



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:14 PM UTC

PDB ID : 7E59 / pdb_00007e59
Title : interferon-inducible anti-viral protein truncated
Authors : Cui, W.; Wang, W.; Chen, C.; Slater, B.; Xiong, Y.; Ji, X.Y.; Yang, H.T.
Deposited on : 2021-02-18
Resolution : 3.00 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

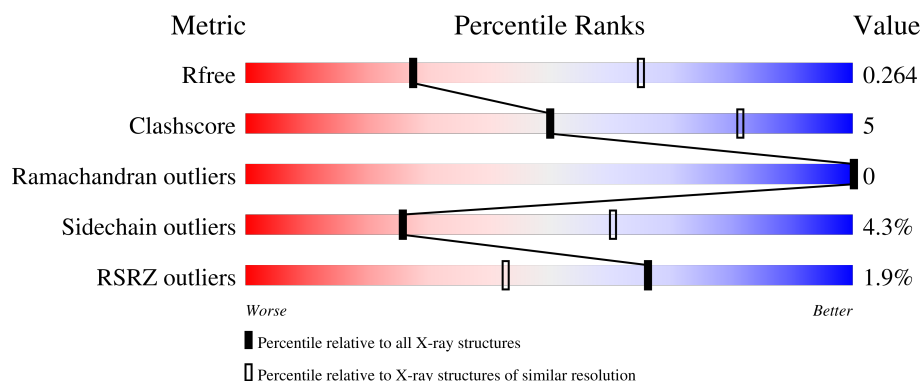
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	487	2% 67% 12% • 20%
1	B	487	2% 69% 14% • 15%
1	C	487	2% 70% 12% • 17%
1	G	487	• 75% 11% • 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13005 atoms, of which 0 are hydrogens and 0 are deuteriums.

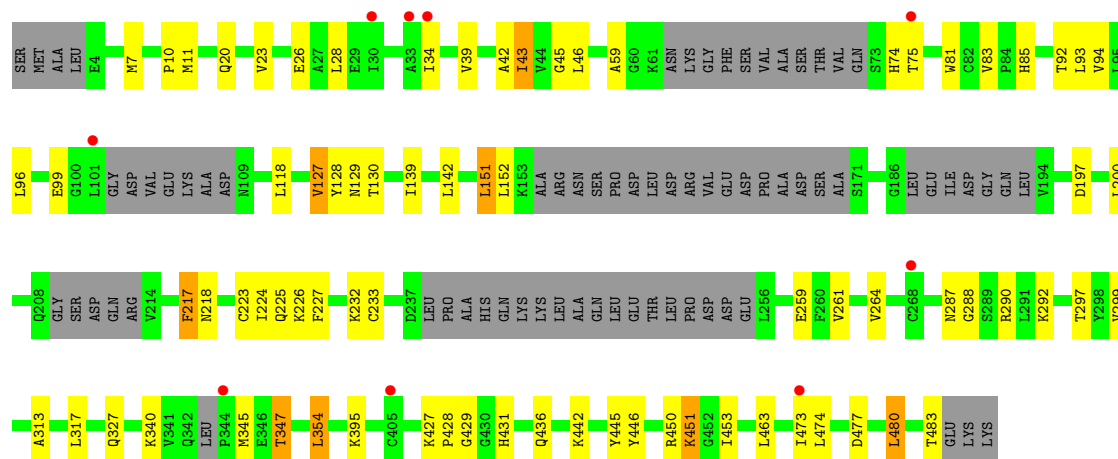
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Guanylate-binding protein 5.

