Residue-property plots [i](#)

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: Mannose/glucose-specific lectin



- Molecule 1: Mannose/glucose-specific lectin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.60Å 68.51Å 208.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.85 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.8 (30.00-2.50) 95.5 (29.85-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.73 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.214 , 0.243 0.211 , 0.242	Depositor DCC
R_{free} test set	1625 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6819	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

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	0.92	5/3419 (0.1%)	0.94	18/4639 (0.4%)
1	B	0.87	7/3419 (0.2%)	1.34	26/4639 (0.6%)
All	All	0.90	12/6838 (0.2%)	1.16	44/9278 (0.5%)

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	A	0	2
1	B	0	4
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	ASP	C-N	-27.44	0.82	1.34
1	B	296	ASP	C-N	14.38	1.67	1.34
1	A	298	GLU	C-N	12.70	1.55	1.33
1	B	433	TYR	CB-CG	12.38	1.70	1.51
1	B	379	TYR	C-N	-9.92	1.15	1.33
1	B	413	SER	C-N	-7.63	1.16	1.34
1	B	388	PHE	C-N	6.83	1.49	1.34
1	B	298	GLU	C-N	-6.68	1.21	1.33
1	B	115	GLY	N-CA	-5.75	1.37	1.46
1	A	223	LEU	CG-CD2	5.48	1.72	1.51
1	A	299	GLY	N-CA	5.44	1.54	1.46
1	A	61	GLU	C-N	-5.33	1.21	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	TYR	CB-CG-CD1	-37.38	98.57	121.00
1	B	433	TYR	CB-CG-CD2	36.88	143.13	121.00
1	B	379	TYR	C-N-CA	-18.06	84.37	122.30
1	B	379	TYR	CA-C-N	-15.32	85.56	116.20
1	B	379	TYR	O-C-N	14.94	148.60	123.20
1	B	334	LYS	N-CA-CB	-14.24	84.97	110.60
1	A	58	ASP	CA-C-N	-14.23	77.26	117.10
1	B	413	SER	O-C-N	-9.43	107.62	122.70
1	B	351	GLY	N-CA-C	-9.22	90.05	113.10
1	B	328	TYR	CB-CG-CD1	8.72	126.23	121.00
1	A	58	ASP	C-N-CA	-8.59	85.90	122.00
1	B	296	ASP	C-N-CA	-8.16	101.29	121.70
1	A	194	ASP	CB-CG-OD2	8.14	125.62	118.30
1	B	202	LYS	N-CA-C	-7.90	89.68	111.00
1	B	298	GLU	O-C-N	-7.56	110.35	123.20
1	A	296	ASP	N-CA-C	-7.26	91.40	111.00
1	B	355	LYS	CA-C-N	-7.18	101.41	117.20
1	A	298	GLU	C-N-CA	-6.60	108.43	122.30
1	A	62	ASN	N-CA-C	-6.59	93.21	111.00
1	B	296	ASP	CA-C-N	-6.57	102.75	117.20
1	A	298	GLU	CA-C-N	6.56	129.32	116.20
1	B	194	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	388	PHE	O-C-N	-6.37	112.51	122.70
1	A	298	GLU	O-C-N	-6.24	112.59	123.20
1	B	354	PRO	CA-N-CD	-6.10	102.96	111.50
1	A	444	ASP	CB-CG-OD2	5.82	123.54	118.30
1	B	165	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	184	ASP	CB-CG-OD2	5.71	123.43	118.30
1	A	435	ASP	CB-CG-OD2	5.68	123.42	118.30
1	B	435	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	286	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	340	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	328	TYR	CB-CG-CD2	-5.39	117.76	121.00
1	B	413	SER	C-N-CA	5.38	135.15	121.70
1	B	286	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	312	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	223	LEU	CD1-CG-CD2	-5.34	94.47	110.50
1	B	298	GLU	CA-C-N	5.31	126.81	116.20
1	B	413	SER	CA-C-N	5.27	128.79	117.20
1	A	125	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	140	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	444	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	194	ASP	CB-CG-OD1	-5.16	113.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	ASP	CB-CG-OD2	5.13	122.91	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	GLY	Peptide
1	A	58	ASP	Mainchain
1	B	201	GLY	Peptide
1	B	298	GLU	Mainchain
1	B	388	PHE	Mainchain
1	B	413	SER	Mainchain

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	3325	0	3189	50	0
1	B	3325	0	3189	77	0
2	A	97	0	0	4	0
2	B	72	0	0	5	0
All	All	6819	0	6378	127	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 10.

