



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:04 AM UTC

PDB ID : 3H84 / pdb_00003h84
Title : Crystal structure of GET3
Authors : Hu, J.; Li, J.; Qian, X.; Sha, B.
Deposited on : 2009-04-28
Resolution : 2.30 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

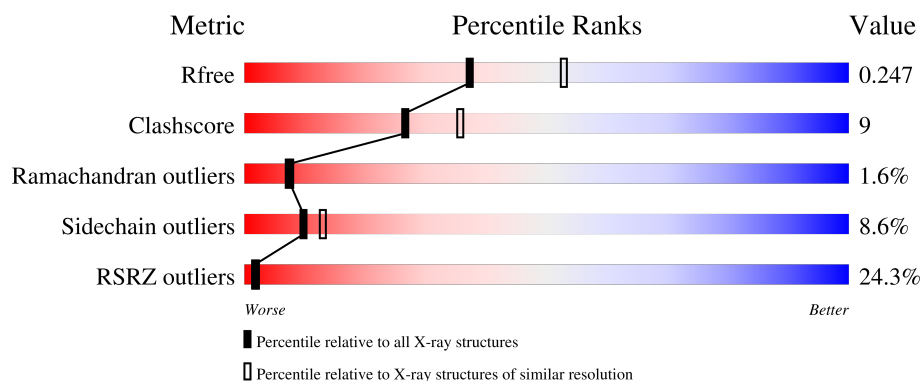
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	354	14% 68% 20% • 8%
1	B	354	31% 69% 19% • 9%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5405 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2547	1600	428	502	17			
1	B	323	Total	C	N	O	S	0	0	0
			2526	1598	420	491	17			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Na	0	0
			3	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		

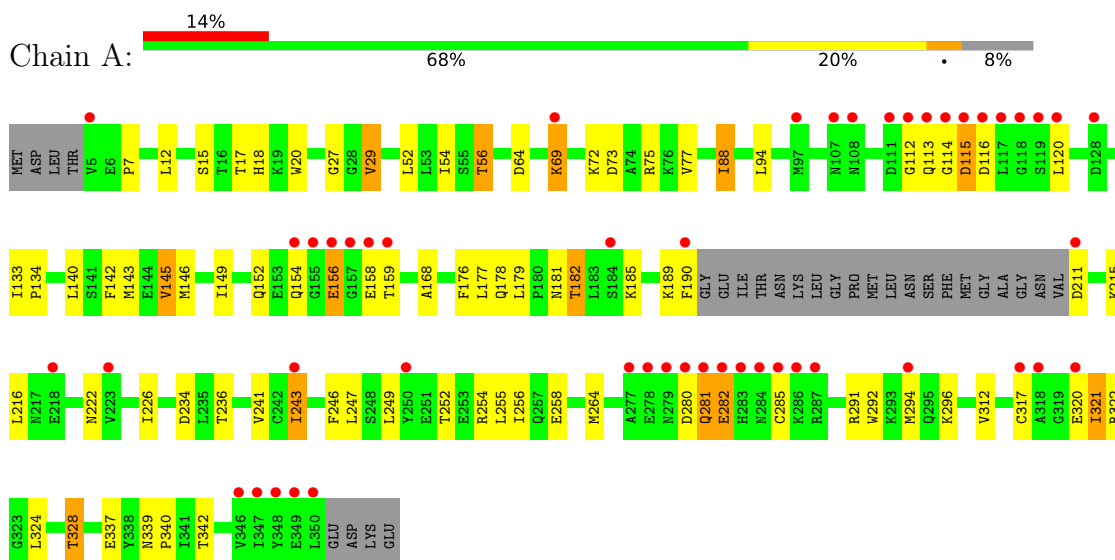
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	202	Total 202	O 202	0	0
6	B	122	Total 122	O 122	0	0

