



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:16 am GMT

PDB ID : 4FOX
Title : Crystal Structure of Mtb ThyA in complex with dUMP and Raltitrexed
Authors : Reddy, M.C.M.; Bruning, J.B.; Sacchettini, J.C.; Harshbarger, W.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2012-06-21
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

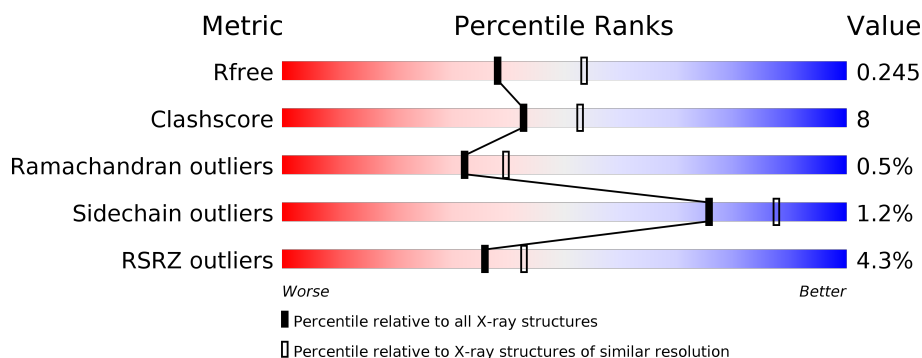
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	<div> <div>9%</div> <div>84% 15%</div> </div>
1	B	263	<div> <div>87% 12%</div> </div>
1	C	263	<div> <div>9%</div> <div>83% 15%</div> </div>
1	D	263	<div> <div>3%</div> <div>87% 13%</div> </div>
1	E	263	<div> <div>2%</div> <div>81% 16%</div> </div>
1	F	263	<div> <div>3%</div> <div>85% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	263	
1	H	263	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	D16	D	301	-	-	X	-
2	D16	F	301	-	-	X	-
2	D16	G	301	-	-	X	-
2	D16	H	301	-	-	X	-
3	UMP	A	302	-	-	-	X

2 Entry composition

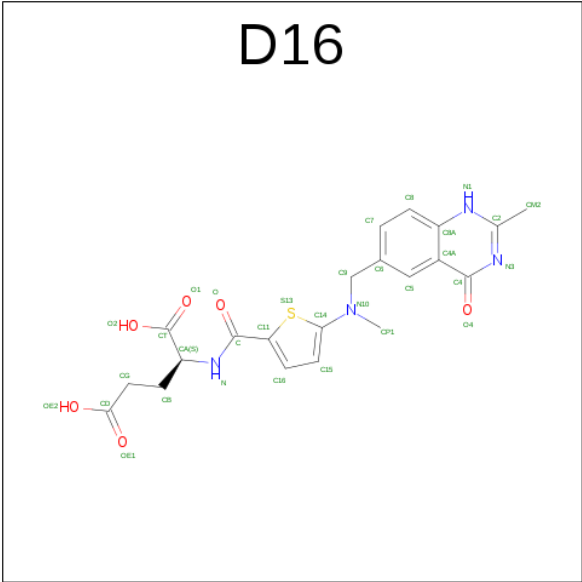
There are 4 unique types of molecules in this entry. The entry contains 17259 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thymidylate synthase.

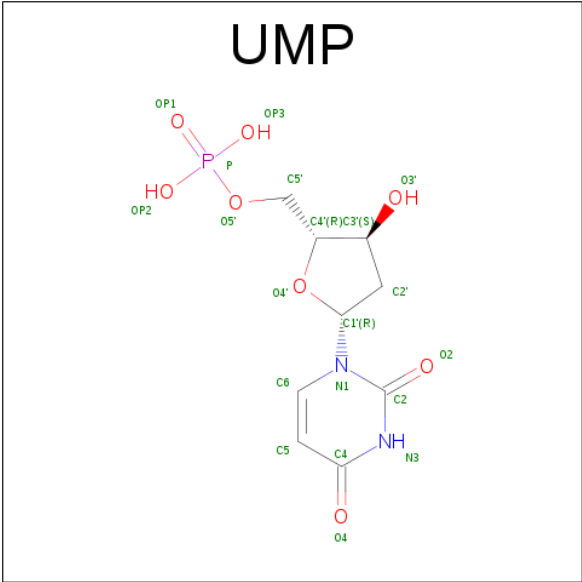
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	1	0
			2093	1347	357	382	7			
1	B	261	Total	C	N	O	S	0	0	0
			2087	1342	357	381	7			
1	C	261	Total	C	N	O	S	0	1	0
			2038	1306	355	370	7			
1	D	263	Total	C	N	O	S	0	0	0
			2085	1345	358	374	8			
1	E	260	Total	C	N	O	S	0	2	0
			2075	1338	356	374	7			
1	F	261	Total	C	N	O	S	0	0	0
			2049	1321	350	371	7			
1	G	260	Total	C	N	O	S	0	0	0
			2058	1323	354	374	7			
1	H	259	Total	C	N	O	S	0	0	0
			2006	1289	354	355	8			

- Molecule 2 is TOMUDEX (three-letter code: D16) (formula: $C_{21}H_{22}N_4O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	B	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	C	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	D	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	E	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	F	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	G	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	H	1	Total	C	N	O	S	0	0
			32	21	4	6	1		

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C₉H₁₃N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	F	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	G	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	H	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	77	Total	O	0	0
			77	77		
4	B	53	Total	O	0	0
			53	53		
4	C	18	Total	O	0	0
			18	18		
4	D	90	Total	O	0	0
			90	90		