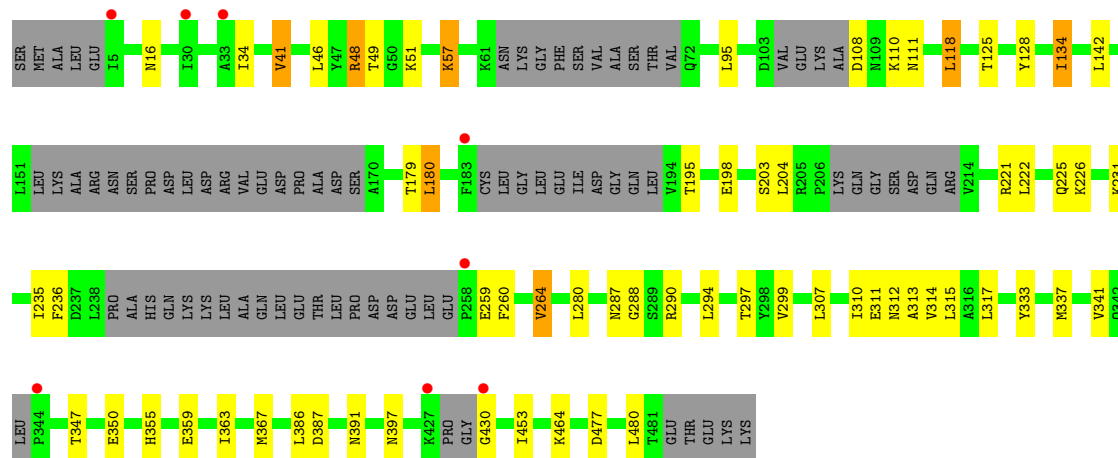
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	422	Total	C	N	O	S	0	0	0
			3358	2141	562	638	17			
1	A	391	Total	C	N	O	S	0	0	0
			3111	1992	515	588	16			
1	B	414	Total	C	N	O	S	0	0	0
			3301	2112	549	623	17			
1	C	406	Total	C	N	O	S	0	0	0
			3235	2068	538	613	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	expression tag	UNP Q96PP8
G	356	ALA	ARG	engineered mutation	UNP Q96PP8
A	0	SER	-	expression tag	UNP Q96PP8
A	356	ALA	ARG	engineered mutation	UNP Q96PP8
B	0	SER	-	expression tag	UNP Q96PP8
B	356	ALA	ARG	engineered mutation	UNP Q96PP8
C	0	SER	-	expression tag	UNP Q96PP8
C	356	ALA	ARG	engineered mutation	UNP Q96PP8



• Molecule 1: Guanylate-binding protein 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	90.87Å 137.31Å 203.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 3.00 48.23 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.23-3.00) 99.9 (48.23-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.218 , 0.259 0.224 , 0.264	Depositor DCC
R_{free} test set	2614 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.3	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	0.94	EDS
Total number of atoms	13005	wwPDB-VP
Average B, all atoms (Å ²)	107.0	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 41.33 % 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 2.4002e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.08	0/3164	0.24	0/4276
1	B	0.13	0/3359	0.28	1/4536 (0.0%)
1	C	0.08	0/3291	0.23	0/4445
1	G	0.08	0/3416	0.25	1/4616 (0.0%)
All	All	0.10	0/13230	0.25	2/17873 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	449	PRO	N-CA-C	5.44	121.24	113.47
1	B	225	GLN	O-C-N	5.21	127.44	122.07

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	3111	0	3125	32	0
1	B	3301	0	3316	45	0
1	C	3235	0	3235	36	0
1	G	3358	0	3359	25	0
All	All	13005	0	13035	137	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 5.

