



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:40 AM UTC

PDB ID : 7ESO / pdb_00007eso
Title : Structure and mutation analysis of the hexameric P4 from Pseudomonas aeruginosa phage phiYY
Authors : Zhang, C.Y.; Jin, T.C.
Deposited on : 2021-05-11
Resolution : 2.45 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

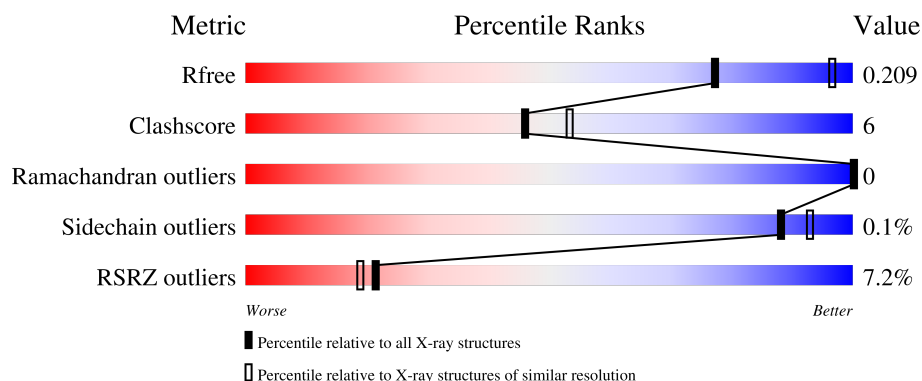
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	5% 64% 11% 25%
1	B	354	5% 62% 10% 27%
1	C	354	6% 67% 8% 25%
1	D	354	5% 64% 9% 27%
1	E	354	6% 66% 10% 25%

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Mol	Chain	Length	Quality of chain
1	F	354	 5% 66% 7% 22%
1	G	354	 4% 64% 8% 24%
1	H	354	 7% 61% 14% 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15697 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 Packaging NTPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			1964	1242	339	371	12			
1	B	257	Total	C	N	O	S	0	0	0
			1899	1201	325	361	12			
1	H	266	Total	C	N	O	S	0	0	0
			1964	1242	339	371	12			
1	G	257	Total	C	N	O	S	0	0	0
			1899	1201	325	361	12			
1	C	266	Total	C	N	O	S	0	0	0
			1964	1242	339	371	12			
1	D	257	Total	C	N	O	S	0	0	0
			1899	1201	325	361	12			
1	E	266	Total	C	N	O	S	0	0	0
			1964	1242	339	371	12			
1	F	257	Total	C	N	O	S	0	0	0
			1899	1201	325	361	12			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A1U9AK63
A	-2	SER	-	expression tag	UNP A0A1U9AK63
A	-1	VAL	-	expression tag	UNP A0A1U9AK63
A	0	ASP	-	expression tag	UNP A0A1U9AK63
B	-3	GLY	-	expression tag	UNP A0A1U9AK63
B	-2	SER	-	expression tag	UNP A0A1U9AK63
B	-1	VAL	-	expression tag	UNP A0A1U9AK63
B	0	ASP	-	expression tag	UNP A0A1U9AK63
H	-3	GLY	-	expression tag	UNP A0A1U9AK63
H	-2	SER	-	expression tag	UNP A0A1U9AK63
H	-1	VAL	-	expression tag	UNP A0A1U9AK63
H	0	ASP	-	expression tag	UNP A0A1U9AK63
G	-3	GLY	-	expression tag	UNP A0A1U9AK63