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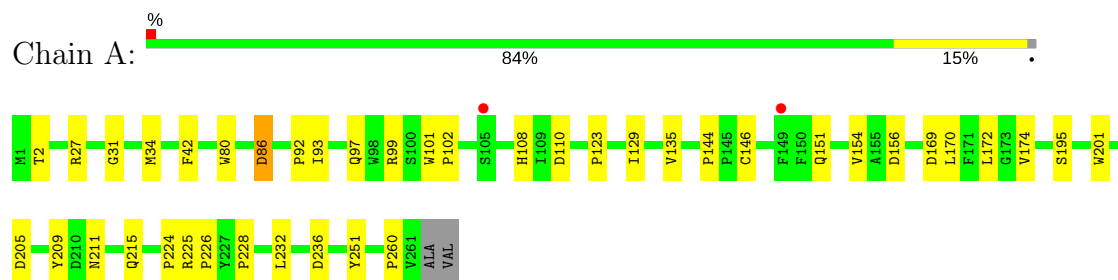
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	35	Total 35	O 35	0	0
4	F	34	Total 34	O 34	0	0
4	G	23	Total 23	O 23	0	0
4	H	22	Total 22	O 22	0	0

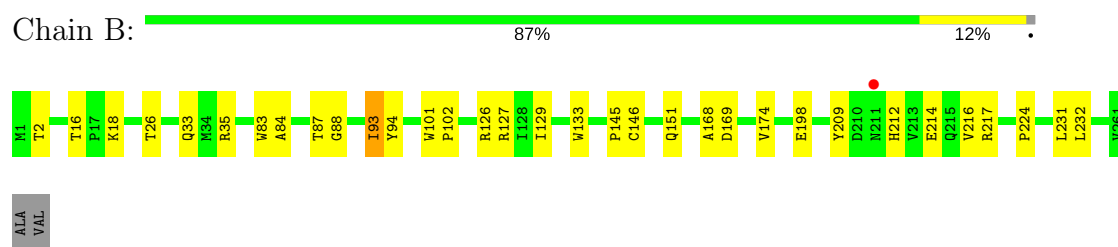
3 Residue-property plots [i](#)

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.

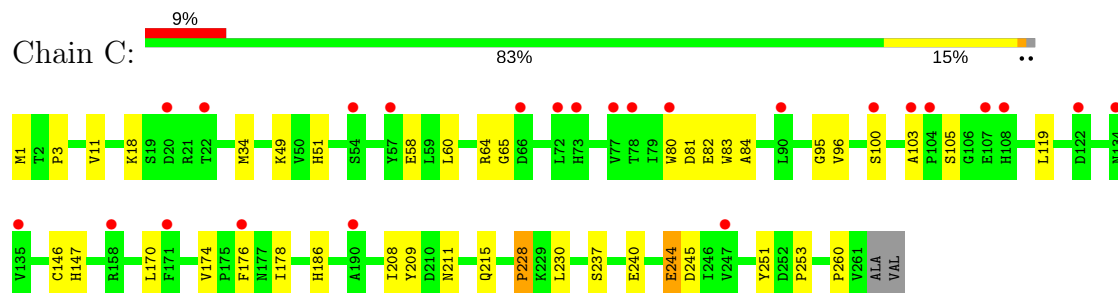
• Molecule 1: Thymidylate synthase



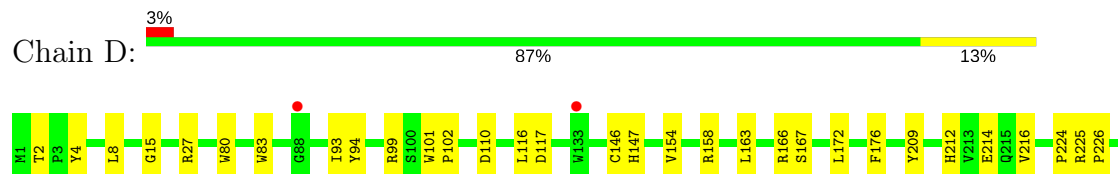
• Molecule 1: Thymidylate synthase

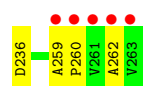


• Molecule 1: Thymidylate synthase

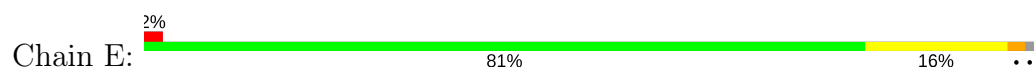


• Molecule 1: Thymidylate synthase

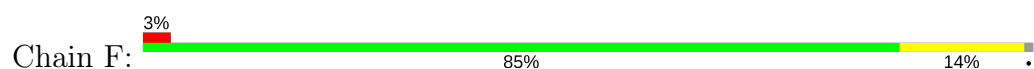




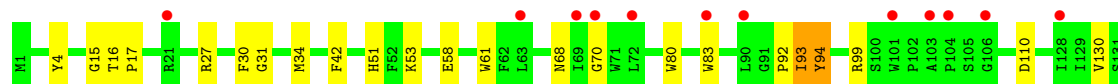
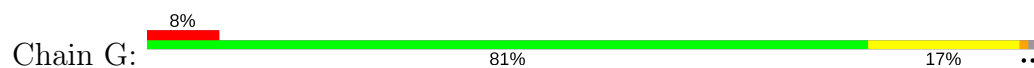
• Molecule 1: Thymidylate synthase



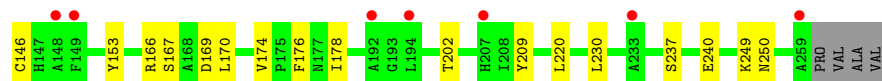
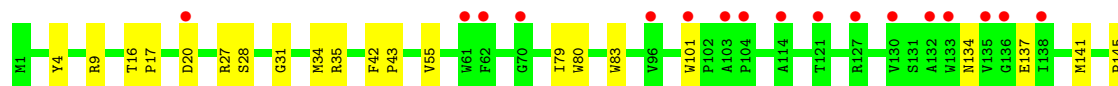
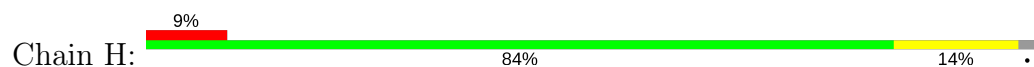
• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.34Å 138.44Å 99.95Å 90.00° 107.00° 90.00°	Depositor
Resolution (Å)	45.01 – 2.30 69.22 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (45.01-2.30) 97.8 (69.22-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.213 , 0.258 0.197 , 0.245	Depositor DCC
R_{free} test set	5133 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17259	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: D16, UMP

