



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:32 am BST

PDB ID : 6IUS
Title : A higher kcat Rubisco
Authors : Li, Y.; Cai, Z.
Deposited on : 2018-11-30
Resolution : 2.12 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

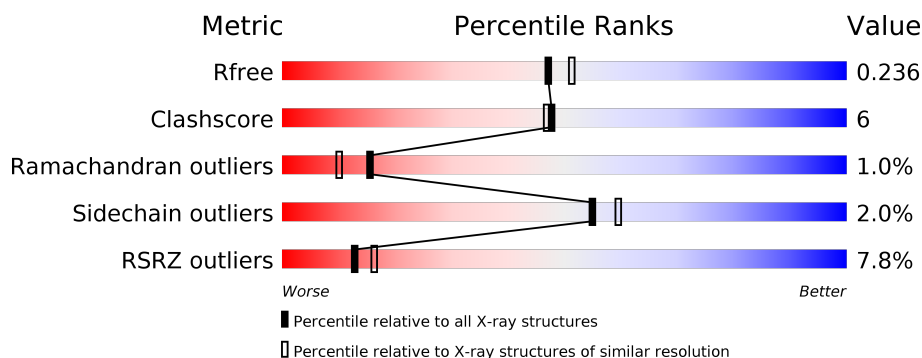
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	461	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>8%</div> </div> </div>
1	B	461	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>9%</div> </div> </div>
1	C	461	<div> <div>10%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10515 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 Ribulose-1,5-bisphosphate carboxylase/oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3294	2103	553	620	18			
1	B	419	Total	C	N	O	S	0	0	0
			3244	2072	545	610	17			
1	C	422	Total	C	N	O	S	0	1	0
			3271	2086	553	615	17			

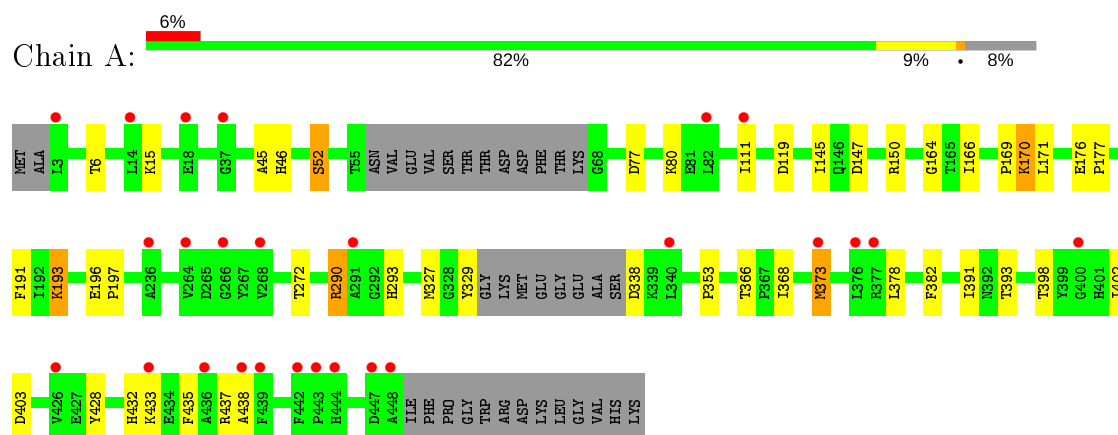
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	237	Total	O	0	0
			237	237		
2	B	225	Total	O	0	0
			225	225		
2	C	244	Total	O	0	0
			244	244		

