



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:55 AM UTC

PDB ID : 4HUD / pdb_00004hud
Title : Structure of the bacteriophage T4 tail terminator protein, gp15.
Authors : Fokine, A.; Zhang, Z.; Kanamaru, S.; Bowman, V.D.; Aksyuk, A.; Arisaka, F.;
Rao, V.B.; Rossmann, M.G.
Deposited on : 2012-11-02
Resolution : 2.70 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

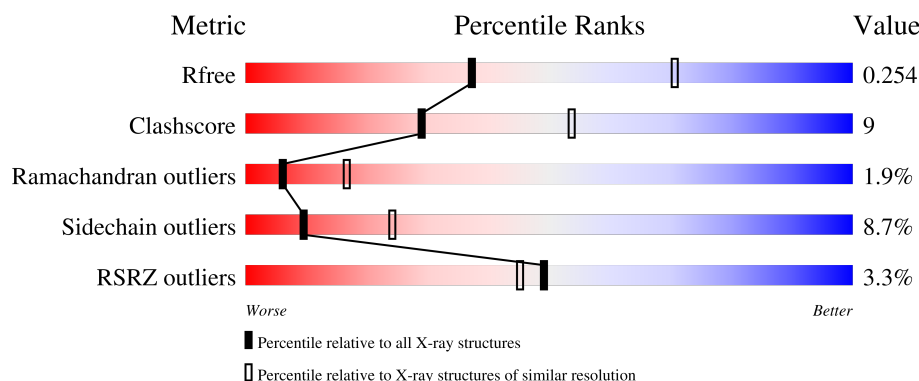
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



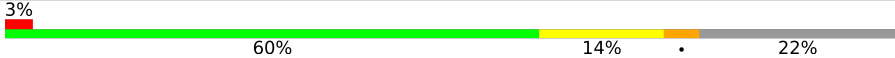
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	272	57% 16% • 22%
1	B	272	59% 14% • 22%
1	C	272	3% 56% 18% • 22%
1	D	272	4% 60% 13% • 22%
1	E	272	3% 58% 14% 5% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	272	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: red (3%), green (60%), yellow (14%), and grey (22%). The segments are labeled with their respective percentages: 3%, 60%, 14%, and 22%. A small black dot is located on the yellow segment.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10524 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 Tail connector protein Gp15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1742	1123	283	328	8			
1	B	211	Total	C	N	O	S	0	0	0
			1742	1123	283	328	8			
1	C	211	Total	C	N	O	S	0	0	0
			1742	1123	283	328	8			
1	D	211	Total	C	N	O	S	0	0	0
			1742	1123	283	328	8			
1	E	211	Total	C	N	O	S	0	0	0
			1742	1123	283	328	8			
1	F	211	Total	C	N	O	S	0	0	0
			1742	1123	283	328	8			

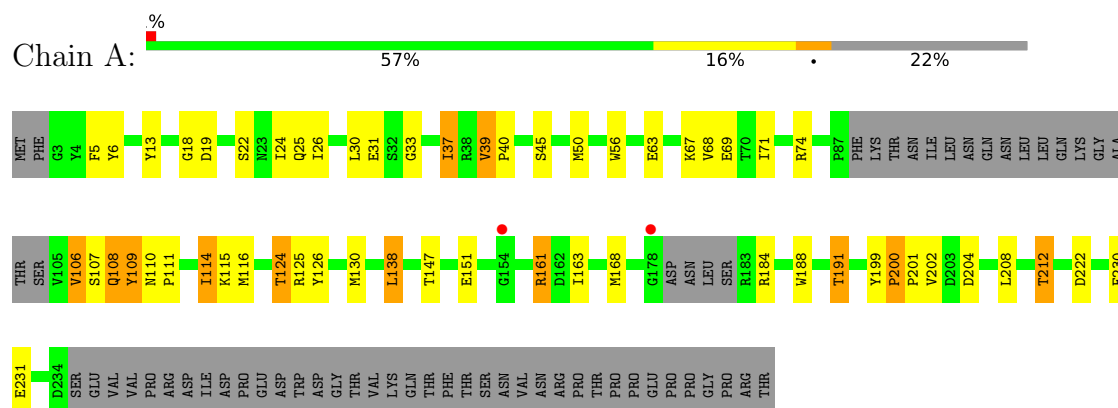
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	8	Total	O	0	0
			8	8		
2	C	8	Total	O	0	0
			8	8		
2	D	12	Total	O	0	0
			12	12		
2	E	14	Total	O	0	0
			14	14		
2	F	18	Total	O	0	0
			18	18		

