Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2024 – 08:11 pm BST

PDB ID	:	7QPB
Title	:	Catalytic C-lobe of the HECT-type ubiquitin ligase E6AP in complex with a hybrid foldamer-peptide macrocycle
Authors	:	Dengler, S.; Howard, R.T.; Morozov, V.; Tsiamantas, C.; Douat, C.; Suga, H.; Huc, I.
Deposited on	:	2022-01-03
Resolution	:	2.34 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:

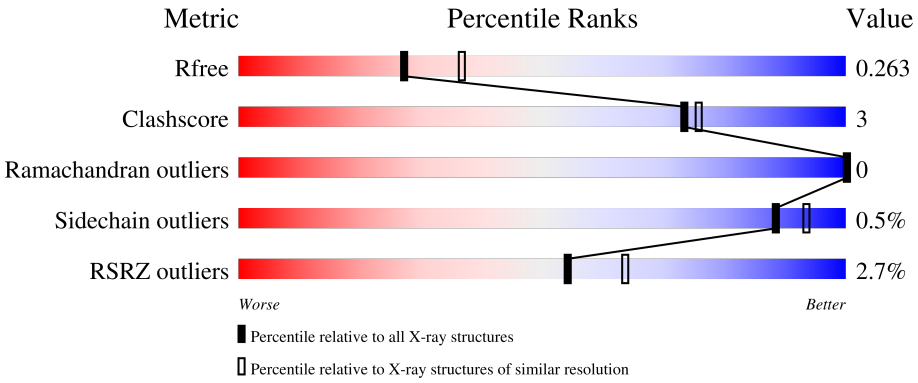
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	114	84% 9% 7%
1	B	114	3% 84% 9% 7%
1	C	114	3% 85% 8% 7%
1	D	114	5% 86% 5% 9%
2	H	15	20% 67% 13%

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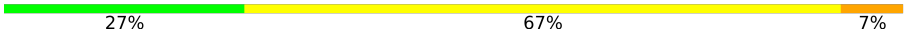
Mol	Chain	Length	Quality of chain
2	I	15	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3753 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 Isoform I of Ubiquitin-protein ligase E3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	0	1	0
			862	552	145	163	2			
1	B	106	Total	C	N	O	S	0	0	0
			854	547	142	163	2			
1	C	106	Total	C	N	O	S	0	0	0
			849	544	139	164	2			
1	D	104	Total	C	N	O	S	0	0	0
			825	529	135	159	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	739	GLY	-	expression tag	UNP Q05086
A	740	PRO	-	expression tag	UNP Q05086
B	739	GLY	-	expression tag	UNP Q05086
B	740	PRO	-	expression tag	UNP Q05086
C	739	GLY	-	expression tag	UNP Q05086
C	740	PRO	-	expression tag	UNP Q05086
D	739	GLY	-	expression tag	UNP Q05086
D	740	PRO	-	expression tag	UNP Q05086

- Molecule 2 is a protein called hybrid foldamer-peptide macrocycle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	15	Total	C	N	O	S	0	0	0
			153	105	27	20	1			
2	I	15	Total	C	N	O	S	0	0	0
			153	105	27	20	1			

- Molecule 3 is water.

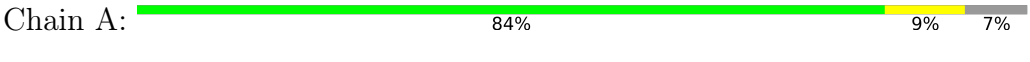
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	4	Total O 4 4	0	0
3	C	16	Total O 16 16	0	0
3	D	14	Total O 14 14	0	0
3	H	1	Total O 1 1	0	0

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.

