Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:00 am BST

PDB ID	:	2YIA
Title	:	Structure of the RNA polymerase VP1 from Infectious Pancreatic Necrosis Virus
Authors	:	Graham, S.C.; Sarin, L.P.; Bahar, M.W.; Myers, R.A.; Stuart, D.I.; Bamford, D.H.; Grimes, J.M.
Deposited on	:	2011-05-11
Resolution	:	3.02 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 following versions of software and data (see references ①) were used in the production of this report:

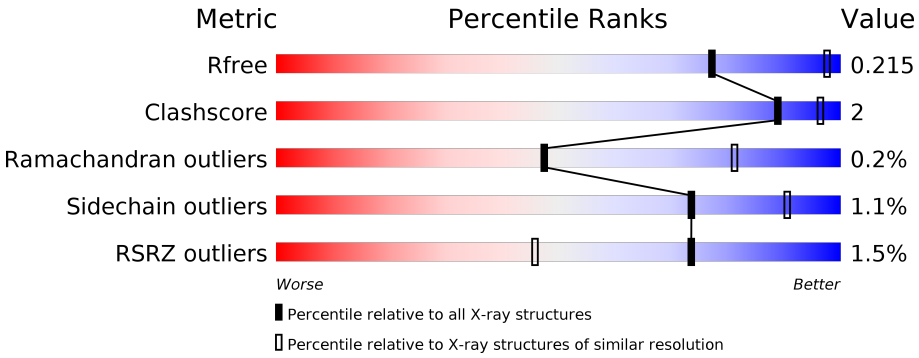
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 >=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 <=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	799	% 93% 6% •
1	B	799	% 92% 6% •
1	C	799	3% 92% 6% •
1	D	799	93% 6% •
1	E	799	92% 6% •
1	F	799	91% 6% •

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Mol	Chain	Length	Quality of chain
1	G	799	
1	H	799	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 49237 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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	5	0
			6202	3927	1047	1202	26			
1	B	790	Total	C	N	O	S	0	5	0
			6185	3916	1041	1202	26			
1	C	790	Total	C	N	O	S	0	5	0
			6193	3922	1043	1202	26			
1	D	790	Total	C	N	O	S	0	5	0
			6193	3922	1043	1202	26			
1	E	790	Total	C	N	O	S	0	5	0
			6189	3919	1042	1202	26			
1	F	782	Total	C	N	O	S	0	5	0
			6136	3887	1033	1190	26			
1	G	762	Total	C	N	O	S	0	0	0
			5966	3782	1007	1152	25			
1	H	790	Total	C	N	O	S	0	0	0
			6165	3907	1037	1195	26			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	791	LYS	-	expression tag	UNP P22173
A	792	THR	-	expression tag	UNP P22173
A	793	GLY	-	expression tag	UNP P22173
A	794	HIS	-	expression tag	UNP P22173
A	795	HIS	-	expression tag	UNP P22173
A	796	HIS	-	expression tag	UNP P22173
A	797	HIS	-	expression tag	UNP P22173
A	798	HIS	-	expression tag	UNP P22173
A	799	HIS	-	expression tag	UNP P22173
B	791	LYS	-	expression tag	UNP P22173
B	792	THR	-	expression tag	UNP P22173
B	793	GLY	-	expression tag	UNP P22173
B	794	HIS	-	expression tag	UNP P22173

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Chain	Residue	Modelled	Actual	Comment	Reference
B	795	HIS	-	expression tag	UNP P22173
B	796	HIS	-	expression tag	UNP P22173
B	797	HIS	-	expression tag	UNP P22173
B	798	HIS	-	expression tag	UNP P22173
B	799	HIS	-	expression tag	UNP P22173
C	791	LYS	-	expression tag	UNP P22173
C	792	THR	-	expression tag	UNP P22173
C	793	GLY	-	expression tag	UNP P22173
C	794	HIS	-	expression tag	UNP P22173
C	795	HIS	-	expression tag	UNP P22173
C	796	HIS	-	expression tag	UNP P22173
C	797	HIS	-	expression tag	UNP P22173
C	798	HIS	-	expression tag	UNP P22173
C	799	HIS	-	expression tag	UNP P22173
D	791	LYS	-	expression tag	UNP P22173
D	792	THR	-	expression tag	UNP P22173
D	793	GLY	-	expression tag	UNP P22173
D	794	HIS	-	expression tag	UNP P22173
D	795	HIS	-	expression tag	UNP P22173
D	796	HIS	-	expression tag	UNP P22173
D	797	HIS	-	expression tag	UNP P22173
D	798	HIS	-	expression tag	UNP P22173
D	799	HIS	-	expression tag	UNP P22173
E	791	LYS	-	expression tag	UNP P22173
E	792	THR	-	expression tag	UNP P22173
E	793	GLY	-	expression tag	UNP P22173
E	794	HIS	-	expression tag	UNP P22173
E	795	HIS	-	expression tag	UNP P22173
E	796	HIS	-	expression tag	UNP P22173
E	797	HIS	-	expression tag	UNP P22173
E	798	HIS	-	expression tag	UNP P22173
E	799	HIS	-	expression tag	UNP P22173
F	791	LYS	-	expression tag	UNP P22173
F	792	THR	-	expression tag	UNP P22173
F	793	GLY	-	expression tag	UNP P22173
F	794	HIS	-	expression tag	UNP P22173
F	795	HIS	-	expression tag	UNP P22173
F	796	HIS	-	expression tag	UNP P22173
F	797	HIS	-	expression tag	UNP P22173
F	798	HIS	-	expression tag	UNP P22173
F	799	HIS	-	expression tag	UNP P22173
G	791	LYS	-	expression tag	UNP P22173