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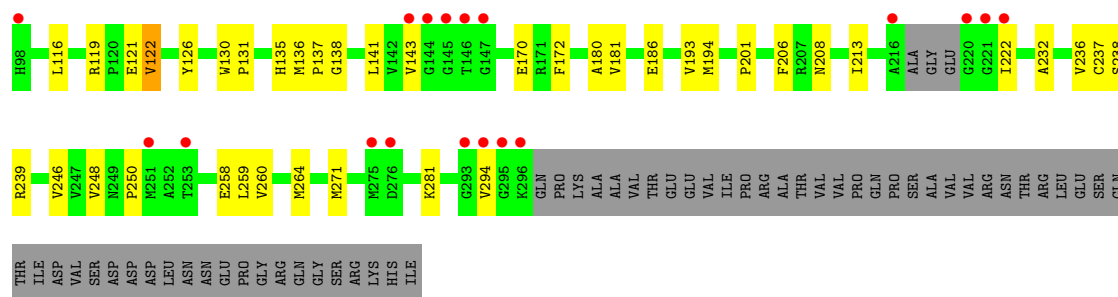
Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	SER	-	expression tag	UNP A0A1U9AK63
G	-1	VAL	-	expression tag	UNP A0A1U9AK63
G	0	ASP	-	expression tag	UNP A0A1U9AK63
C	-3	GLY	-	expression tag	UNP A0A1U9AK63
C	-2	SER	-	expression tag	UNP A0A1U9AK63
C	-1	VAL	-	expression tag	UNP A0A1U9AK63
C	0	ASP	-	expression tag	UNP A0A1U9AK63
D	-3	GLY	-	expression tag	UNP A0A1U9AK63
D	-2	SER	-	expression tag	UNP A0A1U9AK63
D	-1	VAL	-	expression tag	UNP A0A1U9AK63
D	0	ASP	-	expression tag	UNP A0A1U9AK63
E	-3	GLY	-	expression tag	UNP A0A1U9AK63
E	-2	SER	-	expression tag	UNP A0A1U9AK63
E	-1	VAL	-	expression tag	UNP A0A1U9AK63
E	0	ASP	-	expression tag	UNP A0A1U9AK63
F	-3	GLY	-	expression tag	UNP A0A1U9AK63
F	-2	SER	-	expression tag	UNP A0A1U9AK63
F	-1	VAL	-	expression tag	UNP A0A1U9AK63
F	0	ASP	-	expression tag	UNP A0A1U9AK63

- Molecule 2 is water.

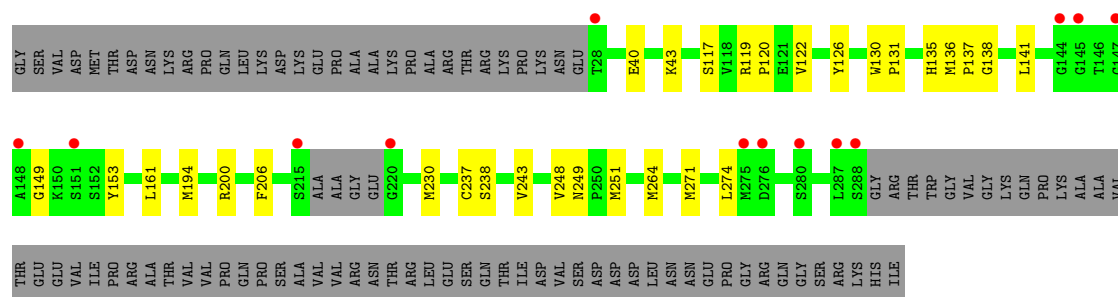
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	37	Total O 37 37	0	0
2	B	39	Total O 39 39	0	0
2	H	24	Total O 24 24	0	0
2	G	34	Total O 34 34	0	0
2	C	33	Total O 33 33	0	0
2	D	25	Total O 25 25	0	0
2	E	27	Total O 27 27	0	0
2	F	26	Total O 26 26	0	0