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	0.46	0/2160	0.60	0/2945
1	B	0.44	0/2151	0.61	0/2933
1	C	0.39	0/2104	0.56	0/2872
1	D	0.48	0/2149	0.62	0/2933
1	E	0.42	0/2145	0.57	0/2925
1	F	0.41	0/2113	0.57	0/2890
1	G	0.38	0/2122	0.52	0/2897
1	H	0.37	0/2069	0.54	0/2824
All	All	0.42	0/17013	0.58	0/23219

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	2093	0	2017	33	0
1	B	2087	0	2003	29	0
1	C	2038	0	1900	37	0
1	D	2085	0	2005	30	0
1	E	2075	0	1995	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2049	0	1930	27	0
1	G	2058	0	1938	40	0
1	H	2006	0	1860	33	0
2	A	32	0	22	7	0
2	B	32	0	22	6	0
2	C	32	0	22	8	0
2	D	32	0	22	15	0
2	E	32	0	22	7	0
2	F	32	0	22	10	0
2	G	32	0	22	9	0
2	H	32	0	22	15	0
3	A	20	0	11	2	0
3	B	20	0	11	2	0
3	C	20	0	11	1	0
3	D	20	0	11	1	0
3	E	20	0	11	1	0
3	F	20	0	11	3	0
3	G	20	0	11	4	0
3	H	20	0	11	2	0
4	A	77	0	0	3	0
4	B	53	0	0	1	0
4	C	18	0	0	0	0
4	D	90	0	0	2	0
4	E	35	0	0	0	0
4	F	34	0	0	0	0
4	G	23	0	0	1	0
4	H	22	0	0	0	0
All	All	17259	0	15912	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (257) 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:146:CYS:SG	3:A:302:UMP:C6	2.68	0.87
1:B:146:CYS:SG	3:B:301:UMP:C6	2.70	0.85
1:D:146:CYS:SG	3:D:302:UMP:C6	2.76	0.78
1:H:146:CYS:SG	3:H:302:UMP:C6	2.79	0.76
1:A:215:GLN:NE2	1:A:260:PRO:HG3	2.04	0.72
1:E:228:PRO:HG3	1:E:251:TYR:HD1	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:HIS:O	1:B:216:VAL:HG23	1.89	0.71
1:F:146:CYS:SG	3:F:302:UMP:C6	2.84	0.71
1:B:209:TYR:CE2	2:B:302:D16:HM21	2.24	0.71
1:G:92:PRO:HG3	1:G:140:ARG:HH12	1.58	0.69
1:C:60:LEU:O	1:C:64:ARG:HG3	1.93	0.69
1:D:83:TRP:CZ2	2:D:301:D16:H8	2.28	0.68
1:A:209:TYR:CE2	2:A:301:D16:HM21	2.29	0.68
1:F:209:TYR:CE2	2:F:301:D16:HM21	2.29	0.67
1:B:83:TRP:CZ2	2:B:302:D16:H8	2.30	0.67
1:E:228:PRO:HG3	1:E:251:TYR:CD1	2.30	0.67
1:F:83:TRP:NE1	2:F:301:D16:H8	2.09	0.67
1:C:80:TRP:CZ2	2:C:301:D16:H91	2.30	0.67
1:C:251:TYR:CZ	1:C:253:PRO:HG3	2.30	0.66
1:H:83:TRP:CZ2	2:H:301:D16:H8	2.30	0.66
1:C:146:CYS:SG	3:C:302:UMP:C6	2.88	0.66
1:H:209:TYR:CE2	2:H:301:D16:HM21	2.31	0.65
1:G:146:CYS:SG	3:G:302:UMP:C6	2.89	0.65
1:B:214:GLU:OE2	1:G:27:ARG:NH1	2.30	0.64
1:E:146:CYS:SG	3:E:302:UMP:C6	2.90	0.64
1:H:141:MET:SD	1:H:145:PRO:HD3	2.37	0.64
1:C:83:TRP:NE1	2:C:301:D16:H8	2.12	0.63
1:H:80:TRP:CE2	2:H:301:D16:H91	2.34	0.63
1:D:83:TRP:CH2	2:D:301:D16:C8	2.82	0.63
1:E:48[B]:LYS:HE3	1:E:257:ILE:H	1.64	0.62
1:H:176:PHE:CE2	2:H:301:D16:H16	2.34	0.62
1:E:79:ILE:HB	2:E:301:D16:S13	2.40	0.62
1:A:80:TRP:CZ2	2:A:301:D16:H91	2.35	0.61
1:A:27:ARG:HG3	4:A:449:HOH:O	2.00	0.60
1:H:249:LYS:HG2	1:H:250:ASN:OD1	2.01	0.60
1:F:251:TYR:CE2	1:F:253:PRO:HG3	2.38	0.58
1:G:83:TRP:CZ2	2:G:301:D16:H8	2.38	0.58
2:A:301:D16:H5	2:A:301:D16:C14	2.33	0.57
1:D:2:THR:HG21	1:D:224:PRO:HG2	1.86	0.57
1:B:214:GLU:OE1	1:G:217:ARG:NH2	2.35	0.57
1:H:176:PHE:CD1	2:H:301:D16:H15	2.40	0.57
1:A:211:ASN:O	1:A:260:PRO:HG2	2.06	0.56
2:F:301:D16:HP12	3:F:302:UMP:C4	2.41	0.56
1:A:228:PRO:HG3	1:A:251:TYR:CD1	2.41	0.55
1:B:35:ARG:NH1	1:B:198:GLU:OE1	2.39	0.55
1:E:92:PRO:HG3	1:E:140:ARG:NH1	2.21	0.55
1:B:83:TRP:CZ2	2:B:302:D16:C8	2.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:HIS:HB2	1:F:163:LEU:HD11	1.88	0.55
