



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 PM GMT

PDB ID : 4HUD  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

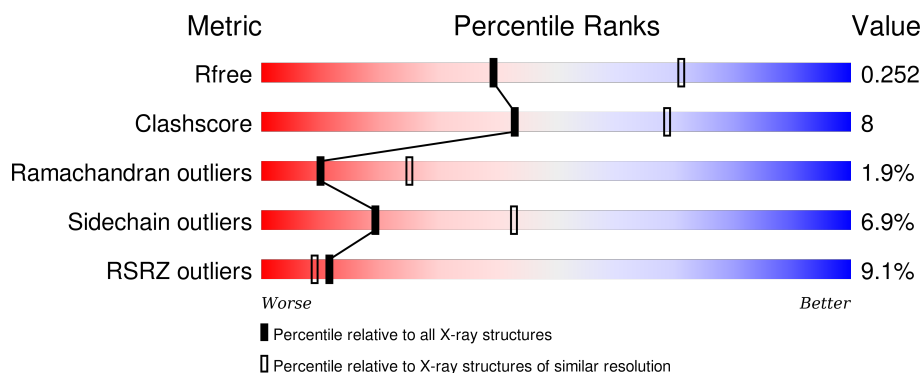
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>58%</div> <div>17%</div> <div>•</div> <div>22%</div> </div>
1	B	272	<div> <div>8%</div> <div>61%</div> <div>14%</div> <div>•</div> <div>22%</div> </div>
1	C	272	<div> <div>7%</div> <div>58%</div> <div>16%</div> <div>•</div> <div>22%</div> </div>
1	D	272	<div> <div>7%</div> <div>62%</div> <div>12%</div> <div>•</div> <div>22%</div> </div>
1	E	272	<div> <div>7%</div> <div>60%</div> <div>14%</div> <div>•</div> <div>22%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	272	<div><div></div><div>8%</div><div>62%</div><div>13%</div><div>•</div><div>22%</div></div>

## 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			

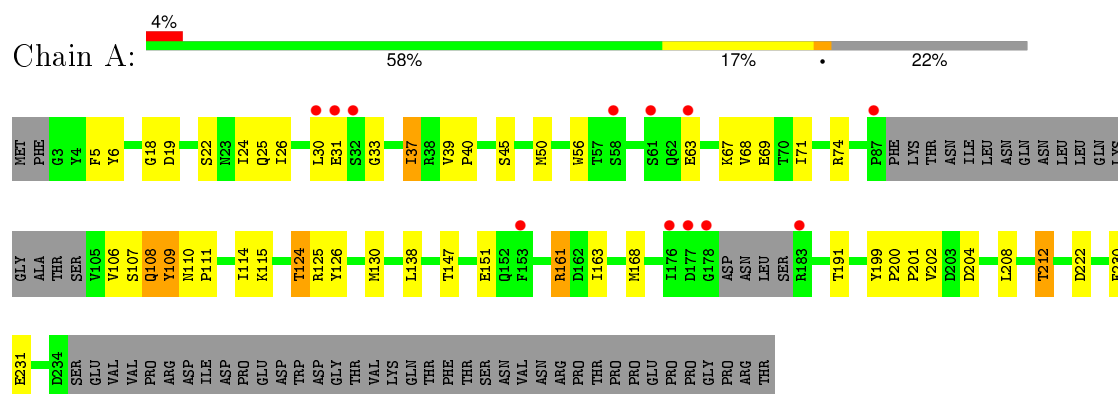
- Molecule 2 is water.