- Molecule 1: Packaging NTPase

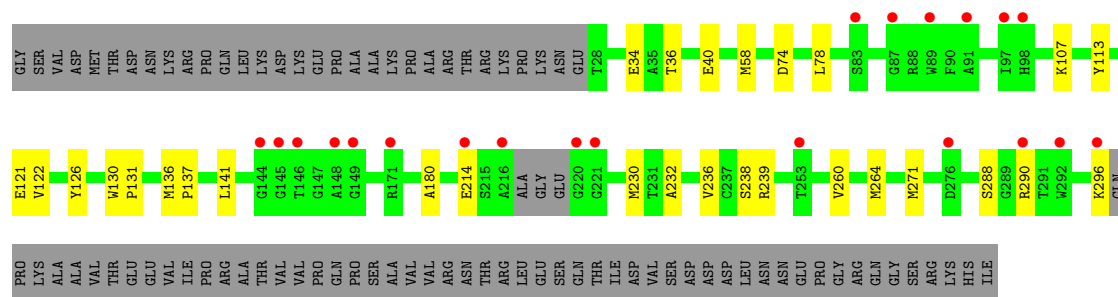




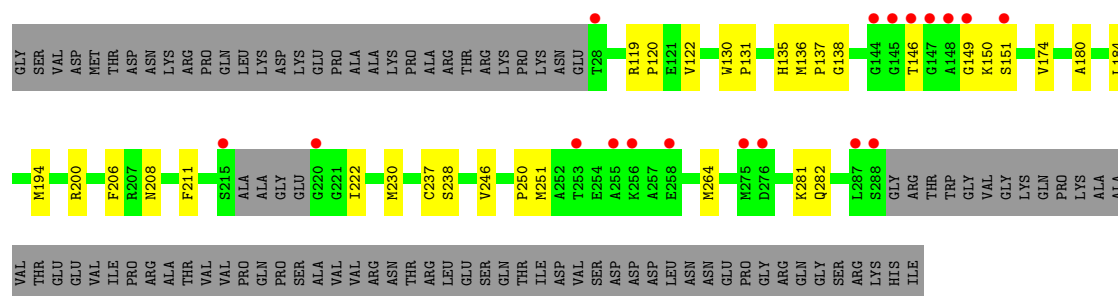
• Molecule 1: Packaging NTPase



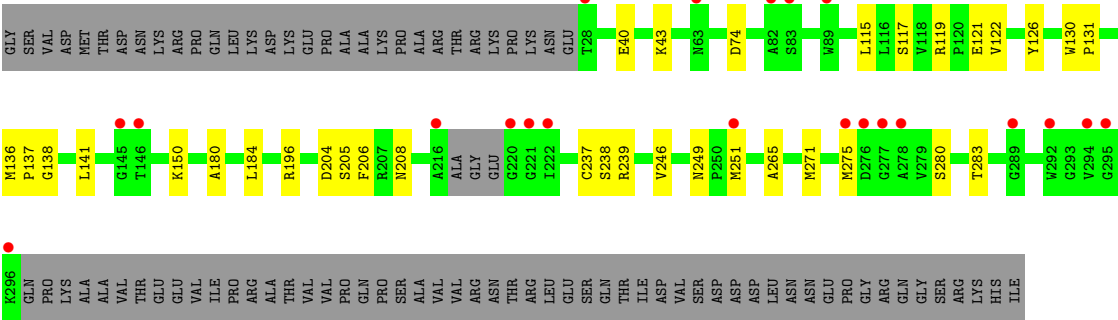
• Molecule 1: Packaging NTPase



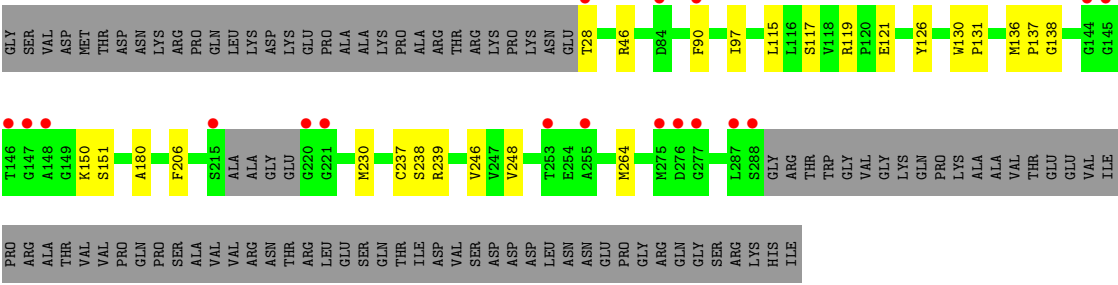
• Molecule 1: Packaging NTPase



• Molecule 1: Packaging NTPase



• Molecule 1: Packaging NTPase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	241.07Å 241.07Å 152.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.13 – 2.45 41.13 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (41.13-2.45) 96.0 (41.13-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.180 , 0.208 0.182 , 0.209	Depositor DCC
R_{free} test set	6080 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for $-1/3^*h+1/3^*k+4/3^*l, -k, 2/3^*h+1/3^*k+1/3^*l$ 0.008 for $-2/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+4/3^*l, -1/3^*h+1/3^*k+1/3^*l$ 0.008 for $-h, 1/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+1/3^*l$ 0.059 for $-1/3^*h-2/3^*k+4/3^*l, -2/3^*h-1/3^*k-4/3^*l, 1/3^*h-1/3^*k-1/3^*l$ 0.039 for $-h, 2/3^*h+1/3^*k+4/3^*l, 1/3^*h+2/3^*k-1/3^*l$ 0.023 for $1/3^*h+2/3^*k-4/3^*l, -k, -2/3^*h-1/3^*k-1/3^*l$ 0.018 for $h, -h-k, -l$	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15697	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 [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	0.24	0/2000	0.46	0/2724
1	B	0.34	1/1933 (0.1%)	0.54	0/2634
1	C	0.31	1/2000 (0.1%)	0.48	0/2724
1	D	0.25	0/1933	0.48	0/2634
1	E	0.25	0/2000	0.48	0/2724
1	F	0.28	0/1933	0.47	0/2634
1	G	0.27	0/1933	0.49	0/2634
1	H	0.29	1/2000 (0.1%)	0.48	0/2724
All	All	0.28	3/15732 (0.0%)	0.49	0/21432

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	290	ARG	C-O	-6.13	1.16	1.23
1	B	75	LYS	C-O	-5.54	1.17	1.24
1	H	122	VAL	CA-C	5.19	1.57	1.52

There are no bond angle outliers.

