Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 05:09 AM EST

PDB ID	:	7RY2
Title	:	mSandy2
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Deposited on	:	2021-08-24
Resolution	:	2.05 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:

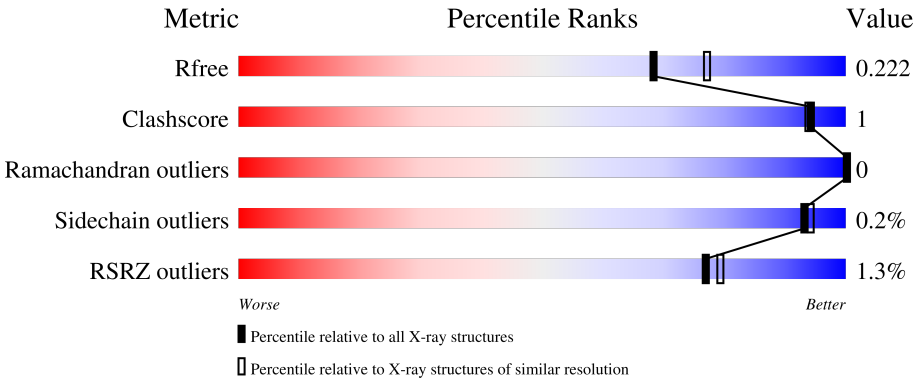
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	242	86% · 11%
1	B	242	86% · 11%
1	C	242	88% · 11%
1	D	242	87% · 11%
1	F	242	88% · 11%

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Mol	Chain	Length	Quality of chain
1	G	242	2% 85% 11%
2	E	242	% 82% 7% 11%
2	H	242	2% 86% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28461 atoms, of which 13724 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 mSandy2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	H	N	O	S	0	11	0
			3514	1133	1736	297	337	11			
1	B	215	Total	C	H	N	O	S	0	9	0
			3477	1123	1716	293	335	10			
1	C	216	Total	C	H	N	O	S	0	10	0
			3485	1128	1717	296	333	11			
1	D	215	Total	C	H	N	O	S	0	6	0
			3455	1118	1706	294	327	10			
1	F	216	Total	C	H	N	O	S	0	5	0
			3442	1114	1696	290	332	10			
1	G	215	Total	C	H	N	O	S	0	8	0
			3492	1125	1727	298	332	10			

- Molecule 2 is a protein called mSandy2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	216	Total	C	H	N	O	S	0	9	0
			3486	1126	1722	294	334	10			
2	H	214	Total	C	H	N	O	S	0	9	0
			3458	1118	1704	294	332	10			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	93	Total	O	0	0
			93	93		
3	B	99	Total	O	0	0
			99	99		
3	C	89	Total	O	0	0
			89	89		
3	D	73	Total	O	0	0
			73	73		

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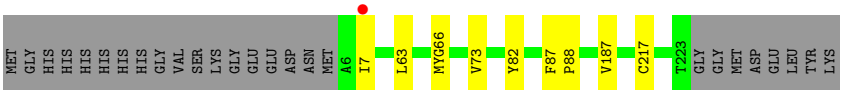
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	103	Total O 103 103	0	0
3	F	100	Total O 100 100	0	0
3	G	46	Total O 46 46	0	0
3	H	49	Total O 49 49	0	0

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: mSandy2

Chain A:

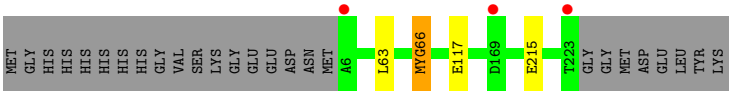


- Molecule 1: mSandy2

Chain B:

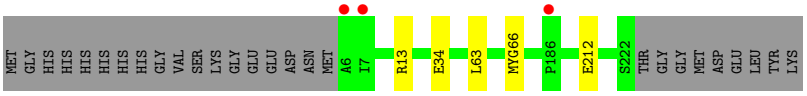
- Molecule 1: mSandy2

Chain C:



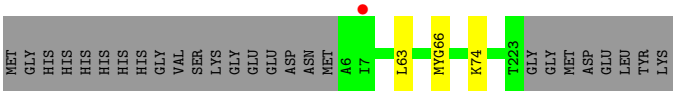
- Molecule 1: mSandy2

Chain D:



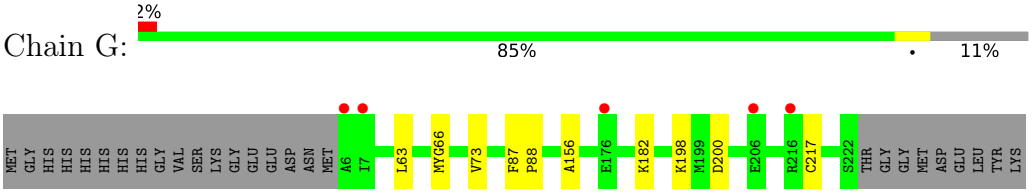
- Molecule 1: mSandy2

Chain F:



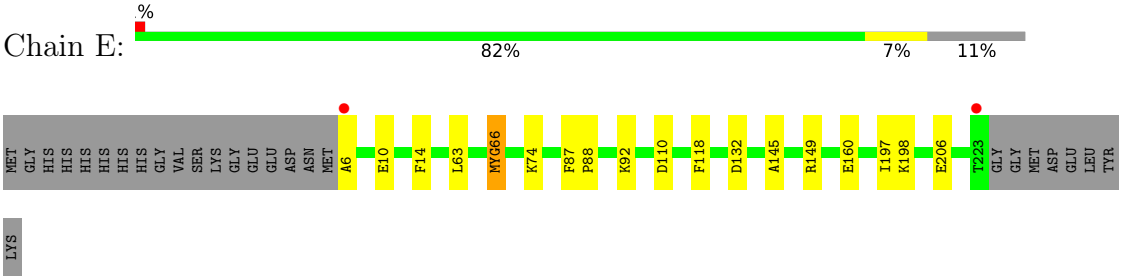
• Molecule 1: mSandy2

Chain G:



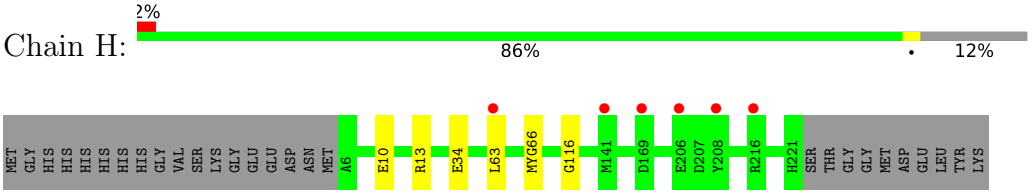
• Molecule 2: mSandy2

Chain E:



• Molecule 2: mSandy2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.68Å 147.21Å 240.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.50 – 2.05 80.31 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (70.50-2.05) 99.7 (80.31-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.190 , 0.223 0.189 , 0.222	Depositor DCC
R_{free} test set	6672 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 35.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	28461	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: NRQ, CH6

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	0.26	0/1843	0.48	0/2475
1	B	0.26	0/1822	0.48	0/2449
1	C	0.26	0/1839	0.48	0/2472
1	D	0.26	0/1798	0.48	0/2417
1	F	0.26	0/1788	0.48	0/2406
1	G	0.25	0/1819	0.46	0/2444
2	E	0.25	0/1829	0.48	0/2461
2	H	0.26	0/1805	0.47	0/2428
All	All	0.26	0/14543	0.48	0/19552

There are no bond length outliers.

There are no bond angle outliers.

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	1778	1736	1691	5	0
1	B	1761	1716	1678	5	0
1	C	1768	1717	1662	3	0
1	D	1749	1706	1679	3	0
1	F	1746	1696	1677	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1765	1727	1698	6	0
2	E	1764	1722	1685	9	1
2	H	1754	1704	1679	3	0
3	A	93	0	0	0	0
3	B	99	0	0	2	0
3	C	89	0	0	1	0
3	D	73	0	0	1	0
3	E	103	0	0	2	0
3	F	100	0	0	1	0
3	G	46	0	0	0	0
3	H	49	0	0	1	0
All	All	14737	13724	13449	36	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 1.

