Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 03:40 am GMT

PDB ID	:	5A97
Title	:	Hazara virus nucleocapsid protain
Authors	:	Surtees, R.; Ariza, A.; Hewson, R.; Barr, J.N.; Edwards, T.A.
Deposited on	:	2015-07-17
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 (i) 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 (1)) were used in the production of this report:

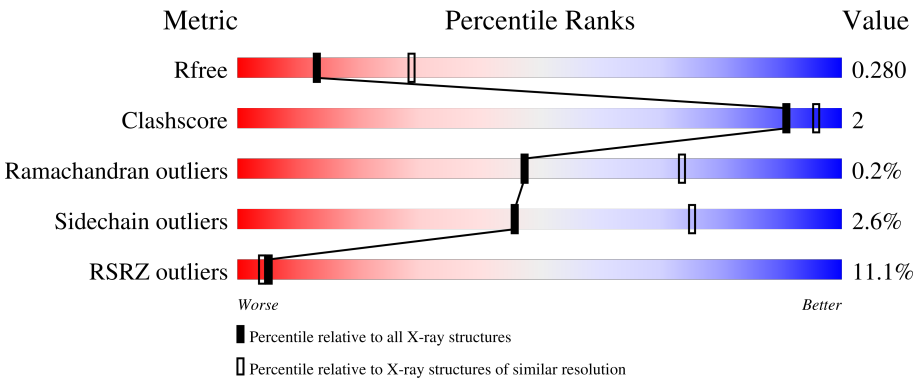
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	489	34% 92% 5% •
1	B	489	% 93% 5% •
1	C	489	5% 94% • •
1	D	489	3% 92% 5% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15226 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 NUCLEOCAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	473	3760	2393	641	708	18	0	3	0
1	B	477	3800	2416	648	718	18	0	6	0
1	C	479	3808	2421	653	716	18	0	5	0
1	D	477	3788	2408	648	714	18	0	4	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PRO	-	expression tag	UNP M4PWE6
A	-2	LEU	-	expression tag	UNP M4PWE6
A	-1	GLY	-	expression tag	UNP M4PWE6
A	0	SER	-	expression tag	UNP M4PWE6
B	-3	PRO	-	expression tag	UNP M4PWE6
B	-2	LEU	-	expression tag	UNP M4PWE6
B	-1	GLY	-	expression tag	UNP M4PWE6
B	0	SER	-	expression tag	UNP M4PWE6
C	-3	PRO	-	expression tag	UNP M4PWE6
C	-2	LEU	-	expression tag	UNP M4PWE6
C	-1	GLY	-	expression tag	UNP M4PWE6
C	0	SER	-	expression tag	UNP M4PWE6
D	-3	PRO	-	expression tag	UNP M4PWE6
D	-2	LEU	-	expression tag	UNP M4PWE6
D	-1	GLY	-	expression tag	UNP M4PWE6
D	0	SER	-	expression tag	UNP M4PWE6

- Molecule 2 is water.

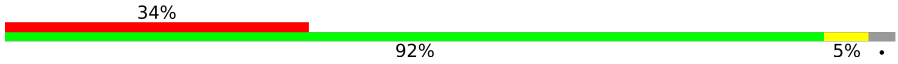
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	6	6	6	0	0
			Total	O		
2	B	26	26	26	0	0
			Total	O		
2	C	24	24	24	0	0
			Total	O		
2	D	14	14	14	0	0