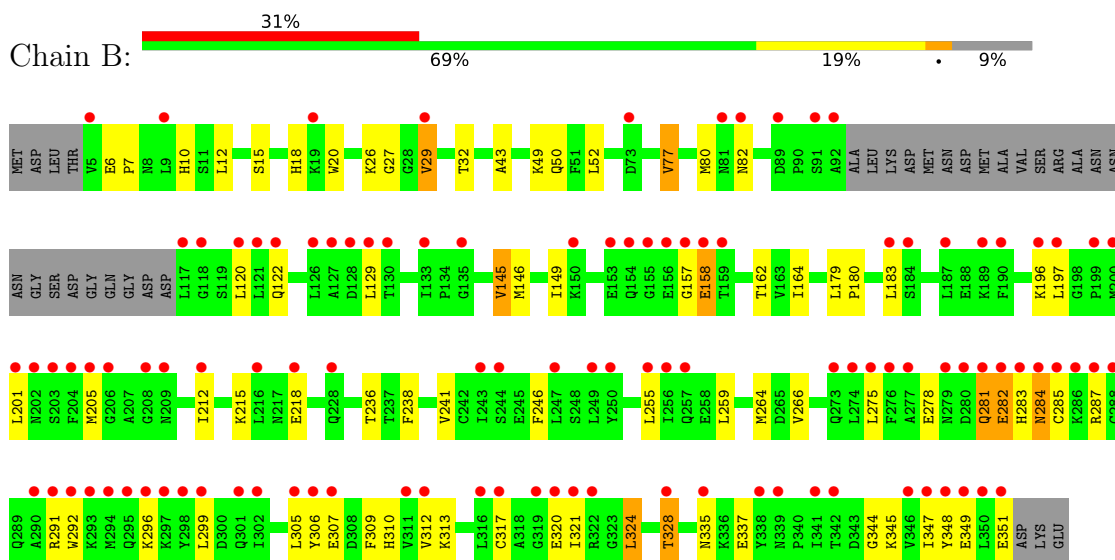
3 Residue-property plots

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: ATPase GET3



• Molecule 1: ATPase GET3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	219.40Å 113.74Å 48.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.30) 99.3 (50.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.247 0.220 , 0.247	Depositor DCC
R_{free} test set	2763 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.1	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	0.92	EDS
Total number of atoms	5405	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG, NA, ZN

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	0.51	0/2588	0.87	0/3491
1	B	0.48	0/2569	0.82	0/3466
All	All	0.49	0/5157	0.85	0/6957

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	2547	0	2514	48	0
1	B	2526	0	2512	49	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	0	0
5	B	2	0	0	0	0
6	A	202	0	0	0	0
6	B	122	0	0	1	0
All	All	5405	0	5026	94	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 9.

