Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 11:08 PM JST

PDB ID	:	7E59
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:

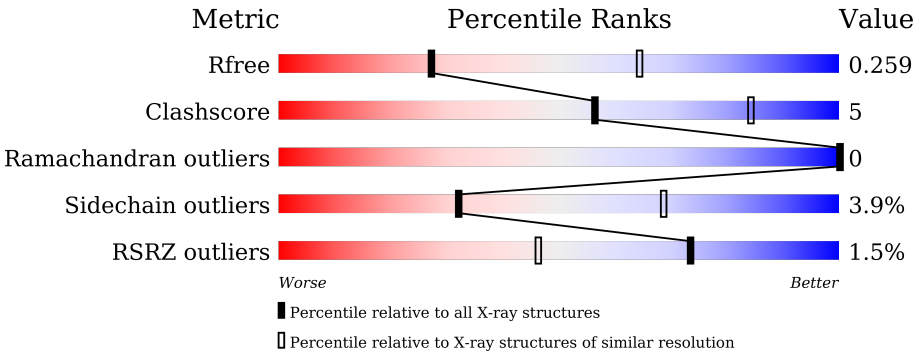
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	67% 12% • 20%
1	B	487	70% 14% • 15%
1	C	487	71% 11% • 17%
1	G	487	75% 11% • 13%

2 Entry composition (i)

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:

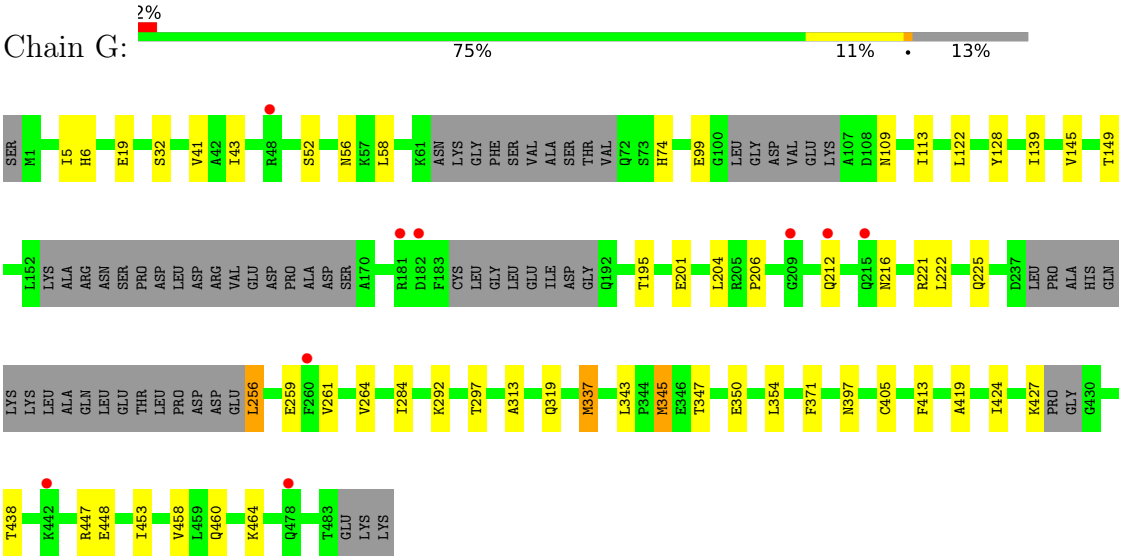
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	SER	-	expression tag	UNP Q96PP8
G	356	ALA	ARG	engineered mutation	UNP Q96PP8
A	0	SER	-	expression tag	UNP Q96PP8
A	356	ALA	ARG	engineered mutation	UNP Q96PP8
B	0	SER	-	expression tag	UNP Q96PP8
B	356	ALA	ARG	engineered mutation	UNP Q96PP8
C	0	SER	-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

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.

