



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 03:51 PM UTC

PDB ID : 6IUS / pdb_00006ius
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

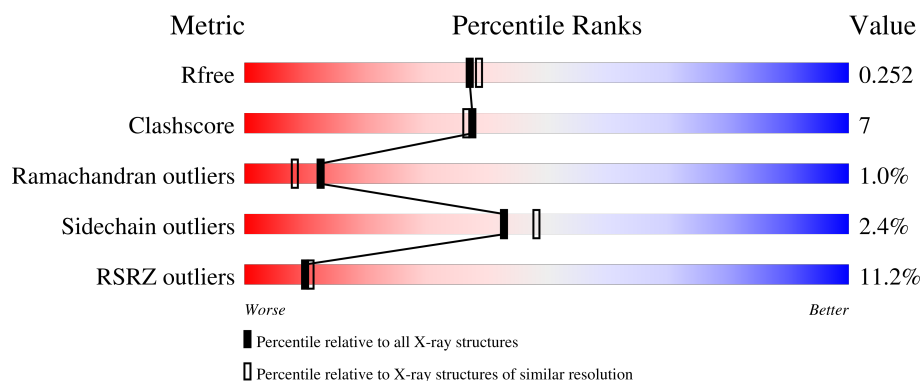
1 Overall quality at a glance

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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 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 $\leq 5\%$. 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	9% 81% 10% • 8%
1	B	461	9% 76% 13% • 9%
1	C	461	13% 77% 13% • 8%

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.

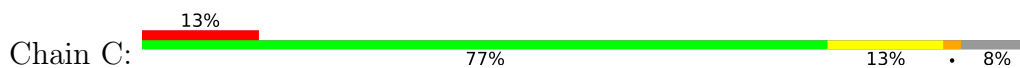
- Molecule 1 is a protein called Ribulose-1,5-bisphosphate carboxylase/oxygenase.

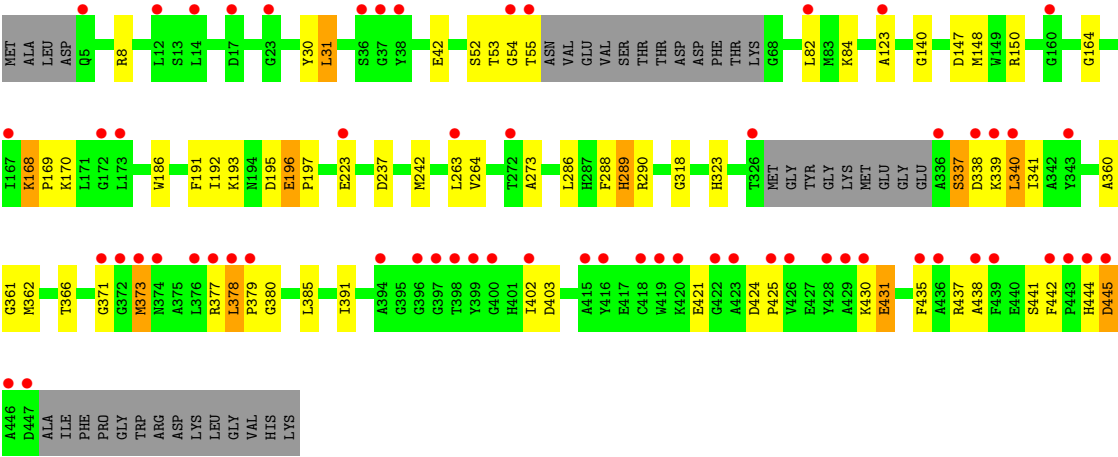
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3294	2103	553	620	18			
1	B	419	Total	C	N	O	S	0	0	0
			3244	2072	545	610	17			
1	C	422	Total	C	N	O	S	0	1	0
			3271	2086	553	615	17			