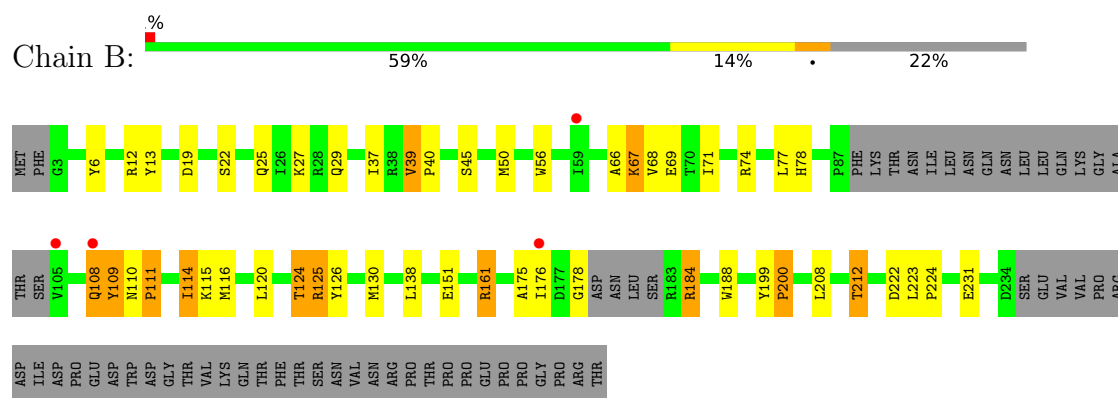
3 Residue-property plots [i](#)

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.

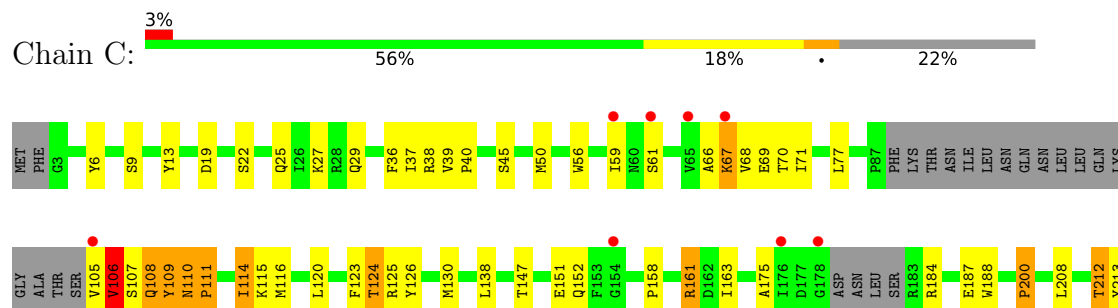
• Molecule 1: Tail connector protein Gp15