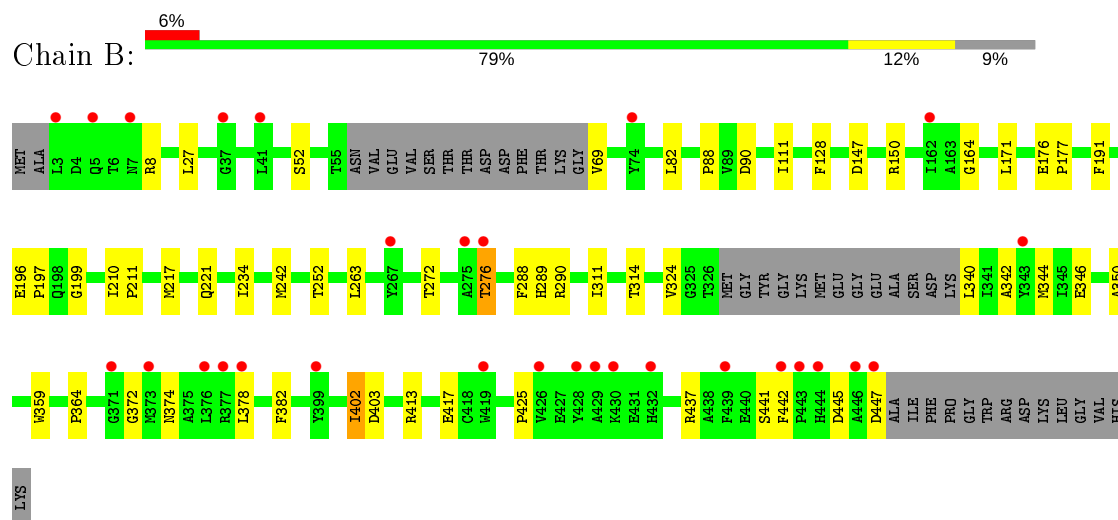
3 Residue-property plots [i](#)

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.

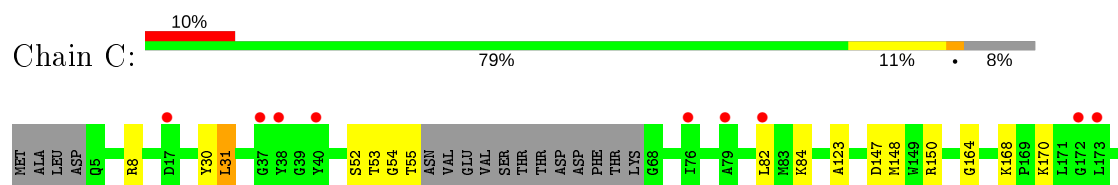
- Molecule 1: Ribulose-1,5-bisphosphate carboxylase/oxygenase

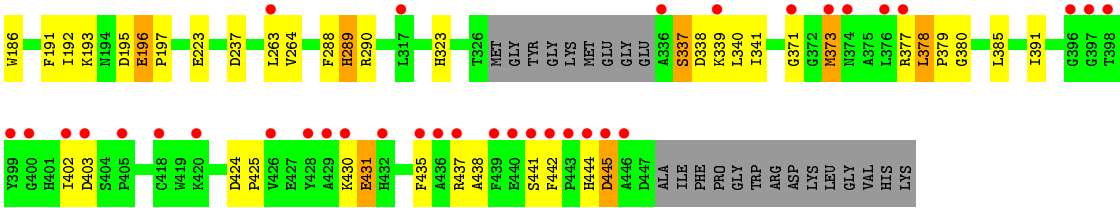


- Molecule 1: Ribulose-1,5-bisphosphate carboxylase/oxygenase



- Molecule 1: Ribulose-1,5-bisphosphate carboxylase/oxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.50Å 107.84Å 112.31Å 90.00° 130.04° 90.00°	Depositor
Resolution (Å)	46.99 – 2.12 46.94 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.1 (46.99-2.12) 96.1 (46.94-2.12)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.192 , 0.231 0.202 , 0.236	Depositor DCC
R_{free} test set	1926 reflections (2.32%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.003 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10515	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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	0.73	0/3378	0.85	0/4573
1	B	0.74	0/3327	0.87	0/4506
1	C	0.73	0/3354	0.88	1/4540 (0.0%)
All	All	0.74	0/10059	0.87	1/13619 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	TYR	CB-CA-C	-6.48	97.44	110.40

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	3294	0	3176	27	0
1	B	3244	0	3130	43	0
1	C	3271	0	3157	51	0
2	A	237	0	0	2	0
2	B	225	0	0	3	0
2	C	244	0	0	2	0
All	All	10515	0	9463	118	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 6.