1:E:166:ARG:HG3	1:E:167:SER:N	2.22	0.55
1:A:42:PHE:O	1:A:228:PRO:HD2	2.07	0.54
1:E:158:ARG:HG2	1:E:197:GLY:CA	2.37	0.54
1:C:215:GLN:NE2	1:C:260:PRO:HG3	2.22	0.54
1:F:35:ARG:NH1	1:F:198:GLU:OE1	2.40	0.54
2:G:301:D16:C14	2:G:301:D16:H5	2.37	0.54
1:H:9:ARG:NH2	1:H:220:LEU:HD22	2.23	0.54
1:C:11:VAL:HG12	1:C:208:ILE:HD12	1.89	0.54
1:H:83:TRP:CZ2	2:H:301:D16:C8	2.91	0.53
1:E:209:TYR:CE2	2:E:301:D16:HM21	2.44	0.53
1:B:169:ASP:OD2	2:B:302:D16:N3	2.42	0.53
1:C:81:ASP:HA	1:C:84:ALA:CB	2.39	0.53
1:G:228:PRO:HG3	1:G:251:TYR:CD1	2.44	0.53
1:H:83:TRP:CH2	2:H:301:D16:C8	2.91	0.53
2:F:301:D16:H5	2:F:301:D16:C14	2.38	0.52
1:C:215:GLN:HE22	1:C:260:PRO:HG3	1.74	0.52
2:E:301:D16:H5	2:E:301:D16:C14	2.39	0.52
1:G:209:TYR:CE2	2:G:301:D16:HM21	2.45	0.52
1:B:129:ILE:HD13	1:B:151:GLN:HB2	1.92	0.52
1:B:87:THR:O	1:B:87:THR:HG22	2.08	0.52
1:G:83:TRP:CZ2	2:G:301:D16:C8	2.93	0.52
1:A:169:ASP:OD2	2:A:301:D16:N3	2.43	0.52
1:D:176:PHE:CD1	2:D:301:D16:H15	2.44	0.52
1:E:48[B]:LYS:HE2	1:E:49:LYS:O	2.10	0.52
1:G:147:HIS:CD2	1:G:147:HIS:H	2.26	0.52
1:G:211:ASN:O	1:G:260:PRO:HG2	2.10	0.52
2:G:301:D16:HM23	3:G:302:UMP:H4'	1.92	0.52
1:D:214:GLU:CB	4:D:465:HOH:O	2.57	0.51
1:D:176:PHE:CE2	2:D:301:D16:H16	2.46	0.51
1:G:92:PRO:HG3	1:G:140:ARG:NH1	2.25	0.51
1:A:34:MET:HE2	1:A:201:TRP:CE3	2.46	0.51
1:B:2:THR:HG21	1:B:224:PRO:HG2	1.92	0.51
1:D:80:TRP:CZ2	2:D:301:D16:H91	2.45	0.51
1:H:83:TRP:CE2	2:H:301:D16:H8	2.46	0.51
1:C:211:ASN:O	1:C:260:PRO:HG2	2.10	0.51
1:C:251:TYR:CE2	1:C:253:PRO:HG3	2.45	0.50
1:F:254:HIS:HB3	1:F:255:PRO:CD	2.41	0.50
1:H:80:TRP:CZ2	2:H:301:D16:H91	2.46	0.50
1:D:225:ARG:HB3	1:D:226:PRO:HD2	1.93	0.50
1:E:5:GLU:OE1	1:E:5:GLU:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:PHE:CZ	2:H:301:D16:H16	2.46	0.50
1:C:237:SER:HB3	1:C:240:GLU:HG3	1.94	0.50
1:A:146:CYS:SG	3:A:302:UMP:C5	3.05	0.50
1:A:225:ARG:HB3	1:A:226:PRO:HD2	1.94	0.50
1:D:166:ARG:HG3	1:D:167:SER:N	2.27	0.49
1:D:83:TRP:CZ2	2:D:301:D16:C8	2.95	0.49
1:G:202:THR:HG21	1:H:202:THR:HG21	1.94	0.49
1:G:158:ARG:HG2	1:G:197:GLY:CA	2.43	0.49
1:H:34:MET:CE	1:H:178:ILE:HD11	2.43	0.49
1:B:133:TRP:CZ3	1:B:145:PRO:HD2	2.48	0.49
1:E:83:TRP:NE1	2:E:301:D16:H8	2.28	0.49
1:A:144:PRO:HG2	1:B:127:ARG:HD3	1.94	0.48
1:B:83:TRP:CH2	2:B:302:D16:C8	2.96	0.48
1:C:83:TRP:CE2	2:C:301:D16:H8	2.48	0.48
1:D:102:PRO:HG3	4:D:453:HOH:O	2.12	0.48
1:F:183:LEU:HG	1:F:187:MET:HE3	1.94	0.48
1:F:83:TRP:CE2	2:F:301:D16:H8	2.48	0.48
1:H:79:ILE:HB	2:H:301:D16:S13	2.53	0.48
1:D:176:PHE:CD1	2:D:301:D16:C15	2.97	0.48
1:E:230:LEU:O	1:E:231:LEU:HD23	2.13	0.48
1:A:195:SER:OG	1:D:236:ASP:HB3	2.13	0.48
1:E:105:SER:HB2	1:E:107:GLU:HG2	1.95	0.48
1:E:172:LEU:HA	1:E:172:LEU:HD23	1.70	0.48
1:A:99:ARG:NH1	1:A:110:ASP:OD2	2.47	0.48
2:A:301:D16:C5	2:A:301:D16:C14	2.92	0.48
1:E:259:ALA:HA	1:E:260:PRO:HD3	1.74	0.48
1:F:186:HIS:CG	1:F:230:LEU:HD23	2.49	0.47
1:G:99:ARG:O	1:G:110:ASP:HA	2.13	0.47
1:C:81:ASP:HA	1:C:84:ALA:HB2	1.96	0.47
1:F:50:VAL:O	1:F:52:PHE:N	2.48	0.47
1:B:26:THR:HG22	1:B:209:TYR:CD1	2.49	0.47
2:B:302:D16:H5	2:B:302:D16:C14	2.43	0.47
1:C:228:PRO:HG3	1:C:251:TYR:HD1	1.79	0.47
1:D:209:TYR:CE2	2:D:301:D16:HM21	2.50	0.47