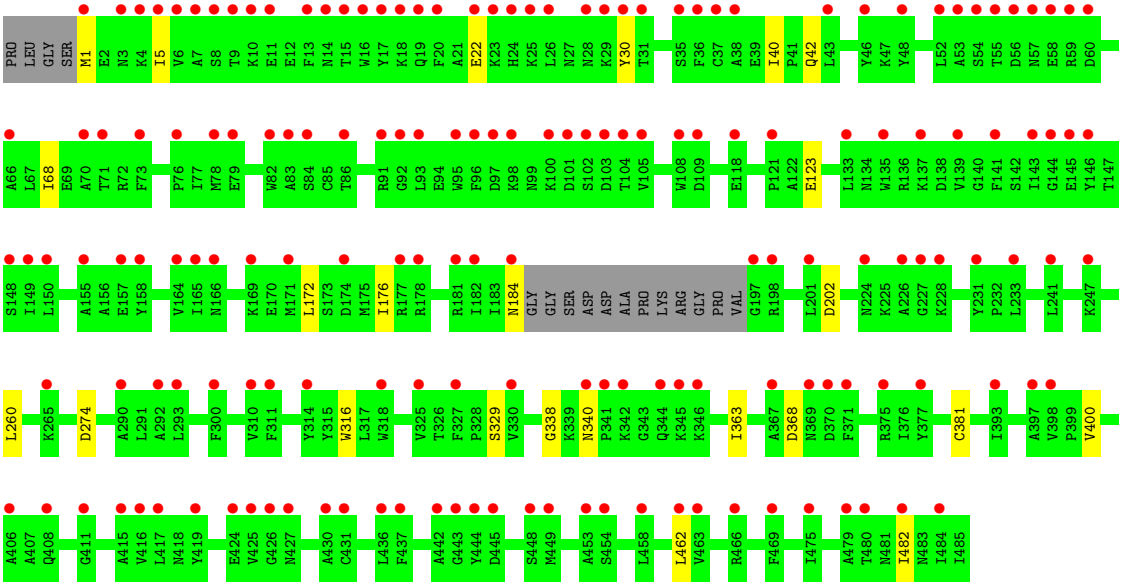
3 Residue-property plots (i)

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: NUCLEOCAPSID PROTEIN

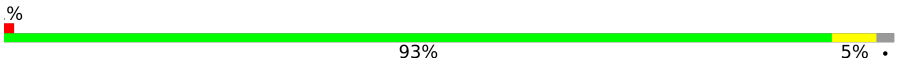
Chain A:

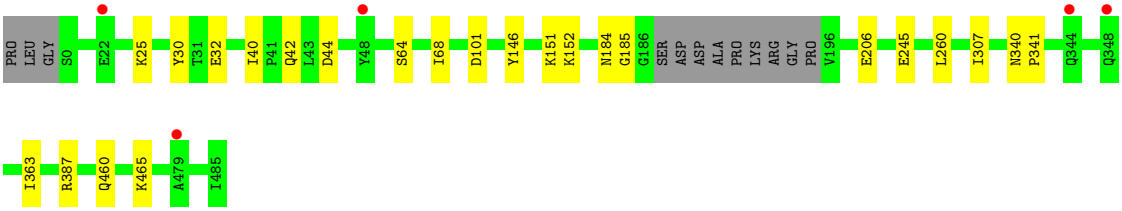




• Molecule 1: NUCLEOCAPSID PROTEIN

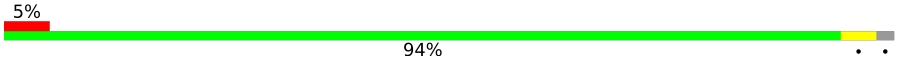
Chain B:

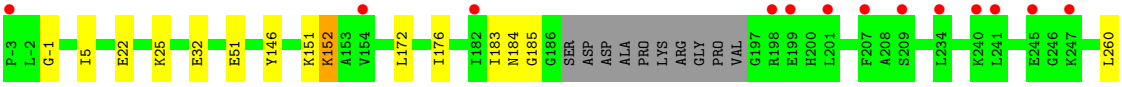




• Molecule 1: NUCLEOCAPSID PROTEIN

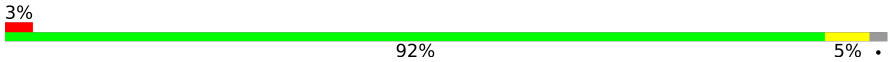
Chain C:

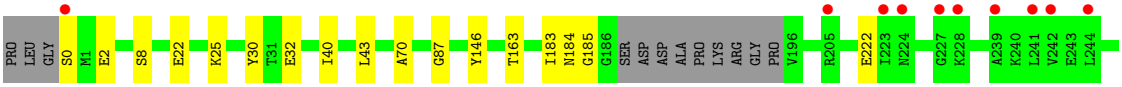


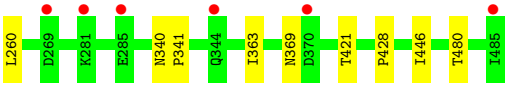


- Molecule 1: NUCLEOCAPSID PROTEIN

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.99Å 76.10Å 449.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.64 – 2.70 74.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (224.64-2.70) 98.5 (74.88-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.242 , 0.282 0.242 , 0.280	Depositor DCC
R_{free} test set	3125 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15226	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 (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	0.39	0/3842	0.52	0/5185
1	B	0.38	0/3885	0.56	0/5242
1	C	0.39	0/3891	0.58	0/5249
1	D	0.39	0/3867	0.56	0/5218
All	All	0.38	0/15485	0.56	0/20894

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	-1	GLY	Peptide

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	3760	0	3760	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3800	0	3796	20	0
1	C	3808	0	3809	13	0
1	D	3788	0	3784	13	0
2	A	6	0	0	0	0
2	B	26	0	0	0	0
2	C	24	0	0	0	0
2	D	14	0	0	0	0
All	All	15226	0	15149	52	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 2.

All (52) 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:B:184[B]:ASN:CB	1:B:185[B]:GLY:HA3	1.27	1.47
1:C:184[B]:ASN:CB	1:C:185[B]:GLY:HA3	1.31	1.42
1:D:184[B]:ASN:CB	1:D:185[B]:GLY:HA3	1.21	1.42
1:D:184[B]:ASN:CB	1:D:185[B]:GLY:CA	2.11	1.29
1:D:184[B]:ASN:HB2	1:D:185[B]:GLY:CA	1.66	1.21
1:B:184[B]:ASN:CB	1:B:185[B]:GLY:CA	2.17	1.20
1:C:184[B]:ASN:HB3	1:C:185[B]:GLY:CA	1.73	1.19
1:C:184[B]:ASN:CB	1:C:185[B]:GLY:CA	2.21	1.17
1:D:184[B]:ASN:HB3	1:D:185[B]:GLY:HA3	1.21	1.16
1:C:184[B]:ASN:HB2	1:C:185[B]:GLY:HA3	1.26	1.10
1:B:184[B]:ASN:HB3	1:B:185[B]:GLY:HA3	1.09	1.09
1:B:184[B]:ASN:HB2	1:B:185[B]:GLY:CA	1.80	1.05
1:B:184[B]:ASN:HB2	1:B:185[B]:GLY:HA3	1.03	1.01
1:C:184[B]:ASN:HB3	1:C:185[B]:GLY:HA3	0.92	0.91
1:D:184[B]:ASN:HB3	1:D:185[B]:GLY:CA	1.90	0.89
1:B:184[B]:ASN:HB3	1:B:185[B]:GLY:CA	1.89	0.89
1:C:151[B]:LYS:O	1:C:152[B]:LYS:HB2	1.70	0.89
1:D:184[B]:ASN:HB2	1:D:185[B]:GLY:HA3	0.82	0.81
1:C:151[B]:LYS:O	1:C:152[B]:LYS:CB	2.29	0.79
1:B:206[B]:GLU:HA	1:B:206[B]:GLU:OE1	1.84	0.78
1:B:151[B]:LYS:O	1:B:152[B]:LYS:CB	2.40	0.69
1:B:151[B]:LYS:O	1:B:152[B]:LYS:HB2	1.93	0.68
1:C:184[B]:ASN:HB2	1:C:185[B]:GLY:CA	2.05	0.67
1:B:151[B]:LYS:H	1:B:152[B]:LYS:HE3	1.64	0.62
1:B:151[B]:LYS:C	1:B:152[B]:LYS:HG3	2.25	0.57
1:D:43:LEU:HD11	1:D:70:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HD12	1:A:400:VAL:HG12	1.89	0.55
1:B:151[B]:LYS:C	1:B:152[B]:LYS:CG	2.76	0.52
1:B:30:TYR:CD1	1:B:40:ILE:HD11	2.45	0.52
1:B:307:ILE:HD11	1:B:387:ARG:NE	2.28	0.49
1:B:206[B]:GLU:OE1	1:B:206[B]:GLU:CA	2.58	0.48
1:D:183:ILE:O	1:D:184[A]:ASN:HB2	2.13	0.48
1:D:8:SER:HA	1:D:87:GLY:HA3	1.95	0.48
1:B:64:SER:O	1:B:68:ILE:HG12	2.15	0.47
1:A:316:TRP:NE1	1:A:381:CYS:O	2.46	0.46
1:C:5:ILE:HD12	1:C:400:VAL:HG12	1.98	0.45
1:D:32:GLU:HG3	1:D:146:TYR:OH	2.17	0.44
1:D:30:TYR:CD1	1:D:40:ILE:HD11	2.52	0.44
1:A:172:LEU:O	1:A:176:ILE:HG12	2.18	0.44
1:B:460:GLN:HE21	1:B:465:LYS:HE2	1.82	0.43
1:C:151[B]:LYS:O	1:C:152[B]:LYS:CG	2.65	0.43
1:D:40:ILE:HD12	1:D:428:PRO:HB3	2.01	0.43
1:A:30:TYR:CD1	1:A:40:ILE:HD11	2.54	0.43
1:D:184[A]:ASN:HA	1:D:185[A]:GLY:HA2	1.59	0.42
1:C:183:ILE:O	1:C:184[A]:ASN:HB2	2.20	0.41
1:A:462:LEU:HD22	1:A:482:ILE:HG21	2.02	0.41
1:B:32:GLU:HG3	1:B:146:TYR:OH	2.20	0.41
1:C:32:GLU:HG3	1:C:146:TYR:CZ	2.56	0.41
1:B:151[B]:LYS:O	1:B:152[B]:LYS:CG	2.69	0.41
1:C:172:LEU:O	1:C:176:ILE:HG12	2.21	0.40
1:B:32:GLU:HG3	1:B:146:TYR:CZ	2.55	0.40
1:A:68:ILE:HD12	1:A:338:GLY:O	2.22	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	472/489 (96%)	464 (98%)	8 (2%)	0	100	100
1	B	479/489 (98%)	462 (96%)	16 (3%)	1 (0%)	47	73
1	C	480/489 (98%)	468 (98%)	9 (2%)	3 (1%)	25	50
1	D	477/489 (98%)	464 (97%)	12 (2%)	1 (0%)	47	73
All	All	1908/1956 (98%)	1858 (97%)	45 (2%)	5 (0%)	47	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	152[A]	LYS
1	C	152[B]	LYS
1	C	341	PRO
1	B	341	PRO
1	D	341	PRO