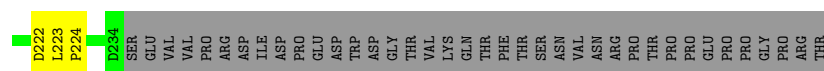


• Molecule 1: Tail connector protein Gp15

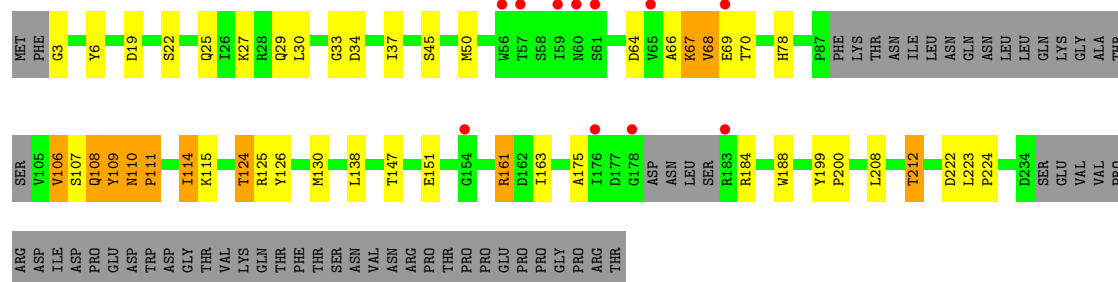


• Molecule 1: Tail connector protein Gp15

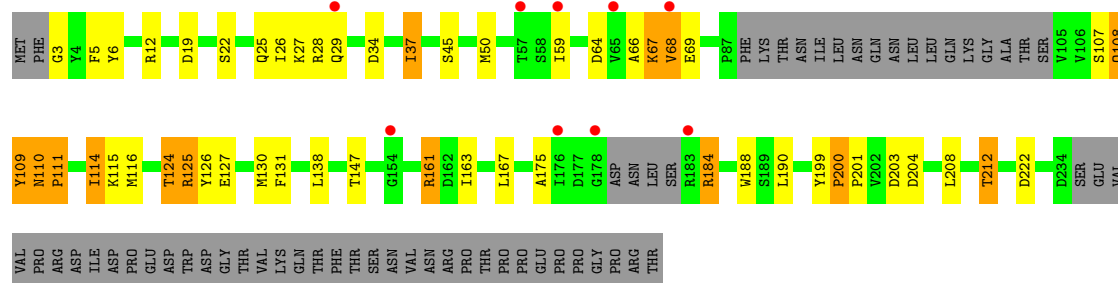




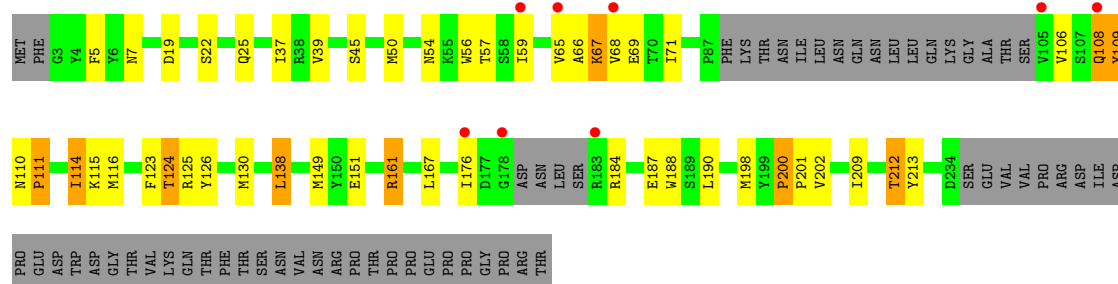
• Molecule 1: Tail connector protein Gp15



• Molecule 1: Tail connector protein Gp15



• Molecule 1: Tail connector protein Gp15



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	100.68Å 100.68Å 155.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.96 – 2.70 32.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (32.96-2.70) 93.5 (32.96-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.207 , 0.252 0.210 , 0.254	Depositor DCC
R_{free} test set	2554 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	1.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.127 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10524	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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 30.38 % 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 1.3202e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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	0.60	1/1787 (0.1%)	0.97	3/2421 (0.1%)
1	B	0.61	1/1787 (0.1%)	0.97	4/2421 (0.2%)
1	C	0.60	1/1787 (0.1%)	0.99	4/2421 (0.2%)
1	D	0.61	0/1787	0.94	1/2421 (0.0%)
1	E	0.63	1/1787 (0.1%)	0.95	1/2421 (0.0%)
1	F	0.63	1/1787 (0.1%)	1.02	5/2421 (0.2%)
All	All	0.61	5/10722 (0.0%)	0.97	18/14526 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	200	PRO	CA-C	6.84	1.55	1.51
1	B	200	PRO	CA-C	6.20	1.55	1.51
1	F	200	PRO	CA-C	5.50	1.54	1.51
1	A	200	PRO	CA-C	5.41	1.54	1.51
1	C	200	PRO	CA-C	5.37	1.54	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	39	VAL	CA-C-N	10.63	130.39	119.76
1	F	39	VAL	C-N-CA	10.63	130.39	119.76
1	C	39	VAL	CA-C-N	8.43	128.19	119.76
1	C	39	VAL	C-N-CA	8.43	128.19	119.76
1	C	61	SER	N-CA-C	7.74	118.20	108.45
1	A	39	VAL	CA-C-N	7.02	126.78	119.76
1	A	39	VAL	C-N-CA	7.02	126.78	119.76
1	F	138	LEU	CA-C-N	-6.01	113.49	119.56
1	F	138	LEU	C-N-CA	-6.01	113.49	119.56
1	D	70	THR	N-CA-C	-5.93	106.20	113.50
1	B	39	VAL	CA-C-N	5.84	125.60	119.76
1	B	39	VAL	C-N-CA	5.84	125.60	119.76
1	C	70	THR	N-CA-C	-5.52	106.71	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	LEU	N-CA-C	5.49	121.95	109.81
1	F	65	VAL	N-CA-C	5.38	116.01	110.36
1	E	29	GLN	N-CA-C	5.36	117.47	109.59
1	B	200	PRO	CA-C-N	5.13	125.04	119.76
1	B	200	PRO	C-N-CA	5.13	125.04	119.76