All (94) 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:157:GLY:H	1:B:158:GLU:HA	1.26	0.97
1:A:17:THR:HG22	1:A:234:ASP:O	1.69	0.92
1:A:324:LEU:O	1:A:328:THR:HG23	1.71	0.90
1:A:189:LYS:CB	1:A:190:PHE:HA	2.02	0.88
1:B:10:HIS:HD2	1:B:335:ASN:HD21	1.22	0.88
1:A:189:LYS:HB2	1:A:190:PHE:HA	1.56	0.87
1:B:324:LEU:O	1:B:328:THR:HG23	1.84	0.77
1:A:291:ARG:O	1:A:294:MET:HG3	1.88	0.74
1:B:157:GLY:N	1:B:158:GLU:HA	1.94	0.69
1:B:146:MET:HA	1:B:146:MET:HE2	1.82	0.62
1:B:196:LYS:HG2	1:B:197:LEU:H	1.65	0.62
1:A:29:VAL:HG13	1:A:241:VAL:HG12	1.82	0.62
1:B:15:SER:OG	1:B:18:HIS:HD2	1.84	0.61
1:B:7:PRO:HG2	1:B:337:GLU:HG2	1.83	0.61
1:B:10:HIS:CD2	1:B:335:ASN:HD21	2.11	0.60
1:B:196:LYS:CG	1:B:197:LEU:H	2.16	0.58
1:B:317:CYS:SG	1:B:321:ILE:HD11	2.43	0.58
1:A:320:GLU:HG2	1:A:321:ILE:N	2.18	0.57
1:A:7:PRO:HG2	1:A:337:GLU:HG2	1.85	0.57
1:A:56:THR:CG2	1:A:168:ALA:HB2	2.34	0.57
1:A:152:GLN:C	1:A:154:GLN:H	2.14	0.55
1:B:259:LEU:HD13	1:B:266:VAL:HG11	1.89	0.55
1:A:142:PHE:HA	1:A:145:VAL:HG13	1.89	0.55
1:B:196:LYS:CG	1:B:197:LEU:N	2.70	0.54
1:A:189:LYS:CB	1:A:190:PHE:CA	2.83	0.54
1:B:281:GLN:O	1:B:282:GLU:HB3	2.06	0.54
1:B:299:LEU:HD22	1:B:313:LYS:HE2	1.89	0.54
1:A:317:CYS:SG	1:A:321:ILE:HD11	2.48	0.54
1:A:246:PHE:HE2	1:B:26:LYS:HE2	1.73	0.53
1:A:320:GLU:HG3	1:A:322:ARG:HG3	1.90	0.53
1:A:15:SER:OG	1:A:18:HIS:HD2	1.92	0.53
1:A:252:THR:O	1:A:256:ILE:HG12	2.10	0.52
1:A:29:VAL:HA	1:A:243:ILE:HD13	1.90	0.52
1:B:281:GLN:NE2	1:B:281:GLN:HA	2.25	0.52
1:A:20:TRP:HB2	1:A:236:THR:HG23	1.91	0.52
1:B:145:VAL:O	1:B:149:ILE:HG12	2.10	0.52
1:A:324:LEU:O	1:A:328:THR:CG2	2.54	0.51
1:A:146:MET:HA	1:A:146:MET:HE2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLN:O	1:A:282:GLU:HB2	2.10	0.51
1:B:49:LYS:O	1:B:82:ASN:OD1	2.29	0.51
1:B:284:ASN:HD22	1:B:284:ASN:N	2.09	0.51
1:B:122:GLN:HE21	1:B:215:LYS:HB2	1.75	0.51
1:B:281:GLN:HA	1:B:281:GLN:HE21	1.76	0.50
1:B:179:LEU:N	1:B:180:PRO:HD2	2.26	0.50
1:A:246:PHE:CD2	1:B:27:GLY:HA2	2.47	0.50
1:B:201:LEU:HG	1:B:205:MET:HE3	1.94	0.50
1:B:157:GLY:N	1:B:158:GLU:CA	2.72	0.50
1:A:69:LYS:H	1:A:69:LYS:CD	2.24	0.49
1:B:238:PHE:HB3	1:B:266:VAL:HG12	1.95	0.48
1:B:29:VAL:HG13	1:B:241:VAL:HG12	1.94	0.48
1:A:292:TRP:NE1	1:A:296:LYS:HD2	2.29	0.48
1:B:281:GLN:O	1:B:282:GLU:CB	2.61	0.48
1:A:27:GLY:HA2	1:B:246:PHE:CD2	2.49	0.48