All (118) 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:344:MET:CE	1:B:359:TRP:HE1	1.53	1.20
1:B:344:MET:HE1	1:B:359:TRP:HE1	1.27	0.99
1:B:344:MET:HE2	1:B:359:TRP:HE1	1.29	0.95
1:B:344:MET:HE3	1:B:350:ALA:HB3	1.52	0.90
1:B:342:ALA:O	1:B:346:GLU:HG2	1.73	0.89
1:B:344:MET:CE	1:B:359:TRP:NE1	2.35	0.88
1:C:338:ASP:O	1:C:341:ILE:HB	1.77	0.85
1:B:82:LEU:HD21	2:B:681:HOH:O	1.78	0.83
1:C:263:LEU:HD21	1:C:289:HIS:CD2	2.13	0.82
1:C:196:GLU:HB3	1:C:289:HIS:CD2	2.16	0.81
1:A:290:ARG:HG3	1:A:293:HIS:CD2	2.16	0.80
1:B:344:MET:HE1	1:B:359:TRP:NE1	1.96	0.80
1:B:344:MET:HE2	1:B:359:TRP:NE1	1.96	0.78
1:A:169:PRO:HB3	1:C:55:THR:HG22	1.67	0.75
1:B:272:THR:O	1:B:276:THR:HG23	1.92	0.70
1:C:263:LEU:HD11	1:C:289:HIS:CD2	2.28	0.68
1:C:147:ASP:OD1	1:C:150:ARG:NH2	2.25	0.68
1:C:444:HIS:O	1:C:445:ASP:HB2	1.95	0.65
1:C:377:ARG:NH1	2:C:503:HOH:O	2.29	0.63
1:A:170:LYS:HE2	2:A:522:HOH:O	1.96	0.63
1:C:170:LYS:HG2	1:C:195:ASP:CG	2.19	0.63
1:C:193:LYS:CE	1:C:289:HIS:CE1	2.82	0.62
1:C:402:ILE:HD12	1:C:403:ASP:N	2.14	0.62
1:C:263:LEU:C	1:C:263:LEU:HD23	2.20	0.62
1:B:344:MET:HE2	1:B:344:MET:O	2.00	0.62
1:C:263:LEU:HD11	1:C:289:HIS:NE2	2.14	0.62
1:A:147:ASP:OD1	1:A:150:ARG:NH2	2.33	0.61
1:C:193:LYS:HE3	1:C:289:HIS:HE1	1.66	0.61
1:B:176:GLU:HB2	1:B:177:PRO:HD3	1.82	0.61
1:B:263:LEU:HD11	1:B:289:HIS:HD2	1.65	0.60
1:C:377:ARG:NH2	1:C:380:GLY:HA3	2.16	0.60
1:A:403:ASP:OD2	1:A:437:ARG:HD3	2.03	0.59
1:C:263:LEU:HD21	1:C:289:HIS:HD2	1.65	0.57
1:C:338:ASP:HB3	1:C:341:ILE:HD12	1.85	0.57
1:C:193:LYS:HE3	1:C:289:HIS:CE1	2.39	0.57
1:B:196:GLU:HG2	1:B:197:PRO:HD3	1.85	0.57
1:B:164:GLY:HA2	1:B:191:PHE:O	2.05	0.56
1:A:15:LYS:NZ	2:A:508:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD11	1:A:197:PRO:HB2	1.86	0.56
1:B:344:MET:HA	1:B:344:MET:HE3	1.88	0.56
1:C:170:LYS:HG2	1:C:195:ASP:OD2	2.06	0.55