All (127) 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:B:355:LYS:HE2	1:B:356:ASP:H	1.14	1.11
1:B:335:SER:HB3	1:B:350:GLY:O	1.47	1.11
1:B:355:LYS:HE2	1:B:356:ASP:N	1.68	1.07
1:B:37:ASN:H	1:B:37:ASN:HD22	1.00	1.00
1:A:250:ASN:H	1:A:250:ASN:HD22	1.13	0.96
1:A:37:ASN:H	1:A:37:ASN:HD22	1.12	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ILE:HD11	1:A:110:PHE:CE1	2.04	0.92
1:B:334:LYS:O	1:B:350:GLY:O	1.88	0.90
1:B:102:THR:HG22	1:B:104:LEU:H	1.34	0.90
1:B:335:SER:CB	1:B:350:GLY:O	2.22	0.88
1:B:70:ILE:HD11	1:B:110:PHE:CE1	2.12	0.83
1:B:29:GLU:OE1	1:B:44:LYS:NZ	2.12	0.81
1:B:37:ASN:H	1:B:37:ASN:ND2	1.80	0.80
1:B:77:GLU:OE1	1:B:102:THR:HG21	1.81	0.79
1:B:355:LYS:O	1:B:356:ASP:CB	2.31	0.78
1:A:443:PRO:O	1:A:444:ASP:HB2	1.84	0.77
1:A:194:ASP:HB3	1:A:196:ASN:H	1.49	0.77
1:B:61:GLU:C	1:B:63:GLU:H	1.89	0.75
1:A:37:ASN:HD21	1:A:39:LYS:NZ	1.86	0.72
1:A:224:GLU:HA	1:A:250:ASN:HD21	1.54	0.72
1:B:355:LYS:HA	1:B:355:LYS:HE2	1.73	0.71
1:B:34:VAL:HG22	1:B:38:ILE:HD13	1.71	0.71
1:B:355:LYS:O	1:B:356:ASP:HB2	1.93	0.68
1:A:250:ASN:H	1:A:250:ASN:ND2	1.91	0.67
1:A:37:ASN:H	1:A:37:ASN:ND2	1.88	0.67
1:A:70:ILE:CD1	1:A:110:PHE:CE1	2.78	0.65
1:A:159:TRP:HH2	1:A:267:ILE:HD12	1.62	0.65
1:A:57:LYS:HG3	1:A:136:GLY:O	1.97	0.65
1:B:29:GLU:CD	1:B:44:LYS:NZ	2.50	0.64
1:A:159:TRP:CH2	1:A:267:ILE:HD12	2.33	0.64
1:B:37:ASN:N	1:B:37:ASN:HD22	1.81	0.63
1:B:25:HIS:O	1:B:45:ASP:HB2	1.98	0.63
1:B:102:THR:CG2	1:B:104:LEU:H	2.11	0.62
1:B:102:THR:HG22	1:B:104:LEU:N	2.12	0.62
1:A:34:VAL:HG21	1:A:111:GLY:HA2	1.81	0.61
1:B:224:GLU:HA	1:B:250:ASN:HD21	1.65	0.61
1:A:25:HIS:CD2	1:A:47:SER:HB3	2.36	0.61
1:A:183:ALA:HA	1:A:188:ASN:HD22	1.65	0.60
1:B:96:ARG:HE	1:B:115:GLY:HA3	1.66	0.59
1:A:16:GLY:O	1:A:134:ARG:NH1	2.35	0.58
1:B:355:LYS:CE	1:B:355:LYS:HA	2.32	0.57
1:B:29:GLU:CD	1:B:44:LYS:HZ3	2.06	0.57
1:B:355:LYS:CA	1:B:355:LYS:HE2	2.35	0.57