- 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		

- 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 46.99 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.1 (46.99-2.12) 96.2 (46.99-2.12)	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 (Not available) , 0.252	Depositor DCC
R_{free} test set	1926 reflections (2.23%)	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)	0.35 , 41.8	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	1.09	0/3378	1.38	3/4573 (0.1%)
1	B	1.09	1/3327 (0.0%)	1.40	2/4506 (0.0%)
1	C	1.09	0/3354	1.44	7/4540 (0.2%)
All	All	1.09	1/10059 (0.0%)	1.41	12/13619 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	390	VAL	C-O	5.75	1.29	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	PHE	CA-CB-CG	6.64	120.44	113.80
1	A	47	PHE	CA-CB-CG	5.90	119.70	113.80
1	C	30	TYR	CB-CA-C	-5.71	97.44	109.38
1	C	169	PRO	CA-C-N	5.43	128.34	120.79
1	C	169	PRO	C-N-CA	5.43	128.34	120.79
1	C	366	THR	CA-CB-OG1	-5.41	101.48	109.60
1	C	360	ALA	CA-C-O	-5.41	115.70	122.03
1	A	395	GLY	CA-C-N	5.10	125.64	119.98
1	A	395	GLY	C-N-CA	5.10	125.64	119.98
1	B	108	THR	CA-CB-OG1	-5.06	102.01	109.60
1	C	42	GLU	CA-C-N	5.02	126.96	120.44
1	C	42	GLU	C-N-CA	5.02	126.96	120.44

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	30	0
1	B	3244	0	3130	52	0
1	C	3271	0	3157	56	0
2	A	237	0	0	2	0
2	B	225	0	0	4	0
2	C	244	0	0	2	0
All	All	10515	0	9463	135	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 7.

All (135) 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:HE2	1:B:359:TRP:HE1	1.07	1.15
1:B:344:MET:HE2	1:B:359:TRP:NE1	1.71	1.05
1:B:342:ALA:O	1:B:346:GLU:HG2	1.73	0.89
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:B:344:MET:HE3	1:B:344:MET:HA	1.61	0.81
1:A:290:ARG:HG3	1:A:293:HIS:CD2	2.16	0.80
1:B:344:MET:CE	1:B:359:TRP:NE1	2.35	0.78
1:A:169:PRO:HB3	1:C:55:THR:HG22	1.67	0.75
1:B:344:MET:HE1	1:B:359:TRP:HE1	1.51	0.71
1:B:272:THR:O	1:B:276:THR:HG23	1.92	0.70
1:B:344:MET:HE2	1:B:359:TRP:CE2	2.27	0.69
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:170:LYS:HG2	1:C:195:ASP:CG	2.19	0.67
1:C:263:LEU:C	1:C:263:LEU:HD23	2.20	0.67
1:B:344:MET:HE3	1:B:350:ALA:HB3	1.78	0.66
1:C:444:HIS:O	1:C:445:ASP:HB2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:171:LEU:HD11	1:A:197:PRO:HB2	1.86	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: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: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:344:MET:CE	1:B:350:ALA:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:B:413:ARG:HG2	1.79	0.47