All (36) 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)
2:H:116:GLY:O	3:H:301:HOH:O	2.04	0.74
1:B:94[B]:GLU:OE1	3:B:301:HOH:O	2.10	0.69
2:E:10:GLU:OE1	3:E:301:HOH:O	2.14	0.64
1:C:117:GLU:OE1	3:C:301:HOH:O	2.15	0.64
1:C:63[B]:LEU:H	1:C:63[B]:LEU:HD23	1.62	0.63
1:G:198:LYS:NZ	1:G:200:ASP:OD1	2.33	0.62
1:D:212:GLU:OE1	3:D:301:HOH:O	2.16	0.60
1:D:13:ARG:NH1	1:D:34:GLU:OE1	2.37	0.57
2:E:92[A]:LYS:NZ	2:E:110:ASP:OD2	2.22	0.57
1:F:74:LYS:NZ	3:F:302:HOH:O	2.38	0.56
2:H:63[B]:LEU:HD23	2:H:63[B]:LEU:H	1.71	0.55
2:H:13:ARG:NH1	2:H:34:GLU:OE1	2.41	0.54
1:A:63[B]:LEU:H	1:A:63[B]:LEU:HD23	1.72	0.54
1:D:63[B]:LEU:HD23	1:D:63[B]:LEU:H	1.74	0.53
2:E:149:ARG:NH2	2:E:160:GLU:OE1	2.41	0.51
2:E:6:ALA:N	3:E:303:HOH:O	2.44	0.51
2:E:63[B]:LEU:H	2:E:63[B]:LEU:HD23	1.74	0.51
1:G:63[B]:LEU:HD23	1:G:63[B]:LEU:H	1.77	0.49
1:B:138:LYS:NZ	3:B:308:HOH:O	2.49	0.46
1:A:82:TYR:CD1	1:A:187:VAL:HG23	2.51	0.45
2:E:145:ALA:HB2	2:E:198:LYS:HD3	1.99	0.45
2:E:66:NRQ:CD2	2:E:197:ILE:HG21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:73:VAL:HG13	1:G:217[B]:CYS:SG	2.57	0.44
1:B:66:CH6:N2	1:B:215:GLU:OE2	2.51	0.44
1:F:63[B]:LEU:H	1:F:63[B]:LEU:HD23	1.83	0.42
1:B:87:PHE:HB3	1:B:88:PRO:HA	2.02	0.42
1:A:73:VAL:HG22	1:A:217[B]:CYS:SG	2.60	0.41
2:E:87:PHE:HB3	2:E:88:PRO:HA	2.03	0.41
1:G:87:PHE:HB3	1:G:88:PRO:HA	2.03	0.41
1:C:66:CH6:N2	1:C:215:GLU:OE2	2.53	0.41
1:G:73:VAL:HG22	1:G:217[B]:CYS:SG	2.61	0.41
1:A:7:ILE:HD12	1:A:7:ILE:H	1.86	0.41
1:G:156:ALA:HB2	1:G:182:LYS:HD3	2.04	0.40
1:B:63[B]:LEU:HD23	1:B:63[B]:LEU:H	1.86	0.40
1:A:87:PHE:HB3	1:A:88:PRO:HA	2.04	0.40
2:E:14:PHE:HB3	2:E:118:PHE:HB2	2.02	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)
2:E:74:LYS:HZ2	2:E:132:ASP:OD2[4_554]	1.56	0.04

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	222/242 (92%)	218 (98%)	4 (2%)	0	100	100
1	B	219/242 (90%)	216 (99%)	3 (1%)	0	100	100
1	C	221/242 (91%)	217 (98%)	4 (2%)	0	100	100
1	D	216/242 (89%)	211 (98%)	5 (2%)	0	100	100
1	F	216/242 (89%)	212 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	218/242 (90%)	213 (98%)	5 (2%)	0	100	100
2	E	220/242 (91%)	215 (98%)	5 (2%)	0	100	100
2	H	218/242 (90%)	214 (98%)	4 (2%)	0	100	100
All	All	1750/1936 (90%)	1716 (98%)	34 (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	193/204 (95%)	193 (100%)	0	100	100
1	B	191/204 (94%)	190 (100%)	1 (0%)	88	89
1	C	190/204 (93%)	190 (100%)	0	100	100
1	D	186/204 (91%)	186 (100%)	0	100	100
1	F	187/204 (92%)	187 (100%)	0	100	100
1	G	190/204 (93%)	190 (100%)	0	100	100
2	E	191/204 (94%)	190 (100%)	1 (0%)	88	89
2	H	188/204 (92%)	187 (100%)	1 (0%)	88	89
All	All	1516/1632 (93%)	1513 (100%)	3 (0%)	93	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	213	GLN
2	E	206	GLU
2	H	10	GLU