1:E:101:TRP:CE2	1:F:135:VAL:HB	2.49	0.47
1:C:228:PRO:HG3	1:C:251:TYR:CD1	2.49	0.47
1:D:4:TYR:CE1	1:D:8:LEU:HD22	2.49	0.47
1:A:123:PRO:HD2	4:A:444:HOH:O	2.13	0.47
1:F:254:HIS:HB3	1:F:255:PRO:HD2	1.97	0.47
1:D:176:PHE:CG	2:D:301:D16:H15	2.50	0.47
1:A:170:LEU:HD23	1:A:174:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PRO:HG3	1:A:251:TYR:HD1	1.79	0.46
1:A:92:PRO:HB2	1:A:97:GLN:HE21	1.80	0.46
1:A:205:ASP:OD2	1:B:126:ARG:HG2	2.15	0.46
1:F:169:ASP:OD2	2:F:301:D16:N3	2.48	0.46
1:F:44:LEU:HD11	1:F:50:VAL:HB	1.98	0.46
1:D:83:TRP:CE2	2:D:301:D16:H8	2.49	0.46
1:H:4:TYR:HA	1:H:34:MET:SD	2.56	0.46
1:F:2:THR:HG21	1:F:224:PRO:HG2	1.98	0.46
1:H:42:PHE:HA	1:H:43:PRO:HD3	1.83	0.46
1:A:236:ASP:CG	1:D:158:ARG:HH21	2.20	0.46
1:H:169:ASP:OD2	2:H:301:D16:N3	2.49	0.46
1:A:86:ASP:OD1	1:A:86:ASP:N	2.43	0.46
1:C:186:HIS:CD2	1:C:230:LEU:HD23	2.50	0.45
1:D:80:TRP:CE2	2:D:301:D16:H91	2.51	0.45
1:F:141:MET:SD	1:F:145:PRO:HD3	2.56	0.45
1:E:135:VAL:HB	1:F:101:TRP:CE2	2.51	0.45
1:C:49:LYS:HE3	1:C:49:LYS:HB2	1.80	0.45
2:D:301:D16:HP11	2:D:301:D16:H15	1.82	0.45
1:G:93:ILE:O	1:G:94:TYR:C	2.54	0.45
1:F:103:ALA:HB1	1:F:104:PRO:HD2	1.98	0.45
1:G:200:ILE:HD13	1:H:31:GLY:HA3	1.97	0.45
1:A:135:VAL:HB	1:B:101:TRP:CE2	2.52	0.45
1:E:93:ILE:H	1:E:93:ILE:HD13	1.81	0.45
1:A:80:TRP:CE2	2:A:301:D16:H91	2.51	0.45
1:G:169:ASP:HB2	3:G:302:UMP:OP2	1.98	0.45
2:F:301:D16:HB2	2:F:301:D16:O	2.17	0.45
1:G:58:GLU:O	1:G:61:TRP:HB3	2.17	0.44
1:B:84:ALA:HB1	1:B:88:GLY:HA2	1.99	0.44
1:C:186:HIS:CG	1:C:230:LEU:HD23	2.52	0.44
1:D:212:HIS:O	1:D:216:VAL:HG23	2.17	0.44
1:C:18:LYS:HE3	1:D:154:VAL:O	2.17	0.44
1:G:166:ARG:NH1	3:G:302:UMP:OP2	2.50	0.44
1:D:262:ALA:HB3	2:D:301:D16:HM22	1.99	0.44
1:E:83:TRP:HE1	2:E:301:D16:H8	1.83	0.44
1:E:223:GLU:HA	1:E:224:PRO:HD3	1.85	0.44
1:H:170:LEU:HD23	1:H:174:VAL:HG21	1.99	0.44
1:C:58:GLU:OE1	2:C:301:D16:HP13	2.17	0.44
1:E:100:SER:HB2	1:E:108:HIS:HD2	1.83	0.44
1:C:244[B]:GLU:HG2	1:C:245:ASP:N	2.33	0.44
1:C:251:TYR:CE1	1:C:253:PRO:HG3	2.53	0.44
1:D:83:TRP:CH2	2:D:301:D16:H8	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:ARG:HG3	1:H:167:SER:N	2.32	0.44
2:H:301:D16:HP12	3:H:302:UMP:C4	2.52	0.44
1:B:146:CYS:SG	3:B:301:UMP:C5	3.11	0.43
1:G:83:TRP:CE2	2:G:301:D16:H8	2.53	0.43
1:E:130:VAL:HB	1:E:150:PHE:CZ	2.53	0.43
1:G:186:HIS:HE1	4:G:402:HOH:O	2.00	0.43
1:G:99:ARG:NH1	1:G:239:PHE:CZ	2.86	0.43
1:F:209:TYR:CZ	2:F:301:D16:HM21	2.53	0.43
1:G:228:PRO:HG3	1:G:251:TYR:HD1	1.82	0.43
1:H:176:PHE:CD1	2:H:301:D16:C15	3.01	0.43
1:H:55:VAL:HG22	1:H:176:PHE:CD1	2.53	0.43
1:C:176:PHE:CD1	2:C:301:D16:H16	2.53	0.43
1:A:129:ILE:HD13	1:A:151:GLN:HB2	1.99	0.43
1:A:31:GLY:O	1:B:35:ARG:NH2	2.51	0.43
1:D:99:ARG:O	1:D:110:ASP:HA	2.18	0.43
1:D:147:HIS:HB2	1:D:163:LEU:HD11	2.00	0.43
1:C:147:HIS:H	1:C:147:HIS:CD2	2.36	0.43
1:G:147:HIS:HB2	1:G:163:LEU:HD11	2.01	0.42
1:G:135:VAL:HB	1:H:101:TRP:CE2	2.54	0.42
1:G:31:GLY:O	1:H:35:ARG:NH2	2.49	0.42
1:H:237:SER:HB3	1:H:240:GLU:HG3	2.01	0.42
1:E:93:ILE:H	1:E:93:ILE:CD1	2.31	0.42
1:E:129:ILE:HD13	1:E:151:GLN:HB2	2.01	0.42
1:E:57:TYR:HB2	1:E:77:VAL:HG21	2.01	0.42
1:E:80:TRP:CZ2	2:E:301:D16:H91	2.54	0.42
1:F:60:LEU:O	1:F:64:ARG:HG3	2.19	0.42
