



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:09 AM UTC

PDB ID : 5FEI / pdb_00005fei
Title : Crystal structure of the bacteriophage phi29 tail knob protein gp9 truncation variant
Authors : Xu, J.W.; Gui, M.; Wang, D.H.; Xiang, Y.
Deposited on : 2015-12-17
Resolution : 2.60 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

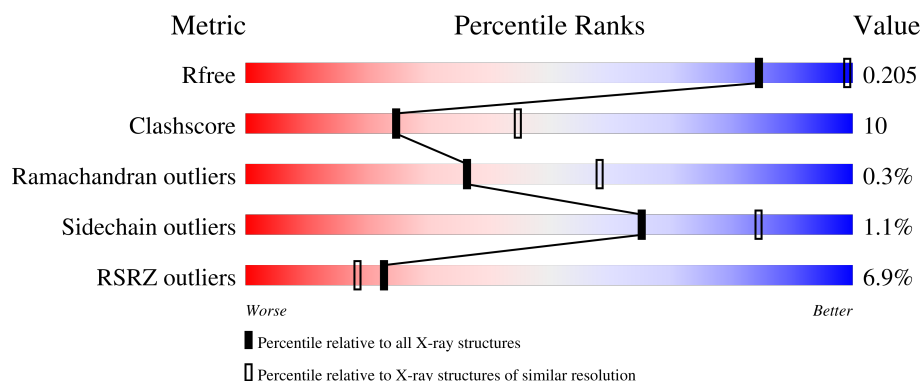
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	605	4% 70% 13% • 16%
1	B	605	7% 69% 14% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8628 atoms, of which 20 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 Distal tube protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			4122	2627	683	795	17			
1	B	512	Total	C	N	O	S	0	0	0
			4145	2640	688	799	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	SER	ARG	see sequence details	UNP P04331
A	121	ILE	MET	see sequence details	UNP P04331
A	600	HIS	-	expression tag	UNP P04331
A	601	HIS	-	expression tag	UNP P04331
A	602	HIS	-	expression tag	UNP P04331
A	603	HIS	-	expression tag	UNP P04331
A	604	HIS	-	expression tag	UNP P04331
A	605	HIS	-	expression tag	UNP P04331
B	41	SER	ARG	see sequence details	UNP P04331
B	121	ILE	MET	see sequence details	UNP P04331
B	600	HIS	-	expression tag	UNP P04331
B	601	HIS	-	expression tag	UNP P04331
B	602	HIS	-	expression tag	UNP P04331
B	603	HIS	-	expression tag	UNP P04331
B	604	HIS	-	expression tag	UNP P04331
B	605	HIS	-	expression tag	UNP P04331

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	A	1	Total	C	H	O	0	0
			17	4	10	3		

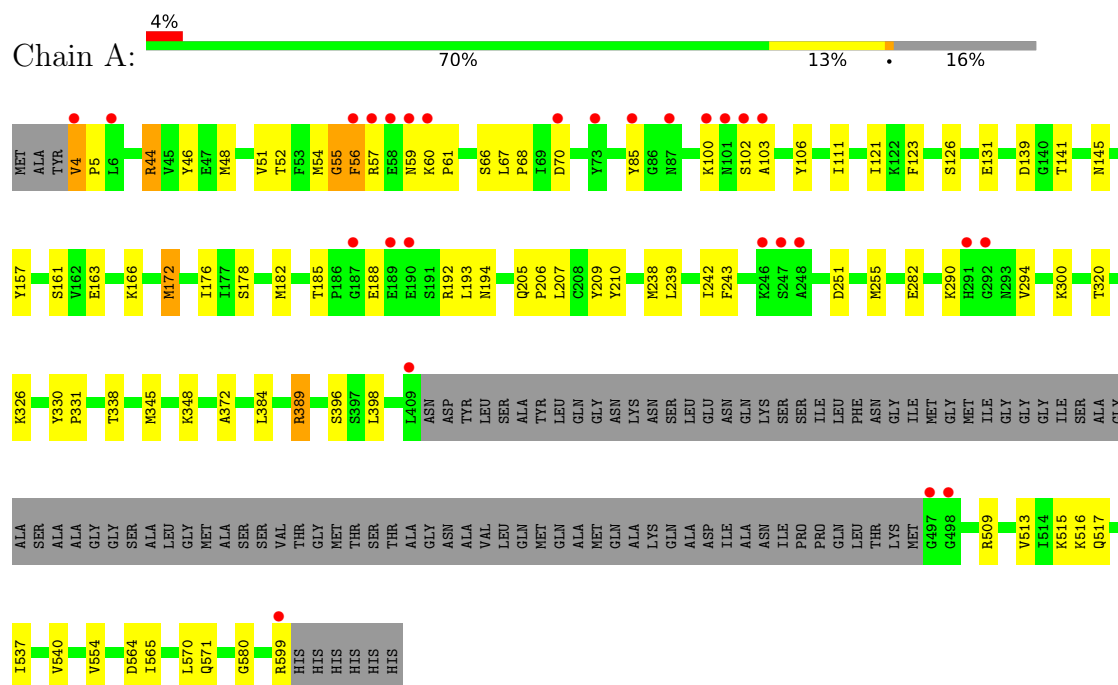
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	172	Total	O	0	0
			172	172		
3	B	155	Total	O	0	0
			155	155		