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Chain	Residue	Modelled	Actual	Comment	Reference
G	792	THR	-	expression tag	UNP P22173
G	793	GLY	-	expression tag	UNP P22173
G	794	HIS	-	expression tag	UNP P22173
G	795	HIS	-	expression tag	UNP P22173
G	796	HIS	-	expression tag	UNP P22173
G	797	HIS	-	expression tag	UNP P22173
G	798	HIS	-	expression tag	UNP P22173
G	799	HIS	-	expression tag	UNP P22173
H	791	LYS	-	expression tag	UNP P22173
H	792	THR	-	expression tag	UNP P22173
H	793	GLY	-	expression tag	UNP P22173
H	794	HIS	-	expression tag	UNP P22173
H	795	HIS	-	expression tag	UNP P22173
H	796	HIS	-	expression tag	UNP P22173
H	797	HIS	-	expression tag	UNP P22173
H	798	HIS	-	expression tag	UNP P22173
H	799	HIS	-	expression tag	UNP P22173

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

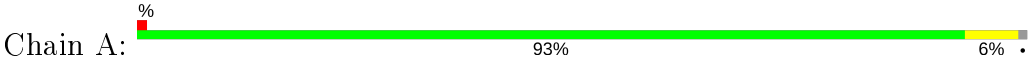
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0

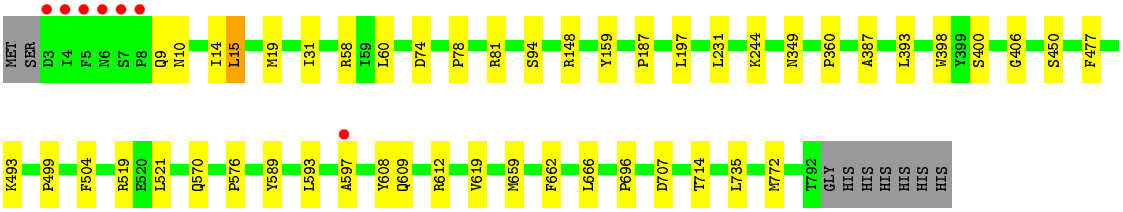
3 Residue-property plots (i)

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

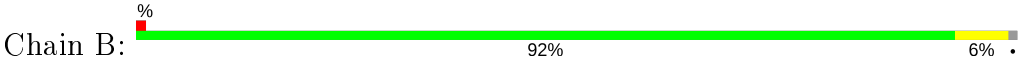
Chain A:

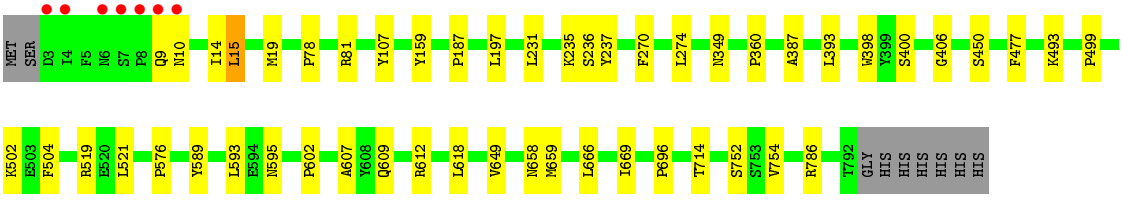




- Molecule 1: RNA-DIRECTED RNA POLYMERASE

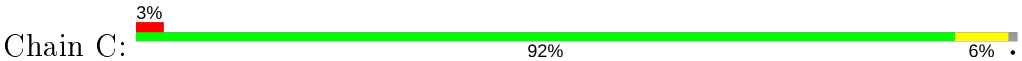
Chain B:

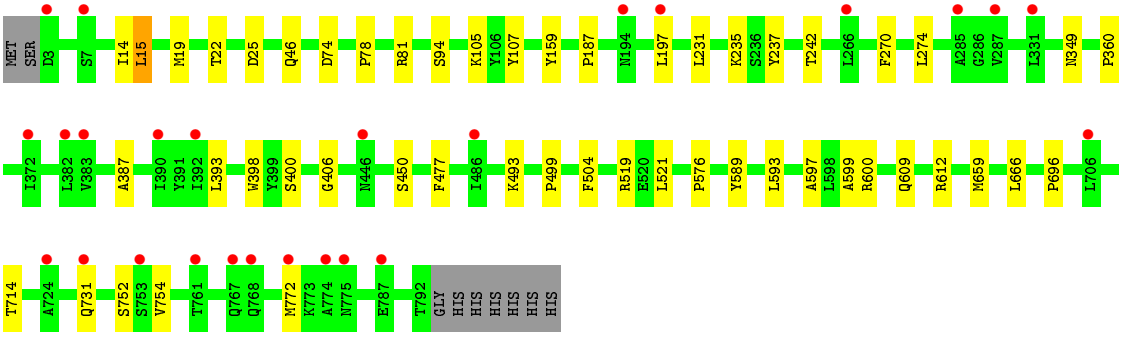




- Molecule 1: RNA-DIRECTED RNA POLYMERASE

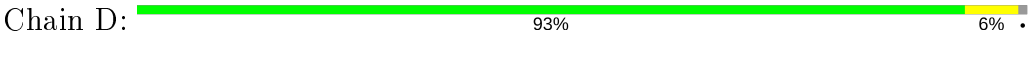
Chain C:

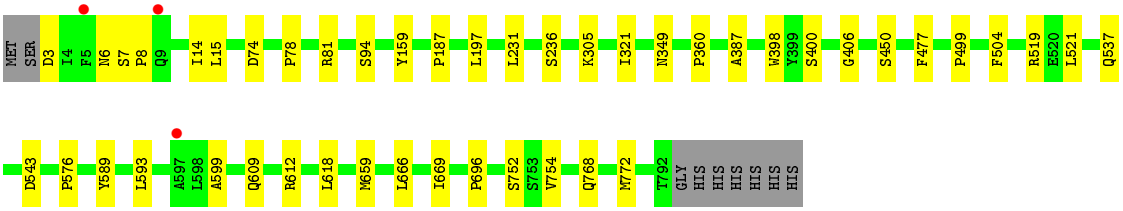




- Molecule 1: RNA-DIRECTED RNA POLYMERASE

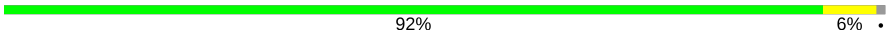
Chain D:

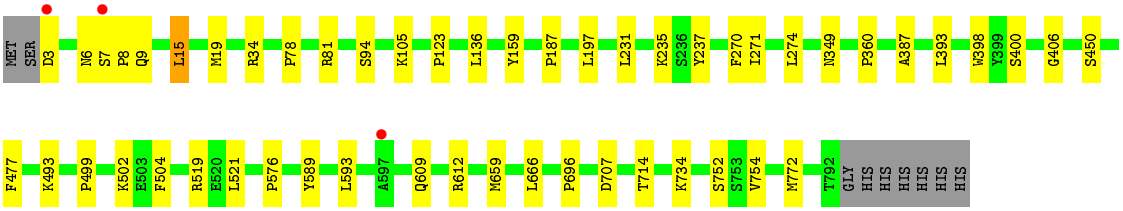




• Molecule 1: RNA-DIRECTED RNA POLYMERASE

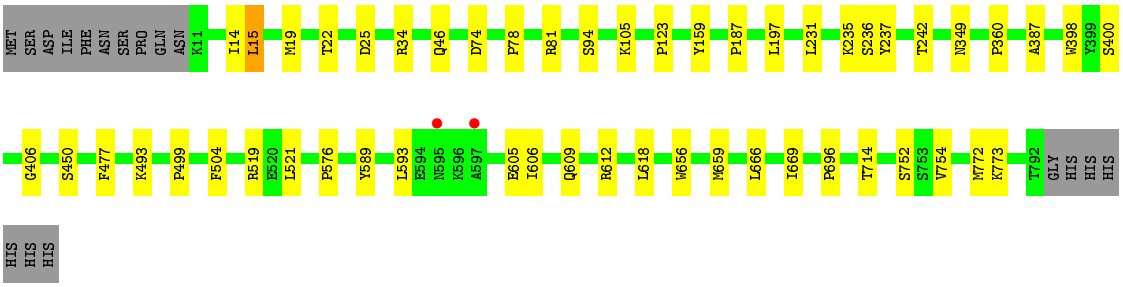
Chain E:





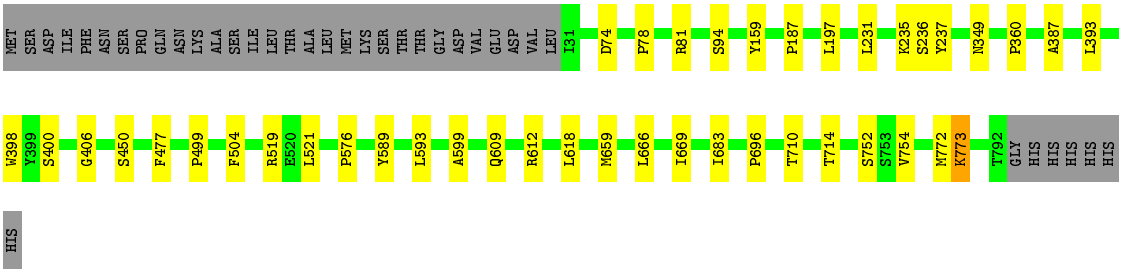
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain F:



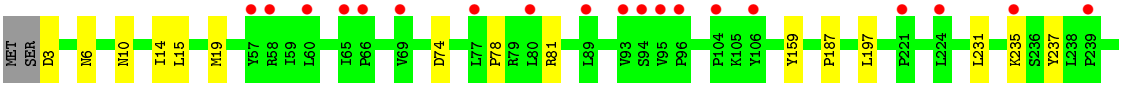
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

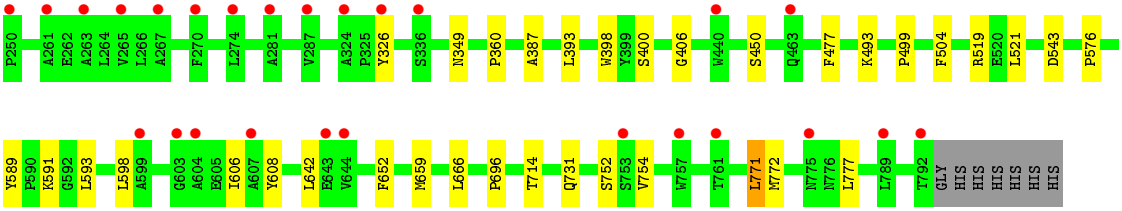
Chain G:



• Molecule 1: RNA-DIRECTED RNA POLYMERASE

Chain H:




P250
A261
E262
A263
L264
V265
L266
A267
F270
L274
A281
V287
A324
P325
Y326
S336
N349
P360
A387
L393
W398
Y399
S400
G406
W440
S450
Q463
F477
K493
P499
F504
R519
E520
L521
D543
P576
Y589
P590
K591
G592
L593
L598
A599
G603
A604
E605
I606
A607
Y608
L642
E643
V644
F652
M659
L666
P696
T714
Q731
S752
S753
V754
W757
T761
L771
M772
N775
N776
L777
L789
T792
GLY
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	200.94Å 209.47Å 243.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.01 – 3.02 145.01 – 3.02	Depositor EDS
% Data completeness (in resolution range)	(Not available) (145.01-3.02) 100.0 (145.01-3.02)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.187 , 0.216 0.193 , 0.215	Depositor DCC
R_{free} test set	2029 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	49237	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: K

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	0.55	0/6347	0.68	0/8643
1	B	0.55	0/6330	0.69	0/8625
1	C	0.52	0/6338	0.68	0/8633
1	D	0.56	0/6338	0.69	0/8633
1	E	0.55	0/6334	0.69	0/8629
1	F	0.55	0/6279	0.69	0/8550
1	G	0.55	0/6102	0.68	1/8310 (0.0%)
1	H	0.48	0/6303	0.66	0/8585
All	All	0.54	0/50371	0.68	1/68608 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	772	MET	CA-CB-CG	-5.76	103.51	113.30

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	6202	0	6117	26	0
1	B	6185	0	6075	26	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6193	0	6097	25	0
1	D	6193	0	6097	23	0
1	E	6189	0	6086	23	0
1	F	6136	0	6056	25	0
1	G	5966	0	5889	22	0
1	H	6165	0	6085	22	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
All	All	49237	0	48502	183	1

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 2.