2:E:301:D16:C5	2:E:301:D16:C14	2.97	0.42
1:E:92:PRO:HA	1:E:96:VAL:HG21	2.02	0.42
1:H:27:ARG:HE	1:H:27:ARG:HB2	1.72	0.42
1:C:34:MET:CE	1:C:178:ILE:HD11	2.50	0.42
1:A:108:HIS:HD2	4:A:416:HOH:O	2.02	0.42
1:F:42:PHE:HA	1:F:43:PRO:HD3	1.73	0.42
1:F:4:TYR:HA	1:F:34:MET:SD	2.60	0.42
1:A:215:GLN:HE22	1:A:260:PRO:HG3	1.80	0.42
1:E:42:PHE:HA	1:E:43:PRO:HD3	1.85	0.42
1:E:67:SER:HB3	1:E:96:VAL:CG2	2.50	0.42
1:C:80:TRP:C	1:C:82:GLU:H	2.23	0.42
2:F:301:D16:HP12	3:F:302:UMP:C5	2.55	0.42
1:B:217:ARG:NH2	1:G:15:GLY:O	2.45	0.42
2:A:301:D16:H15	2:A:301:D16:HP11	2.00	0.41
1:C:103:ALA:HB3	1:C:105:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:ASN:C	1:G:70:GLY:H	2.23	0.41
1:B:168:ALA:HB1	1:B:174:VAL:CG2	2.50	0.41
1:E:35:ARG:NH2	1:E:198:GLU:OE1	2.47	0.41
1:G:4:TYR:HA	1:G:34:MET:SD	2.59	0.41
1:B:101:TRP:HA	1:B:102:PRO:HD3	1.84	0.41
1:B:87:THR:O	1:B:87:THR:CG2	2.68	0.41
1:C:119:LEU:HA	1:C:119:LEU:HD23	1.93	0.41
1:G:170:LEU:HD23	1:G:174:VAL:HG21	2.01	0.41
1:G:51:HIS:CE1	1:G:53:LYS:HB3	2.55	0.41
1:A:101:TRP:CD1	1:A:101:TRP:C	2.94	0.41
1:D:259:ALA:HA	1:D:260:PRO:HD3	1.79	0.41
1:A:2:THR:HG21	1:A:224:PRO:HG2	2.02	0.41
1:C:81:ASP:HA	1:C:84:ALA:HB3	2.03	0.41
1:G:42:PHE:O	1:G:228:PRO:HD2	2.21	0.41
1:G:176:PHE:CD2	2:G:301:D16:H15	2.55	0.41
1:C:65:GLY:HA2	1:C:95:GLY:O	2.19	0.41
1:G:80:TRP:CZ2	2:G:301:D16:H91	2.56	0.41
1:H:134:ASN:CG	1:H:137:GLU:HG3	2.40	0.41
1:G:30:PHE:HB2	1:H:153:TYR:CE2	2.55	0.41
2:C:301:D16:HP11	2:C:301:D16:H15	1.99	0.41
1:G:16:THR:HA	1:G:17:PRO:HD3	1.92	0.41
1:H:16:THR:HA	1:H:17:PRO:HD3	1.93	0.41
1:C:1:MET:O	1:C:3:PRO:HD3	2.20	0.41
1:A:154:VAL:O	1:B:18:LYS:NZ	2.54	0.41
1:C:170:LEU:HD23	1:C:174:VAL:HG21	2.03	0.41
1:C:176:PHE:CE1	2:C:301:D16:H16	2.56	0.41
1:C:34:MET:HE3	1:C:178:ILE:HD11	2.03	0.41
1:D:15:GLY:HA3	1:D:27:ARG:HG2	2.02	0.41
1:G:99:ARG:NH1	1:G:110:ASP:OD2	2.54	0.41
1:B:93:ILE:O	1:B:94:TYR:C	2.59	0.41
1:F:168:ALA:HB1	1:F:174:VAL:CG2	2.51	0.41
1:C:96:VAL:O	1:C:100:SER:N	2.43	0.41
1:D:101:TRP:C	1:D:101:TRP:CD1	2.94	0.41
1:F:83:TRP:HE1	2:F:301:D16:H8	1.83	0.41
1:G:130:VAL:HB	1:G:150:PHE:CZ	2.56	0.41
1:G:172:LEU:HA	1:G:172:LEU:HD23	1.90	0.41
1:G:176:PHE:CD2	2:G:301:D16:C15	3.04	0.40
1:A:101:TRP:HA	1:A:102:PRO:HD3	1.89	0.40
1:A:135:VAL:HB	1:B:101:TRP:CD2	2.57	0.40
1:E:231:LEU:HB2	1:E:247:VAL:HB	2.02	0.40
1:F:147:HIS:H	1:F:147:HIS:CD2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LEU:HD13	4:B:453:HOH:O	2.22	0.40
1:D:172:LEU:HD22	2:D:301:D16:N	2.37	0.40
1:F:251:TYR:CZ	1:F:253:PRO:HG3	2.57	0.40
1:H:79:ILE:HG22	2:H:301:D16:O	2.22	0.40
1:C:209:TYR:CE2	2:C:301:D16:HM21	2.56	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	260/263 (99%)	251 (96%)	8 (3%)	1 (0%)	38	47
1	B	259/263 (98%)	250 (96%)	8 (3%)	1 (0%)	38	47
1	C	260/263 (99%)	247 (95%)	12 (5%)	1 (0%)	38	47
1	D	261/263 (99%)	252 (97%)	7 (3%)	2 (1%)	22	26
1	E	260/263 (99%)	248 (95%)	11 (4%)	1 (0%)	38	47
1	F	259/263 (98%)	246 (95%)	11 (4%)	2 (1%)	22	26
1	G	258/263 (98%)	248 (96%)	8 (3%)	2 (1%)	22	26
1	H	257/263 (98%)	246 (96%)	11 (4%)	0	100	100
All	All	2074/2104 (99%)	1988 (96%)	76 (4%)	10 (0%)	32	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	HIS
1	F	94	TYR
1	E	94	TYR
1	G	94	TYR
1	D	94	TYR