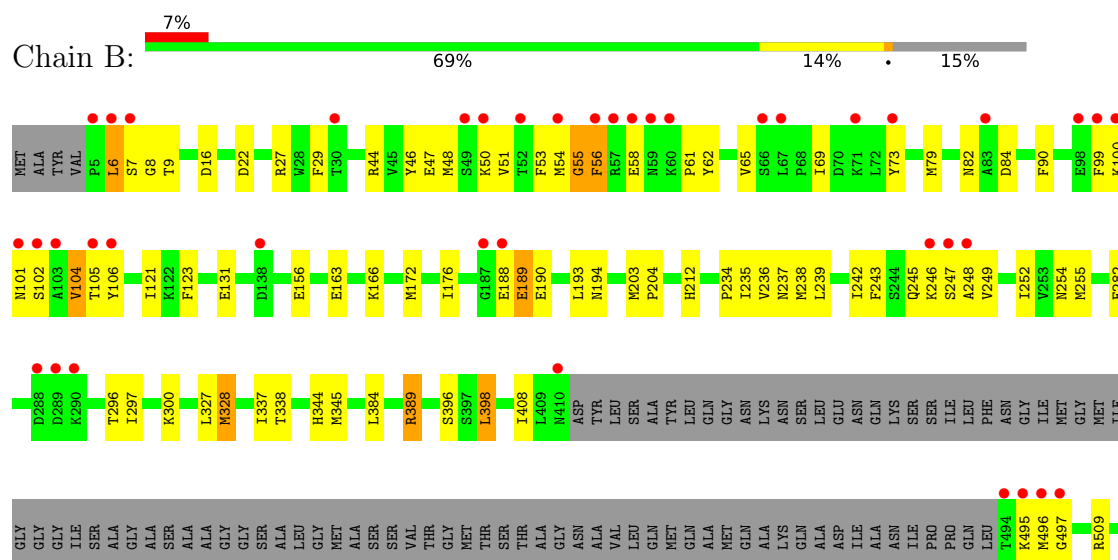
3 Residue-property plots [i](#)

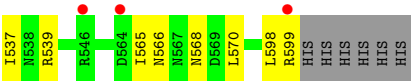
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Distal tube protein



• Molecule 1: Distal tube protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	184.67Å 184.67Å 184.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.35 – 2.60 49.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.35-2.60) 97.3 (49.35-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.85 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.166 , 0.201 0.173 , 0.205	Depositor DCC
R_{free} test set	3256 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8628	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: PEG

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	0.53	0/4218	0.86	5/5707 (0.1%)
1	B	0.51	0/4241	0.86	6/5735 (0.1%)
All	All	0.52	0/8459	0.86	11/11442 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	8	GLY	N-CA-C	6.57	120.73	111.14
1	A	4	VAL	CA-C-N	6.54	126.50	120.03
1	A	4	VAL	C-N-CA	6.54	126.50	120.03
1	B	55	GLY	N-CA-C	-6.29	106.40	115.27
1	B	166	LYS	CA-C-N	5.75	125.22	119.24
1	B	166	LYS	C-N-CA	5.75	125.22	119.24
1	A	166	LYS	CA-C-N	5.46	124.92	119.24
1	A	166	LYS	C-N-CA	5.46	124.92	119.24
1	A	290	LYS	N-CA-C	-5.36	106.05	113.18
1	B	16	ASP	CA-C-N	-5.01	119.19	122.60
1	B	16	ASP	C-N-CA	-5.01	119.19	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	GLY	Peptide

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	4122	0	3988	66	0
1	B	4145	0	4010	96	0
2	A	14	20	20	0	0
3	A	172	0	0	3	0
3	B	155	0	0	2	0
All	All	8608	20	8018	159	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 10.