All (137) 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:A:131:VAL:HG23	1:A:181:ARG:HB2	1.71	0.73
1:B:7:MET:HA	1:B:81:TRP:HE1	1.54	0.73
1:A:413:PHE:HB3	1:A:441:LEU:HD13	1.72	0.70
1:C:310:ILE:HG23	1:C:312:ASN:H	1.60	0.67
1:B:226:LYS:O	1:B:227:PHE:HB3	1.94	0.65
1:C:222:LEU:HG	1:C:226:LYS:HE3	1.77	0.65
1:G:212:GLN:O	1:G:216:ASN:ND2	2.33	0.61
1:G:52:SER:O	1:G:56:ASN:ND2	2.33	0.61
1:A:32:SER:HB3	1:A:292:LYS:HD2	1.82	0.61
1:A:7:MET:HE3	1:A:82:CYS:H	1.66	0.60
1:C:280:LEU:HD21	1:C:294:LEU:HD21	1.83	0.60
1:A:257:GLU:HB2	1:A:260:PHE:HB3	1.85	0.59
1:C:41:VAL:HG12	1:C:125:THR:HB	1.82	0.59
1:G:32:SER:HB2	1:G:292:LYS:HD2	1.86	0.58
1:A:363:ILE:HG22	1:A:367:MET:HE2	1.86	0.57
1:C:16:ASN:HD21	1:C:111:ASN:HB3	1.68	0.57
1:B:45:GLY:HA2	1:B:129:ASN:HB3	1.87	0.56
1:C:430:GLY:N	1:C:477:ASP:OD1	2.39	0.56
1:B:43:ILE:HD13	1:B:127:VAL:HG11	1.86	0.56
1:B:34:ILE:HD13	1:B:92:THR:HG21	1.88	0.56
1:C:307:LEU:H	1:C:307:LEU:HD23	1.72	0.55
1:G:206:PRO:HG3	1:G:222:LEU:HD21	1.87	0.55
1:A:206:PRO:HB2	1:A:217:PHE:HE2	1.70	0.55
1:B:297:THR:HG21	1:B:313:ALA:HA	1.89	0.55
1:G:343:LEU:O	1:G:397:ASN:ND2	2.40	0.54
1:C:225:GLN:HA	1:C:231:LYS:HZ1	1.72	0.54
1:A:143:HIS:NE2	1:A:147:GLU:OE2	2.41	0.54
1:B:11:MET:HE1	1:B:26:GLU:HG3	1.89	0.54
1:C:387:ASP:O	1:C:391:ASN:ND2	2.40	0.54
1:B:429:GLY:N	1:B:477:ASP:OD1	2.41	0.53
1:A:195:THR:HG23	1:A:198:GLU:H	1.72	0.53
1:B:28:LEU:HG	1:B:292:LYS:HG3	1.90	0.53
1:A:34:ILE:HD13	1:A:92:THR:HG21	1.91	0.52
1:C:363:ILE:HG22	1:C:367:MET:HE2	1.90	0.52
1:G:113:ILE:HG23	1:G:145:VAL:HG12	1.92	0.51
1:G:363:ILE:HG22	1:G:367:MET:HE2	1.93	0.51
1:A:113:ILE:HG22	1:A:148:LEU:HD22	1.93	0.51
1:C:290:ARG:HB3	1:C:317:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD11	1:A:291:LEU:HD23	1.93	0.50
1:B:223:CYS:O	1:B:226:LYS:O	2.28	0.50
1:C:347:THR:HG23	1:C:350:GLU:H	1.77	0.50
1:B:142:LEU:HD23	1:B:224:ILE:HD13	1.92	0.49
1:B:427:LYS:HA	1:B:480:LEU:HD11	1.94	0.49
1:G:297:THR:HG21	1:G:313:ALA:HA	1.94	0.49
1:B:43:ILE:HA	1:B:127:VAL:HG13	1.93	0.49
1:B:226:LYS:O	1:B:227:PHE:CB	2.60	0.49
1:G:11:MET:HE1	1:G:26:GLU:HG2	1.95	0.48
1:A:40:VAL:HB	1:A:123:SER:HA	1.96	0.48
1:B:428:PRO:HD3	1:B:480:LEU:HD12	1.94	0.48