5.3.2 Protein sidechains (i)

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	401/409 (98%)	388 (97%)	13 (3%)	39	68
1	B	405/409 (99%)	397 (98%)	8 (2%)	55	81
1	C	405/409 (99%)	397 (98%)	8 (2%)	55	81
1	D	403/409 (98%)	390 (97%)	13 (3%)	39	68
All	All	1614/1636 (99%)	1572 (97%)	42 (3%)	46	75

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	22	GLU
1	A	42	GLN
1	A	123	GLU
1	A	184	ASN
1	A	202	ASP

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Mol	Chain	Res	Type
1	A	260	LEU
1	A	274[A]	ASP
1	A	274[B]	ASP
1	A	329	SER
1	A	340	ASN
1	A	363	ILE
1	A	368	ASP
1	B	25	LYS
1	B	42	GLN
1	B	44	ASP
1	B	101	ASP
1	B	245	GLU
1	B	260	LEU
1	B	340	ASN
1	B	363	ILE
1	C	22	GLU
1	C	25	LYS
1	C	51	GLU
1	C	260	LEU
1	C	340	ASN
1	C	363	ILE
1	C	370	ASP
1	C	421	THR
1	D	0	SER
1	D	2	GLU
1	D	22	GLU
1	D	25	LYS
1	D	163	THR
1	D	222	GLU
1	D	260	LEU
1	D	340	ASN
1	D	363	ILE
1	D	369	ASN
1	D	421	THR
1	D	446	ILE
1	D	480	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	344	GLN