1:A:176:GLU:HB2	1:A:177:PRO:HD3	1.95	0.47
1:B:344:MET:HE2	1:B:359:TRP:CZ2	2.50	0.47
1:C:193:LYS:CE	1:C:289:HIS:HE1	2.24	0.47
1:C:263:LEU:C	1:C:263:LEU:CD2	2.88	0.47
1:C:371:GLY:CA	1:C:373:MET:HE2	2.44	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:HH11	1:C:290[B]:ARG:HG3	1.80	0.46
1:C:377:ARG:HD2	1:C:377:ARG:O	2.15	0.46
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:82:LEU:CD2	2:B:681:HOH:O	2.49	0.45
1:B:289:HIS:HD1	1:B:290:ARG:H	1.65	0.45
1:B:234:ILE:O	1:B:242:MET:HG2	2.16	0.45
1:B:90:ASP:OD1	2:B:501:HOH:O	2.21	0.45
1:B:340:LEU:HD22	1:B:340:LEU:C	2.42	0.45
1:B:8:ARG:HH11	1:B:55:THR:C	2.25	0.44
1:B:413:ARG:NH2	1:B:417:GLU:OE1	2.50	0.44
1:A:290:ARG:O	1:A:291:ALA:C	2.60	0.44
1:A:168:LYS:HA	1:A:169:PRO:C	2.43	0.44
1:C:148:MET:SD	1:C:391:ILE:HD11	2.58	0.44
1:C:242:MET:HE1	1:C:273:ALA:O	2.18	0.44
1:B:110:THR:OG1	1:B:125:MET:HE1	2.17	0.44
1:B:69:VAL:HA	1:B:88:PRO:HG2	1.99	0.44
1:B:402:ILE:HD13	1:B:437:ARG:CZ	2.47	0.44
1:C:424:ASP:O	1:C:425:PRO:C	2.60	0.43
1:C:140:GLY:C	1:C:318:GLY:HA2	2.43	0.43
1:C:288:PHE:C	1:C:288:PHE:CD1	2.95	0.43
1:B:293:HIS:ND1	1:B:297:THR:OG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:263:LEU:HD23	1:C:264:VAL:N	2.32	0.43
1:B:171:LEU:HD11	1:B:197:PRO:HB2	2.01	0.43
1:B:344:MET:CE	1:B:344:MET:HA	2.42	0.43
1:A:164:GLY:HA2	1:A:191:PHE:O	2.18	0.43
1:A:378:LEU:HD12	1:A:378:LEU:HA	1.83	0.43
1:B:290:ARG:O	1:B:291:ALA:C	2.61	0.43
1:A:6:THR:HA	1:A:45:ALA:CB	2.49	0.43
1:A:327:MET:HA	1:A:338:ASP:CB	2.49	0.43
1:C:53:THR:O	1:C:55:THR:N	2.52	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: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:B:207:LYS:NZ	2:B:521:HOH:O	2.53	0.42
1:C:196:GLU:N	1:C:197:PRO:HD3	2.35	0.42
1:B:8:ARG:NH1	1:B:55:THR:C	2.78	0.41
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:373:MET:HE2	1:B:378:LEU:HA	2.02	0.41
1:B:288:PHE:CE2	1:B:314:THR:HG22	2.56	0.41
1:A:32:MET:HB2	1:A:83:MET:HE2	2.03	0.40
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:361:GLY:O	1:C:362:MET:C	2.65	0.40
1:A:329:TYR:HB2	1:A:373:MET:HE1	2.03	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%)	18	15
1	B	413/461 (90%)	388 (94%)	20 (5%)	5 (1%)	10	6
1	C	417/461 (90%)	400 (96%)	12 (3%)	5 (1%)	10	6
All	All	1250/1383 (90%)	1191 (95%)	46 (4%)	13 (1%)	12	8