1:C:203:SER:O	1:C:221:ARG:NH2	2.47	0.48
1:B:152:LEU:HD22	1:B:227:PHE:HD2	1.77	0.48
1:G:284:ILE:HD13	1:G:371:PHE:HZ	1.79	0.48
1:A:409:LEU:HD22	1:A:413:PHE:CZ	2.49	0.48
1:G:447:ARG:HA	1:G:447:ARG:HD3	1.70	0.48
1:C:333:TYR:CZ	1:C:337:MET:HG3	2.49	0.48
1:C:46:LEU:O	1:C:49:THR:OG1	2.28	0.47
1:G:256:LEU:HD12	1:G:261:VAL:HG13	1.96	0.47
1:G:405:CYS:HB3	1:G:458:VAL:HG11	1.97	0.47
1:B:290:ARG:HD3	1:B:317:LEU:HD21	1.96	0.47
1:C:34:ILE:HB	1:C:288:GLY:HA3	1.95	0.47
1:A:176:LEU:HB2	1:A:228:PHE:CG	2.50	0.47
1:C:195:THR:HG23	1:C:198:GLU:H	1.79	0.47
1:G:419:ALA:HB1	1:G:424:ILE:HG21	1.97	0.46
1:G:460:GLN:O	1:G:464:LYS:HG2	2.15	0.46
1:B:42:ALA:HA	1:B:96:LEU:HB2	1.97	0.46
1:C:236:PHE:HB3	1:C:260:PHE:HE1	1.79	0.46
1:C:48:ARG:HH12	1:C:51:LYS:HG3	1.81	0.46
1:C:108:ASP:N	1:C:108:ASP:OD1	2.49	0.46
1:C:359:GLU:HG3	1:C:386:LEU:HD13	1.98	0.46
1:G:139:ILE:HG21	1:G:221:ARG:HG2	1.97	0.46
1:C:118:LEU:HD11	1:C:299:VAL:HG22	1.97	0.45
1:B:227:PHE:CD1	1:B:227:PHE:O	2.69	0.45
1:B:197:ASP:OD2	1:B:232:LYS:NZ	2.39	0.45
1:B:227:PHE:CD1	1:B:227:PHE:C	2.94	0.45
1:B:10:PRO:HB3	1:B:81:TRP:HB2	1.97	0.45
1:A:202:ASN:HA	1:A:205:ARG:HD2	1.99	0.45
1:B:139:ILE:HG23	1:B:224:ILE:HD12	1.99	0.44
1:C:48:ARG:HH22	1:C:51:LYS:HA	1.81	0.44
1:C:310:ILE:HG13	1:C:311:GLU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:OG1	1:A:150:ASP:N	2.50	0.44
1:C:110:LYS:HD2	1:C:110:LYS:H	1.83	0.44
1:C:314:VAL:HG13	1:C:315:LEU:HD12	1.99	0.44
1:A:337:MET:HE1	1:A:354:LEU:HB3	1.99	0.44
1:B:39:VAL:HG21	1:B:85:HIS:HD2	1.83	0.44
1:C:128:TYR:CE2	1:C:142:LEU:HB2	2.52	0.44
1:A:357:THR:HG22	1:A:360:ARG:NH2	2.33	0.43
1:B:431:HIS:CD2	1:B:474:LEU:HD13	2.53	0.43
1:B:445:TYR:O	1:B:451:LYS:NZ	2.42	0.43
1:A:46:LEU:HD11	1:A:141:LEU:HD21	1.99	0.43
1:C:57:LYS:HZ3	1:C:264:VAL:HG22	1.82	0.43
1:C:179:THR:HB	1:C:236:PHE:HE2	1.83	0.43
1:B:74:HIS:O	1:B:99:GLU:N	2.51	0.43
1:A:257:GLU:OE1	1:A:257:GLU:N	2.48	0.43
1:B:151:LEU:HD11	1:B:227:PHE:CE2	2.53	0.43
1:C:333:TYR:OH	1:C:355:HIS:ND1	2.38	0.43
1:G:347:THR:HG23	1:G:350:GLU:H	1.83	0.43
1:C:16:ASN:ND2	1:C:111:ASN:HB3	2.32	0.43
1:B:446:TYR:HA	1:B:451:LYS:HE3	2.01	0.43
1:G:413:PHE:HE2	1:G:438:THR:HG23	1.84	0.43
1:G:261:VAL:HA	1:G:264:VAL:HG12	2.00	0.42