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		

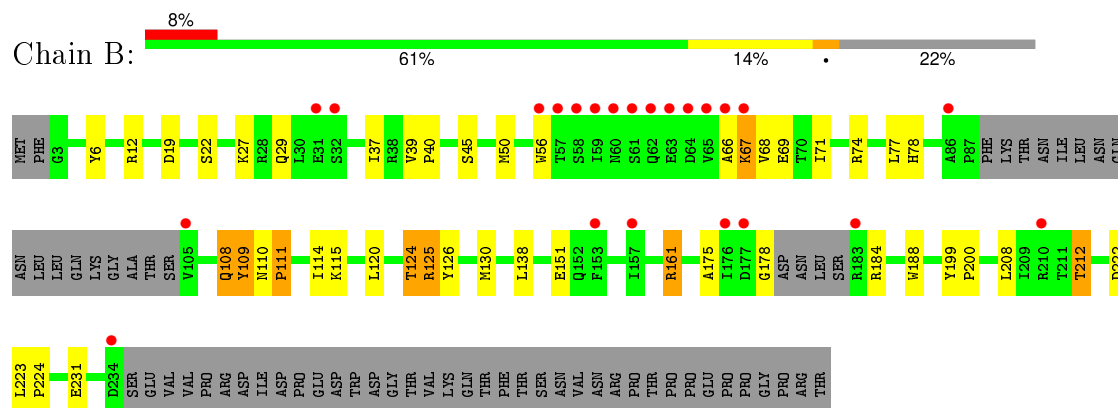
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

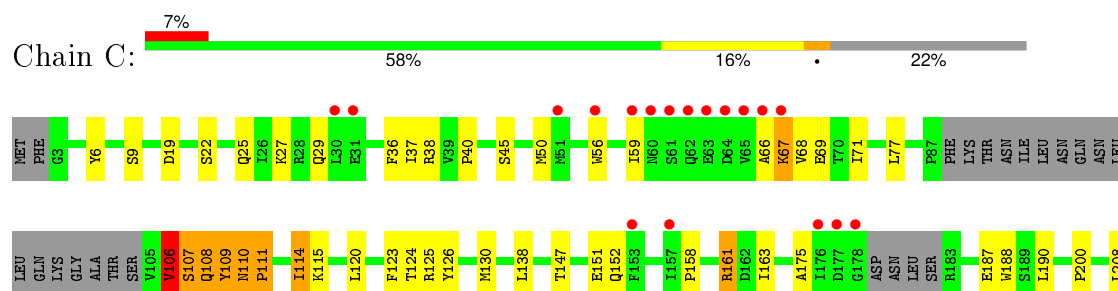
#### • Molecule 1: Tail connector protein Gp15



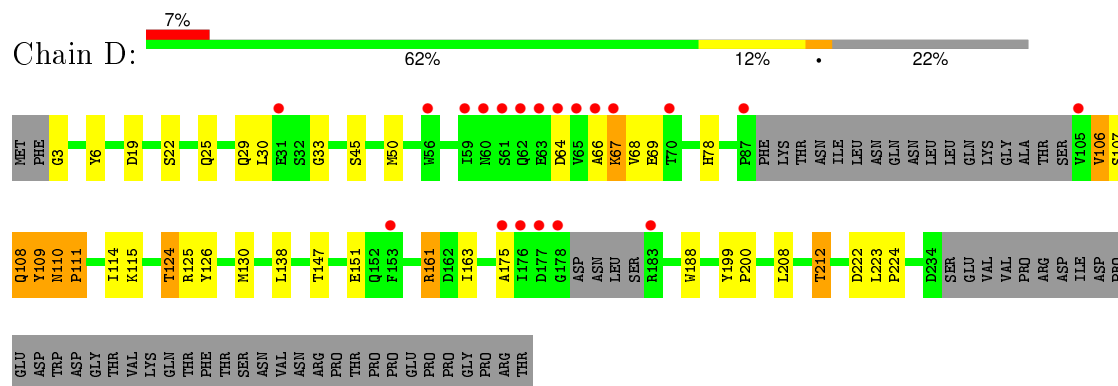
#### • Molecule 1: Tail connector protein Gp15