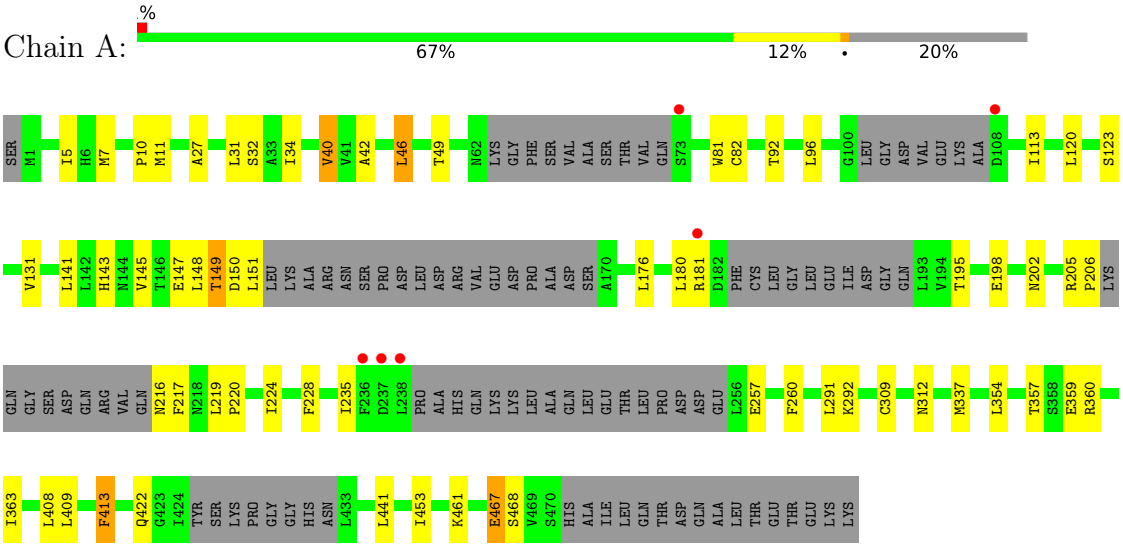
• Molecule 1: Guanylate-binding protein 5

Chain G:



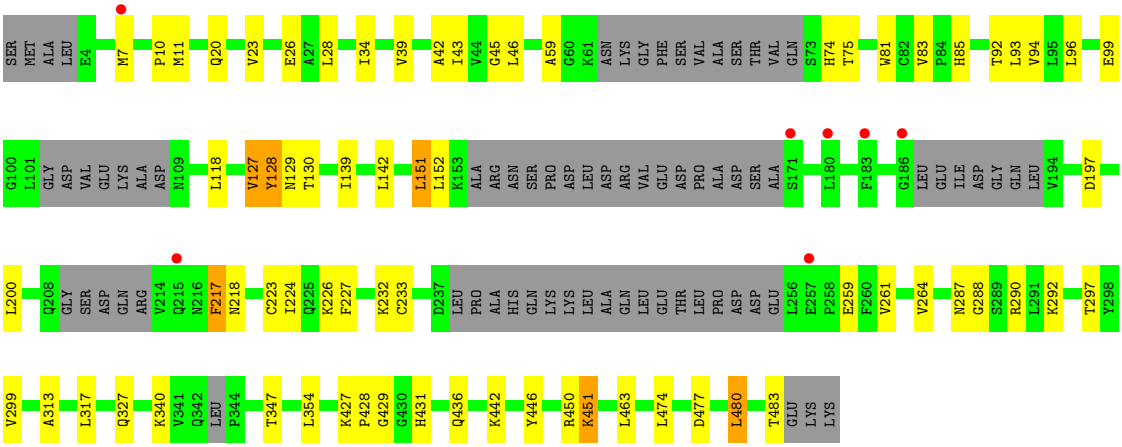
• Molecule 1: Guanylate-binding protein 5

Chain A:



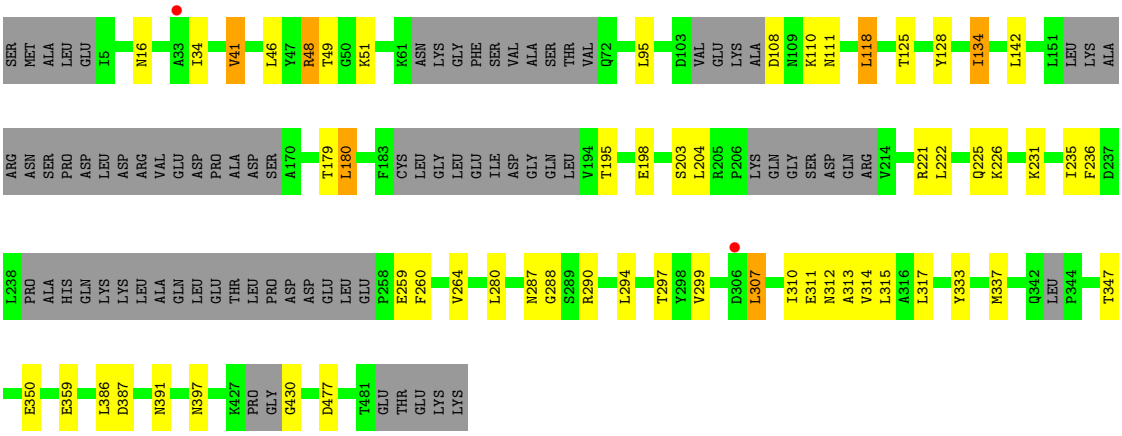
• Molecule 1: Guanylate-binding protein 5

Chain B:



• Molecule 1: Guanylate-binding protein 5

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	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 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.23-3.00) 99.6 (48.23-2.99)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.218 , 0.259 0.220 , 0.259	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)	0.29 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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

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	0.24	0/3164	0.38	0/4276
1	B	0.25	0/3359	0.39	0/4536
1	C	0.24	0/3291	0.37	0/4445
1	G	0.24	0/3416	0.38	0/4616
All	All	0.24	0/13230	0.38	0/17873

There are no bond length outliers.