1:C:378:LEU:N	1:C:379:PRO:CD	2.70	0.55
1:C:337:SER:O	1:C:340:LEU:HB2	2.06	0.55
1:B:402:ILE:HG13	1:B:441:SER:OG	2.07	0.54
1:C:8:ARG:NH1	1:C:55:THR:HG21	2.22	0.54
1:B:210:ILE:HG22	1:B:252:THR:HG21	1.89	0.54
1:C:402:ILE:HG13	1:C:441:SER:OG	2.08	0.53
1:B:27:LEU:O	1:B:128:PHE:HA	2.09	0.52
1:C:430:LYS:O	1:C:431:GLU:HB2	2.09	0.52
1:A:378:LEU:HG	1:A:382:PHE:CE2	2.44	0.52
1:B:272:THR:O	1:B:276:THR:CG2	2.58	0.51
1:C:371:GLY:HA3	1:C:373:MET:CE	2.40	0.51
1:C:290[B]:ARG:HG2	1:C:323:HIS:HB2	1.92	0.50
1:B:344:MET:CE	1:B:344:MET:HA	2.42	0.50
1:B:196:GLU:HG2	1:B:197:PRO:CD	2.42	0.50
1:B:403:ASP:OD2	1:B:437:ARG:HD3	2.12	0.50
1:A:77:ASP:OD2	1:A:80:LYS:HG3	2.12	0.49
1:C:339:LYS:HE2	2:C:514:HOH:O	2.11	0.49
1:A:329:TYR:HB2	1:A:373:MET:HE1	1.93	0.49
1:B:147:ASP:OD1	1:B:150:ARG:NH2	2.45	0.49
1:A:52:SER:O	1:C:170:LYS:HE3	2.13	0.49
1:B:196:GLU:N	1:B:197:PRO:HD3	2.28	0.49
1:C:402:ILE:HD13	1:C:437:ARG:HH21	1.78	0.49
1:A:193:LYS:HD3	1:A:393:THR:HG21	1.95	0.48
1:B:413:ARG:O	1:B:417:GLU:HG2	2.13	0.48
1:C:196:GLU:HG2	1:C:197:PRO:HD3	1.94	0.48
1:C:186:TRP:CE2	1:C:192:ILE:HD12	2.48	0.48
1:C:168:LYS:HA	1:C:168:LYS:HE2	1.96	0.48
1:B:378:LEU:HG	1:B:382:PHE:CE2	2.49	0.47
1:A:46:HIS:ND1	1:A:119:ASP:OD2	2.43	0.47
1:B:413:ARG:HG2	1:B:413:ARG:HH11	1.79	0.47
1:A:176:GLU:HB2	1:A:177:PRO:HD3	1.95	0.47
1:C:193:LYS:CE	1:C:289:HIS:HE1	2.24	0.47
1:C:164:GLY:HA2	1:C:191:PHE:O	2.15	0.46
1:A:166:ILE:HD11	1:A:193:LYS:HE3	1.97	0.46
1:B:196:GLU:N	1:B:197:PRO:CD	2.79	0.46
1:B:311:ILE:HD13	1:B:324:VAL:HG23	1.96	0.46
1:C:290[B]:ARG:HG3	1:C:290[B]:ARG:HH11	1.80	0.46
1:C:377:ARG:O	1:C:377:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ARG:HH12	1:C:55:THR:HG21	1.81	0.46
1:B:346:GLU:HA	1:B:364:PRO:HB3	1.97	0.46
1:B:442:PHE:O	1:B:445:ASP:O	2.33	0.46
1:C:31:LEU:O	1:C:123:ALA:HA	2.15	0.46
1:C:373:MET:HG2	1:C:377:ARG:HG3	1.97	0.45