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	1964	0	1977	25	0
1	B	1899	0	1911	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1964	0	1977	23	0
1	D	1899	0	1911	27	0
1	E	1964	0	1977	24	0
1	F	1899	0	1911	18	0
1	G	1899	0	1911	20	0
1	H	1964	0	1977	36	0
2	A	37	0	0	0	0
2	B	39	0	0	0	0
2	C	33	0	0	1	0
2	D	25	0	0	0	0
2	E	27	0	0	0	0
2	F	26	0	0	0	0
2	G	34	0	0	1	0
2	H	24	0	0	0	0
All	All	15697	0	15552	179	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 6.

All (179) 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:D:230:MET:HE1	1:D:264:MET:HG2	1.55	0.87
1:H:181:VAL:HB	1:H:186:GLU:HG3	1.66	0.77
1:A:181:VAL:HB	1:A:186:GLU:HG3	1.65	0.77
1:F:230:MET:HE1	1:F:264:MET:HG2	1.73	0.71
1:B:137:PRO:HB2	1:B:238:SER:HA	1.74	0.69
1:B:248:VAL:HG11	1:B:264:MET:HE1	1.75	0.68
1:F:137:PRO:HB2	1:F:238:SER:HA	1.75	0.68
1:B:174:VAL:HG22	1:C:122:VAL:HG11	1.74	0.67
1:B:254:GLU:HA	1:B:257:ALA:HB2	1.75	0.67
1:C:264:MET:HB3	1:C:271:MET:HE1	1.75	0.67
1:H:206:PHE:HB2	1:H:248:VAL:HG22	1.76	0.67
1:E:275:MET:HB2	1:E:280:SER:HB2	1.75	0.67
1:H:119:ARG:NE	1:H:121:GLU:OE1	2.24	0.66
1:H:137:PRO:HB2	1:H:238:SER:HA	1.79	0.65
1:C:230:MET:HE1	1:C:264:MET:HG2	1.79	0.65
1:G:161:LEU:HD22	1:G:194:MET:HE2	1.77	0.65
1:C:264:MET:CB	1:C:271:MET:HE1	2.27	0.64
1:D:208:ASN:ND2	1:E:117:SER:HB2	2.13	0.64
1:A:137:PRO:HB2	1:A:238:SER:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:250:PRO:HG3	1:H:264:MET:HE1	1.80	0.64
1:H:281:LYS:HG3	1:H:294:VAL:HG22	1.81	0.63
1:A:171:ARG:HD3	1:B:288:SER:HB2	1.80	0.62
1:D:130:TRP:CE2	1:D:200:ARG:HD3	2.35	0.62
1:D:146:THR:HB	1:D:149:GLY:H	1.66	0.61
1:G:137:PRO:HB2	1:G:238:SER:HA	1.83	0.61
1:E:208:ASN:ND2	1:F:117:SER:HB2	2.17	0.59
1:F:136:MET:HE3	1:F:137:PRO:HD2	1.85	0.59
1:H:40:GLU:HA	1:H:43:LYS:HE2	1.84	0.59
1:H:260:VAL:HG12	1:H:264:MET:HE2	1.84	0.59
1:E:138:GLY:HA2	1:E:237:CYS:HB2	1.84	0.59
1:B:130:TRP:CD1	1:B:131:PRO:HA	2.39	0.58
1:G:130:TRP:CD1	1:G:131:PRO:HA	2.39	0.57
1:C:137:PRO:HB2	1:C:238:SER:HA	1.87	0.57
1:F:121:GLU:HB2	1:F:239:ARG:HG2	1.86	0.56
1:H:121:GLU:HB2	1:H:239:ARG:HG2	1.87	0.56
1:B:265:ALA:HB2	1:B:271:MET:HE2	1.87	0.56
1:D:281:LYS:HG3	1:D:282:GLN:N	2.21	0.55
1:H:61:VAL:HG12	1:H:213:ILE:HD11	1.87	0.55
1:H:250:PRO:HG3	1:H:264:MET:CE	2.37	0.55
1:F:206:PHE:HB2	1:F:248:VAL:HG22	1.89	0.55
1:D:130:TRP:CD1	1:D:131:PRO:HA	2.42	0.55
1:D:208:ASN:HD21	1:E:117:SER:HB2	1.72	0.54
1:A:230:MET:HE1	1:A:264:MET:HG2	1.89	0.54
1:E:208:ASN:HD21	1:F:117:SER:HB2	1.72	0.54
1:F:126:TYR:CE2	1:F:137:PRO:HD3	2.43	0.53
1:G:206:PHE:HB2	1:G:248:VAL:HG22	1.90	0.53