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	1742	0	1673	32	0
1	B	1742	0	1673	31	0
1	C	1742	0	1673	29	0
1	D	1742	0	1673	27	0
1	E	1742	0	1673	33	0
1	F	1742	0	1673	28	0
2	A	12	0	0	1	0
2	B	8	0	0	1	0
2	C	8	0	0	0	0
2	D	12	0	0	0	0
2	E	14	0	0	0	0
2	F	18	0	0	0	0
All	All	10524	0	10038	178	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 (178) 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:109:TYR:HB3	1:D:161:ARG:HH22	1.39	0.87
1:C:109:TYR:HB3	1:C:161:ARG:HH22	1.41	0.86
1:B:109:TYR:HB3	1:B:161:ARG:HH22	1.44	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:TYR:HB3	1:A:161:ARG:HH22	1.44	0.82
1:F:108:GLN:HB3	1:F:200:PRO:HD2	1.70	0.72
1:E:69:GLU:OE2	1:E:126:TYR:OH	2.09	0.69
1:F:124:THR:HG21	1:F:130:MET:HG2	1.73	0.69
1:B:108:GLN:HB3	1:B:200:PRO:HD2	1.75	0.68
1:F:109:TYR:HB3	1:F:161:ARG:HH22	1.59	0.68
1:D:124:THR:HG21	1:D:130:MET:HG2	1.75	0.67
1:A:124:THR:HG21	1:A:130:MET:HG2	1.77	0.67
1:F:19:ASP:HA	1:F:22:SER:HB2	1.77	0.67
1:A:108:GLN:HB3	1:A:200:PRO:HD2	1.80	0.62
1:E:108:GLN:HB3	1:E:200:PRO:HD2	1.81	0.62
1:E:66:ALA:O	1:E:68:VAL:N	2.32	0.62
1:E:130:MET:HE2	1:E:188:TRP:CD2	2.35	0.61
1:D:130:MET:HE2	1:D:188:TRP:CD2	2.36	0.61
1:C:69:GLU:OE2	1:C:126:TYR:OH	2.13	0.61
1:E:124:THR:HG21	1:E:130:MET:HG2	1.81	0.61
1:B:124:THR:HG21	1:B:130:MET:HG2	1.83	0.60
1:D:108:GLN:HB3	1:D:200:PRO:HD2	1.83	0.60
1:E:125:ARG:HH21	1:E:184:ARG:HG2	1.68	0.59
1:F:66:ALA:O	1:F:68:VAL:N	2.32	0.59
1:D:69:GLU:OE2	1:D:126:TYR:OH	2.12	0.58
1:B:69:GLU:OE2	1:B:126:TYR:OH	2.18	0.58
1:E:109:TYR:HB3	1:E:161:ARG:HH22	1.69	0.58
1:F:69:GLU:OE2	1:F:126:TYR:OH	2.11	0.58
1:B:151:GLU:OE2	1:B:161:ARG:NH1	2.33	0.57
1:F:19:ASP:OD2	1:F:213:TYR:OH	2.22	0.57
1:C:130:MET:HE2	1:C:188:TRP:CD2	2.40	0.57
1:C:114:ILE:HG12	1:C:115:LYS:N	2.17	0.57
1:F:114:ILE:HG12	1:F:115:LYS:H	1.68	0.57
1:A:151:GLU:OE2	1:A:161:ARG:NH1	2.30	0.57
1:C:151:GLU:OE2	1:C:161:ARG:NH1	2.37	0.57
1:E:124:THR:HG23	1:E:126:TYR:H	1.70	0.57
1:F:114:ILE:HG12	1:F:115:LYS:N	2.20	0.56
1:F:66:ALA:C	1:F:68:VAL:H	2.13	0.56
1:F:130:MET:HE2	1:F:188:TRP:CD2	2.41	0.56
1:E:66:ALA:C	1:E:68:VAL:H	2.13	0.56
1:A:109:TYR:HB3	1:A:161:ARG:NH2	2.18	0.56
1:C:114:ILE:HG12	1:C:115:LYS:H	1.71	0.55
1:B:130:MET:HE2	1:B:188:TRP:CD2	2.41	0.55
1:E:19:ASP:HA	1:E:22:SER:HB2	1.89	0.55
1:D:124:THR:HG23	1:D:126:TYR:H	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ALA:O	1:B:68:VAL:N	2.38	0.55
1:C:109:TYR:HB3	1:C:161:ARG:NH2	2.18	0.55
1:D:114:ILE:HG12	1:D:115:LYS:H	1.71	0.55
1:A:6:TYR:CD2	1:A:208:LEU:HG	2.42	0.54
1:F:124:THR:CG2	1:F:130:MET:HG2	2.37	0.54
1:B:109:TYR:HB3	1:B:161:ARG:NH2	2.20	0.54
1:B:125:ARG:HH21	1:B:184:ARG:HG2	1.73	0.53
1:A:6:TYR:N	1:A:204:ASP:OD2	2.38	0.53
1:A:130:MET:HE2	1:A:188:TRP:CD2	2.44	0.53
1:D:124:THR:CG2	1:D:130:MET:HG2	2.39	0.53
1:A:56:TRP:HB3	1:A:71:ILE:HD13	1.91	0.52