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Mol	Chain	Res	Type
1	A	460	GLN
1	B	57	ASN
1	B	166	ASN
1	B	167	ASN
1	B	344	GLN
1	B	460	GLN
1	C	57	ASN
1	C	344	GLN
1	C	369	ASN
1	D	42	GLN
1	D	57	ASN
1	D	166	ASN
1	D	344	GLN
1	D	460	GLN

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	473/489 (96%)	1.83	168 (35%)	0	0	75, 136, 191, 246	0
1	B	477/489 (97%)	0.14	5 (1%)	82	83	42, 61, 87, 144	0
1	C	479/489 (97%)	0.32	23 (4%)	30	28	35, 62, 110, 140	0
1	D	477/489 (97%)	0.26	16 (3%)	45	45	45, 71, 120, 147	0
All	All	1906/1956 (97%)	0.63	212 (11%)	5	4	35, 73, 162, 246	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	SER	17.9
1	A	7	ALA	13.1
1	A	5	ILE	10.2
1	A	416	VAL	8.6
1	A	54	SER	8.5
1	A	425	VAL	8.2
1	A	419	TYR	8.0
1	C	480	THR	7.6
1	A	16	TRP	7.4
1	A	479	ALA	7.3
1	A	141	PHE	7.3
1	A	17	TYR	7.2
1	A	93	LEU	7.1
1	A	38	ALA	6.7
1	A	52	LEU	6.3
1	A	103	ASP	6.3
1	A	78	MET	6.1
1	A	13	PHE	6.0
1	A	158	TYR	5.9
1	A	327	PHE	5.9
1	A	444	TYR	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	20	PHE	5.8
1	A	139	VAL	5.8
1	A	415	ALA	5.8
1	A	6	VAL	5.7
1	A	36	PHE	5.6
1	A	96	PHE	5.4
1	A	293	LEU	5.3
1	A	443	GLY	5.3
1	A	73	PHE	5.2
1	C	-3	PRO	5.2
1	A	482	ILE	5.1
1	C	479	ALA	5.1
1	A	398	VAL	5.1
1	A	137	LYS	5.0
1	A	442	ALA	4.9
1	A	449	MET	4.9
1	A	231	TYR	4.8
1	A	22	GLU	4.8
1	A	370	ASP	4.8
1	A	427	ASN	4.7
1	C	198	ARG	4.7
1	A	466	ARG	4.6
1	A	411	GLY	4.5
1	A	95	TRP	4.5
1	D	0	SER	4.4
1	A	18	LYS	4.4
1	A	57	ASN	4.4
1	A	37	CYS	4.4
1	A	102	SER	4.4
1	A	82	TRP	4.4
1	A	171	MET	4.4
1	A	445	ASP	4.4
1	A	24	HIS	4.3
1	A	424	GLU	4.2
1	A	133	LEU	4.2
1	C	154	VAL	4.1
1	A	10	LYS	4.1
1	A	228	LYS	4.1
1	A	417	LEU	4.0
1	A	150	LEU	4.0
1	C	265	LYS	4.0
1	A	56	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	25	LYS	3.9
1	A	145	GLU	3.8
1	D	370	ASP	3.8
1	D	285	GLU	3.8
1	A	148	SER	3.8
1	A	166	ASN	3.7
1	A	178	ARG	3.7
1	A	310	VAL	3.7
1	A	11	GLU	3.7
1	A	43	LEU	3.7
1	A	325	VAL	3.6
1	A	371	PHE	3.5
1	A	426	GLY	3.5
1	A	469	PHE	3.5
1	A	342	LYS	3.5
1	A	92	GLY	3.4
1	A	105	VAL	3.4
1	A	144	GLY	3.4
1	A	53	ALA	3.4
1	A	169	LYS	3.4
1	A	292	ALA	3.3
1	C	478	ASN	3.3
1	A	345	LYS	3.3
1	A	14	ASN	3.3
1	A	397	ALA	3.3
1	B	48	TYR	3.2
1	C	269	ASP	3.2
1	A	30	TYR	3.2