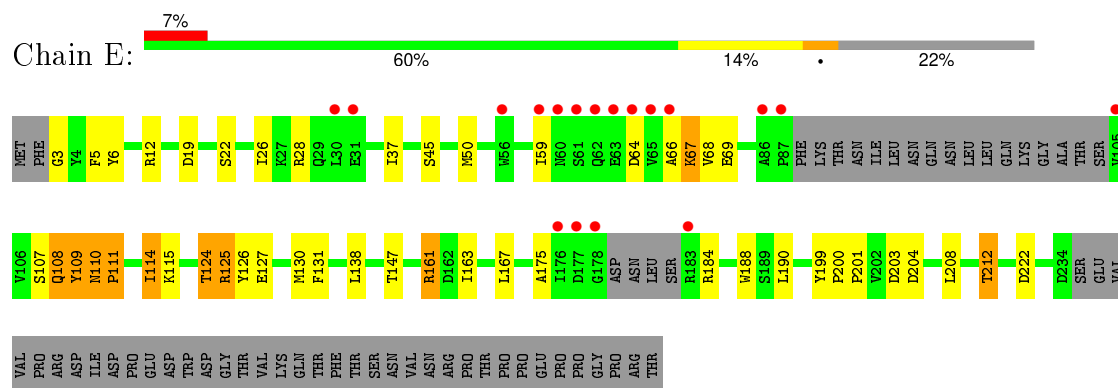
#### • Molecule 1: Tail connector protein Gp15



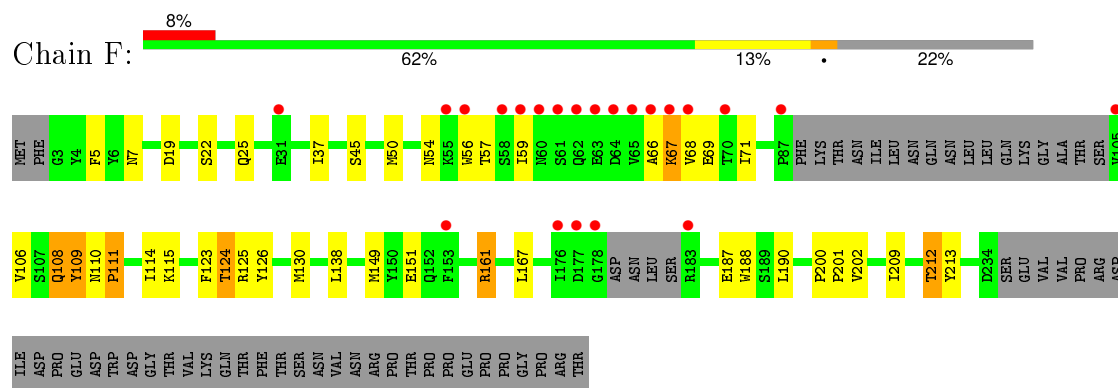
- Molecule 1: Tail connector protein Gp15



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.207 , 0.252 0.207 , 0.252	Depositor DCC
$R_{free}$ test set	2534 reflections (5.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.8	Xtriage
Anisotropy	1.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.9	EDS
Estimated twinning fraction	0.127 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 45407 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.47	0/1787	0.63	0/2421
1	B	0.45	0/1787	0.63	0/2421
1	C	0.46	0/1787	0.63	1/2421 (0.0%)
1	D	0.47	0/1787	0.62	0/2421
1	E	0.48	0/1787	0.63	0/2421
1	F	0.49	0/1787	0.64	0/2421
All	All	0.47	0/10722	0.63	1/14526 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	LEU	CA-CB-CG	5.07	126.97	115.30

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	1742	0	1673	30	0
1	B	1742	0	1673	29	0
1	C	1742	0	1673	28	0
1	D	1742	0	1673	26	0
1	E	1742	0	1673	31	0
1	F	1742	0	1673	25	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	167	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 8.