1:C:136:MET:HE3	1:C:137:PRO:HD2	1.91	0.53
1:F:130:TRP:CD1	1:F:131:PRO:HA	2.43	0.53
1:E:121:GLU:HB2	1:E:239:ARG:HG2	1.91	0.52
1:E:130:TRP:CD1	1:E:131:PRO:HA	2.44	0.52
1:G:230:MET:HE1	1:G:264:MET:HG2	1.90	0.52
1:B:122:VAL:HG21	1:B:136:MET:HE1	1.91	0.52
1:D:137:PRO:HB2	1:D:238:SER:HA	1.91	0.52
1:C:180:ALA:HB1	1:D:119:ARG:HB2	1.93	0.51
1:H:180:ALA:HB1	1:G:119:ARG:HB2	1.92	0.51
1:B:146:THR:HG23	1:B:149:GLY:H	1.76	0.51
1:B:206:PHE:HB2	1:B:248:VAL:HG22	1.93	0.51
1:B:145:GLY:N	1:B:274:LEU:O	2.44	0.51
1:B:260:VAL:O	1:B:264:MET:HG3	2.11	0.51
1:H:136:MET:HE3	1:H:137:PRO:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:HA	1:A:43:LYS:HE2	1.93	0.51
1:E:126:TYR:CE2	1:E:137:PRO:HD3	2.46	0.50
1:E:74:ASP:OD1	1:E:196:ARG:NH1	2.44	0.50
1:G:130:TRP:CE2	1:G:200:ARG:HD3	2.45	0.50
1:C:141:LEU:HD12	1:C:271:MET:HE3	1.93	0.50
1:D:250:PRO:HB3	1:D:264:MET:HE1	1.94	0.49
1:H:222:ILE:HD13	1:H:250:PRO:HB2	1.95	0.49
1:G:131:PRO:HD3	1:G:243:VAL:HG11	1.94	0.49
1:H:143:VAL:HG11	1:H:271:MET:HE3	1.95	0.49
1:H:264:MET:HE3	1:H:271:MET:HE1	1.94	0.49
1:G:149:GLY:HA3	2:G:405:HOH:O	2.12	0.49
1:F:90:PHE:CD1	1:F:97:ILE:HD13	2.47	0.49
1:A:214:GLU:OE2	1:B:215:SER:HB2	2.13	0.48
1:A:265:ALA:HB1	1:A:283:THR:HG21	1.95	0.48
1:A:85:ASP:HB3	1:A:88:ARG:HB3	1.94	0.48
1:G:122:VAL:HG21	1:G:136:MET:HE1	1.96	0.48
1:C:74:ASP:O	1:C:78:LEU:HD23	2.13	0.48
1:H:90:PHE:HZ	1:H:194:MET:HG3	1.79	0.48
1:C:214:GLU:N	1:C:214:GLU:OE1	2.47	0.48
1:H:85:ASP:HB3	1:H:88:ARG:HB3	1.96	0.48
1:H:138:GLY:HA2	1:H:237:CYS:HB2	1.94	0.48
1:C:122:VAL:HG23	1:C:137:PRO:HG3	1.96	0.48
1:A:141:LEU:HD22	1:A:248:VAL:HG21	1.95	0.48
1:A:265:ALA:HB2	1:A:271:MET:HE2	1.96	0.48
1:G:153:TYR:HB2	1:G:274:LEU:HD21	1.95	0.48
1:D:130:TRP:CD2	1:D:200:ARG:HD3	2.49	0.48
1:B:170:GLU:HG3	1:B:172:PHE:H	1.79	0.48
1:D:131:PRO:HD2	1:D:135:HIS:CD2	2.49	0.48
1:D:211:PHE:HZ	1:D:251:MET:HE3	1.78	0.47
1:A:209:LEU:HD11	1:A:213:ILE:HD11	1.95	0.47
1:G:138:GLY:HA2	1:G:237:CYS:HB2	1.96	0.47
1:A:120:PRO:HD2	1:F:180:ALA:HB1	1.95	0.47
1:A:121:GLU:HB2	1:A:239:ARG:HG2	1.96	0.47
1:H:122:VAL:HG21	1:H:136:MET:HE1	1.96	0.47
1:B:118:VAL:HG21	1:B:236:VAL:HG23	1.95	0.47
1:D:130:TRP:CG	1:D:131:PRO:HA	2.49	0.47
1:D:174:VAL:HG22	1:E:122:VAL:HG21	1.97	0.47
1:C:126:TYR:CE2	1:C:137:PRO:HD3	2.50	0.47
1:G:130:TRP:CG	1:G:131:PRO:HA	2.50	0.47
1:B:130:TRP:CG	1:B:131:PRO:HA	2.50	0.47
1:B:38:GLU:O	1:B:42:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:TRP:CD1	1:C:131:PRO:HA	2.50	0.46
1:C:296:LYS:N	2:C:402:HOH:O	2.47	0.46
1:C:58:MET:HE1	1:C:113:TYR:CD2	2.50	0.46