All (183) 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:244:LYS:HE3	1:A:597[B]:ALA:HB2	1.39	1.02
1:A:10:ASN:OD1	1:B:658:ASN:ND2	2.10	0.82
1:H:606:ILE:HG21	1:H:642:LEU:HD21	1.60	0.81
1:E:3:ASP:OD1	1:E:6:ASN:ND2	2.25	0.69
1:H:493:LYS:HE3	1:H:714:THR:HG22	1.76	0.68
1:G:669:ILE:HG21	1:G:683:ILE:HG22	1.76	0.67
1:A:244:LYS:CE	1:A:597[B]:ALA:HB2	2.23	0.64
1:A:244:LYS:HE3	1:A:597[B]:ALA:CB	2.20	0.64
1:F:493:LYS:HE3	1:F:714:THR:HG22	1.79	0.63
1:H:3:ASP:OD1	1:H:6:ASN:ND2	2.31	0.63
1:C:187:PRO:HB3	1:C:197:LEU:HD11	1.82	0.62
1:C:493:LYS:HE3	1:C:714:THR:HG22	1.84	0.60
1:A:187:PRO:HB3	1:A:197:LEU:HD11	1.84	0.59
1:H:187:PRO:HB3	1:H:197:LEU:HD11	1.85	0.59
1:E:734:LYS:HD3	1:E:772:MET:HE1	1.85	0.58
1:G:593:LEU:HD23	1:G:599:ALA:HA	1.85	0.58
1:E:187:PRO:HB3	1:E:197:LEU:HD11	1.86	0.57
1:F:400:SER:HB3	1:F:519:ARG:HB3	1.87	0.56
1:F:187:PRO:HB3	1:F:197:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:398:TRP:HB3	1:G:521:LEU:HB3	1.88	0.56
1:E:398:TRP:HB3	1:E:521:LEU:HB3	1.88	0.56
1:G:187:PRO:HB3	1:G:197:LEU:HD11	1.89	0.55
1:G:618:LEU:HD11	1:G:669:ILE:HD11	1.88	0.55
1:H:598:LEU:HD11	1:H:652:PHE:CE1	2.41	0.55
1:A:609:GLN:OE1	1:A:612:ARG:NH2	2.40	0.54
1:D:398:TRP:HB3	1:D:521:LEU:HB3	1.90	0.54
1:C:398:TRP:HB3	1:C:521:LEU:HB3	1.90	0.54
1:H:731:GLN:HG2	1:H:772:MET:SD	2.48	0.54
1:D:400:SER:HB3	1:D:519:ARG:HB3	1.90	0.54
1:B:593:LEU:CD1	1:B:659:MET:HB2	2.37	0.53
1:B:400:SER:HB3	1:B:519:ARG:HB3	1.89	0.53
1:B:398:TRP:HB3	1:B:521:LEU:HB3	1.89	0.53
1:E:593:LEU:CD1	1:E:659:MET:HB2	2.38	0.53
1:B:187:PRO:HB3	1:B:197:LEU:HD11	1.89	0.53
1:F:398:TRP:HB3	1:F:521:LEU:HB3	1.91	0.53
1:D:187:PRO:HB3	1:D:197:LEU:HD11	1.89	0.53
1:D:609:GLN:OE1	1:D:612:ARG:NH2	2.42	0.53
1:A:593:LEU:CD1	1:A:659:MET:HB2	2.39	0.52
1:D:3:ASP:OD1	1:D:6:ASN:ND2	2.43	0.52
1:F:609:GLN:OE1	1:F:612:ARG:NH2	2.42	0.52
1:B:609:GLN:OE1	1:B:612:ARG:NH2	2.43	0.52
1:A:398:TRP:HB3	1:A:521:LEU:HB3	1.91	0.52
1:A:400:SER:HB3	1:A:519:ARG:HB3	1.92	0.51
1:H:349:ASN:O	1:H:696:PRO:HD2	2.11	0.51
1:G:593:LEU:CD1	1:G:659:MET:HB2	2.40	0.51
1:G:609:GLN:OE1	1:G:612:ARG:NH2	2.43	0.51
1:E:609:GLN:OE1	1:E:612:ARG:NH2	2.43	0.51
1:F:593:LEU:CD1	1:F:659:MET:HB2	2.40	0.51
1:E:493:LYS:HE3	1:E:714:THR:HG22	1.93	0.50
1:D:593:LEU:CD1	1:D:659:MET:HB2	2.40	0.50
1:H:398:TRP:HB3	1:H:521:LEU:HB3	1.92	0.50
1:C:609:GLN:OE1	1:C:612:ARG:NH2	2.45	0.50
1:E:400:SER:HB3	1:E:519:ARG:HB3	1.93	0.50
1:H:591:LYS:O	1:H:608:TYR:OH	2.22	0.50
1:H:771:LEU:HD13	1:H:777:LEU:HD13	1.93	0.50
1:D:537:GLN:OE1	1:F:46:GLN:OE1	2.30	0.49
1:C:400:SER:HB3	1:C:519:ARG:HB3	1.92	0.49
1:G:618:LEU:HD11	1:G:669:ILE:CD1	2.41	0.49
1:H:400:SER:HB3	1:H:519:ARG:HB3	1.94	0.49
1:A:31:ILE:CD1	1:B:602:PRO:HG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:ASN:O	1:E:696:PRO:HD2	2.12	0.49
1:A:735:LEU:HD21	1:A:772:MET:HG3	1.93	0.48
1:B:618:LEU:HD11	1:B:669:ILE:HD11	1.95	0.48
1:C:593:LEU:CD1	1:C:659:MET:HB2	2.42	0.48
1:C:349:ASN:O	1:C:696:PRO:HD2	2.14	0.48
1:D:387:ALA:HB2	1:D:477:PHE:CD2	2.48	0.48
1:A:349:ASN:O	1:A:696:PRO:HD2	2.14	0.47
1:B:349:ASN:O	1:B:696:PRO:HD2	2.13	0.47
1:A:58:ARG:NH2	1:A:60:LEU:HD22	2.30	0.47
1:G:400:SER:HB3	1:G:519:ARG:HB3	1.96	0.47
1:F:360:PRO:HB2	1:F:576:PRO:HB3	1.97	0.47
1:H:387:ALA:HB2	1:H:477:PHE:CD2	2.50	0.47
1:C:387:ALA:HB2	1:C:477:PHE:CD2	2.49	0.47
1:C:105:LYS:HD2	1:C:107:TYR:HE1	1.79	0.47
1:G:349:ASN:O	1:G:696:PRO:HD2	2.15	0.47
1:E:136:LEU:HD11	1:F:606:ILE:HG12	1.97	0.47
1:F:349:ASN:O	1:F:696:PRO:HD2	2.15	0.47
1:B:78:PRO:O	1:B:81:ARG:HG3	2.15	0.46
1:A:387:ALA:HB2	1:A:477:PHE:CD2	2.50	0.46
1:B:159:TYR:HB2	1:B:589:TYR:HB3	1.98	0.46
1:A:9:GLN:HA	1:B:595[A]:ASN:OD1	2.16	0.46
1:D:78:PRO:O	1:D:81:ARG:HG3	2.16	0.46
1:G:387:ALA:HB2	1:G:477:PHE:CD2	2.51	0.46
1:C:593:LEU:HD23	1:C:599:ALA:HA	1.97	0.46
1:F:78:PRO:O	1:F:81:ARG:HG3	2.16	0.46
1:H:499:PRO:HA	1:H:504:PHE:CG	2.51	0.46
1:D:752:SER:HB2	1:D:754:VAL:HG13	1.98	0.45
1:F:618:LEU:HD11	1:F:669:ILE:HD11	1.98	0.45
1:B:387:ALA:HB2	1:B:477:PHE:CD2	2.51	0.45
1:E:499:PRO:HA	1:E:504:PHE:CG	2.52	0.45
1:G:159:TYR:HB2	1:G:589:TYR:HB3	1.98	0.45