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 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	$\#\|Z\| > 2$
1	CH6	B	66	1	24,24,25	2.71	8 (33%)	28,32,34	3.12	9 (32%)
1	CH6	C	66	1	24,24,25	2.72	8 (33%)	28,32,34	3.06	7 (25%)
1	CH6	F	66	1	24,24,25	2.73	7 (29%)	28,32,34	2.83	10 (35%)
2	NRQ	H	66	2	23,24,25	2.45	8 (34%)	23,32,34	3.02	8 (34%)
1	CH6	D	66	1	24,24,25	2.67	8 (33%)	28,32,34	2.96	10 (35%)
1	CH6	G	66	1	24,24,25	2.70	8 (33%)	28,32,34	2.98	8 (28%)
1	CH6	A	66	1	24,24,25	2.69	8 (33%)	28,32,34	2.98	8 (28%)
2	NRQ	E	66	2	23,24,25	2.47	8 (34%)	23,32,34	3.14	8 (34%)

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
1	CH6	B	66	1	-	3/12/31/32	0/2/2/2
1	CH6	C	66	1	-	3/12/31/32	0/2/2/2
1	CH6	F	66	1	-	5/12/31/32	0/2/2/2
2	NRQ	H	66	2	-	4/9/31/32	0/2/2/2
1	CH6	D	66	1	-	4/12/31/32	0/2/2/2
1	CH6	G	66	1	-	5/12/31/32	0/2/2/2
1	CH6	A	66	1	-	3/12/31/32	0/2/2/2
2	NRQ	E	66	2	-	3/9/31/32	0/2/2/2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CH6	C1-N2	7.89	1.43	1.32
1	C	66	CH6	C1-N2	7.82	1.43	1.32
1	F	66	CH6	C1-N2	7.80	1.43	1.32
1	D	66	CH6	C1-N2	7.68	1.43	1.32
1	G	66	CH6	C1-N2	7.66	1.43	1.32
1	A	66	CH6	C1-N2	7.39	1.43	1.32
1	F	66	CH6	CA2-C2	6.01	1.54	1.48
2	H	66	NRQ	CA2-C2	5.90	1.54	1.48
2	E	66	NRQ	CA2-C2	5.85	1.54	1.48
1	C	66	CH6	CA2-C2	5.79	1.54	1.48
1	A	66	CH6	CA2-C2	5.73	1.54	1.48
1	G	66	CH6	CA2-C2	5.66	1.54	1.48
1	A	66	CH6	C1-N3	5.58	1.46	1.37
1	B	66	CH6	CA2-C2	5.44	1.54	1.48
1	G	66	CH6	C1-N3	5.43	1.46	1.37
1	C	66	CH6	C1-N3	5.39	1.46	1.37
1	B	66	CH6	C1-N3	5.38	1.46	1.37
1	D	66	CH6	C1-N3	5.36	1.46	1.37
2	E	66	NRQ	C1-N3	5.34	1.47	1.38
1	D	66	CH6	CA2-C2	5.26	1.53	1.48
2	H	66	NRQ	C1-N3	5.25	1.47	1.38
1	F	66	CH6	C1-N3	5.22	1.46	1.37
2	H	66	NRQ	C1-N2	4.58	1.43	1.33
2	E	66	NRQ	C1-N2	4.45	1.43	1.33
2	E	66	NRQ	C2-N3	3.84	1.48	1.39
1	C	66	CH6	C2-N3	3.74	1.48	1.39
1	G	66	CH6	C2-N3	3.74	1.48	1.39
1	F	66	CH6	C2-N3	3.70	1.48	1.39
2	H	66	NRQ	C2-N3	3.68	1.48	1.39
1	B	66	CH6	C2-N3	3.66	1.48	1.39
1	A	66	CH6	C2-N3	3.65	1.48	1.39
2	E	66	NRQ	CB2-CA2	-3.65	1.32	1.35
1	D	66	CH6	C2-N3	3.58	1.48	1.39
1	A	66	CH6	CG2-CB2	3.55	1.53	1.46
1	F	66	CH6	CG2-CB2	3.52	1.53	1.46
1	G	66	CH6	CG2-CB2	3.51	1.53	1.46
2	E	66	NRQ	CG2-CB2	3.46	1.53	1.46
2	H	66	NRQ	CG2-CB2	3.44	1.53	1.46
1	C	66	CH6	CG2-CB2	3.42	1.53	1.46
1	B	66	CH6	CG2-CB2	3.41	1.53	1.46
1	D	66	CH6	CB2-CA2	-3.41	1.32	1.35
2	H	66	NRQ	CB2-CA2	-3.35	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	CH6	CG2-CB2	3.31	1.53	1.46
1	A	66	CH6	CB2-CA2	-3.29	1.32	1.35
1	B	66	CH6	CB2-CA2	-3.10	1.32	1.35
1	C	66	CH6	CB2-CA2	-2.97	1.32	1.35
1	F	66	CH6	CB2-CA2	-2.94	1.32	1.35
1	G	66	CH6	CB2-CA2	-2.90	1.32	1.35
1	F	66	CH6	CA2-N2	2.54	1.44	1.38
1	D	66	CH6	CA2-N2	2.50	1.43	1.38
1	B	66	CH6	CA2-N2	2.44	1.43	1.38
1	G	66	CH6	CA2-N2	2.44	1.43	1.38
1	A	66	CH6	CA2-N2	2.39	1.43	1.38
1	C	66	CH6	CA2-N2	2.33	1.43	1.38
2	H	66	NRQ	CA2-N2	2.22	1.43	1.38
2	E	66	NRQ	CA2-N2	2.17	1.43	1.38
1	B	66	CH6	O2-C2	-2.15	1.18	1.23
2	H	66	NRQ	O2-C2	-2.15	1.18	1.23
1	C	66	CH6	O2-C2	-2.14	1.18	1.23
2	E	66	NRQ	O2-C2	-2.10	1.18	1.23
1	D	66	CH6	O2-C2	-2.07	1.18	1.23
1	A	66	CH6	O2-C2	-2.07	1.18	1.23
1	G	66	CH6	O2-C2	-2.07	1.18	1.23