All (159) 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:57:ARG:HD2	1:A:60:LYS:HE2	1.28	1.12
1:B:101:ASN:HB3	1:B:104:VAL:HG22	1.33	1.05
1:A:176:ILE:HG12	1:A:255:MET:HE2	1.47	0.97
1:B:176:ILE:HG12	1:B:255:MET:HE2	1.45	0.95
1:A:55:GLY:HA2	1:A:56:PHE:HB2	1.53	0.89
1:B:188:GLU:HA	1:B:189:GLU:CB	2.03	0.88
1:B:176:ILE:HD12	1:B:238:MET:HE1	1.57	0.85
1:B:6:LEU:HD21	1:B:82:ASN:HB2	1.58	0.85
1:A:57:ARG:CD	1:A:60:LYS:HE2	2.08	0.84
1:B:246:LYS:C	1:B:248:ALA:HA	2.02	0.83
1:B:188:GLU:HA	1:B:189:GLU:HB3	1.63	0.81
1:B:328:MET:HA	1:B:328:MET:HE2	1.62	0.80
1:B:254:ASN:HA	1:B:408:ILE:HD11	1.64	0.79
1:B:9:THR:HG22	1:B:50:LYS:HG3	1.69	0.75
1:B:246:LYS:O	1:B:248:ALA:HA	1.87	0.75
1:B:56:PHE:HB2	1:B:58:GLU:OE1	1.90	0.72
1:B:69:ILE:CA	1:B:105:THR:HG21	2.20	0.71
1:B:176:ILE:CG1	1:B:255:MET:HE2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ASN:CB	1:B:104:VAL:HG22	2.16	0.69
1:A:205:GLN:NE2	1:A:207:LEU:HB2	2.07	0.69
1:B:495:LYS:HA	3:B:701:HOH:O	1.91	0.69
1:A:54:MET:HB3	1:A:56:PHE:CE2	2.29	0.68
1:A:384:LEU:O	1:A:389:ARG:HD2	1.93	0.68
1:A:185:THR:HG22	1:A:188:GLU:HB3	1.75	0.68
1:A:176:ILE:CG1	1:A:255:MET:HE2	2.22	0.68
1:B:7:SER:HA	1:B:53:PHE:CD2	2.29	0.67
1:B:69:ILE:HB	1:B:105:THR:HG21	1.76	0.67
1:A:100:LYS:HD2	1:A:106:TYR:CZ	2.29	0.67
1:B:6:LEU:H	1:B:6:LEU:HD13	1.61	0.65
1:A:205:GLN:HE21	1:A:207:LEU:HB2	1.62	0.64
1:B:46:TYR:CD2	1:B:48:MET:HE2	2.32	0.64
1:B:188:GLU:HA	1:B:189:GLU:HB2	1.79	0.64
1:B:328:MET:HA	1:B:328:MET:CE	2.28	0.63
1:A:205:GLN:HG2	1:A:206:PRO:HD2	1.81	0.63
1:B:69:ILE:CB	1:B:105:THR:HG21	2.30	0.62
1:B:46:TYR:HD2	1:B:48:MET:HE2	1.63	0.62
1:A:571:GLN:HG2	1:B:22:ASP:OD2	2.00	0.61
1:B:495:LYS:HE3	1:B:497:GLY:H	1.65	0.60
1:A:57:ARG:HD2	1:A:60:LYS:CE	2.19	0.60
1:A:185:THR:CG2	1:A:188:GLU:HB3	2.31	0.60
1:A:55:GLY:CA	1:A:56:PHE:HB2	2.31	0.60
1:B:189:GLU:HG2	1:B:190:GLU:H	1.65	0.60
1:B:188:GLU:CA	1:B:189:GLU:CB	2.79	0.59
1:A:205:GLN:NE2	1:A:207:LEU:H	2.00	0.59
1:A:348:LYS:NZ	1:B:156:GLU:OE1	2.36	0.58
1:A:44:ARG:HD2	3:A:810:HOH:O	2.04	0.58
1:B:82:ASN:OD1	1:B:84:ASP:HB2	2.04	0.57
1:B:384:LEU:O	1:B:389:ARG:HD2	2.04	0.57
1:A:384:LEU:HD23	1:A:389:ARG:HG3	1.87	0.56
1:B:243:PHE:CZ	1:B:255:MET:HE1	2.40	0.56
1:B:55:GLY:HA3	1:B:61:PRO:HA	1.86	0.56
1:B:238:MET:HE2	1:B:242:ILE:HD11	1.88	0.56
1:B:238:MET:HE2	1:B:242:ILE:CD1	2.35	0.56
1:A:66:SER:O	1:A:67:LEU:HD23	2.06	0.55
1:A:131:GLU:HG2	1:A:537:ILE:HG13	1.89	0.55