All (167) 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
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:E:108:GLN:HB3	1:E:200:PRO:HD2	1.81	0.62
1:A:108:GLN:HB3	1:A:200:PRO:HD2	1.80	0.62
1:E:66:ALA:O	1:E:68:VAL:N	2.32	0.62
1:E:124:THR:HG21	1:E:130:MET:HG2	1.81	0.61
1:C:69:GLU:OE2	1:C:126:TYR:OH	2.13	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:C:114:ILE:HG12	1:C:115:LYS:N	2.17	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:F:124:THR:HG23	1:F:126:TYR:H	1.73	0.52
1:B:19:ASP:HA	1:B:22:SER:HB2	1.90	0.52
1:F:5:PHE:CE2	1:F:201:PRO:HB3	2.45	0.52
1:A:106:VAL:HG12	1:A:107:SER:H	1.74	0.52
1:E:26:ILE:HD11	1:E:37:ILE:HD11	1.92	0.52
1:A:212:THR:HA	1:A:222:ASP:HA	1.91	0.52
1:F:66:ALA:C	1:F:68:VAL:H	2.13	0.52
1:C:19:ASP:OD2	1:C:213:TYR:OH	2.25	0.52
1:E:66:ALA:C	1:E:68:VAL:H	2.13	0.51
1:D:223:LEU:HD12	1:D:224:PRO:HD2	1.92	0.51
1:F:19:ASP:OD2	1:F:213:TYR:OH	2.22	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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:114:ILE:HG12	1:E:115:LYS:H	1.76	0.49
1:D:147:THR:HG23	1:D:163:ILE:HB	1.94	0.49
1:B:6:TYR:CD2	1:B:208:LEU:HG	2.48	0.48
1:E:167:LEU:HD11	1:E:190:LEU:HD12	1.95	0.48
1:D:66:ALA:O	1:D:68:VAL:N	2.45	0.48
1:C:124:THR:HG21	1:C:130:MET:HG2	1.95	0.48
1:A:114:ILE:HG12	1:A:115:LYS:N	2.29	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
1:F:54:ASN:HA	1:F:57:THR:HG22	1.95	0.48
1:E:130:MET:HE2	1:E:188:TRP:CD2	2.48	0.48
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:E:107:SER:O	1:E:107:SER:OG	2.31	0.46
1:E:5:PHE:CE2	1:E:201:PRO:HB3	2.50	0.46
1:D:114:ILE:HG12	1:D:115:LYS:N	2.30	0.46
1:A:74:ARG:NH2	1:A:231:GLU:OE2	2.48	0.46
1:E:147:THR:HG23	1:E:163:ILE:HB	1.97	0.46
1:C:130:MET:HE2	1:C:188:TRP:CD2	2.50	0.46
1:D:151:GLU:OE2	1:D:161:ARG:NH1	2.39	0.46
1:C:6:TYR:CD2	1:C:208:LEU:HG	2.51	0.46
1:A:19:ASP:HA	1:A:22:SER:HB2	1.98	0.46
1:E:125:ARG:NH2	1:E:184:ARG:HG2	2.30	0.46
1:E:6:TYR:CD2	1:E:208:LEU:HG	2.51	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:E:114:ILE:HG12	1:E:115:LYS:N	2.31	0.45
1:D:64:ASP:O	1:D:68:VAL:HG23	2.16	0.45
1:D:19:ASP:HA	1:D:22:SER:HB2	1.98	0.45
1:B:66:ALA:C	1:B:68:VAL:H	2.20	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:109:TYR:HB3	1:D:161:ARG:NH2	2.18	0.45
1:D:29:GLN:OE1	1:E:3:GLY:N	2.49	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:LEU:HD12	1:B:224:PRO:HD2	1.98	0.45
1:B:110:ASN:HA	1:B:111:PRO:HD3	1.71	0.45
1:D:130:MET:HE2	1:D:188:TRP:CD2	2.52	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:F:110:ASN:HA	1:F:111:PRO:HD3	1.69	0.44
1:C:29:GLN:OE1	1:D:3:GLY:N	2.51	0.44
1:B:114:ILE:HG12	1:B:115:LYS:H	1.81	0.44
1:D:67:LYS:HG2	1:D:67:LYS:O	2.18	0.44
1:A:26:ILE:HG13	1:A:37:ILE:HG12	2.00	0.44
1:B:178:GLY:O	2:B:303:HOH:O	2.21	0.44
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: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:D:108:GLN:HB3	1:D:199:TYR:HB2	2.02	0.42
1:A:168:MET:HB2	1:A:191:THR:HG22	2.01	0.42
1:E:212:THR:HA	1:E:222:ASP:HA	2.00	0.42
1:B:12:ARG:NH2	1:B:199:TYR:OH	2.52	0.42
1:A:108:GLN:HB3	1:A:199:TYR:HB2	2.00	0.42
1:B:130:MET:HE2	1:B:188:TRP:CD2	2.54	0.42
1:F:130:MET:HE2	1:F:188:TRP:CD2	2.54	0.42
1:B:222:ASP:OD1	1:B:222:ASP:N	2.53	0.42
1:C:212:THR:HA	1:C:222:ASP:HA	2.00	0.42
1:A:39:VAL:HA	1:A:40:PRO:HD2	1.87	0.42
1:F:7:ASN:HB3	1:F:209:ILE:HD12	2.01	0.42
1:C:38:ARG:O	1:C:40:PRO:HD3	2.19	0.42
1:E:64:ASP:O	1:E:68:VAL:HG23	2.20	0.42
1:C:27:LYS:HB2	1:C:36:PHE:HE2	1.83	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:124:THR:CB	1:C:130:MET:HG2	2.50	0.42
1:C:56:TRP:HB3	1:C:71:ILE:HD13	2.01	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:66:ALA:C	1:C:68:VAL:H	2.23	0.41
1:E:222:ASP:OD1	1:E:222:ASP:N	2.53	0.41
1:E:203:ASP:OD1	1:E:204:ASP:N	2.54	0.41
1:B:39:VAL:HA	1:B:40:PRO:HD2	1.93	0.41
1:E:124:THR:HG23	1:E:126:TYR:N	2.35	0.41
1:A:222:ASP:N	1:A:222:ASP:OD1	2.54	0.41
1:D:66:ALA:C	1:D:68:VAL:H	2.22	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: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:E:108:GLN:HB3	1:E:199:TYR:HB2	2.03	0.41
1:C:77:LEU:HD13	1:C:120:LEU:HD23	2.03	0.41
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