1:H:60:PRO:HG3	1:H:116:LEU:HG	1.98	0.46
1:H:232:ALA:O	1:H:236:VAL:HG23	2.15	0.46
1:G:141:LEU:HB2	1:G:271:MET:HG3	1.97	0.46
1:D:122:VAL:HG21	1:D:136:MET:HE1	1.97	0.46
1:D:184:LEU:HD22	1:E:115:LEU:HD12	1.97	0.46
1:A:290:ARG:HE	1:A:292:TRP:HZ2	1.64	0.46
1:H:258:GLU:HG3	1:H:259:LEU:N	2.31	0.45
1:E:136:MET:HE3	1:E:137:PRO:HD2	1.98	0.45
1:F:28:THR:HG23	1:F:46:ARG:HH11	1.81	0.45
1:G:40:GLU:HA	1:G:43:LYS:HE2	1.98	0.45
1:H:90:PHE:CZ	1:H:194:MET:HG3	2.51	0.45
1:H:194:MET:HE2	1:H:201:PRO:HB3	1.97	0.45
1:C:141:LEU:HD12	1:C:271:MET:CE	2.47	0.45
1:C:260:VAL:HG12	1:C:264:MET:HE2	1.98	0.45
1:E:40:GLU:HA	1:E:43:LYS:HE3	1.98	0.45
1:H:130:TRP:CD1	1:H:131:PRO:HA	2.52	0.45
1:C:121:GLU:HB2	1:C:239:ARG:HG2	1.98	0.45
1:A:261:TYR:O	1:A:271:MET:HE1	2.16	0.45
1:A:131:PRO:HD3	1:A:243:VAL:HG11	1.99	0.44
1:H:143:VAL:HG21	1:H:271:MET:HE2	1.99	0.44
1:A:126:TYR:CE2	1:A:137:PRO:HD3	2.52	0.44
1:A:138:GLY:HA2	1:A:237:CYS:HB2	1.98	0.44
1:C:264:MET:HB2	1:C:271:MET:HE1	1.98	0.44
1:C:34:GLU:OE1	1:C:107:LYS:HG2	2.18	0.44
1:F:130:TRP:CG	1:F:131:PRO:HA	2.52	0.44
1:H:88:ARG:O	1:H:92:GLU:HG2	2.18	0.44
1:A:130:TRP:CD1	1:A:131:PRO:HA	2.53	0.43
1:H:206:PHE:CD2	1:H:246:VAL:HG11	2.52	0.43
1:D:250:PRO:HB3	1:D:264:MET:CE	2.48	0.43
1:F:138:GLY:HA2	1:F:237:CYS:HB2	2.00	0.43
1:H:126:TYR:OH	1:H:135:HIS:O	2.36	0.43
1:E:141:LEU:HB2	1:E:271:MET:HG3	1.98	0.43
1:E:180:ALA:HB1	1:F:119:ARG:HB2	2.00	0.43
1:B:126:TYR:CE2	1:B:137:PRO:HD3	2.54	0.43
1:G:131:PRO:HD2	1:G:135:HIS:CD2	2.53	0.43
1:F:150:LYS:HD2	1:F:151:SER:N	2.33	0.43
1:A:206:PHE:CD2	1:A:246:VAL:HG11	2.54	0.43
1:H:170:GLU:HG3	1:H:172:PHE:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:LYS:HD2	1:D:151:SER:N	2.34	0.43
1:H:141:LEU:HB2	1:H:271:MET:HG3	2.01	0.43
1:B:171:ARG:HD3	1:C:288:SER:HA	2.00	0.42
1:D:146:THR:HB	1:D:149:GLY:N	2.34	0.42
1:G:126:TYR:CE2	1:G:137:PRO:HD3	2.53	0.42
1:H:208:ASN:ND2	1:G:117:SER:HB2	2.35	0.42
1:E:249:ASN:HD21	1:E:251:MET:HE3	1.84	0.42
1:F:206:PHE:CD2	1:F:246:VAL:HG11	2.54	0.42
1:A:284:VAL:HB	1:A:291:THR:OG1	2.19	0.42
1:G:249:ASN:CG	1:G:251:MET:HE2	2.45	0.42
1:D:194:MET:HE3	1:D:194:MET:HB3	1.79	0.42
1:E:184:LEU:HD22	1:F:115:LEU:HD12	2.02	0.42
1:D:180:ALA:HB1	1:E:119:ARG:HB2	2.01	0.42
1:E:206:PHE:CD2	1:E:246:VAL:HG11	2.55	0.42
1:B:265:ALA:HB2	1:B:271:MET:CE	2.50	0.42
1:C:232:ALA:O	1:C:236:VAL:HG23	2.20	0.42
1:E:137:PRO:HB2	1:E:238:SER:HA	2.01	0.41
1:E:265:ALA:HB1	1:E:283:THR:HG21	2.02	0.41
1:A:131:PRO:HD2	1:A:135:HIS:CD2	2.55	0.41
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.88	0.41
1:B:59:ILE:HG12	1:B:236:VAL:HG21	2.03	0.41