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	CH6	O2-C2-CA2	-9.85	125.43	130.96
1	D	66	CH6	O2-C2-CA2	-9.10	125.85	130.96
1	C	66	CH6	O2-C2-CA2	-9.09	125.86	130.96
2	H	66	NRQ	CA2-C2-N3	9.00	107.63	103.37
1	C	66	CH6	CA2-C2-N3	8.86	107.56	103.37
1	B	66	CH6	CA2-C2-N3	8.80	107.53	103.37
2	E	66	NRQ	CA2-C2-N3	8.77	107.52	103.37
1	A	66	CH6	CA2-C2-N3	8.59	107.43	103.37
2	E	66	NRQ	O2-C2-CA2	-8.56	126.15	130.96
1	G	66	CH6	CA2-C2-N3	8.55	107.41	103.37
1	G	66	CH6	O2-C2-CA2	-8.47	126.21	130.96
1	A	66	CH6	O2-C2-CA2	-8.28	126.31	130.96
1	D	66	CH6	CA2-C2-N3	8.10	107.20	103.37
2	H	66	NRQ	O2-C2-CA2	-7.95	126.50	130.96
1	F	66	CH6	CA2-C2-N3	7.83	107.07	103.37
1	F	66	CH6	O2-C2-CA2	-7.81	126.57	130.96
2	E	66	NRQ	CG2-CB2-CA2	-5.64	123.03	129.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	CH6	C2-N3-C1	-5.63	105.11	107.97
1	B	66	CH6	C2-N3-C1	-5.03	105.42	107.97
1	C	66	CH6	C2-N3-C1	-5.02	105.42	107.97
1	G	66	CH6	CA2-N2-C1	4.93	109.40	105.77
1	C	66	CH6	CA2-N2-C1	4.73	109.25	105.77
2	H	66	NRQ	CG2-CB2-CA2	-4.60	124.30	129.94
1	D	66	CH6	C2-N3-C1	-4.57	105.65	107.97
1	G	66	CH6	C2-N3-C1	-4.52	105.68	107.97
1	F	66	CH6	C2-N3-C1	-4.17	105.86	107.97
1	F	66	CH6	CA2-N2-C1	4.14	108.82	105.77
1	B	66	CH6	CA2-N2-C1	4.10	108.80	105.77
1	G	66	CH6	CG2-CB2-CA2	-3.97	125.07	129.94
1	A	66	CH6	CA2-N2-C1	3.95	108.68	105.77
1	C	66	CH6	CG2-CB2-CA2	-3.84	125.24	129.94
1	A	66	CH6	CG2-CB2-CA2	-3.77	125.33	129.94
1	D	66	CH6	CA2-N2-C1	3.76	108.54	105.77
1	G	66	CH6	C2-CA2-N2	-3.74	106.31	108.93
1	C	66	CH6	C2-CA2-N2	-3.72	106.33	108.93
1	F	66	CH6	CA1-C1-N3	-3.55	120.23	124.85
1	D	66	CH6	CG2-CB2-CA2	-3.43	125.75	129.94
2	H	66	NRQ	C2-CA2-N2	-3.35	106.59	108.93
1	D	66	CH6	CA1-C1-N3	-3.29	120.56	124.85
1	B	66	CH6	C2-CA2-N2	-3.27	106.64	108.93
2	E	66	NRQ	C2-CA2-N2	-3.24	106.66	108.93
1	F	66	CH6	C2-CA2-N2	-3.22	106.68	108.93
1	B	66	CH6	O3-C3-CA3	-3.17	116.81	126.39
1	F	66	CH6	CG2-CB2-CA2	-3.17	126.06	129.94
1	C	66	CH6	O3-C3-CA3	-3.16	116.85	126.39
1	F	66	CH6	O3-C3-CA3	-3.14	116.90	126.39
1	A	66	CH6	C2-CA2-N2	-3.12	106.75	108.93
1	A	66	CH6	O3-C3-CA3	-3.05	117.17	126.39
2	H	66	NRQ	O3-C3-CA3	-2.95	117.47	126.39
1	D	66	CH6	O3-C3-CA3	-2.91	117.59	126.39
1	D	66	CH6	C2-CA2-N2	-2.82	106.96	108.93
2	E	66	NRQ	O3-C3-CA3	-2.80	117.92	126.39
1	F	66	CH6	CE-SD-CG1	2.72	109.75	100.40
1	G	66	CH6	O3-C3-CA3	-2.70	118.23	126.39
1	B	66	CH6	CG2-CB2-CA2	-2.66	126.68	129.94
1	D	66	CH6	CE-SD-CG1	2.65	109.51	100.40
2	E	66	NRQ	CA2-N2-C1	2.63	109.14	104.33
2	H	66	NRQ	CA2-N2-C1	2.56	109.02	104.33
1	G	66	CH6	CE-SD-CG1	2.55	109.16	100.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	CH6	CA1-C1-N3	-2.49	121.60	124.85
2	H	66	NRQ	CE-SD-CG1	2.46	108.86	100.40
2	E	66	NRQ	CB2-CA2-C2	2.45	125.20	122.28
2	E	66	NRQ	CE-SD-CG1	2.36	108.51	100.40
1	B	66	CH6	CE-SD-CG1	2.31	108.33	100.40
1	F	66	CH6	CA1-C1-N2	2.30	128.19	123.56
1	A	66	CH6	CB1-CA1-N1	-2.24	104.29	110.17
1	D	66	CH6	CA1-C1-N2	2.10	127.79	123.56
2	H	66	NRQ	CB2-CA2-C2	2.03	124.70	122.28