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	205/272 (75%)	185 (90%)	17 (8%)	3 (2%)	13	32
1	B	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	9	24
1	C	205/272 (75%)	184 (90%)	16 (8%)	5 (2%)	7	19
1	D	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	9	24
1	E	205/272 (75%)	184 (90%)	17 (8%)	4 (2%)	9	24
1	F	205/272 (75%)	184 (90%)	18 (9%)	3 (2%)	13	32
All	All	1230/1632 (75%)	1105 (90%)	102 (8%)	23 (2%)	10	25

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
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%)	177 (92%)	15 (8%)	16	35
1	B	192/250 (77%)	181 (94%)	11 (6%)	25	53
1	C	192/250 (77%)	176 (92%)	16 (8%)	14	31
1	D	192/250 (77%)	180 (94%)	12 (6%)	22	48
1	E	192/250 (77%)	180 (94%)	12 (6%)	22	48
1	F	192/250 (77%)	179 (93%)	13 (7%)	20	43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1152/1500 (77%)	1073 (93%)	79 (7%)	19	43

All (79) 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	109	TYR
1	A	110	ASN
1	A	124	THR
1	A	125	ARG
1	A	138	LEU
1	A	161	ARG
1	A	212	THR
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	124	THR
1	B	125	ARG
1	B	138	LEU
1	B	161	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	106	VAL
1	C	107	SER
1	C	109	TYR
1	C	110	ASN