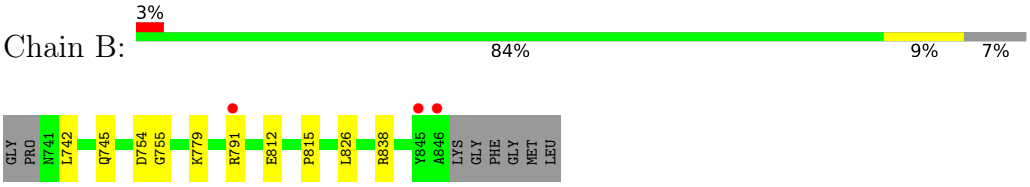
• Molecule 1: Isoform I of Ubiquitin-protein ligase E3A

Chain A:



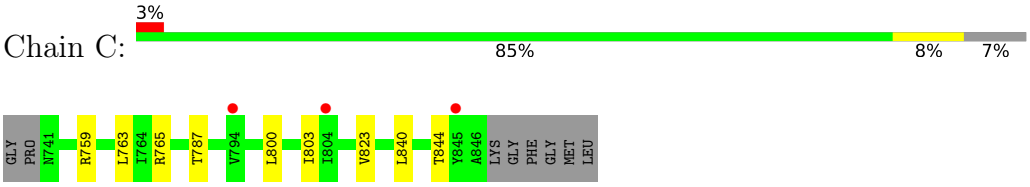
• Molecule 1: Isoform I of Ubiquitin-protein ligase E3A

Chain B:



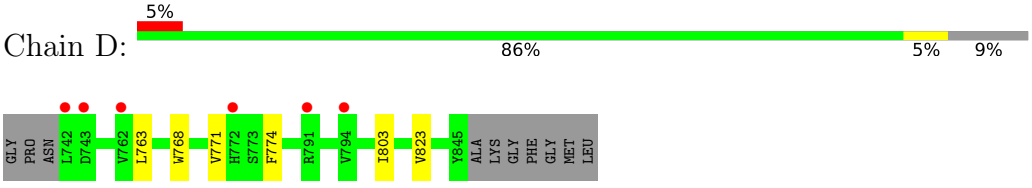
• Molecule 1: Isoform I of Ubiquitin-protein ligase E3A

Chain C:



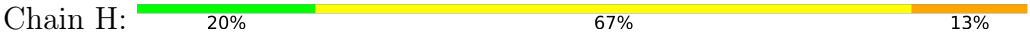
• Molecule 1: Isoform I of Ubiquitin-protein ligase E3A

Chain D:



• Molecule 2: hybrid foldamer-peptide macrocycle

Chain H:



• Molecule 2: hybrid foldamer-peptide macrocycle

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	149.91Å 59.05Å 67.30Å 90.00° 95.47° 90.00°	Depositor
Resolution (Å)	29.53 – 2.34 29.53 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.53-2.34) 98.4 (29.53-2.34)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.215 , 0.263 0.216 , 0.263	Depositor DCC
R_{free} test set	1225 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3753	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.01% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: 9JC, ZY9, GM1, CCS, 9JV

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	0.28	0/879	0.42	0/1186
1	B	0.31	0/871	0.46	0/1176
1	C	0.25	0/866	0.43	0/1171
1	D	0.25	0/841	0.42	0/1137
2	H	2.83	11/93 (11.8%)	1.04	0/124
2	I	2.81	10/93 (10.8%)	1.09	0/124
All	All	0.69	21/3643 (0.6%)	0.48	0/4918