1:B:19:ASP:HA	1:B:22:SER:HB2	1.90	0.52
1:F:124:THR:HG23	1:F:126:TYR:H	1.73	0.52
1:A:106:VAL:HG12	1:A:107:SER:H	1.74	0.52
1:F:5:PHE:CE2	1:F:201:PRO:HB3	2.45	0.52
1:A:212:THR:HA	1:A:222:ASP:HA	1.91	0.52
1:E:26:ILE:HD11	1:E:37:ILE:HD11	1.92	0.52
1:D:223:LEU:HD12	1:D:224:PRO:HD2	1.92	0.51
1:B:74:ARG:NH2	1:B:231:GLU:OE2	2.43	0.51
1:A:124:THR:CG2	1:A:130:MET:HG2	2.40	0.51
1:C:108:GLN:HB3	1:C:200:PRO:HD2	1.91	0.51
1:E:124:THR:CG2	1:E:130:MET:HG2	2.41	0.51
1:B:27:LYS:HE2	1:B:29:GLN:HG2	1.91	0.51
1:A:147:THR:HG23	1:A:163:ILE:HB	1.93	0.50
1:B:66:ALA:C	1:B:68:VAL:H	2.20	0.50
1:C:19:ASP:HA	1:C:22:SER:HB2	1.93	0.50
1:B:77:LEU:HD13	1:B:120:LEU:HD23	1.93	0.50
1:E:12:ARG:NH2	1:E:199:TYR:OH	2.45	0.49
1:B:212:THR:HA	1:B:222:ASP:HA	1.95	0.49
1:A:124:THR:HG23	1:A:126:TYR:H	1.77	0.49
1:C:66:ALA:O	1:C:68:VAL:N	2.45	0.49
1:C:147:THR:HG23	1:C:163:ILE:HB	1.93	0.49
1:D:147:THR:HG23	1:D:163:ILE:HB	1.94	0.49
1:E:114:ILE:HG12	1:E:115:LYS:H	1.76	0.49
1:B:6:TYR:CD2	1:B:208:LEU:HG	2.48	0.48
1:D:66:ALA:O	1:D:68:VAL:N	2.45	0.48
1:E:167:LEU:HD11	1:E:190:LEU:HD12	1.95	0.48
1:A:114:ILE:HG12	1:A:115:LYS:N	2.29	0.48
1:C:124:THR:HG21	1:C:130:MET:HG2	1.95	0.48
1:C:110:ASN:HA	1:C:111:PRO:HD3	1.71	0.48
1:D:110:ASN:HA	1:D:111:PRO:HD3	1.69	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:ASN:HA	1:F:57:THR:HG22	1.95	0.48
1:C:19:ASP:OD2	1:C:213:TYR:OH	2.25	0.47
1:D:6:TYR:CD2	1:D:208:LEU:HG	2.49	0.47
1:A:5:PHE:CE2	1:A:201:PRO:HB3	2.50	0.47
1:D:106:VAL:HG12	1:D:107:SER:H	1.80	0.47
1:C:13:TYR:CD2	1:C:116:MET:HE1	2.50	0.47
1:E:5:PHE:CE2	1:E:201:PRO:HB3	2.50	0.46
1:E:107:SER:O	1:E:107:SER:OG	2.31	0.46
1:A:74:ARG:NH2	1:A:231:GLU:OE2	2.48	0.46
1:D:114:ILE:HG12	1:D:115:LYS:N	2.30	0.46
1:E:147:THR:HG23	1:E:163:ILE:HB	1.97	0.46
1:C:66:ALA:C	1:C:68:VAL:H	2.23	0.46
1:A:13:TYR:CD2	1:A:116:MET:HE1	2.51	0.46
1:D:151:GLU:OE2	1:D:161:ARG:NH1	2.39	0.46
1:A:19:ASP:HA	1:A:22:SER:HB2	1.98	0.46
1:C:6:TYR:CD2	1:C:208:LEU:HG	2.51	0.46
1:D:66:ALA:C	1:D:68:VAL:H	2.22	0.46
1:E:6:TYR:CD2	1:E:208:LEU:HG	2.51	0.46
1:E:125:ARG:NH2	1:E:184:ARG:HG2	2.30	0.46
1:C:27:LYS:HB2	1:C:36:PHE:CE2	2.51	0.46
1:A:18:GLY:HA3	1:A:230:PHE:CZ	2.51	0.46
1:D:19:ASP:HA	1:D:22:SER:HB2	1.98	0.45
1:D:64:ASP:O	1:D:68:VAL:HG23	2.16	0.45
1:E:114:ILE:HG12	1:E:115:LYS:N	2.31	0.45
1:C:223:LEU:HA	1:C:224:PRO:HD3	1.81	0.45
1:F:56:TRP:HB3	1:F:71:ILE:HD13	1.99	0.45
1:D:29:GLN:OE1	1:E:3:GLY:N	2.49	0.45
1:D:109:TYR:HB3	1:D:161:ARG:NH2	2.18	0.45
1:C:152:GLN:HA	1:C:158:PRO:HA	1.99	0.45
1:A:30:LEU:HB2	1:A:33:GLY:O	2.17	0.45
1:B:124:THR:CG2	1:B:130:MET:HG2	2.46	0.45
1:C:106:VAL:HG12	1:C:107:SER:H	1.82	0.45
1:B:110:ASN:HA	1:B:111:PRO:HD3	1.71	0.45
1:B:223:LEU:HD12	1:B:224:PRO:HD2	1.98	0.45
1:A:114:ILE:HG12	1:A:115:LYS:H	1.82	0.45
1:F:124:THR:HG23	1:F:126:TYR:N	2.33	0.44
1:D:212:THR:HA	1:D:222:ASP:HA	1.98	0.44
1:F:123:PHE:CE1	1:F:187:GLU:HG3	2.52	0.44