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 ⓘ

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%)	328 (99%)	4 (1%)	63	71
1	B	328/361 (91%)	319 (97%)	9 (3%)	39	44
1	C	330/361 (91%)	319 (97%)	11 (3%)	33	36
All	All	990/1083 (91%)	966 (98%)	24 (2%)	43	48

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	290	ARG
1	A	398	THR
1	A	433	LYS
1	B	8	ARG
1	B	170	LYS
1	B	223	GLU
1	B	276	THR
1	B	340	LEU
1	B	344	MET
1	B	374	ASN
1	B	402	ILE
1	B	447	ASP
1	C	31	LEU
1	C	168	LYS
1	C	196	GLU
1	C	223	GLU
1	C	286	LEU
1	C	289	HIS
1	C	337	SER
1	C	340	LEU
1	C	378	LEU
1	C	385	LEU
1	C	421	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	259	GLN
1	B	146	GLN
1	B	259	GLN
1	B	392	ASN
1	C	146	GLN
1	C	289	HIS
1	C	384	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 oligosaccharides 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%)	0.67	40 (9%)	14 15	22, 35, 68, 100	0
1	B	419/461 (90%)	0.78	40 (9%)	14 15	24, 37, 70, 94	0
1	C	422/461 (91%)	0.93	62 (14%)	6 6	16, 40, 69, 96	1 (0%)
All	All	1267/1383 (91%)	0.80	142 (11%)	10 11	16, 38, 69, 100	1 (0%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	446	ALA	6.4
1	C	376	LEU	6.2
1	C	443	PRO	6.0
1	B	446	ALA	5.4
1	C	442	PHE	5.1
1	C	399	TYR	5.0
1	C	439	PHE	4.9
1	B	340	LEU	4.8
1	C	373	MET	4.7
1	B	3	LEU	4.4
1	C	371	GLY	4.4
1	B	439	PHE	4.4
1	A	3	LEU	4.3
1	C	377	ARG	4.3
1	A	448	ALA	4.2
1	A	82	LEU	3.9
1	B	422	GLY	3.9
1	B	373	MET	3.9
1	C	436	ALA	3.8
1	B	162	ILE	3.8
1	A	394	ALA	3.8
1	B	399	TYR	3.7
1	C	37	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	435	PHE	3.7
1	C	55	THR	3.7
1	B	425	PRO	3.6
1	A	172	GLY	3.6
1	A	223	GLU	3.6
1	B	396	GLY	3.6
1	B	5	GLN	3.5
1	B	171	LEU	3.4
1	A	444	HIS	3.4
1	A	433	LYS	3.4
1	C	428	TYR	3.4
1	B	394	ALA	3.3
1	B	402	ILE	3.3
1	B	426	VAL	3.3
1	C	444	HIS	3.2
1	C	397	GLY	3.2
1	C	418	CYS	3.2
1	C	426	VAL	3.1
1	C	429	ALA	3.1
1	B	223	GLU	3.1
1	A	400	GLY	3.1
1	C	398	THR	3.1
1	A	373	MET	3.1
1	B	376	LEU	3.1
1	B	400	GLY	3.1
1	C	400	GLY	3.1
1	A	40	TYR	3.1
1	B	343	TYR	3.0
1	C	172	GLY	3.0
1	A	113	ASN	3.0
1	A	371	GLY	3.0
1	A	377	ARG	3.0
1	A	438	ALA	3.0
1	C	396	GLY	3.0
1	C	326	THR	3.0
1	C	420	LYS	3.0
1	C	423	ALA	3.0
1	B	371	GLY	3.0
1	A	397	GLY	2.9
1	C	374	ASN	2.9
1	A	37	GLY	2.9
1	C	425	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	2.8
1	C	339	LYS	2.8
1	B	372	GLY	2.8
1	B	409	ALA	2.8
1	C	336	ALA	2.8
1	A	376	LEU	2.8
1	A	442	PHE	2.7
1	B	423	ALA	2.7
1	C	223	GLU	2.7
1	A	145	ILE	2.7
1	A	68	GLY	2.7
1	C	23	GLY	2.7
1	A	340	LEU	2.6
1	C	36	SER	2.6
1	C	447	ASP	2.6
1	C	82	LEU	2.6
1	C	422	GLY	2.6
1	A	421	GLU	2.5
1	B	374	ASN	2.5
1	C	445	ASP	2.5
1	B	82	LEU	2.5
1	C	173	LEU	2.5
1	C	419	TRP	2.5
1	C	416	TYR	2.5
1	C	14	LEU	2.5
1	A	372	GLY	2.5
1	C	438	ALA	2.5
1	C	402	ILE	2.5
1	A	399	TYR	2.4
1	A	429	ALA	2.4
1	C	415	ALA	2.4
1	C	430	LYS	2.4
1	B	428	TYR	2.4
1	B	443	PRO	2.4
1	C	343	TYR	2.4
1	B	429	ALA	2.4
1	A	5	GLN	2.4
1	C	5	GLN	2.4
1	C	372	GLY	2.4
1	C	12	LEU	2.3
1	A	167	ILE	2.3
1	B	444	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	272	THR	2.3
1	C	379	PRO	2.3
1	B	38	TYR	2.3
1	C	123	ALA	2.3
1	B	424	ASP	2.3
1	C	338	ASP	2.3
1	C	394	ALA	2.3
1	C	340	LEU	2.3
1	C	378	LEU	2.3
1	A	43	ALA	2.3
1	A	395	GLY	2.3
1	A	42	GLU	2.2
1	A	439	PHE	2.2
1	A	38	TYR	2.2
1	B	69	VAL	2.2
1	C	17	ASP	2.2
1	B	395	GLY	2.2
1	C	160	GLY	2.2
1	B	31	LEU	2.2
1	C	263	LEU	2.2
1	B	324	VAL	2.1
1	B	33	LYS	2.1
1	A	426	VAL	2.1
1	C	54	GLY	2.1
1	B	418	CYS	2.1
1	A	422	GLY	2.1
1	B	378	LEU	2.1
1	A	419	TRP	2.1
1	A	326	THR	2.0
1	C	38	TYR	2.0
1	B	120	ILE	2.0
1	C	167	ILE	2.0
1	A	431	GLU	2.0
1	A	396	GLY	2.0
1	B	172	GLY	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 oligosaccharides 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.