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Mol	Chain	Res	Type
1	G	93	ILE
1	A	93	ILE
1	B	93	ILE
1	D	93	ILE
1	F	93	ILE

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	221/224 (99%)	217 (98%)	4 (2%)	64	79
1	B	219/224 (98%)	216 (99%)	3 (1%)	71	85
1	C	203/224 (91%)	200 (98%)	3 (2%)	70	83
1	D	216/224 (96%)	214 (99%)	2 (1%)	82	91
1	E	216/224 (96%)	210 (97%)	6 (3%)	49	65
1	F	208/224 (93%)	207 (100%)	1 (0%)	91	96
1	G	209/224 (93%)	209 (100%)	0	100	100
1	H	194/224 (87%)	191 (98%)	3 (2%)	70	83
All	All	1686/1792 (94%)	1664 (99%)	22 (1%)	75	86

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	A	156	ASP
1	A	172	LEU
1	A	232	LEU
1	B	16	THR
1	B	33	GLN
1	B	232	LEU
1	C	228	PRO
1	C	244[A]	GLU
1	C	244[B]	GLU

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Mol	Chain	Res	Type
1	D	116	LEU
1	D	117	ASP
1	E	73	HIS
1	E	92	PRO
1	E	93	ILE
1	E	105	SER
1	E	117	ASP
1	E	260	PRO
1	F	73	HIS
1	H	20	ASP
1	H	28	SER
1	H	230	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	250	ASN
1	E	108	HIS
1	F	162	GLN
1	H	108	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 ligands 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	D16	A	301	-	24,34,34	6.30	16 (66%)	26,48,48	2.73	8 (30%)
3	UMP	A	302	-	17,21,21	5.15	9 (52%)	23,31,31	1.27	1 (4%)
3	UMP	B	301	-	17,21,21	5.15	7 (41%)	23,31,31	1.69	1 (4%)
2	D16	B	302	-	24,34,34	6.52	17 (70%)	26,48,48	2.34	7 (26%)
2	D16	C	301	-	24,34,34	6.55	17 (70%)	26,48,48	2.32	8 (30%)
3	UMP	C	302	-	17,21,21	5.18	8 (47%)	23,31,31	1.30	1 (4%)
2	D16	D	301	-	24,34,34	6.33	16 (66%)	26,48,48	2.58	10 (38%)
3	UMP	D	302	-	17,21,21	5.08	7 (41%)	23,31,31	1.75	2 (8%)
2	D16	E	301	-	24,34,34	6.54	17 (70%)	26,48,48	2.31	5 (19%)
3	UMP	E	302	-	17,21,21	5.27	7 (41%)	23,31,31	1.63	1 (4%)
2	D16	F	301	-	24,34,34	6.59	17 (70%)	26,48,48	2.72	10 (38%)
3	UMP	F	302	-	17,21,21	5.21	9 (52%)	23,31,31	1.77	1 (4%)
2	D16	G	301	-	24,34,34	6.55	17 (70%)	26,48,48	2.47	6 (23%)
3	UMP	G	302	-	17,21,21	5.25	7 (41%)	23,31,31	1.49	1 (4%)
2	D16	H	301	-	24,34,34	6.45	17 (70%)	26,48,48	2.42	9 (34%)
3	UMP	H	302	-	17,21,21	5.20	7 (41%)	23,31,31	1.59	1 (4%)

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	D16	A	301	-	-	0/13/25/25	0/3/3/3
3	UMP	A	302	-	-	0/6/22/22	0/2/2/2
3	UMP	B	301	-	-	0/6/22/22	0/2/2/2
2	D16	B	302	-	-	0/13/25/25	0/3/3/3
2	D16	C	301	-	-	0/13/25/25	0/3/3/3
3	UMP	C	302	-	-	0/6/22/22	0/2/2/2
2	D16	D	301	-	-	0/13/25/25	0/3/3/3
3	UMP	D	302	-	-	0/6/22/22	0/2/2/2
2	D16	E	301	-	-	0/13/25/25	0/3/3/3
3	UMP	E	302	-	-	0/6/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	D16	F	301	-	-	0/13/25/25	0/3/3/3
3	UMP	F	302	-	-	0/6/22/22	0/2/2/2
2	D16	G	301	-	-	0/13/25/25	0/3/3/3
3	UMP	G	302	-	-	0/6/22/22	0/2/2/2
2	D16	H	301	-	-	0/13/25/25	0/3/3/3
3	UMP	H	302	-	-	0/6/22/22	0/2/2/2