1:A:37:ASN:HD22	1:A:37:ASN:N	1.92	0.57
1:B:352:VAL:O	1:B:352:VAL:HG12	2.05	0.57
1:B:334:LYS:C	1:B:350:GLY:O	2.43	0.56
1:A:225:HIS:H	1:A:250:ASN:ND2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASN:HD21	1:A:39:LYS:HZ2	1.52	0.56
1:B:178:ASP:HB2	1:B:193:LYS:HB2	1.86	0.55
1:B:335:SER:CA	1:B:350:GLY:O	2.53	0.55
1:B:327:ILE:HG23	1:B:336:VAL:HG12	1.88	0.55
1:A:34:VAL:CG2	1:A:111:GLY:HA2	2.36	0.55
1:A:122:PRO:HG3	2:A:527:HOH:O	2.07	0.55
1:B:443:PRO:O	1:B:444:ASP:HB2	2.08	0.54
1:A:58:ASP:OD2	1:A:58:ASP:N	2.39	0.53
1:B:353:ASN:O	1:B:354:PRO:C	2.43	0.53
1:B:335:SER:HB2	1:B:348:THR:HG22	1.91	0.52
1:B:77:GLU:CG	1:B:102:THR:CG2	2.88	0.52
1:B:439:ILE:HD12	1:B:441:VAL:CG1	2.41	0.50
1:A:15:GLY:O	1:A:134:ARG:HD3	2.11	0.50
1:B:112:SER:OG	1:B:114:SER:O	2.30	0.50
1:A:33:HIS:HD2	2:A:473:HOH:O	1.94	0.50
1:B:70:ILE:CD1	1:B:100:PHE:CD1	2.94	0.50
1:A:198:HIS:HB2	2:A:482:HOH:O	2.12	0.50
1:B:61:GLU:C	1:B:63:GLU:N	2.61	0.49
1:A:250:ASN:N	1:A:250:ASN:HD22	1.92	0.49
1:B:29:GLU:HB3	1:B:44:LYS:HB3	1.94	0.49
1:A:73:HIS:HD2	1:A:77:GLU:OE2	1.95	0.49
1:A:29:GLU:HB3	1:A:44:LYS:HB3	1.95	0.49
1:B:323:ASN:OD1	1:B:341:THR:HG22	2.13	0.48
1:B:225:HIS:H	1:B:250:ASN:ND2	2.12	0.48
1:B:77:GLU:CG	1:B:102:THR:HG21	2.43	0.48
1:B:13:GLY:HA2	1:B:93:LEU:HD12	1.96	0.48
1:B:205:GLY:HA2	2:B:462:HOH:O	2.13	0.48
1:A:80:LYS:HE2	1:A:101:ILE:HG22	1.97	0.47
1:B:306:TRP:CH2	1:B:416:ILE:HG12	2.49	0.47
1:B:79:LEU:HB3	1:B:128:VAL:HB	1.97	0.47
1:B:77:GLU:HG3	1:B:102:THR:CG2	2.45	0.46
1:A:37:ASN:HD21	1:A:39:LYS:HZ3	1.58	0.46
1:B:134:ARG:NH2	2:B:494:HOH:O	2.48	0.46
1:B:37:ASN:HD21	1:B:39:LYS:NZ	2.13	0.46
1:A:97:SER:HA	1:A:110:PHE:O	2.16	0.45
1:B:350:GLY:HA2	1:B:352:VAL:HG23	1.98	0.45
1:B:77:GLU:CG	1:B:102:THR:HG23	2.47	0.45
1:B:175:TRP:CE2	1:B:195:ALA:HB2	2.51	0.45
1:B:353:ASN:C	1:B:355:LYS:N	2.68	0.45
1:A:23:ALA:HB1	1:A:25:HIS:O	2.17	0.45