1:A:493:LYS:HG3	1:A:714:THR:HG21	1.98	0.45
1:B:752:SER:HB2	1:B:754:VAL:HG13	1.99	0.45
1:A:499:PRO:HA	1:A:504:PHE:CG	2.52	0.44
1:H:593:LEU:CD1	1:H:659:MET:HB2	2.47	0.44
1:B:15:LEU:O	1:B:19:MET:HG2	2.17	0.44
1:B:618:LEU:HD11	1:B:669:ILE:CD1	2.47	0.44
1:C:499:PRO:HA	1:C:504:PHE:CG	2.53	0.44
1:G:360:PRO:HB2	1:G:576:PRO:HB3	1.98	0.44
1:F:387:ALA:HB2	1:F:477:PHE:CD2	2.52	0.44
1:A:78:PRO:O	1:A:81:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:593:LEU:HD12	1:D:593:LEU:HA	1.87	0.44
1:E:78:PRO:O	1:E:81:ARG:HG3	2.17	0.44
1:G:618:LEU:HD13	1:G:666:LEU:HD13	1.99	0.44
1:A:15:LEU:O	1:A:19:MET:HG2	2.18	0.44
1:F:15:LEU:O	1:F:19:MET:HG2	2.18	0.44
1:D:519:ARG:HE	1:D:519:ARG:HB2	1.71	0.44
1:B:360:PRO:HB2	1:B:576:PRO:HB3	1.99	0.44
1:F:499:PRO:HA	1:F:504:PHE:CG	2.52	0.44
1:D:349:ASN:O	1:D:696:PRO:HD2	2.18	0.43
1:D:768:GLN:O	1:D:772:MET:HG3	2.18	0.43
1:D:543:ASP:O	1:F:105:LYS:HE2	2.18	0.43
1:F:656:TRP:HE1	1:F:669:ILE:HG13	1.83	0.43
1:E:34:ARG:HD3	1:E:123:PRO:HD2	2.00	0.43
1:B:499:PRO:HA	1:B:504:PHE:CG	2.53	0.43
1:D:360:PRO:HB2	1:D:576:PRO:HB3	2.00	0.43
1:G:499:PRO:HA	1:G:504:PHE:CG	2.53	0.43
1:C:731:GLN:HG2	1:C:772:MET:SD	2.58	0.43
1:E:387:ALA:HB2	1:E:477:PHE:CD2	2.53	0.43
1:E:159:TYR:HB2	1:E:589:TYR:HB3	2.01	0.43
1:B:9:GLN:HB3	1:C:242:THR:HG23	2.00	0.43
1:F:235:LYS:HD3	1:F:237:TYR:CZ	2.54	0.43
1:A:619:VAL:HG11	1:A:662:PHE:CD1	2.54	0.43
1:A:74:ASP:HB2	1:A:81:ARG:HG2	2.00	0.43
1:C:360:PRO:HB2	1:C:576:PRO:HB3	2.00	0.43
1:G:618:LEU:CD1	1:G:669:ILE:HD11	2.48	0.43
1:D:159:TYR:HB2	1:D:589:TYR:HB3	2.01	0.43
1:F:752:SER:HB2	1:F:754:VAL:HG13	2.01	0.43
1:C:78:PRO:O	1:C:81:ARG:HG3	2.18	0.42
1:D:74:ASP:HB2	1:D:81:ARG:HG2	2.00	0.42
1:D:499:PRO:HA	1:D:504:PHE:CG	2.53	0.42
1:E:270:PHE:O	1:E:274:LEU:HB2	2.19	0.42
1:F:22:THR:HG23	1:F:25:ASP:OD2	2.19	0.42
1:C:752:SER:HB2	1:C:754:VAL:HG13	2.01	0.42
1:D:593:LEU:HD23	1:D:599:ALA:HA	2.02	0.42
1:G:710:THR:O	1:G:714:THR:HG23	2.18	0.42
1:E:360:PRO:HB2	1:E:576:PRO:HB3	2.01	0.42
1:C:15:LEU:O	1:C:19:MET:HG2	2.20	0.42
1:E:752:SER:HB2	1:E:754:VAL:HG13	2.01	0.42
1:F:159:TYR:HB2	1:F:589:TYR:HB3	2.02	0.42
1:B:235:LYS:HD3	1:B:237:TYR:CZ	2.54	0.42
1:B:493:LYS:HE3	1:B:714:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:LEU:O	1:E:19:MET:HG2	2.18	0.42
1:E:7:SER:HA	1:E:8:PRO:HD3	1.94	0.42
1:H:360:PRO:HB2	1:H:576:PRO:HB3	2.00	0.42
1:H:78:PRO:O	1:H:81:ARG:HG3	2.19	0.42
1:A:360:PRO:HB2	1:A:576:PRO:HB3	2.01	0.42
1:F:618:LEU:HD11	1:F:669:ILE:CD1	2.49	0.42
1:G:78:PRO:O	1:G:81:ARG:HG3	2.19	0.42
1:F:74:ASP:HB2	1:F:81:ARG:HG2	2.01	0.42
1:A:187:PRO:CB	1:A:197:LEU:HD11	2.50	0.41
1:B:607:ALA:HB2	1:B:649:VAL:HB	2.02	0.41
1:H:235:LYS:HD3	1:H:237:TYR:CZ	2.55	0.41
1:C:597[A]:ALA:O	1:C:600:ARG:HG2	2.20	0.41
1:H:606:ILE:CG2	1:H:642:LEU:HD21	2.42	0.41
1:E:9:GLN:HB3	1:F:242:THR:HG23	2.01	0.41
1:A:570:GLN:HG3	1:C:46:GLN:NE2	2.36	0.41
1:B:786:ARG:HG2	1:B:786:ARG:HH11	1.85	0.41
1:F:34:ARG:HD3	1:F:123:PRO:HD2	2.03	0.41
1:G:74:ASP:HB2	1:G:81:ARG:HG2	2.02	0.41
1:H:752:SER:HB2	1:H:754:VAL:HG13	2.02	0.41
1:H:159:TYR:HB2	1:H:589:TYR:HB3	2.02	0.41
1:A:608:TYR:HB2	1:A:659:MET:HE2	2.02	0.41
1:C:74:ASP:HB2	1:C:81:ARG:HG2	2.03	0.41
1:G:752:SER:HB2	1:G:754:VAL:HG13	2.02	0.41
1:G:773:LYS:HE2	1:G:773:LYS:HB2	1.95	0.41
1:C:22:THR:HG23	1:C:25:ASP:OD2	2.20	0.41
1:D:618:LEU:HD11	1:D:669:ILE:HD11	2.03	0.41
1:C:270:PHE:O	1:C:274:LEU:HB2	2.21	0.40
1:D:305:LYS:HG3	1:D:321:ILE:HD11	2.03	0.40
1:G:235:LYS:HD3	1:G:237:TYR:CZ	2.56	0.40
1:B:270:PHE:O	1:B:274:LEU:HB2	2.20	0.40
1:D:7:SER:HA	1:D:8:PRO:HD3	1.94	0.40
1:H:74:ASP:HB2	1:H:81:ARG:HG2	2.03	0.40
1:C:159:TYR:HB2	1:C:589:TYR:HB3	2.04	0.40
1:C:235:LYS:HD3	1:C:237:TYR:CZ	2.56	0.40
1:A:159:TYR:HB2	1:A:589:TYR:HB3	2.03	0.40
1:B:593:LEU:HD12	1:B:593:LEU:HA	1.83	0.40
1:B:595[A]:ASN:ND2	1:B:658:ASN:HB3	2.37	0.40
1:C:15:LEU:HD12	1:C:15:LEU:HA	1.91	0.40
1:E:235:LYS:HD3	1:E:237:TYR:CZ	2.56	0.40
1:E:519:ARG:HE	1:E:519:ARG:HB2	1.72	0.40
1:H:15:LEU:O	1:H:19:MET:HG2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TYR:OH	1:H:543:ASP:O[1_545]	2.13	0.07