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CH6	N2-CA2-CB2-CG2
1	A	66	CH6	C2-CA2-CB2-CG2
1	B	66	CH6	N2-CA2-CB2-CG2
1	B	66	CH6	C2-CA2-CB2-CG2
1	C	66	CH6	CA1-CB1-CG1-SD
1	C	66	CH6	N2-CA2-CB2-CG2
1	C	66	CH6	C2-CA2-CB2-CG2
1	D	66	CH6	N1-CA1-CB1-CG1
1	D	66	CH6	C1-CA1-CB1-CG1
1	D	66	CH6	N2-CA2-CB2-CG2
1	D	66	CH6	C2-CA2-CB2-CG2
1	F	66	CH6	N1-CA1-CB1-CG1
1	F	66	CH6	C1-CA1-CB1-CG1
1	F	66	CH6	N2-CA2-CB2-CG2
1	F	66	CH6	C2-CA2-CB2-CG2
1	G	66	CH6	N1-CA1-CB1-CG1
1	G	66	CH6	N2-CA2-CB2-CG2
1	G	66	CH6	C2-CA2-CB2-CG2
2	E	66	NRQ	C1-CA1-CB1-CG1
2	E	66	NRQ	N2-CA2-CB2-CG2
2	E	66	NRQ	C2-CA2-CB2-CG2
2	H	66	NRQ	C1-CA1-CB1-CG1
2	H	66	NRQ	N2-CA2-CB2-CG2
2	H	66	NRQ	C2-CA2-CB2-CG2
1	G	66	CH6	CB1-CG1-SD-CE
1	G	66	CH6	C1-CA1-CB1-CG1
1	B	66	CH6	CA1-CB1-CG1-SD
2	H	66	NRQ	CA1-CB1-CG1-SD