1:C:29:GLN:OE1	1:D:3:GLY:N	2.51	0.44
1:F:110:ASN:HA	1:F:111:PRO:HD3	1.69	0.44
1:B:114:ILE:HG12	1:B:115:LYS:H	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HG13	1:A:37:ILE:HG12	2.00	0.44
1:D:67:LYS:O	1:D:67:LYS:HG2	2.18	0.44
1:F:114:ILE:HD12	1:F:198:MET:HE3	2.00	0.44
1:B:178:GLY:O	2:B:303:HOH:O	2.21	0.44
1:F:114:ILE:HG23	1:F:116:MET:HE2	2.00	0.43
1:C:123:PHE:CE1	1:C:187:GLU:HG3	2.54	0.43
1:B:108:GLN:CB	1:B:199:TYR:HB2	2.49	0.43
1:B:124:THR:HG23	1:B:126:TYR:H	1.84	0.43
1:E:110:ASN:HA	1:E:111:PRO:HD3	1.73	0.43
1:F:149:MET:HG3	1:F:212:THR:O	2.18	0.43
1:B:114:ILE:HG12	1:B:115:LYS:N	2.33	0.43
1:B:13:TYR:CD2	1:B:116:MET:HE1	2.54	0.43
1:D:30:LEU:HB2	1:D:33:GLY:O	2.18	0.43
1:E:127:GLU:HG2	1:E:131:PHE:CZ	2.54	0.43
1:B:56:TRP:HB3	1:B:71:ILE:HD13	2.00	0.43
1:F:109:TYR:OH	1:F:202:VAL:HG21	2.19	0.42
1:A:168:MET:HB2	1:A:191:THR:HG22	2.01	0.42
1:D:108:GLN:HB3	1:D:199:TYR:HB2	2.02	0.42
1:E:212:THR:HA	1:E:222:ASP:HA	2.00	0.42
1:A:108:GLN:HB3	1:A:199:TYR:HB2	2.00	0.42
1:B:12:ARG:NH2	1:B:199:TYR:OH	2.52	0.42
1:A:39:VAL:HA	1:A:40:PRO:HD2	1.87	0.42
1:B:222:ASP:OD1	1:B:222:ASP:N	2.53	0.42
1:C:38:ARG:O	1:C:40:PRO:HD3	2.19	0.42
1:C:212:THR:HA	1:C:222:ASP:HA	2.00	0.42
1:E:114:ILE:HG23	1:E:116:MET:HE2	2.01	0.42
1:F:7:ASN:HB3	1:F:209:ILE:HD12	2.01	0.42
1:C:27:LYS:HB2	1:C:36:PHE:HE2	1.83	0.42
1:E:64:ASP:O	1:E:68:VAL:HG23	2.20	0.42
1:A:200:PRO:HA	1:A:201:PRO:HD3	1.94	0.42
1:A:109:TYR:OH	1:A:202:VAL:HG21	2.20	0.42
1:C:56:TRP:HB3	1:C:71:ILE:HD13	2.01	0.42
1:C:124:THR:CB	1:C:130:MET:HG2	2.50	0.42
1:B:108:GLN:HB3	1:B:199:TYR:HB2	2.02	0.42
1:F:167:LEU:HD11	1:F:190:LEU:HD12	2.02	0.42
1:E:27:LYS:HE3	1:E:34:ASP:CG	2.44	0.42
1:D:27:LYS:HE3	1:D:34:ASP:CG	2.45	0.41
1:E:203:ASP:OD1	1:E:204:ASP:N	2.54	0.41
1:E:222:ASP:OD1	1:E:222:ASP:N	2.53	0.41
1:B:39:VAL:HA	1:B:40:PRO:HD2	1.93	0.41
1:A:222:ASP:OD1	1:A:222:ASP:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:THR:HG23	1:E:126:TYR:N	2.35	0.41
1:E:28:ARG:HD3	1:E:28:ARG:HA	1.89	0.41
1:A:108:GLN:CB	1:A:199:TYR:HB2	2.50	0.41
1:C:77:LEU:HD13	1:C:120:LEU:HD23	2.03	0.41
1:E:108:GLN:HB3	1:E:199:TYR:HB2	2.03	0.41
1:F:109:TYR:HB3	1:F:161:ARG:NH2	2.33	0.41
1:F:151:GLU:OE2	1:F:161:ARG:NH1	2.52	0.41
1:F:66:ALA:C	1:F:68:VAL:N	2.79	0.40
1:A:24:ILE:HB	2:A:302:HOH:O	2.22	0.40
1:A:115:LYS:HE3	1:A:115:LYS:HB2	1.84	0.40
1:B:13:TYR:CG	1:B:116:MET:HE1	2.56	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	205/272 (75%)	185 (90%)	17 (8%)	3 (2%)	8	22
1	B	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	6	16
1	C	205/272 (75%)	184 (90%)	16 (8%)	5 (2%)	4	12
1	D	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	6	16
1	E	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	6	16
1	F	205/272 (75%)	184 (90%)	18 (9%)	3 (2%)	8	22
All	All	1230/1632 (75%)	1105 (90%)	102 (8%)	23 (2%)	6	17