1:B:20:GLN:N	1:B:20:GLN:OE1	2.52	0.42
1:B:59:ALA:HB1	1:B:83:VAL:HG21	2.01	0.42
1:B:287:ASN:OD1	1:B:290:ARG:HG3	2.19	0.42
1:B:200:LEU:HD12	1:B:233:CYS:HB2	2.02	0.42
1:C:297:THR:HG21	1:C:313:ALA:HA	2.01	0.42
1:G:43:ILE:HD11	1:G:58:LEU:HD12	2.02	0.42
1:A:42:ALA:HA	1:A:96:LEU:HB2	2.02	0.42
1:B:128:TYR:CE2	1:B:142:LEU:HB2	2.55	0.42
1:C:180:LEU:HD11	1:C:235:ILE:HG12	2.02	0.42
1:B:151:LEU:HD11	1:B:227:PHE:HE2	1.85	0.41
1:G:337:MET:HE3	1:G:337:MET:HA	2.03	0.41
1:B:39:VAL:HG23	1:B:93:LEU:HA	2.01	0.41
1:A:309:CYS:SG	1:A:312:ASN:ND2	2.93	0.41
1:A:359:GLU:O	1:A:363:ILE:HG12	2.20	0.41
1:A:113:ILE:HG23	1:A:145:VAL:HG12	2.03	0.41
1:B:34:ILE:HB	1:B:288:GLY:HA3	2.01	0.41
1:C:41:VAL:HG23	1:C:95:LEU:HD23	2.03	0.41
1:B:345:MET:C	1:B:347:THR:H	2.28	0.41
1:A:5:ILE:HD11	1:A:34:ILE:HD11	2.02	0.41
1:A:180:LEU:HB2	1:A:235:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:LYS:HB2	1:B:428:PRO:HD2	2.02	0.41
1:B:23:VAL:HG21	1:B:299:VAL:HG11	2.02	0.41
1:B:46:LEU:HD12	1:B:130:THR:HG22	2.03	0.41
1:B:261:VAL:HA	1:B:264:VAL:HG12	2.02	0.41
1:A:219:LEU:HB3	1:A:220:PRO:HD3	2.03	0.41
1:A:467:GLU:OE2	1:A:468:SER:N	2.54	0.41
1:B:442:LYS:HD3	1:B:463:LEU:HD11	2.03	0.41
1:C:134:ILE:HG23	1:C:180:LEU:HD23	2.03	0.41
1:C:287:ASN:OD1	1:C:290:ARG:HG3	2.21	0.41
1:G:74:HIS:O	1:G:99:GLU:HG2	2.20	0.40
1:B:217:PHE:HD1	1:B:217:PHE:HA	1.68	0.40
1:G:343:LEU:O	1:G:345:MET:N	2.55	0.40
1:A:150:ASP:HB2	1:A:151:LEU:H	1.70	0.40
1:G:5:ILE:HG12	1:A:5:ILE:HG22	2.04	0.40
1:A:10:PRO:HB3	1:A:81:TRP:HB2	2.03	0.40
1:G:204:LEU:HD23	1:G:225:GLN:HG2	2.04	0.40
1:B:354:LEU:HD13	1:B:354:LEU:HA	1.92	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	375/487 (77%)	353 (94%)	22 (6%)	0	100	100
1	B	398/487 (82%)	378 (95%)	20 (5%)	0	100	100
1	C	388/487 (80%)	366 (94%)	22 (6%)	0	100	100
1	G	408/487 (84%)	393 (96%)	15 (4%)	0	100	100
All	All	1569/1948 (80%)	1490 (95%)	79 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	349/433 (81%)	334 (96%)	15 (4%)	26	60
1	B	371/433 (86%)	350 (94%)	21 (6%)	18	52
1	C	363/433 (84%)	349 (96%)	14 (4%)	28	62
1	G	375/433 (87%)	363 (97%)	12 (3%)	34	67
All	All	1458/1732 (84%)	1396 (96%)	62 (4%)	26	60