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	793/799 (99%)	770 (97%)	21 (3%)	2 (0%)	41	75
1	B	793/799 (99%)	769 (97%)	22 (3%)	2 (0%)	41	75
1	C	793/799 (99%)	772 (97%)	19 (2%)	2 (0%)	41	75
1	D	793/799 (99%)	768 (97%)	23 (3%)	2 (0%)	41	75
1	E	793/799 (99%)	771 (97%)	20 (2%)	2 (0%)	41	75
1	F	785/799 (98%)	764 (97%)	19 (2%)	2 (0%)	41	75
1	G	760/799 (95%)	741 (98%)	18 (2%)	1 (0%)	51	85
1	H	788/799 (99%)	766 (97%)	20 (2%)	2 (0%)	41	75
All	All	6298/6392 (98%)	6121 (97%)	162 (3%)	15 (0%)	47	81

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLY
1	B	406	GLY
1	C	406	GLY
1	D	406	GLY
1	E	406	GLY
1	F	406	GLY
1	G	406	GLY
1	H	406	GLY
1	A	666	LEU

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Mol	Chain	Res	Type
1	B	666	LEU
1	C	666	LEU
1	D	666	LEU
1	E	666	LEU
1	F	666	LEU
1	H	666	LEU

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	676/692 (98%)	668 (99%)	8 (1%)	71	89
1	B	672/692 (97%)	664 (99%)	8 (1%)	71	89
1	C	674/692 (97%)	668 (99%)	6 (1%)	78	92
1	D	674/692 (97%)	668 (99%)	6 (1%)	78	92
1	E	673/692 (97%)	664 (99%)	9 (1%)	69	88
1	F	668/692 (96%)	659 (99%)	9 (1%)	69	88
1	G	648/692 (94%)	642 (99%)	6 (1%)	78	92
1	H	671/692 (97%)	664 (99%)	7 (1%)	76	91
All	All	5356/5536 (97%)	5297 (99%)	59 (1%)	73	90

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	15	LEU
1	A	94	SER
1	A	148	ARG
1	A	231	LEU
1	A	393	LEU
1	A	450	SER
1	A	707	ASP
1	B	10	ASN

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Mol	Chain	Res	Type
1	B	14	ILE
1	B	15	LEU
1	B	231	LEU
1	B	236	SER
1	B	393	LEU
1	B	450	SER
1	B	502	LYS
1	C	14	ILE
1	C	15	LEU
1	C	94	SER
1	C	231	LEU
1	C	393	LEU
1	C	450	SER
1	D	14	ILE
1	D	15	LEU
1	D	94	SER
1	D	231	LEU
1	D	236	SER
1	D	450	SER
1	E	15	LEU
1	E	94	SER
1	E	105	LYS
1	E	231	LEU
1	E	271	ILE
1	E	393	LEU
1	E	450	SER
1	E	502	LYS
1	E	707	ASP
1	F	14	ILE
1	F	15	LEU
1	F	94	SER
1	F	231	LEU
1	F	236	SER
1	F	450	SER
1	F	605	GLU
1	F	772	MET
1	F	773	LYS
1	G	94	SER
1	G	231	LEU
1	G	236	SER
1	G	393	LEU
1	G	450	SER