1:B:188:GLU:CA	1:B:189:GLU:HB3	2.35	0.54
1:A:172:MET:HG2	1:A:509:ARG:NH1	2.23	0.54
1:A:68:PRO:HB2	1:A:70:ASP:OD1	2.08	0.53
1:B:566:ASN:OD1	1:B:568:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:MET:HG2	1:B:509:ARG:NH1	2.24	0.52
1:B:69:ILE:HA	1:B:105:THR:HG21	1.90	0.52
1:A:59:ASN:C	1:A:61:PRO:HD3	2.34	0.52
1:B:6:LEU:HD13	1:B:6:LEU:N	2.25	0.52
1:B:44:ARG:NH1	1:B:47:GLU:OE1	2.40	0.52
1:B:344:HIS:HA	1:B:398:LEU:HD11	1.91	0.51
1:B:537:ILE:HG22	1:B:539:ARG:HB2	1.92	0.51
1:B:54:MET:HB2	1:B:62:TYR:CZ	2.46	0.51
1:B:121:ILE:HG22	1:B:565:ILE:CD1	2.41	0.51
1:A:163:GLU:HG2	3:A:859:HOH:O	2.10	0.51
1:B:6:LEU:HD21	1:B:82:ASN:CB	2.34	0.51
1:B:495:LYS:HE3	1:B:497:GLY:N	2.27	0.50
1:B:384:LEU:HD23	1:B:389:ARG:HG3	1.94	0.50
1:A:205:GLN:NE2	1:A:209:TYR:HE1	2.08	0.50
1:A:345:MET:SD	1:A:396:SER:O	2.70	0.50
1:A:100:LYS:HD2	1:A:106:TYR:CE1	2.48	0.49
1:B:176:ILE:CD1	1:B:255:MET:HE2	2.43	0.49
1:A:121:ILE:HG22	1:A:565:ILE:HD11	1.95	0.49
1:A:565:ILE:HD12	1:A:570:LEU:HD13	1.94	0.48
1:B:46:TYR:CE2	1:B:65:VAL:HG13	2.48	0.48
1:A:121:ILE:HG22	1:A:565:ILE:CD1	2.43	0.48
1:B:27:ARG:HG2	1:B:29:PHE:CZ	2.49	0.48
1:B:131:GLU:HG2	1:B:537:ILE:HG13	1.96	0.48
1:A:239:LEU:O	1:A:242:ILE:HG22	2.13	0.48
1:A:55:GLY:HA2	1:A:56:PHE:CB	2.36	0.48
1:A:178:SER:HB2	1:A:251:ASP:HB3	1.96	0.48
1:A:4:VAL:HA	1:A:5:PRO:HD3	1.67	0.47
1:B:6:LEU:HD22	1:B:6:LEU:O	2.14	0.47
1:A:163:GLU:HG3	1:A:513:VAL:HB	1.95	0.47
1:B:495:LYS:HE3	1:B:497:GLY:CA	2.45	0.47
1:B:193:LEU:O	1:B:194:ASN:HB2	2.15	0.47
1:B:245:GLN:O	1:B:249:VAL:HG13	2.14	0.47
1:A:4:VAL:HG11	1:A:111:ILE:HG13	1.97	0.47
1:A:243:PHE:CZ	1:A:255:MET:HE1	2.50	0.47
1:A:205:GLN:HG2	1:A:206:PRO:CD	2.44	0.47
1:B:337:ILE:HG22	1:B:398:LEU:HD22	1.97	0.47
1:B:234:PRO:HG2	1:B:237:ASN:OD1	2.15	0.47
1:A:85:TYR:CE2	1:B:73:TYR:HD2	2.34	0.46
1:B:100:LYS:HD2	1:B:106:TYR:CE2	2.50	0.46
1:B:99:PHE:CE1	1:B:102:SER:HA	2.50	0.46
1:B:121:ILE:HG22	1:B:565:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LEU:HD23	1:B:327:LEU:HA	1.78	0.46
1:B:282:GLU:HB3	1:B:300:LYS:HD2	1.98	0.46
1:B:54:MET:HB2	1:B:62:TYR:CE1	2.51	0.46
1:B:6:LEU:HD22	1:B:6:LEU:C	2.41	0.46
1:B:212:HIS:HD2	1:B:296:THR:OG1	1.98	0.45
1:B:6:LEU:HD23	1:B:82:ASN:ND2	2.31	0.45
1:A:345:MET:HE2	1:A:398:LEU:CD1	2.46	0.45
1:B:345:MET:SD	1:B:396:SER:O	2.75	0.45
1:A:176:ILE:CD1	1:A:255:MET:HE2	2.46	0.45
1:B:598:LEU:O	1:B:599:ARG:HB3	2.17	0.44