*Continued on next page...*

*Continued from previous page...*

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



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	152	GLN
1	F	78	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	211/272 (77%)	0.15	12 (5%) 27 26	27, 58, 105, 140	0
1	B	211/272 (77%)	0.48	23 (10%) 7 5	35, 65, 136, 170	0
1	C	211/272 (77%)	0.48	20 (9%) 10 8	35, 67, 137, 198	0
1	D	211/272 (77%)	0.36	20 (9%) 10 8	23, 58, 134, 189	0
1	E	211/272 (77%)	0.29	18 (8%) 13 10	17, 47, 122, 177	0
1	F	211/272 (77%)	0.29	22 (10%) 8 6	18, 47, 130, 163	0
All	All	1266/1632 (77%)	0.34	115 (9%) 11 9	17, 58, 130, 198	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	ASN	12.9
1	C	61	SER	11.2
1	D	60	ASN	8.8
1	F	60	ASN	8.8
1	F	61	SER	8.0
1	E	63	GLU	7.6
1	D	61	SER	7.4
1	E	61	SER	7.4
1	B	61	SER	7.3
1	C	63	GLU	7.3
1	C	64	ASP	7.3
1	D	62	GLN	7.1
1	E	64	ASP	6.8
1	E	60	ASN	6.4
1	E	176	ILE	6.2
1	F	59	ILE	5.9
1	B	65	VAL	5.8
1	F	62	GLN	5.7
1	C	60	ASN	5.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	62	GLN	5.5
1	E	183	ARG	5.3
1	F	183	ARG	5.3
1	E	177	ASP	5.3
1	D	176	ILE	5.3
1	C	62	GLN	5.1
1	D	64	ASP	5.1
1	D	63	GLU	5.1
1	F	63	GLU	5.0
1	D	183	ARG	5.0
1	F	65	VAL	5.0
1	D	56	TRP	4.9
1	B	66	ALA	4.9
1	B	62	GLN	4.7
1	E	87	PRO	4.6
1	B	63	GLU	4.6
1	D	59	ILE	4.5
1	B	59	ILE	4.5
1	C	66	ALA	4.4
1	F	64	ASP	4.3
1	B	183	ARG	4.3
1	C	67	LYS	4.1
1	D	65	VAL	4.0
1	B	67	LYS	4.0
1	F	67	LYS	3.9
1	C	176	ILE	3.8
1	F	177	ASP	3.7
1	F	31	GLU	3.7
1	B	58	SER	3.7
1	D	178	GLY	3.6
1	E	31	GLU	3.6
1	B	157	ILE	3.6
1	F	176	ILE	3.6
1	C	59	ILE	3.6
1	A	177	ASP	3.5
1	B	64	ASP	3.4
1	F	66	ALA	3.4
1	D	105	VAL	3.4
1	B	31	GLU	3.4
1	C	157	ILE	3.3
1	E	105	VAL	3.3
1	F	105	VAL	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	87	PRO	3.2
1	E	66	ALA	3.2
1	D	70	THR	3.2
1	B	153	PHE	3.1
1	D	66	ALA	3.1
1	B	105	VAL	3.1
1	B	177	ASP	3.1
1	D	177	ASP	3.1
1	A	183	ARG	3.0
1	D	153	PHE	3.0
1	B	56	TRP	3.0
1	F	70	THR	3.0
1	A	30	LEU	3.0
1	B	86	ALA	2.9
1	C	56	TRP	2.9
1	A	176	ILE	2.9
1	C	31	GLU	2.9
1	A	153	PHE	2.9
1	D	67	LYS	2.9
1	A	87	PRO	2.8
1	B	210	ARG	2.8
1	C	51	MET	2.8
1	D	87	PRO	2.8
1	C	153	PHE	2.8
1	B	176	ILE	2.8
1	E	86	ALA	2.8
1	C	30	LEU	2.7
1	C	210	ARG	2.7
1	F	55	LYS	2.7
1	A	63	GLU	2.7
1	F	68	VAL	2.6
1	E	59	ILE	2.6
1	E	65	VAL	2.6
1	C	65	VAL	2.6
1	C	178	GLY	2.5
1	C	177	ASP	2.5
1	F	56	TRP	2.5
1	F	178	GLY	2.5
1	A	178	GLY	2.5
1	E	30	LEU	2.5
1	E	56	TRP	2.5
1	D	31	GLU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	58	SER	2.3
1	C	227	GLU	2.3
1	B	234	ASP	2.3
1	A	31	GLU	2.2
1	A	61	SER	2.2
1	E	178	GLY	2.1
1	A	32	SER	2.1
1	F	58	SER	2.1
1	D	175	ALA	2.1
1	B	57	THR	2.0
1	F	153	PHE	2.0
1	B	32	SER	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 carbohydrates 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.