1:A:70:ILE:HD12	1:A:100:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:SER:O	1:B:269:ILE:HA	2.17	0.45
1:B:38:ILE:HG13	1:B:95:ILE:HG22	1.99	0.45
2:A:460:HOH:O	1:B:57:LYS:HE2	2.15	0.44
1:B:45:ASP:OD1	1:B:45:ASP:C	2.56	0.44
1:B:94:VAL:HB	2:B:485:HOH:O	2.17	0.44
1:A:7:SER:O	1:A:269:ILE:HA	2.18	0.44
1:A:159:TRP:CH2	1:A:267:ILE:CD1	3.01	0.44
1:A:306:TRP:CH2	1:A:416:ILE:HG12	2.53	0.43
1:B:194:ASP:OD2	2:B:495:HOH:O	2.21	0.43
1:A:44:LYS:HA	1:A:49:ASP:O	2.18	0.43
1:B:15:GLY:O	1:B:134:ARG:HD3	2.18	0.43
1:B:273:LEU:HB2	1:B:295:ARG:HG2	2.01	0.43
1:B:194:ASP:HB3	1:B:196:ASN:H	1.82	0.43
1:B:37:ASN:ND2	1:B:39:LYS:HE2	2.34	0.43
1:B:202:LYS:NZ	2:B:506:HOH:O	2.21	0.43
1:A:283:TYR:C	1:A:284:TYR:CD2	2.92	0.43
1:A:79:LEU:HB3	1:A:128:VAL:HB	1.99	0.43
1:A:70:ILE:CD1	1:A:100:PHE:CD1	3.02	0.43
1:A:231:GLY:HA3	1:A:244:SER:O	2.19	0.42
1:A:34:VAL:HG21	1:A:111:GLY:CA	2.48	0.42
1:B:16:GLY:O	1:B:134:ARG:NH1	2.53	0.42
1:A:13:GLY:HA3	1:A:93:LEU:O	2.20	0.42
1:B:323:ASN:HD22	1:B:323:ASN:C	2.23	0.42
1:B:102:THR:CG2	1:B:103:ASN:N	2.83	0.42
1:B:80:LYS:HE2	1:B:102:THR:O	2.20	0.42
1:A:214:GLU:OE2	1:A:216:LYS:HE3	2.20	0.41
1:B:355:LYS:O	1:B:356:ASP:HB3	2.16	0.41
1:B:77:GLU:HG3	1:B:102:THR:HG23	2.02	0.41
1:A:89:TYR:CE2	1:A:138:TYR:CE2	3.09	0.41
1:A:393:SER:HA	1:A:406:PHE:O	2.20	0.41
1:B:74:TRP:CD2	1:B:75:PRO:HA	2.55	0.41
1:A:273:LEU:HB2	1:A:295:ARG:CG	2.50	0.41
1:B:250:ASN:H	1:B:250:ASN:HD22	1.67	0.41
1:B:334:LYS:O	1:B:350:GLY:C	2.54	0.41
1:A:9:GLY:HA3	1:A:10:PRO:HA	1.90	0.41
1:B:367:TRP:CG	1:B:368:PRO:HA	2.56	0.41
1:A:70:ILE:HD13	1:A:100:PHE:CD1	2.55	0.41
1:B:179:ILE:HG22	1:B:181:ILE:HD11	2.02	0.40
1:B:77:GLU:CD	1:B:102:THR:HG21	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/447 (98%)	410 (93%)	22 (5%)	7 (2%)	9	17
1	B	439/447 (98%)	401 (91%)	30 (7%)	8 (2%)	8	14
All	All	878/894 (98%)	811 (92%)	52 (6%)	15 (2%)	9	16