1:B:69:ILE:HB	1:B:105:THR:CG2	2.47	0.44
1:B:247:SER:N	1:B:248:ALA:HA	2.32	0.44
1:A:330:TYR:CG	1:A:331:PRO:HA	2.52	0.44
1:A:599:ARG:NH2	1:A:599:ARG:HB2	2.33	0.44
1:B:338:THR:HA	1:B:398:LEU:HD21	1.99	0.44
1:B:495:LYS:HD2	1:B:496:MET:H	1.81	0.44
1:A:145:ASN:O	1:A:326:LYS:HE3	2.18	0.44
1:A:55:GLY:CA	1:A:56:PHE:CB	2.95	0.43
1:B:203:MET:HB2	1:B:204:PRO:HD2	1.99	0.43
1:B:47:GLU:O	1:B:48:MET:HG3	2.18	0.43
1:B:254:ASN:HA	1:B:408:ILE:CD1	2.43	0.43
1:B:565:ILE:HD12	1:B:570:LEU:HD13	2.01	0.43
1:A:126:SER:O	1:A:540:VAL:HA	2.18	0.43
1:A:282:GLU:HB3	1:A:300:LYS:HD2	2.01	0.43
1:B:243:PHE:CE2	1:B:255:MET:HE1	2.53	0.43
1:A:338:THR:HA	1:A:398:LEU:HD21	2.00	0.43
1:A:554:VAL:O	1:A:580:GLY:HA2	2.19	0.43
1:B:203:MET:HB2	1:B:204:PRO:CD	2.49	0.42
1:B:48:MET:HB3	1:B:51:VAL:CG1	2.49	0.42
1:A:193:LEU:O	1:A:194:ASN:HB2	2.19	0.42
1:A:157:TYR:HB3	1:A:516:LYS:HB3	2.01	0.42
1:B:345:MET:HE2	1:B:345:MET:HB3	1.75	0.42
1:A:102:SER:O	1:A:103:ALA:HB3	2.20	0.42
1:B:163:GLU:HG2	3:B:714:HOH:O	2.19	0.42
1:B:242:ILE:CG2	1:B:252:ILE:HD11	2.50	0.42
1:A:161:SER:HB3	1:A:515:LYS:HB2	2.01	0.41
1:A:372:ALA:HA	1:A:398:LEU:O	2.21	0.41
1:B:495:LYS:C	1:B:496:MET:HG3	2.45	0.41
1:B:48:MET:SD	1:B:51:VAL:HG11	2.60	0.41
1:A:51:VAL:HG22	1:A:52:THR:N	2.35	0.41
1:B:79:MET:HA	1:B:90:PHE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ILE:CD1	1:B:238:MET:HE1	2.40	0.41
1:B:235:ILE:HG23	1:B:236:VAL:N	2.35	0.41
1:A:139:ASP:OD1	1:A:141:THR:HG23	2.20	0.41
1:A:192:ARG:NH2	1:A:282:GLU:OE1	2.54	0.41
1:B:48:MET:CB	1:B:51:VAL:CG1	2.99	0.41
1:A:182:MET:HE2	1:A:210:TYR:CE1	2.55	0.41
1:A:238:MET:HG2	1:A:294:VAL:HG13	2.02	0.41
1:B:121:ILE:CG2	1:B:565:ILE:HD11	2.50	0.41
1:B:296:THR:OG1	1:B:297:ILE:N	2.53	0.40
1:A:46:TYR:HD2	1:A:48:MET:HE2	1.86	0.40
1:A:205:GLN:NE2	1:A:207:LEU:N	2.66	0.40
1:A:205:GLN:HG3	3:A:829:HOH:O	2.20	0.40
1:A:320:THR:HG23	1:A:517:GLN:OE1	2.21	0.40
1:A:564:ASP:C	1:A:565:ILE:HG13	2.47	0.40
1:B:6:LEU:N	1:B:6:LEU:CD1	2.85	0.40
1:B:243:PHE:CZ	1:B:255:MET:CE	3.05	0.40
1:B:255:MET:HB2	1:B:255:MET:HE3	1.82	0.40
1:B:239:LEU:HD23	1:B:239:LEU:HA	1.91	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	505/605 (84%)	484 (96%)	20 (4%)	1 (0%)	43	66
1	B	473/605 (78%)	459 (97%)	12 (2%)	2 (0%)	30	51
All	All	978/1210 (81%)	943 (96%)	32 (3%)	3 (0%)	36	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	56	PHE
1	B	189	GLU
1	A	56	PHE