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
2	H	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	8	ARG	NE-CZ	11.05	1.47	1.33
2	I	8	ARG	NE-CZ	11.00	1.47	1.33
2	H	8	ARG	C-N	7.44	1.51	1.34
2	I	8	ARG	C-N	7.30	1.50	1.34
2	I	6	PHE	C-N	7.23	1.50	1.34
2	H	6	PHE	C-N	7.20	1.50	1.34
2	H	9	TYR	C-N	6.96	1.50	1.34
2	I	9	TYR	C-N	6.87	1.49	1.34
2	H	11	TYR	C-N	6.77	1.49	1.34
2	I	11	TYR	C-N	6.72	1.49	1.34
2	H	12	GLN	C-N	6.72	1.49	1.34
2	I	12	GLN	C-N	6.68	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	7	TRP	C-N	6.47	1.49	1.34
2	I	7	TRP	C-N	6.39	1.48	1.34
2	H	5	GLY	C-N	6.19	1.48	1.34
2	I	5	GLY	C-N	6.12	1.48	1.34
2	H	8	ARG	CZ-NH2	-5.92	1.25	1.33
2	I	8	ARG	CZ-NH2	-5.81	1.25	1.33
2	H	12	GLN	CD-NE2	5.67	1.47	1.32
2	I	12	GLN	CD-NE2	5.65	1.47	1.32
2	H	10	VAL	C-N	5.04	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	3	ZY9	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	862	0	864	5	0
1	B	854	0	852	7	0
1	C	849	0	838	8	0
1	D	825	0	814	4	0
2	H	153	0	93	2	0
2	I	153	0	93	2	0
3	A	22	0	0	0	0
3	B	4	0	0	0	0
3	C	16	0	0	0	0
3	D	14	0	0	0	0
3	H	1	0	0	0	0
All	All	3753	0	3554	24	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 3.