1:A:69:LYS:H	1:A:69:LYS:HD3	1.80	0.47
1:B:20:TRP:HB2	1:B:236:THR:HG23	1.95	0.47
1:B:347:ILE:C	1:B:349:GLU:H	2.23	0.47
1:A:254:ARG:NH2	1:A:258:GLU:OE1	2.48	0.47
1:B:77:VAL:HG22	1:B:80:MET:HG3	1.96	0.47
1:A:176:PHE:O	1:A:179:LEU:HB2	2.15	0.47
1:A:64:ASP:OD1	1:A:322:ARG:NH1	2.48	0.47
1:B:324:LEU:O	1:B:328:THR:CG2	2.58	0.46
1:B:345:LYS:O	1:B:349:GLU:HB3	2.16	0.45
1:A:222:ASN:O	1:A:226:ILE:HG12	2.16	0.45
1:A:56:THR:HG22	1:A:168:ALA:HB2	1.98	0.45
1:B:146:MET:HE2	1:B:149:ILE:HG13	1.99	0.45
1:B:10:HIS:HD2	1:B:335:ASN:ND2	2.03	0.45
1:B:278:GLU:OE1	1:B:292:TRP:HZ3	2.00	0.44
1:A:112:GLY:C	1:A:114:GLY:H	2.24	0.44
1:A:94:LEU:HD11	1:A:140:LEU:C	2.42	0.44
1:A:146:MET:CE	1:A:149:ILE:HD12	2.48	0.44
1:B:201:LEU:O	1:B:205:MET:HG2	2.18	0.44
1:B:6:GLU:O	1:B:310:HIS:HD2	2.01	0.44
1:A:72:LYS:HA	1:A:88:ILE:HG22	2.01	0.43
1:B:238:PHE:HB3	1:B:266:VAL:CG1	2.48	0.43
1:A:156:GLU:C	1:A:158:GLU:H	2.26	0.43
1:A:178:GLN:O	1:A:182:THR:HG23	2.19	0.43
1:B:43:ALA:O	1:B:82:ASN:ND2	2.51	0.42
1:A:189:LYS:HB3	1:A:190:PHE:HA	1.96	0.42
1:A:339:ASN:HA	1:A:340:PRO:HD2	1.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HD11	1:A:88:ILE:CD1	2.50	0.42
1:B:196:LYS:HE2	1:B:201:LEU:HD23	2.02	0.42
1:B:50:GLN:NE2	6:B:379:HOH:O	2.53	0.41
1:B:275:LEU:HD11	1:B:291:ARG:HD3	2.01	0.41
1:A:73:ASP:O	1:A:75:ARG:HD3	2.21	0.41
1:A:115:ASP:HA	1:A:116:ASP:HA	1.80	0.41
1:B:259:LEU:CD1	1:B:266:VAL:HG11	2.50	0.41
1:B:306:TYR:HB3	1:B:309:PHE:HB2	2.02	0.41
1:A:292:TRP:CE2	1:A:296:LYS:HD2	2.56	0.41
1:B:292:TRP:CH2	1:B:296:LYS:HD3	2.56	0.41
1:A:181:ASN:O	1:A:185:LYS:HG2	2.20	0.41
1:A:133:ILE:HA	1:A:134:PRO:HD2	1.95	0.40
1:A:211:ASP:O	1:A:215:LYS:HG2	2.21	0.40
1:A:320:GLU:CG	1:A:322:ARG:HG3	2.51	0.40
1:B:344:GLY:O	1:B:348:TYR:HD2	2.03	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	322/354 (91%)	297 (92%)	19 (6%)	6 (2%)	6	5
1	B	319/354 (90%)	303 (95%)	12 (4%)	4 (1%)	9	10
All	All	641/708 (90%)	600 (94%)	31 (5%)	10 (2%)	7	7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	282	GLU
1	B	283	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	113	GLN
1	A	280	ASP
1	B	282	GLU
1	B	285	CYS
1	B	212	ILE
1	A	285	CYS
1	A	321	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	286/309 (93%)	262 (92%)	24 (8%)	10	14
1	B	284/309 (92%)	259 (91%)	25 (9%)	9	12
All	All	570/618 (92%)	521 (91%)	49 (9%)	10	13