1:B:289:HIS:HD1	1:B:290:ARG:H	1.65	0.45
1:B:82:LEU:CD2	2:B:681:HOH:O	2.49	0.45
1:B:234:ILE:O	1:B:242:MET:HG2	2.16	0.45
1:C:371:GLY:CA	1:C:373:MET:HE2	2.47	0.45
1:B:90:ASP:OD1	2:B:501:HOH:O	2.21	0.45
1:B:413:ARG:NH2	1:B:417:GLU:OE1	2.50	0.44
1:C:263:LEU:HD23	1:C:264:VAL:N	2.32	0.44
1:C:148:MET:SD	1:C:391:ILE:HD11	2.58	0.44
1:B:402:ILE:HD13	1:B:437:ARG:CZ	2.47	0.44
1:B:69:VAL:HA	1:B:88:PRO:HG2	1.99	0.44
1:A:196:GLU:N	1:A:197:PRO:CD	2.82	0.43
1:C:82:LEU:HD21	1:C:84:LYS:HE3	2.00	0.43
1:B:171:LEU:HD11	1:B:197:PRO:HB2	2.01	0.43
1:A:164:GLY:HA2	1:A:191:PHE:O	2.18	0.43
1:A:378:LEU:HA	1:A:378:LEU:HD12	1.83	0.43
1:A:327:MET:HA	1:A:338:ASP:CB	2.49	0.43
1:A:6:THR:HA	1:A:45:ALA:CB	2.49	0.43
1:C:438:ALA:O	1:C:442:PHE:HD2	2.02	0.43
1:C:444:HIS:O	1:C:445:ASP:CB	2.67	0.43
1:C:53:THR:O	1:C:55:THR:N	2.52	0.43
1:A:402:ILE:HD13	1:A:437:ARG:NH2	2.34	0.42
1:C:435:PHE:O	1:C:438:ALA:HB3	2.20	0.42
1:A:272:THR:HA	1:C:237:ASP:O	2.20	0.42
1:C:196:GLU:N	1:C:197:PRO:HD3	2.35	0.42
1:B:210:ILE:N	1:B:211:PRO:CD	2.84	0.41
1:A:145:ILE:HB	1:A:366:THR:HG21	2.03	0.41
1:B:217:MET:O	1:B:221:GLN:HG3	2.21	0.41
1:B:288:PHE:CE2	1:B:314:THR:HG22	2.56	0.41
1:A:368:ILE:HA	1:A:391:ILE:O	2.22	0.40
1:C:263:LEU:CD2	1:C:289:HIS:CD2	2.97	0.40
1:A:196:GLU:HG2	1:A:197:PRO:HD3	2.03	0.40
1:A:428:TYR:CE1	1:A:432:HIS:CE1	3.09	0.40
1:C:424:ASP:O	1:C:425:PRO:C	2.60	0.40
1:A:435:PHE:O	1:A:438:ALA:HB3	2.21	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	420/461 (91%)	403 (96%)	14 (3%)	3 (1%)	22	17
1	B	413/461 (90%)	388 (94%)	20 (5%)	5 (1%)	13	8
1	C	417/461 (90%)	400 (96%)	12 (3%)	5 (1%)	13	8
All	All	1250/1383 (90%)	1191 (95%)	46 (4%)	13 (1%)	15	10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	54	GLY
1	C	373	MET
1	C	445	ASP
1	A	52	SER
1	A	373	MET
1	B	52	SER
1	C	52	SER
1	C	431	GLU
1	A	111	ILE
1	B	372	GLY
1	B	199	GLY
1	B	425	PRO
1	B	111	ILE