All (24) 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:C:803:ILE:HB	1:C:823:VAL:HG22	1.72	0.71
1:D:803:ILE:HD12	2:I:9:TYR:HB2	1.84	0.59
1:C:763:LEU:C	1:C:763:LEU:HD13	2.25	0.58
1:C:763:LEU:HD13	1:C:763:LEU:O	2.04	0.57
1:D:768:TRP:HA	1:D:771:VAL:HG22	1.91	0.51
1:D:771:VAL:HG12	1:D:774:PHE:CE2	2.45	0.51
1:B:754:ASP:OD1	1:B:755:GLY:N	2.44	0.51
1:B:742:LEU:HD13	1:B:779:LYS:HD2	1.92	0.51
1:C:759:ARG:O	1:C:765:ARG:NH1	2.43	0.50
1:B:812:GLU:O	1:B:838:ARG:NH1	2.42	0.49
1:D:823:VAL:HG21	2:I:9:TYR:CE1	2.48	0.49
1:A:770:ILE:HD11	1:A:832[A]:LYS:HG3	1.96	0.47
1:B:742:LEU:HD13	1:B:779:LYS:CD	2.45	0.47
1:A:741:ASN:HB2	1:A:792:ALA:HB2	1.97	0.46
1:A:812:GLU:O	1:A:838:ARG:NH1	2.46	0.46
1:A:815:PRO:HB3	1:A:826:LEU:HD12	2.00	0.43
1:A:814:LEU:HD21	1:A:841:LYS:HD3	2.00	0.42
1:C:840:LEU:O	1:C:844:THR:HG23	2.19	0.42
1:B:742:LEU:HD12	1:B:742:LEU:O	2.19	0.42
1:C:823:VAL:HG21	2:H:9:TYR:CE2	2.55	0.41
1:C:823:VAL:HG21	2:H:9:TYR:CD2	2.56	0.41
1:C:787:THR:HG21	1:C:800:LEU:HD13	2.03	0.40
1:B:791:ARG:HA	1:B:791:ARG:HD3	1.93	0.40
1:B:815:PRO:HB3	1:B:826:LEU:HD12	2.02	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	105/114 (92%)	103 (98%)	2 (2%)	0	100	100
1	B	104/114 (91%)	100 (96%)	4 (4%)	0	100	100
1	C	104/114 (91%)	102 (98%)	2 (2%)	0	100	100
1	D	102/114 (90%)	100 (98%)	2 (2%)	0	100	100
2	H	9/15 (60%)	9 (100%)	0	0	100	100
2	I	9/15 (60%)	9 (100%)	0	0	100	100
All	All	433/486 (89%)	423 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	94/99 (95%)	94 (100%)	0	100	100
1	B	93/99 (94%)	92 (99%)	1 (1%)	73	83
1	C	92/99 (93%)	92 (100%)	0	100	100
1	D	89/99 (90%)	88 (99%)	1 (1%)	73	83
2	H	8/8 (100%)	8 (100%)	0	100	100
2	I	8/8 (100%)	8 (100%)	0	100	100
All	All	384/412 (93%)	382 (100%)	2 (0%)	88	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	745	GLN
1	D	763	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	9JC	I	2	2	16,16,17	2.18	3 (18%)	19,22,24	1.72	3 (15%)
2	CCS	H	14	2	7,8,10	0.74	0	3,8,12	1.13	0
2	ZY9	I	1	2	10,10,11	2.32	2 (20%)	11,12,14	1.70	3 (27%)
2	ZY9	I	3	2	10,10,11	2.35	2 (20%)	11,12,14	1.69	2 (18%)
2	CCS	I	14	2	7,8,10	0.73	0	3,8,12	1.20	0
2	9JV	I	4	2	16,16,17	2.20	4 (25%)	19,22,24	2.30	5 (26%)
2	9JC	H	2	2	16,16,17	2.22	3 (18%)	19,22,24	1.63	3 (15%)
2	ZY9	H	3	2	10,10,11	2.32	2 (20%)	11,12,14	1.62	2 (18%)
2	ZY9	H	1	2	10,10,11	2.37	2 (20%)	11,12,14	1.65	2 (18%)
2	9JV	H	4	2	16,16,17	2.24	3 (18%)	19,22,24	2.30	5 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9JC	I	2	2	-	3/4/4/6	0/2/2/2
2	CCS	H	14	2	-	1/4/7/10	-
2	ZY9	I	1	2	-	1/4/4/6	0/1/1/1
2	ZY9	I	3	2	-	0/4/4/6	0/1/1/1
2	CCS	I	14	2	-	1/4/7/10	-
2	9JV	I	4	2	-	0/4/4/6	0/2/2/2
2	9JC	H	2	2	-	3/4/4/6	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZY9	H	3	2	-	0/4/4/6	0/1/1/1
2	ZY9	H	1	2	-	1/4/4/6	0/1/1/1
2	9JV	H	4	2	-	0/4/4/6	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	4	9JV	CA-C	7.33	1.56	1.48
2	I	4	9JV	CA-C	7.10	1.56	1.48
2	H	2	9JC	CA-C	7.07	1.56	1.48
2	I	2	9JC	CA-C	7.00	1.56	1.48
2	H	1	ZY9	CA-C	6.80	1.55	1.48
2	I	1	ZY9	CA-C	6.68	1.55	1.48
2	I	3	ZY9	CA-C	5.33	1.54	1.48
2	H	3	ZY9	CA-C	5.25	1.54	1.48
2	I	3	ZY9	C2-C7	4.68	1.57	1.51
2	H	3	ZY9	C2-C7	4.60	1.57	1.51
2	H	2	9JC	C100-N	3.20	1.48	1.38
2	I	2	9JC	C100-N	3.18	1.48	1.38
2	H	4	9JV	O15-C76	2.96	1.42	1.36
2	I	4	9JV	O15-C76	2.91	1.41	1.36
2	H	2	9JC	C95-C94	2.46	1.41	1.37
2	I	4	9JV	C82-N	2.41	1.46	1.38
2	H	1	ZY9	C2-C7	2.33	1.54	1.51
2	H	4	9JV	C82-N	2.33	1.45	1.38
2	I	2	9JC	C95-C94	2.29	1.41	1.37
2	I	1	ZY9	C2-C7	2.13	1.54	1.51
2	I	4	9JV	C80-C81	-2.06	1.37	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	4	9JV	O15-C76-C80	7.19	121.49	114.46
2	H	4	9JV	O15-C76-C80	7.17	121.47	114.46
2	H	2	9JC	CA-N4-C99	4.35	121.41	118.11
2	I	2	9JC	C-CA-N4	4.30	118.88	114.66
2	I	4	9JV	CA-N2-C81	4.17	121.27	118.11
2	I	2	9JC	CA-N4-C99	4.17	121.27	118.11
2	H	4	9JV	CA-N2-C81	4.03	121.16	118.11
2	H	2	9JC	C-CA-N4	3.77	118.36	114.66
2	I	3	ZY9	O-C-CA	-3.67	120.75	124.22
2	I	1	ZY9	O-C-CA	-3.48	120.93	124.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	9JC	O-C-CA	-3.29	121.11	124.22
2	H	3	ZY9	O-C-CA	-3.20	121.19	124.22
2	H	1	ZY9	O-C-CA	-3.11	121.27	124.22
2	H	2	9JC	O-C-CA	-3.10	121.28	124.22
2	H	4	9JV	C-CA-N2	2.98	117.58	114.66
2	H	4	9JV	O-C-CA	-2.86	121.51	124.22
2	I	3	ZY9	CA-N11-C7	2.81	122.45	118.41
2	H	3	ZY9	CA-N11-C7	2.80	122.44	118.41
2	I	4	9JV	O-C-CA	-2.79	121.58	124.22
2	I	4	9JV	C-CA-N2	2.52	117.13	114.66
2	I	4	9JV	C103-O15-C76	-2.51	114.23	117.75
2	H	1	ZY9	CA-N11-C7	2.48	121.98	118.41
2	H	4	9JV	C103-O15-C76	-2.36	114.45	117.75
2	I	1	ZY9	CA-N11-C7	2.27	121.68	118.41
2	I	1	ZY9	C2-C7-N11	2.00	119.30	115.89