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	29	VAL
1	A	52	LEU
1	A	56	THR
1	A	69	LYS
1	A	77	VAL
1	A	88	ILE
1	A	115	ASP
1	A	120	LEU
1	A	143	MET
1	A	145	VAL
1	A	156	GLU
1	A	159	THR
1	A	177	LEU
1	A	182	THR
1	A	216	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	243	ILE
1	A	247	LEU
1	A	249	LEU
1	A	255	LEU
1	A	264	MET
1	A	312	VAL
1	A	328	THR
1	A	342	THR
1	B	12	LEU
1	B	29	VAL
1	B	32	THR
1	B	52	LEU
1	B	77	VAL
1	B	120	LEU
1	B	129	LEU
1	B	145	VAL
1	B	158	GLU
1	B	162	THR
1	B	164	ILE
1	B	183	LEU
1	B	218	GLU
1	B	255	LEU
1	B	264	MET
1	B	281	GLN
1	B	284	ASN
1	B	287	ARG
1	B	305	LEU
1	B	307	GLU
1	B	312	VAL
1	B	320	GLU
1	B	324	LEU
1	B	328	THR
1	B	351	GLU

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

Mol	Chain	Res	Type
1	A	18	HIS
1	A	60	HIS
1	A	148	HIS
1	A	172	HIS
1	A	257	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	10	HIS
1	B	18	HIS
1	B	41	GLN
1	B	46	GLN
1	B	50	GLN
1	B	122	GLN
1	B	148	HIS
1	B	154	GLN
1	B	202	ASN
1	B	217	ASN
1	B	281	GLN
1	B	284	ASN
1	B	301	GLN
1	B	310	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	326/354 (92%)	1.08	49 (15%) 5 6	39, 47, 68, 76	0
1	B	323/354 (91%)	1.79	109 (33%) 1 1	40, 49, 66, 70	0
All	All	649/708 (91%)	1.44	158 (24%) 2 2	39, 48, 67, 76	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	LEU	9.4
1	B	281	GLN	7.7
1	B	157	GLY	6.6
1	A	114	GLY	6.4
1	A	190	PHE	6.2
1	B	292	TRP	5.9
1	A	113	GLN	5.7
1	B	120	LEU	5.6
1	A	280	ASP	5.3
1	B	5	VAL	5.2
1	B	285	CYS	5.2
1	B	280	ASP	5.1
1	A	112	GLY	5.1
1	A	115	ASP	5.0
1	B	288	CYS	5.0
1	A	155	GLY	4.9
1	A	350	LEU	4.9
1	B	287	ARG	4.9
1	B	158	GLU	4.6
1	B	117	LEU	4.6
1	B	283	HIS	4.5
1	B	350	LEU	4.5
1	A	156	GLU	4.4
1	A	349	GLU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	91	SER	4.4
1	B	200	MET	4.3
1	B	291	ARG	4.3
1	A	157	GLY	4.2
1	B	317	CYS	4.1
1	A	281	GLN	4.1
1	B	155	GLY	4.0
1	B	92	ALA	4.0
1	B	348	TYR	3.8
1	A	283	HIS	3.8
1	A	348	TYR	3.7
1	B	351	GLU	3.7
1	B	127	ALA	3.7
1	B	206	GLY	3.6
1	B	199	PRO	3.6
1	B	302	ILE	3.6
1	A	158	GLU	3.6
1	B	298	TYR	3.5
1	B	201	LEU	3.5
1	B	316	LEU	3.5
1	A	117	LEU	3.5
1	B	276	PHE	3.5
1	B	346	VAL	3.5
1	B	293	LYS	3.4
1	A	108	ASN	3.4
1	B	349	GLU	3.4
1	B	156	GLU	3.4
1	B	154	GLN	3.4
1	B	187	LEU	3.4
1	B	81	ASN	3.4