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Mol	Chain	Res	Type
1	G	773	LYS
1	H	10	ASN
1	H	14	ILE
1	H	231	LEU
1	H	326	TYR
1	H	393	LEU
1	H	450	SER
1	H	771	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	130	GLN
1	C	633	HIS
1	D	130	GLN
1	D	633	HIS
1	E	130	GLN
1	E	633	HIS
1	F	46	GLN
1	F	130	GLN
1	F	633	HIS
1	F	766	GLN
1	G	130	GLN
1	H	130	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 carbohydrates in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95^{th} 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	790/799 (98%)	-0.06	7 (0%) 84 62	24, 50, 84, 112	0
1	B	790/799 (98%)	-0.01	7 (0%) 84 62	29, 51, 87, 121	0
1	C	790/799 (98%)	0.36	26 (3%) 46 20	32, 77, 124, 151	0
1	D	790/799 (98%)	-0.10	3 (0%) 92 78	32, 50, 84, 114	0
1	E	790/799 (98%)	0.09	3 (0%) 92 78	34, 58, 95, 125	0
1	F	782/799 (97%)	0.02	2 (0%) 94 83	30, 52, 79, 107	0
1	G	762/799 (95%)	-0.07	0 100 100	35, 55, 80, 106	0
1	H	790/799 (98%)	0.44	45 (5%) 23 8	45, 96, 185, 209	0
All	All	6284/6392 (98%)	0.08	93 (1%) 73 46	24, 57, 116, 209	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	80	LEU	6.2
1	H	775	ASN	4.9
1	H	463	GLN	4.5
1	H	274	LEU	4.5
1	B	8	PRO	4.4
1	B	4	ILE	4.3
1	H	603	GLY	4.1
1	H	60	LEU	4.1
1	H	94	SER	4.0
1	B	6	ASN	4.0
1	C	768	GLN	4.0
1	H	93	VAL	3.9
1	H	89	LEU	3.8
1	H	644	VAL	3.8
1	B	7	SER	3.8
1	A	6	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	95	VAL	3.7
1	H	604	ALA	3.5
1	H	267	ALA	3.3
1	D	9	GLN	3.2
1	H	287	VAL	3.2
1	H	789	LEU	3.2
1	H	270	PHE	3.2
1	H	753	SER	3.1
1	H	250	PRO	3.1
1	B	9	GLN	3.1
1	H	96	PRO	3.0
1	H	263	ALA	2.9
1	H	235	LYS	2.9
1	C	287	VAL	2.9
1	C	706	LEU	2.9
1	C	331	LEU	2.9
1	H	599	ALA	2.8
1	H	761	THR	2.8
1	C	285	ALA	2.8
1	C	775	ASN	2.8
1	H	224	LEU	2.8
1	A	7	SER	2.7
1	H	69	VAL	2.7
1	C	767	GLN	2.7
1	H	65	ILE	2.6
1	C	787	GLU	2.6
1	C	446	ASN	2.6
1	H	336	SER	2.5
1	C	197	LEU	2.5
1	C	486	ILE	2.5
1	C	7	SER	2.5
1	H	239	PRO	2.5
1	A	3	ASP	2.5
1	C	731	GLN	2.5
1	H	607	ALA	2.5
1	H	792	THR	2.4
1	B	3	ASP	2.4
1	C	724	ALA	2.4
1	H	281	ALA	2.4
1	H	77	LEU	2.4
1	D	5	PHE	2.4
1	A	597[A]	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	597[A]	ALA	2.4
1	A	4	ILE	2.4
1	C	392	ILE	2.4
1	E	3	ASP	2.3
1	F	597[A]	ALA	2.3
1	H	265	VAL	2.3
1	H	57	TYR	2.3
1	H	326	TYR	2.3
1	H	104	PRO	2.3
1	C	772	MET	2.3
1	H	643	GLU	2.3
1	H	261	ALA	2.2
1	A	8	PRO	2.2
1	H	221	PRO	2.2
1	C	383	VAL	2.2
1	C	774	ALA	2.2
1	E	7	SER	2.2
1	C	3	ASP	2.2
1	C	266	LEU	2.1
1	H	440	TRP	2.1
1	A	5	PHE	2.1
1	D	597[A]	ALA	2.1
1	C	194	ASN	2.1
1	H	106	TYR	2.1
1	H	66	PRO	2.1
1	F	595[A]	ASN	2.1
1	C	753	SER	2.1
1	H	58	ARG	2.1
1	H	324	ALA	2.1
1	C	382	LEU	2.0
1	H	757	TRP	2.0
1	C	390	ILE	2.0
1	C	372	ILE	2.0
1	B	10	ASN	2.0
1	C	761	THR	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)

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, 95^{th} 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(Å^2)	Q<0.9
2	K	C	1002	1/1	0.85	0.15	109,109,109,109	0
2	K	H	1002	1/1	0.92	0.21	108,108,108,108	0
2	K	B	1002	1/1	0.94	0.08	74,74,74,74	0
2	K	E	1002	1/1	0.95	0.15	85,85,85,85	0
2	K	F	1002	1/1	0.96	0.16	71,71,71,71	0
2	K	D	1002	1/1	0.97	0.08	67,67,67,67	0
2	K	G	1002	1/1	0.99	0.13	80,80,80,80	0
2	K	A	1002	1/1	0.99	0.13	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.