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	458/528 (87%)	454 (99%)	4 (1%)	70	87
1	B	460/528 (87%)	454 (99%)	6 (1%)	61	82
All	All	918/1056 (87%)	908 (99%)	10 (1%)	65	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	123	PHE
1	A	172	MET
1	A	389	ARG
1	B	6	LEU
1	B	104	VAL
1	B	123	PHE
1	B	328	MET
1	B	389	ARG
1	B	398	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	205	GLN
1	B	212	HIS
1	B	293	ASN
1	B	567	ASN

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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEG	A	701	-	6,6,6	0.67	0	5,5,5	0.59	0
2	PEG	A	702	-	6,6,6	0.86	0	5,5,5	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	701	-	-	2/4/4/4	-
2	PEG	A	702	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	702	PEG	O1-C1-C2-O2
2	A	701	PEG	O1-C1-C2-O2
2	A	701	PEG	O2-C3-C4-O4
2	A	702	PEG	C1-C2-O2-C3

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	509/605 (84%)	-0.36	27 (5%) 32 26	19, 36, 92, 151	0
1	B	512/605 (84%)	-0.10	43 (8%) 17 13	20, 41, 108, 159	0
All	All	1021/1210 (84%)	-0.23	70 (6%) 23 18	19, 38, 103, 159	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	PRO	10.9
1	B	494	THR	8.5
1	A	85	TYR	6.4
1	A	497	GLY	6.1
1	B	7	SER	6.1
1	A	6	LEU	5.5
1	B	410	ASN	5.1
1	B	6	LEU	5.0
1	A	70	ASP	4.3
1	B	60	LYS	4.3
1	B	50	LYS	4.2
1	B	56	PHE	4.0
1	B	495	LYS	3.9
1	A	187	GLY	3.9
1	B	57	ARG	3.8
1	A	189	GLU	3.7
1	B	290	LYS	3.7
1	A	246	LYS	3.7
1	B	188	GLU	3.6
1	A	56	PHE	3.6
1	A	291	HIS	3.5
1	A	73	TYR	3.4
1	A	59	ASN	3.4
1	B	289	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	99	PHE	3.3
1	A	599	ARG	3.3
1	B	564	ASP	3.1
1	B	83	ALA	3.1
1	A	4	VAL	3.1
1	B	248	ALA	3.0
1	B	58	GLU	3.0
1	A	101	ASN	3.0
1	A	409	LEU	2.9
1	B	599	ARG	2.9
1	B	100	LYS	2.9
1	B	187	GLY	2.8
1	A	103	ALA	2.8
1	B	246	LYS	2.7
1	B	497	GLY	2.7
1	A	190	GLU	2.7
1	B	106	TYR	2.7
1	A	60	LYS	2.6
1	B	101	ASN	2.6
1	A	57	ARG	2.6
1	A	58	GLU	2.6
1	A	292	GLY	2.6
1	A	102	SER	2.5
1	B	103	ALA	2.5
1	B	247	SER	2.4
1	B	71	LYS	2.4
1	B	59	ASN	2.4
1	A	247	SER	2.4
1	B	98	GLU	2.4
1	A	248	ALA	2.4
1	B	73	TYR	2.3
1	B	496	MET	2.3
1	B	105	THR	2.3
1	B	52	THR	2.3
1	B	66	SER	2.3
1	A	498	GLY	2.2
1	A	87	ASN	2.2
1	B	288	ASP	2.2
1	B	49	SER	2.2
1	B	546	ARG	2.1
1	B	67	LEU	2.1
1	B	54	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	102	SER	2.1
1	A	100	LYS	2.1
1	B	30	THR	2.1
1	B	138	ASP	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
2	PEG	A	702	7/7	0.85	0.18	43,54,67,67	0
2	PEG	A	701	7/7	0.91	0.12	40,59,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.