1	B	284	ASN	3.4
1	B	121	LEU	3.3
1	B	342	THR	3.3
1	B	286	LYS	3.3
1	B	118	GLY	3.3
1	A	285	CYS	3.2
1	A	284	ASN	3.2
1	A	317	CYS	3.2
1	B	133	ILE	3.2
1	B	159	THR	3.2
1	B	328	THR	3.2
1	B	296	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	111	ASP	3.1
1	A	318	ALA	3.1
1	B	129	LEU	3.1
1	A	294	MET	3.1
1	A	279	ASN	3.1
1	B	275	LEU	3.1
1	A	154	GLN	3.1
1	B	135	GLY	3.1
1	B	190	PHE	3.0
1	B	347	ILE	3.0
1	A	286	LYS	3.0
1	B	196	LYS	3.0
1	B	9	LEU	3.0
1	A	250	TYR	2.9
1	B	204	PHE	2.9
1	B	126	LEU	2.9
1	B	320	GLU	2.9
1	A	320	GLU	2.8
1	B	338	TYR	2.8
1	B	290	ALA	2.8
1	B	243	ILE	2.8
1	B	297	LYS	2.8
1	B	322	ARG	2.8
1	B	277	ALA	2.7
1	B	312	VAL	2.7
1	B	183	LEU	2.7
1	A	5	VAL	2.7
1	B	216	LEU	2.7
1	A	116	ASP	2.7
1	B	301	GLN	2.6
1	B	311	VAL	2.6
1	B	306	TYR	2.6
1	A	223	VAL	2.6
1	B	130	THR	2.6
1	B	244	SER	2.6
1	A	159	THR	2.5
1	B	319	GLY	2.5
1	A	287	ARG	2.5
1	B	208	GLY	2.5
1	B	341	ILE	2.5
1	B	228	GLN	2.5
1	B	247	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	278	GLU	2.4
1	B	307	GLU	2.4
1	B	249	LEU	2.4
1	B	122	GLN	2.4
1	A	118	GLY	2.4
1	A	184	SER	2.4
1	B	82	ASN	2.4
1	B	128	ASP	2.4
1	B	279	ASN	2.4
1	B	203	SER	2.4
1	B	256	ILE	2.4
1	B	299	LEU	2.4
1	B	205	MET	2.3
1	A	347	ILE	2.3
1	B	184	SER	2.3
1	A	282	GLU	2.3
1	B	295	GLN	2.3
1	A	97	MET	2.3
1	B	153	GLU	2.3
1	A	69	LYS	2.3
1	B	274	LEU	2.3
1	A	128	ASP	2.3
1	A	119	SER	2.3
1	B	189	LYS	2.3
1	A	218	GLU	2.2
1	B	321	ILE	2.2
1	B	29	VAL	2.2
1	A	107	ASN	2.2
1	B	209	ASN	2.2
1	B	150	LYS	2.2
1	B	73	ASP	2.2
1	B	89	ASP	2.2
1	B	212	ILE	2.2
1	B	305	LEU	2.2
1	A	346	VAL	2.1
1	B	339	ASN	2.1
1	A	211	ASP	2.1
1	B	218	GLU	2.1
1	B	257	GLN	2.1
1	B	273	GLN	2.1
1	B	294	MET	2.1
1	A	120	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	277	ALA	2.1
1	B	255	LEU	2.1
1	B	202	ASN	2.1
1	B	250	TYR	2.1
1	B	282	GLU	2.0
1	B	335	ASN	2.0
1	A	243	ILE	2.0
1	B	19	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	B	357	1/1	0.86	0.19	67,67,67,67	0
4	NA	A	357	1/1	0.88	0.15	58,58,58,58	0
4	NA	A	359	1/1	0.89	0.22	53,53,53,53	0
5	CL	B	356	1/1	0.89	0.18	73,73,73,73	0
4	NA	A	358	1/1	0.89	0.13	46,46,46,46	0
3	MG	B	355	1/1	0.94	0.23	40,40,40,40	0
3	MG	A	356	1/1	0.96	0.22	30,30,30,30	0
2	ZN	A	355	1/1	0.98	0.10	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.