1	A	35	SER	3.2
1	A	330	VAL	3.1
1	B	479	ALA	3.1
1	A	454	SER	3.1
1	D	344	GLN	3.1
1	A	58	GLU	3.1
1	A	143	ILE	3.1
1	A	31	THR	3.1
1	A	157	GLU	3.1
1	A	318	TRP	3.1
1	A	475	ILE	3.0
1	A	118	GLU	2.9
1	A	377	TYR	2.9
1	D	269	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	431	CYS	2.9
1	A	66	ALA	2.9
1	A	375	ARG	2.9
1	A	55	THR	2.9
1	A	91	ARG	2.9
1	A	1	MET	2.9
1	A	174	ASP	2.9
1	A	70	ALA	2.8
1	A	104	THR	2.8
1	A	224	ASN	2.8
1	C	481	ASN	2.8
1	A	101	ASP	2.8
1	A	314	TYR	2.8
1	A	184	ASN	2.8
1	A	165	ILE	2.8
1	A	86	THR	2.7
1	A	484	ILE	2.7
1	A	60	ASP	2.7
1	C	241	LEU	2.7
1	A	369	ASN	2.7
1	A	48	TYR	2.7
1	A	29	LYS	2.7
1	A	340	ASN	2.6
1	D	227	GLY	2.6
1	A	437	PHE	2.6
1	A	155	ALA	2.6
1	C	270	GLN	2.6
1	A	3	ASN	2.6
1	A	4	LYS	2.6
1	A	23	LYS	2.5
1	A	98	LYS	2.5
1	B	22	GLU	2.5
1	A	453	ALA	2.5
1	C	266	GLU	2.5
1	A	71	THR	2.5
1	C	182	ILE	2.5
1	A	458	LEU	2.5
1	C	245	GLU	2.5
1	A	83	ALA	2.5
1	A	226	ALA	2.5
1	A	430	ALA	2.5
1	A	164	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	463	VAL	2.5
1	A	247	LYS	2.5
1	A	462	LEU	2.5
1	D	224	ASN	2.5
1	C	234	LEU	2.4
1	A	84	SER	2.4
1	C	199	GLU	2.4
1	A	406	ALA	2.4
1	A	100	LYS	2.4
1	A	265	LYS	2.4
1	A	76	PRO	2.4
1	A	28	ASN	2.4
1	A	290	ALA	2.4
1	D	485	ILE	2.4
1	A	241	LEU	2.3
1	A	367	ALA	2.3
1	A	393	ILE	2.3
1	A	436	LEU	2.3
1	A	135	TRP	2.3
1	A	26	LEU	2.3
1	A	300	PHE	2.3
1	A	311	PHE	2.3
1	B	348	GLN	2.3
1	D	242	VAL	2.3
1	A	79	GLU	2.3
1	A	233	LEU	2.3
1	A	181	ARG	2.3
1	A	448	SER	2.3
1	A	346	LYS	2.3
1	A	46	TYR	2.3
1	A	59	ARG	2.3
1	A	177	ARG	2.3
1	C	277	GLU	2.2
1	C	247	LYS	2.2
1	A	121	PRO	2.2
1	A	198	ARG	2.2
1	A	15	THR	2.2
1	A	182	ILE	2.2
1	A	341	PRO	2.2
1	D	228	LYS	2.2
1	D	223	ILE	2.2
1	A	146	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	ILE	2.1
1	D	205	ARG	2.1
1	A	97	ASP	2.1
1	D	281	LYS	2.1
1	A	108	TRP	2.1
1	A	480	THR	2.1
1	A	109	ASP	2.1
1	B	344	GLN	2.1
1	A	201	LEU	2.1
1	D	239	ALA	2.1
1	C	207	PHE	2.1
1	D	241	LEU	2.1
1	C	484	ILE	2.1
1	A	227	GLY	2.1
1	A	19	GLN	2.0
1	C	201	LEU	2.0
1	D	244	LEU	2.0
1	C	240	LYS	2.0
1	A	344	GLN	2.0
1	A	197	GLY	2.0
1	A	408	GLN	2.0
1	C	209	SER	2.0
1	A	9	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 monosaccharides 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.