1:B:119:ARG:HA	1:B:120:PRO:HD3	1.89	0.41
1:E:204:ASP:OD1	1:E:205:SER:HB3	2.20	0.41
1:A:206:PHE:CD2	1:A:209:LEU:HD23	2.56	0.41
1:B:138:GLY:HA2	1:B:237:CYS:HB2	2.03	0.41
1:D:138:GLY:HA2	1:D:237:CYS:HB2	2.01	0.41
1:C:36:THR:HG22	1:C:40:GLU:OE1	2.21	0.41
1:D:200:ARG:HE	1:D:200:ARG:HB2	1.63	0.41
1:B:230:MET:HE3	1:B:230:MET:HB2	1.81	0.40
1:H:32:VAL:HG13	1:H:33:VAL:HG23	2.03	0.40
1:H:80:LEU:HD22	1:H:193:VAL:HG12	2.04	0.40
1:E:150:LYS:HB3	1:E:150:LYS:HE3	1.92	0.40
1:D:119:ARG:HA	1:D:120:PRO:HD3	1.95	0.40
1:D:222:ILE:HD11	1:D:250:PRO:O	2.21	0.40
1:A:66:LEU:HD11	1:A:184:LEU:HD23	2.04	0.40
1:H:180:ALA:HB1	1:G:120:PRO:HD2	2.03	0.40
1:D:206:PHE:CD2	1:D:246:VAL:HG11	2.56	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	262/354 (74%)	253 (97%)	9 (3%)	0	100	100
1	B	253/354 (72%)	246 (97%)	7 (3%)	0	100	100
1	C	262/354 (74%)	256 (98%)	6 (2%)	0	100	100
1	D	253/354 (72%)	247 (98%)	6 (2%)	0	100	100
1	E	262/354 (74%)	257 (98%)	5 (2%)	0	100	100
1	F	253/354 (72%)	250 (99%)	3 (1%)	0	100	100
1	G	253/354 (72%)	247 (98%)	6 (2%)	0	100	100
1	H	262/354 (74%)	255 (97%)	7 (3%)	0	100	100
All	All	2060/2832 (73%)	2011 (98%)	49 (2%)	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	205/281 (73%)	205 (100%)	0	100	100
1	B	200/281 (71%)	199 (100%)	1 (0%)	81	87
1	C	205/281 (73%)	205 (100%)	0	100	100
1	D	200/281 (71%)	200 (100%)	0	100	100
1	E	205/281 (73%)	205 (100%)	0	100	100
1	F	200/281 (71%)	200 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	200/281 (71%)	200 (100%)	0	100	100
1	H	205/281 (73%)	205 (100%)	0	100	100
All	All	1620/2248 (72%)	1619 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	75	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	GLN
1	G	133	GLN
1	D	93	ASN
1	D	262	ASN
1	D	263	ASN
1	D	282	GLN
1	F	133	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 [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	266/354 (75%)	0.09	18 (6%)	23	21	38, 52, 88, 103	0
1	B	257/354 (72%)	0.04	16 (6%)	26	24	35, 50, 87, 105	0
1	C	266/354 (75%)	0.19	21 (7%)	18	16	37, 53, 94, 109	0
1	D	257/354 (72%)	0.16	18 (7%)	22	20	40, 54, 94, 107	0
1	E	266/354 (75%)	0.24	21 (7%)	18	16	41, 59, 95, 110	0
1	F	257/354 (72%)	0.08	18 (7%)	22	20	39, 52, 90, 108	0
1	G	257/354 (72%)	0.02	13 (5%)	33	31	38, 53, 92, 109	0
1	H	266/354 (75%)	0.36	25 (9%)	14	11	40, 57, 95, 113	0
All	All	2092/2832 (73%)	0.15	150 (7%)	21	19	35, 54, 93, 113	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	220	GLY	7.5
1	G	220	GLY	6.7
1	A	220	GLY	6.4
1	E	292	TRP	6.3
1	B	220	GLY	6.3
1	E	220	GLY	6.1