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	41	VAL
1	G	122	LEU
1	G	149	THR
1	G	195	THR
1	G	201	GLU
1	G	256	LEU
1	G	259	GLU
1	G	337	MET
1	G	345	MET
1	G	354	LEU
1	G	448	GLU
1	G	453	ILE
1	A	40	VAL
1	A	49	THR
1	A	120	LEU
1	A	141	LEU
1	A	149	THR
1	A	224	ILE
1	A	235	ILE
1	A	295	VAL
1	A	310	ILE
1	A	337	MET
1	A	408	LEU
1	A	422	GLN

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Mol	Chain	Res	Type
1	A	453	ILE
1	A	467	GLU
1	A	469	VAL
1	B	43	ILE
1	B	75	THR
1	B	94	VAL
1	B	118	LEU
1	B	127	VAL
1	B	151	LEU
1	B	217	PHE
1	B	218	ASN
1	B	259	GLU
1	B	327	GLN
1	B	340	LYS
1	B	347	THR
1	B	354	LEU
1	B	395	LYS
1	B	436	GLN
1	B	450	ARG
1	B	451	LYS
1	B	453	ILE
1	B	473	ILE
1	B	480	LEU
1	B	483	THR
1	C	41	VAL
1	C	48	ARG
1	C	57	LYS
1	C	118	LEU
1	C	134	ILE
1	C	180	LEU
1	C	204	LEU
1	C	259	GLU
1	C	264	VAL
1	C	341	VAL
1	C	397	ASN
1	C	453	ILE
1	C	464	LYS
1	C	480	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	18	ASN
1	G	36	GLN
1	G	91	HIS
1	G	143	HIS
1	G	274	HIS
1	G	390	GLN
1	G	454	GLN
1	A	18	ASN
1	A	36	GLN
1	A	114	GLN
1	A	129	ASN
1	A	312	ASN
1	B	36	GLN
1	B	114	GLN
1	B	397	ASN
1	B	431	HIS
1	C	16	ASN
1	C	376	GLN
1	C	431	HIS
1	C	454	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	391/487 (80%)	-0.10	9 (2%)	61 38	63, 104, 170, 203	0
1	B	414/487 (85%)	0.06	9 (2%)	62 39	62, 106, 170, 242	0
1	C	406/487 (83%)	-0.07	8 (1%)	65 41	59, 97, 153, 207	0
1	G	422/487 (86%)	-0.12	5 (1%)	76 55	59, 102, 159, 201	0
All	All	1633/1948 (83%)	-0.06	31 (1%)	66 43	59, 102, 166, 242	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	LEU	5.3
1	C	33	ALA	5.1
1	C	30	ILE	4.0
1	B	30	ILE	3.8
1	A	56	ASN	3.6
1	A	9	ASP	3.5
1	A	343	LEU	3.0
1	B	405	CYS	2.9
1	G	100	GLY	2.9
1	A	73	SER	2.9
1	B	33	ALA	2.8
1	B	34	ILE	2.7
1	B	473	ILE	2.6
1	C	344	PRO	2.6
1	A	170	ALA	2.5
1	B	344	PRO	2.5
1	G	152	LEU	2.5
1	G	170	ALA	2.5
1	A	424	ILE	2.5
1	A	151	LEU	2.4
1	B	268	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	427	LYS	2.4
1	A	100	GLY	2.3
1	B	75	THR	2.3
1	C	183	PHE	2.3
1	C	430	GLY	2.3
1	C	5	ILE	2.2
1	G	387	ASP	2.2
1	C	258	PRO	2.2
1	A	226	LYS	2.1
1	G	222	LEU	2.1

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 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.