There are no bond angle outliers.

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	3111	0	3125	32	0
1	B	3301	0	3316	43	0
1	C	3235	0	3235	33	0
1	G	3358	0	3359	23	0
All	All	13005	0	13035	130	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 (130) 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	0.67
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: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: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:B:11:MET:HE1	1:B:26:GLU:HG3	1.90	0.54
1:G:343:LEU:O	1:G:397:ASN:ND2	2.40	0.54
1:A:143:HIS:NE2	1:A:147:GLU:OE2	2.41	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:7:MET:HE3	1:A:82:CYS:H	1.74	0.53
1:C:225:GLN:HA	1:C:231:LYS:HZ1	1.74	0.52
1:A:34:ILE:HD13	1:A:92:THR:HG21	1.91	0.52
1:G:113:ILE:HG23	1:G:145:VAL:HG12	1.92	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LYS:O	1:B:227:PHE:CB	2.60	0.49
1:A:337:MET:HE1	1:A:354:LEU:HB3	1.95	0.49
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:G:337:MET:HE1	1:G:354:LEU:HB3	1.96	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: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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LEU:HD11	1:A:141:LEU:HD21	1.99	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: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: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:A:11:MET:HE2	1:A:27:ALA:HB2	2.03	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASP:HB2	1:A:151:LEU:H	1.70	0.40
1:B:227:PHE:CD1	1:B:227:PHE:C	2.94	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 (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	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 (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	349/433 (81%)	336 (96%)	13 (4%)	34	70
1	B	371/433 (86%)	354 (95%)	17 (5%)	27	64
1	C	363/433 (84%)	353 (97%)	10 (3%)	43	77
1	G	375/433 (87%)	358 (96%)	17 (4%)	27	64
All	All	1458/1732 (84%)	1401 (96%)	57 (4%)	32	69

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	6	HIS
1	G	19	GLU
1	G	41	VAL
1	G	109	ASN
1	G	122	LEU
1	G	128	TYR
1	G	149	THR
1	G	195	THR
1	G	201	GLU
1	G	256	LEU
1	G	259	GLU
1	G	319	GLN
1	G	337	MET
1	G	345	MET
1	G	427	LYS
1	G	448	GLU
1	G	453	ILE
1	A	40	VAL
1	A	46	LEU
1	A	49	THR
1	A	120	LEU
1	A	149	THR
1	A	216	ASN
1	A	224	ILE
1	A	408	LEU
1	A	413	PHE
1	A	422	GLN
1	A	453	ILE
1	A	461	LYS
1	A	467	GLU
1	B	75	THR
1	B	94	VAL
1	B	118	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	127	VAL
1	B	128	TYR
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	436	GLN
1	B	450	ARG
1	B	451	LYS
1	B	480	LEU
1	B	483	THR
1	C	41	VAL
1	C	48	ARG
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	307	LEU
1	C	397	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	16	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)

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, 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	391/487 (80%)	0.05	6 (1%)	73	46	63, 104, 170, 203	0
1	B	414/487 (85%)	0.02	7 (1%)	70	41	62, 106, 170, 242	0
1	C	406/487 (83%)	-0.06	2 (0%)	91	75	59, 97, 153, 207	0
1	G	422/487 (86%)	0.02	9 (2%)	63	34	59, 102, 159, 201	0
All	All	1633/1948 (83%)	0.01	24 (1%)	73	46	59, 102, 166, 242	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	ASP	5.9
1	C	306	ASP	4.1
1	G	212	GLN	3.6
1	A	238	LEU	3.4
1	G	215	GLN	2.9
1	B	257	GLU	2.9
1	A	236	PHE	2.8
1	G	182	ASP	2.8
1	G	209	GLY	2.5
1	C	33	ALA	2.5
1	B	186	GLY	2.5
1	B	7	MET	2.4
1	A	237	ASP	2.4
1	B	171	SER	2.3
1	B	180	LEU	2.3
1	G	478	GLN	2.2
1	B	183	PHE	2.2
1	A	73	SER	2.2
1	G	48	ARG	2.2
1	G	181	ARG	2.1
1	G	260	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	181	ARG	2.0
1	G	442	LYS	2.0
1	B	215	GLN	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 monosaccharides 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.