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	67	LYS
1	B	108	GLN
1	C	67	LYS
1	C	108	GLN
1	D	67	LYS
1	E	67	LYS
1	F	67	LYS
1	D	108	GLN
1	E	108	GLN
1	F	108	GLN
1	A	67	LYS
1	F	111	PRO
1	A	111	PRO
1	E	111	PRO
1	B	111	PRO
1	B	175	ALA
1	C	111	PRO
1	D	175	ALA
1	E	175	ALA
1	C	175	ALA
1	D	111	PRO
1	C	106	VAL

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	192/250 (77%)	173 (90%)	19 (10%)	7	19
1	B	192/250 (77%)	177 (92%)	15 (8%)	11	29
1	C	192/250 (77%)	174 (91%)	18 (9%)	8	21
1	D	192/250 (77%)	176 (92%)	16 (8%)	10	26
1	E	192/250 (77%)	176 (92%)	16 (8%)	10	26
1	F	192/250 (77%)	176 (92%)	16 (8%)	10	26
All	All	1152/1500 (77%)	1052 (91%)	100 (9%)	9	24

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	31	GLU
1	A	37	ILE
1	A	45	SER
1	A	50	MET
1	A	63	GLU
1	A	68	VAL
1	A	69	GLU
1	A	106	VAL
1	A	109	TYR
1	A	110	ASN
1	A	114	ILE
1	A	124	THR
1	A	125	ARG
1	A	138	LEU
1	A	161	ARG
1	A	184	ARG
1	A	191	THR
1	A	212	THR
1	B	25	GLN
1	B	37	ILE
1	B	45	SER
1	B	50	MET
1	B	67	LYS
1	B	78	HIS
1	B	109	TYR
1	B	114	ILE
1	B	124	THR
1	B	125	ARG
1	B	138	LEU
1	B	161	ARG
1	B	176	ILE
1	B	184	ARG
1	B	212	THR
1	C	9	SER
1	C	25	GLN
1	C	37	ILE
1	C	45	SER
1	C	50	MET
1	C	59	ILE
1	C	67	LYS
1	C	105	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	106	VAL
1	C	109	TYR
1	C	110	ASN
1	C	114	ILE
1	C	124	THR
1	C	125	ARG
1	C	138	LEU
1	C	161	ARG
1	C	184	ARG
1	C	212	THR
1	D	25	GLN
1	D	37	ILE
1	D	45	SER
1	D	50	MET
1	D	68	VAL
1	D	78	HIS
1	D	106	VAL
1	D	109	TYR
1	D	110	ASN
1	D	114	ILE
1	D	124	THR
1	D	125	ARG
1	D	138	LEU
1	D	161	ARG
1	D	184	ARG
1	D	212	THR
1	E	25	GLN
1	E	37	ILE
1	E	45	SER
1	E	50	MET
1	E	59	ILE
1	E	67	LYS
1	E	68	VAL
1	E	109	TYR
1	E	110	ASN
1	E	114	ILE
1	E	124	THR
1	E	125	ARG
1	E	138	LEU
1	E	161	ARG
1	E	184	ARG
1	E	212	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	25	GLN
1	F	37	ILE
1	F	45	SER
1	F	50	MET
1	F	59	ILE
1	F	67	LYS
1	F	106	VAL
1	F	109	TYR
1	F	114	ILE
1	F	124	THR
1	F	125	ARG
1	F	138	LEU
1	F	161	ARG
1	F	176	ILE
1	F	184	ARG
1	F	212	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	136	GLN
1	B	152	GLN
1	C	62	GLN
1	C	217	HIS
1	D	62	GLN
1	E	108	GLN
1	F	110	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