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	332/361 (92%)	326 (98%)	6 (2%)	59	63
1	B	328/361 (91%)	322 (98%)	6 (2%)	59	63
1	C	330/361 (91%)	322 (98%)	8 (2%)	49	52
All	All	990/1083 (91%)	970 (98%)	20 (2%)	55	59

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	193	LYS
1	A	290	ARG
1	A	353	PRO
1	A	398	THR
1	A	433	LYS
1	B	8	ARG
1	B	276	THR
1	B	340	LEU
1	B	374	ASN
1	B	402	ILE
1	B	447	ASP
1	C	31	LEU
1	C	196	GLU
1	C	223	GLU
1	C	288	PHE
1	C	289	HIS
1	C	337	SER
1	C	378	LEU
1	C	385	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	146	GLN
1	C	289	HIS

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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	426/461 (92%)	0.28	26 (6%) 21 25	22, 35, 68, 100	0
1	B	419/461 (90%)	0.31	29 (6%) 16 20	24, 37, 70, 94	0
1	C	422/461 (91%)	0.67	44 (10%) 6 8	23, 40, 69, 97	0
All	All	1267/1383 (91%)	0.42	99 (7%) 13 16	22, 38, 69, 100	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	443	PRO	9.1
1	C	376	LEU	7.9
1	C	439	PHE	7.2
1	C	442	PHE	7.1
1	C	396	GLY	6.0
1	A	444	HIS	6.0
1	B	3	LEU	5.5
1	C	399	TYR	5.4
1	C	436	ALA	5.2
1	B	439	PHE	5.0
1	C	37	GLY	5.0
1	B	446	ALA	4.7
1	C	445	ASP	4.6
1	C	428	TYR	4.3
1	C	400	GLY	4.1
1	C	430	LYS	4.0
1	C	435	PHE	4.0
1	C	444	HIS	3.9
1	C	373	MET	3.9
1	C	76	ILE	3.8
1	A	3	LEU	3.6
1	C	374	ASN	3.6
1	B	447	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	441	SER	3.5
1	C	446	ALA	3.5
1	C	371	GLY	3.4
1	C	402	ILE	3.4
1	A	439	PHE	3.2
1	B	41	LEU	3.2
1	B	442	PHE	3.2
1	C	82	LEU	3.0
1	A	377	ARG	3.0
1	C	377	ARG	3.0
1	C	336	ALA	3.0
1	B	399	TYR	3.0
1	C	40	TYR	3.0
1	C	397	GLY	3.0
1	C	79	ALA	3.0
1	A	373	MET	2.9
1	A	443	PRO	2.9
1	C	17	ASP	2.9
1	A	433	LYS	2.9
1	B	428	TYR	2.8
1	B	444	HIS	2.8
1	B	371	GLY	2.8
1	C	426	VAL	2.8
1	A	436	ALA	2.7
1	C	405	PRO	2.7
1	B	378	LEU	2.7
1	A	438	ALA	2.7
1	B	376	LEU	2.7
1	C	172	GLY	2.7
1	C	429	ALA	2.7
1	C	173	LEU	2.7
1	A	442	PHE	2.7
1	A	291	ALA	2.7
1	A	37	GLY	2.6
1	A	376	LEU	2.6
1	A	236	ALA	2.5
1	C	440	GLU	2.5
1	B	7	ASN	2.5
1	C	418	CYS	2.5
1	B	162	ILE	2.5
1	B	377	ARG	2.5
1	C	403	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	432	HIS	2.5
1	A	268	VAL	2.4
1	B	373	MET	2.3
1	B	430	LYS	2.3
1	C	398	THR	2.3
1	C	38	TYR	2.3
1	B	443	PRO	2.3
1	B	37	GLY	2.3
1	A	340	LEU	2.2
1	B	432	HIS	2.2
1	B	5	GLN	2.2
1	B	426	VAL	2.2
1	B	276	THR	2.2
1	B	419	TRP	2.2
1	B	74	TYR	2.2
1	A	266	GLY	2.2
1	A	82	LEU	2.2
1	C	437	ARG	2.2
1	B	343	TYR	2.1
1	A	447	ASP	2.1
1	A	14	LEU	2.1
1	C	317	LEU	2.1
1	A	448	ALA	2.1
1	C	339	LYS	2.1
1	C	420	LYS	2.1
1	B	275	ALA	2.0
1	B	429	ALA	2.0
1	A	400	GLY	2.0
1	B	267	TYR	2.0
1	C	263	LEU	2.0
1	A	18	GLU	2.0
1	A	264	VAL	2.0
1	A	426	VAL	2.0
1	A	111	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.