1	D	220	GLY	6.1
1	E	294	VAL	5.8
1	F	145	GLY	5.7
1	F	220	GLY	5.6
1	C	220	GLY	5.0
1	D	144	GLY	4.9
1	D	288	SER	4.8
1	F	144	GLY	4.7
1	E	216	ALA	4.7
1	G	288	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	216	ALA	4.4
1	D	148	ALA	4.3
1	A	216	ALA	4.2
1	B	288	SER	4.0
1	C	221	GLY	4.0
1	E	296	LYS	4.0
1	H	145	GLY	4.0
1	D	287	LEU	3.9
1	D	145	GLY	3.9
1	F	288	SER	3.8
1	D	147	GLY	3.7
1	B	276	ASP	3.7
1	D	146	THR	3.6
1	D	275	MET	3.5
1	B	149	GLY	3.5
1	G	148	ALA	3.5
1	G	145	GLY	3.4
1	C	296	LYS	3.4
1	E	251	MET	3.4
1	A	144	GLY	3.3
1	B	146	THR	3.3
1	H	221	GLY	3.3
1	B	28	THR	3.3
1	G	215	SER	3.2
1	E	275	MET	3.2
1	H	216	ALA	3.2
1	F	287	LEU	3.2
1	F	147	GLY	3.2
1	C	292	TRP	3.1
1	B	275	MET	3.1
1	G	276	ASP	3.1
1	F	276	ASP	3.1
1	A	296	LYS	3.1
1	H	296	LYS	3.1
1	C	145	GLY	3.1
1	F	275	MET	3.0
1	D	215	SER	3.0
1	H	144	GLY	3.0
1	C	149	GLY	3.0
1	A	91	ALA	3.0
1	H	82	ALA	2.9
1	H	28	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	144	GLY	2.9
1	E	221	GLY	2.9
1	H	87	GLY	2.9
1	D	253	THR	2.9
1	F	146	THR	2.8
1	H	146	THR	2.8
1	H	98	HIS	2.8
1	A	276	ASP	2.8
1	A	145	GLY	2.7
1	B	145	GLY	2.7
1	E	295	GLY	2.7
1	D	149	GLY	2.7
1	A	292	TRP	2.7
1	C	171	ARG	2.7
1	E	222	ILE	2.6
1	G	287	LEU	2.6
1	E	28	THR	2.6
1	F	28	THR	2.6
1	E	145	GLY	2.6
1	E	277	GLY	2.6
1	B	215	SER	2.6
1	H	253	THR	2.6
1	E	82	ALA	2.6
1	H	295	GLY	2.6
1	A	146	THR	2.6
1	F	148	ALA	2.6
1	F	253	THR	2.6
1	A	147	GLY	2.6
1	E	276	ASP	2.6
1	F	221	GLY	2.6
1	A	82	ALA	2.6
1	D	28	THR	2.6
1	B	287	LEU	2.5
1	G	280	SER	2.5
1	G	275	MET	2.5
1	A	253	THR	2.5
1	C	83	SER	2.5
1	E	89	TRP	2.5
1	H	275	MET	2.5
1	B	90	PHE	2.4
1	D	258	GLU	2.4
1	A	251	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	78	LEU	2.4
1	H	251	MET	2.4
1	C	148	ALA	2.4
1	F	255	ALA	2.4
1	A	149	GLY	2.4
1	F	90	PHE	2.4
1	A	148	ALA	2.3
1	E	63	ASN	2.3
1	A	222	ILE	2.3
1	H	222	ILE	2.3
1	A	84	ASP	2.3
1	C	214	GLU	2.3
1	G	28	THR	2.3
1	B	147	GLY	2.3
1	H	294	VAL	2.3
1	C	146	THR	2.2
1	C	97	ILE	2.2
1	H	143	VAL	2.2
1	E	278	ALA	2.2
1	B	256	LYS	2.2
1	F	215	SER	2.2
1	B	279	VAL	2.2
1	A	28	THR	2.2
1	C	253	THR	2.2
1	G	147	GLY	2.2
1	C	144	GLY	2.2
1	E	289	GLY	2.2
1	G	151	SER	2.2
1	B	255	ALA	2.2
1	C	91	ALA	2.2
1	H	293	GLY	2.2
1	D	151	SER	2.2
1	H	91	ALA	2.1
1	C	98	HIS	2.1
1	D	255	ALA	2.1
1	C	87	GLY	2.1
1	C	89	TRP	2.1
1	H	147	GLY	2.1
1	C	290	ARG	2.1
1	H	276	ASP	2.1
1	F	84	ASP	2.1
1	D	256	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	144	GLY	2.1
1	F	277	GLY	2.1
1	C	276	ASP	2.1
1	E	83	SER	2.1
1	H	94	GLU	2.0
1	H	90	PHE	2.0
1	E	146	THR	2.0
1	D	276	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.