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Mol	Chain	Res	Type	Atoms
1	F	66	CH6	CA1-CB1-CG1-SD
1	A	66	CH6	C1-CA1-CB1-CG1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	CH6	1	0
1	C	66	CH6	1	0
2	E	66	NRQ	1	0

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	215/242 (88%)	0.42	1 (0%)	91	92	29, 37, 52, 64	0
1	B	214/242 (88%)	0.38	1 (0%)	91	92	30, 39, 53, 69	0
1	C	215/242 (88%)	0.48	3 (1%)	75	78	28, 38, 52, 74	0
1	D	214/242 (88%)	0.52	3 (1%)	75	78	29, 41, 56, 71	0
1	F	215/242 (88%)	0.39	1 (0%)	91	92	32, 40, 53, 73	0
1	G	214/242 (88%)	0.58	5 (2%)	60	64	34, 49, 64, 78	0
2	E	215/242 (88%)	0.40	2 (0%)	84	86	31, 38, 51, 69	0
2	H	213/242 (88%)	0.59	6 (2%)	53	58	32, 50, 65, 76	0
All	All	1715/1936 (88%)	0.47	22 (1%)	77	79	28, 41, 59, 78	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	6	ALA	3.6
2	H	206	GLU	3.3
1	B	7	ILE	3.2
1	D	6	ALA	3.1
2	H	208	TYR	2.9
2	H	141	MET	2.9
1	G	7	ILE	2.9
1	A	7	ILE	2.8
2	E	223	THR	2.7
1	D	7	ILE	2.7
1	G	176	GLU	2.5
1	F	7	ILE	2.5
2	E	6	ALA	2.5
1	G	216[A]	ARG	2.4
1	D	186	PRO	2.2
2	H	169	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	216	ARG	2.2
1	C	6	ALA	2.1
1	C	223	THR	2.1
1	G	206	GLU	2.1
2	H	63[A]	LEU	2.0
1	C	169	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CH6	A	66	23/24	0.85	0.20	33,46,62,66	0
1	CH6	D	66	23/24	0.85	0.21	37,48,64,70	0
2	NRQ	H	66	23/24	0.85	0.21	42,57,72,77	0
1	CH6	F	66	23/24	0.86	0.25	39,49,66,71	0
2	NRQ	E	66	23/24	0.86	0.19	36,46,62,67	0
1	CH6	C	66	23/24	0.86	0.22	35,47,60,65	0
1	CH6	G	66	23/24	0.87	0.21	43,56,69,78	0
1	CH6	B	66	23/24	0.88	0.21	35,47,65,66	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.