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	211/272 (77%)	0.01	2 (0%) 81 80	27, 58, 105, 140	0
1	B	211/272 (77%)	0.21	4 (1%) 66 63	35, 65, 136, 170	0
1	C	211/272 (77%)	0.22	8 (3%) 44 40	35, 67, 137, 198	0
1	D	211/272 (77%)	0.13	11 (5%) 33 29	23, 58, 134, 189	0
1	E	211/272 (77%)	0.11	9 (4%) 40 36	17, 47, 122, 177	0
1	F	211/272 (77%)	0.07	8 (3%) 44 40	18, 47, 130, 163	0
All	All	1266/1632 (77%)	0.13	42 (3%) 49 45	17, 58, 130, 198	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	59	ILE	3.9
1	D	65	VAL	3.7
1	D	59	ILE	3.5
1	E	176	ILE	3.5
1	F	68	VAL	3.5
1	F	183	ARG	3.3
1	C	178	GLY	3.1
1	E	59	ILE	3.1
1	E	154	GLY	3.1
1	C	65	VAL	3.1
1	C	61	SER	3.0
1	F	59	ILE	2.9
1	E	68	VAL	2.9
1	D	154	GLY	2.9
1	F	108	GLN	2.9
1	C	154	GLY	2.8
1	D	176	ILE	2.7
1	B	105	VAL	2.7
1	C	176	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	65	VAL	2.6
1	C	59	ILE	2.6
1	D	183	ARG	2.5
1	E	65	VAL	2.5
1	F	178	GLY	2.5
1	F	105	VAL	2.5
1	E	57	THR	2.4
1	D	56	TRP	2.4
1	C	105	VAL	2.4
1	D	60	ASN	2.3
1	E	29	GLN	2.3
1	E	183	ARG	2.3
1	A	154	GLY	2.3
1	D	57	THR	2.3
1	D	69	GLU	2.3
1	D	178	GLY	2.2
1	B	108	GLN	2.2
1	B	176	ILE	2.2
1	F	176	ILE	2.2
1	C	67	LYS	2.2
1	D	61	SER	2.2
1	A	178	GLY	2.1
1	E	178	GLY	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.