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	ZY9	N-C2-C7-N11
2	H	2	9JC	O-C-CA-C95
2	H	2	9JC	N5-C93-C94-C98
2	I	2	9JC	O-C-CA-C95
2	I	2	9JC	O-C-CA-N4
2	I	2	9JC	N5-C93-C94-C98
2	H	1	ZY9	N-C2-C7-N11
2	H	2	9JC	O-C-CA-N4
2	H	14	CCS	N-CA-CB-SG
2	I	14	CCS	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

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

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	106/114 (92%)	-0.01	0 100 100	36, 47, 62, 74	0
1	B	106/114 (92%)	0.20	3 (2%) 53 63	38, 54, 71, 79	0
1	C	106/114 (92%)	0.13	3 (2%) 53 63	38, 51, 72, 81	0
1	D	104/114 (91%)	0.38	6 (5%) 23 32	41, 56, 74, 82	0
2	H	9/15 (60%)	0.26	0 100 100	40, 41, 54, 56	0
2	I	9/15 (60%)	0.28	0 100 100	39, 44, 57, 57	0
All	All	440/486 (90%)	0.18	12 (2%) 54 64	36, 52, 72, 82	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	845	TYR	3.3
1	B	846	ALA	3.2
1	D	791	ARG	3.1
1	B	791	ARG	2.9
1	D	762	VAL	2.8
1	D	742	LEU	2.7
1	B	845	TYR	2.5
1	D	772	HIS	2.3
1	C	794	VAL	2.2
1	D	794	VAL	2.2
1	D	743	ASP	2.1
1	C	804	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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	9JV	I	4	15/16	0.92	0.16	39,42,51,53	0
2	ZY9	I	1	10/11	0.93	0.17	37,40,44,47	0
2	9JC	H	2	15/16	0.93	0.15	35,42,50,50	0
2	ZY9	I	3	10/11	0.93	0.17	36,39,48,55	0
2	9JV	H	4	15/16	0.93	0.14	36,41,45,45	0
2	ZY9	H	1	10/11	0.93	0.18	33,36,40,45	0
2	9JC	I	2	15/16	0.96	0.13	34,41,48,51	0
2	CCS	H	14	9/11	0.96	0.12	30,40,45,46	0
2	CCS	I	14	9/11	0.96	0.12	32,39,45,48	0
2	ZY9	H	3	10/11	0.97	0.14	32,37,39,47	0

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.