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	64	LYS
1	B	194	ASP
1	B	332	ASN
1	B	356	ASP
1	A	63	GLU
1	B	116	GLY
1	B	26	ALA
1	B	351	GLY
1	A	59	PRO
1	A	194	ASP
1	B	333	ILE
1	A	58	ASP
1	A	299	GLY
1	B	62	ASN

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	352/358 (98%)	327 (93%)	25 (7%)	14	28
1	B	352/358 (98%)	332 (94%)	20 (6%)	20	39
All	All	704/716 (98%)	659 (94%)	45 (6%)	17	33

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	58	ASP
1	A	62	ASN
1	A	68	LYS
1	A	79	LEU
1	A	93	LEU
1	A	113	THR
1	A	117	GLU
1	A	125	ASP
1	A	165	ASP
1	A	226	LEU
1	A	250	ASN
1	A	267	ILE
1	A	283	TYR
1	A	285	LEU
1	A	295	ARG
1	A	298	GLU
1	A	300	SER
1	A	323	ASN
1	A	340	ASP
1	A	373	THR
1	A	386	ASP
1	A	410	SER
1	A	416	ILE
1	A	444	ASP
1	B	36	ASP
1	B	37	ASN
1	B	58	ASP
1	B	79	LEU
1	B	93	LEU
1	B	102	THR
1	B	134	ARG
1	B	155	SER
1	B	215	LYS
1	B	226	LEU

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Mol	Chain	Res	Type
1	B	285	LEU
1	B	300	SER
1	B	323	ASN
1	B	340	ASP
1	B	354	PRO
1	B	355	LYS
1	B	373	THR
1	B	376	SER
1	B	389	THR
1	B	395	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	33	HIS
1	A	37	ASN
1	A	73	HIS
1	A	151	HIS
1	A	188	ASN
1	A	235	ASN
1	A	250	ASN
1	A	323	ASN
1	B	25	HIS
1	B	33	HIS
1	B	37	ASN
1	B	73	HIS
1	B	151	HIS
1	B	188	ASN
1	B	235	ASN
1	B	250	ASN
1	B	319	ASN
1	B	366	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	296:ASP	C	297:VAL	N	1.67
1	B	413:SER	C	414:PHE	N	1.16
1	B	379:TYR	C	380:GLY	N	1.15
1	A	58:ASP	C	59:PRO	N	0.82

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	434/447 (97%)	-0.02	16 (3%) 41 45	17, 29, 49, 59	5 (1%)
1	B	416/447 (93%)	0.24	35 (8%) 11 11	16, 34, 63, 70	5 (1%)
All	All	850/894 (95%)	0.11	51 (6%) 21 22	16, 31, 57, 70	10 (1%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	VAL	6.5
1	B	351	GLY	5.8
1	B	356	ASP	5.1
1	B	222	ASN	5.0
1	B	299	GLY	5.0
1	B	406	PHE	4.9
1	B	59	PRO	4.8
1	B	354	PRO	4.4
1	A	296	ASP	4.1
1	B	360	LYS	3.7
1	B	362	THR	3.6
1	B	355	LYS	3.5
1	B	327	ILE	3.3
1	B	350	GLY	3.3
1	B	328	TYR	3.0
1	A	113	THR	3.0
1	A	209	ASN	3.0
1	A	238	GLY	2.9
1	B	379	TYR	2.9
1	B	221	GLY	2.8
1	A	166	ASP	2.7
1	B	62	ASN	2.7
1	B	308	GLY	2.7
1	A	206	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	395	SER	2.6
1	A	35	LYS	2.6
1	A	92	VAL	2.6
1	B	433	TYR	2.6
1	A	240	GLU	2.6
1	B	404	GLY	2.5
1	B	322	ILE	2.5
1	B	392	THR	2.5
1	B	403	TYR	2.4
1	A	208	PRO	2.4
1	B	389	THR	2.4
1	B	368	PRO	2.3
1	B	393	SER	2.3
1	B	251	VAL	2.3
1	B	394	LEU	2.2
1	A	114	SER	2.2
1	A	235	ASN	2.1
1	A	115	GLY	2.1
1	B	220	ASP	2.1
1	B	309	SER	2.1
1	A	234	GLY	2.1
1	A	381	GLN	2.1
1	B	326	ILE	2.1
1	A	239	PHE	2.1
1	B	353	ASN	2.1
1	B	58	ASP	2.0
1	B	320	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.