All (195) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	D16	C14-S13	-3.90	1.66	1.72
2	E	301	D16	C14-S13	-3.81	1.66	1.72
2	F	301	D16	C14-S13	-3.79	1.66	1.72
2	G	301	D16	C14-S13	-3.65	1.66	1.72
2	D	301	D16	C14-S13	-3.42	1.67	1.72
2	B	302	D16	C14-S13	-3.39	1.67	1.72
2	C	301	D16	C14-S13	-3.18	1.67	1.72
2	A	301	D16	C14-S13	-2.69	1.68	1.72
2	B	302	D16	O-C	-2.58	1.17	1.23
2	C	301	D16	O-C	-2.21	1.18	1.23
2	F	301	D16	O-C	-2.07	1.19	1.23
3	F	302	UMP	P-OP3	-2.07	1.46	1.54
2	G	301	D16	O-C	-2.02	1.19	1.23
3	F	302	UMP	O4'-C1'	2.11	1.47	1.42
2	H	301	D16	C9-C6	2.12	1.55	1.51
3	C	302	UMP	P-O5'	2.17	1.67	1.60
3	A	302	UMP	O4'-C1'	2.19	1.47	1.42
3	A	302	UMP	P-OP2	2.26	1.64	1.54
2	E	301	D16	C9-C6	2.30	1.55	1.51
3	G	302	UMP	P-OP2	2.39	1.64	1.54
3	A	302	UMP	P-O5'	2.40	1.67	1.60
3	D	302	UMP	P-OP2	2.41	1.64	1.54
3	B	301	UMP	P-OP2	2.44	1.64	1.54
3	H	302	UMP	P-OP2	2.48	1.65	1.54
3	E	302	UMP	P-OP2	2.49	1.65	1.54
3	C	302	UMP	P-OP2	2.51	1.65	1.54
3	F	302	UMP	P-OP2	2.79	1.66	1.54
2	D	301	D16	C14-N10	3.23	1.46	1.36
2	F	301	D16	C14-N10	3.31	1.47	1.36
2	H	301	D16	C14-N10	3.39	1.47	1.36
2	C	301	D16	C14-N10	3.45	1.47	1.36
2	G	301	D16	C14-N10	3.47	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	D16	C14-N10	3.49	1.47	1.36
2	B	302	D16	C14-N10	3.50	1.47	1.36
2	E	301	D16	C14-N10	3.74	1.48	1.36
3	D	302	UMP	P-OP1	4.25	1.65	1.50
3	A	302	UMP	P-OP1	4.32	1.65	1.50
3	C	302	UMP	P-OP1	4.37	1.65	1.50
2	D	301	D16	C16-C11	4.53	1.57	1.39
3	G	302	UMP	P-OP1	4.55	1.66	1.50
3	H	302	UMP	P-OP1	4.56	1.66	1.50
3	B	301	UMP	P-OP1	4.61	1.66	1.50
3	E	302	UMP	P-OP1	4.62	1.66	1.50
2	A	301	D16	C16-C11	4.67	1.58	1.39
2	B	302	D16	C16-C11	4.74	1.58	1.39
2	G	301	D16	C16-C11	4.74	1.58	1.39
2	C	301	D16	C16-C11	4.80	1.58	1.39
2	E	301	D16	C16-C11	4.80	1.58	1.39
2	F	301	D16	C16-C11	4.81	1.59	1.39
2	H	301	D16	C16-C11	4.83	1.59	1.39
2	H	301	D16	C4A-C8A	4.87	1.51	1.41
3	F	302	UMP	P-OP1	5.01	1.67	1.50
2	D	301	D16	C4A-C8A	5.12	1.52	1.41
2	B	302	D16	C4A-C8A	5.21	1.52	1.41
2	H	301	D16	C-N	5.23	1.46	1.34
2	D	301	D16	C-N	5.26	1.46	1.34
2	F	301	D16	C4A-C8A	5.27	1.52	1.41
2	C	301	D16	C4A-C8A	5.28	1.52	1.41
2	E	301	D16	C-N	5.30	1.46	1.34
2	G	301	D16	C4A-C8A	5.36	1.52	1.41
2	G	301	D16	C-N	5.41	1.46	1.34
2	E	301	D16	C4A-C8A	5.41	1.52	1.41
2	A	301	D16	C4A-C8A	5.58	1.53	1.41
2	A	301	D16	C-N	5.62	1.46	1.34
2	C	301	D16	C-N	5.67	1.47	1.34
2	F	301	D16	C-N	5.68	1.47	1.34
2	B	302	D16	C-N	5.69	1.47	1.34
2	B	302	D16	O4-C4	5.84	1.39	1.24
2	D	301	D16	O4-C4	5.88	1.39	1.24
2	H	301	D16	O4-C4	6.09	1.39	1.24
3	A	302	UMP	O4-C4	6.18	1.40	1.24
2	E	301	D16	O4-C4	6.21	1.40	1.24
2	A	301	D16	O4-C4	6.24	1.40	1.24
3	B	301	UMP	O4-C4	6.28	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	UMP	O4-C4	6.33	1.40	1.24
2	G	301	D16	O4-C4	6.34	1.40	1.24
2	D	301	D16	C16-C15	6.36	1.71	1.39
3	D	302	UMP	O4-C4	6.40	1.40	1.24
2	F	301	D16	O4-C4	6.45	1.40	1.24
2	C	301	D16	O4-C4	6.59	1.41	1.24
2	A	301	D16	C16-C15	6.62	1.72	1.39
3	E	302	UMP	O4-C4	6.66	1.41	1.24
2	B	302	D16	C16-C15	6.68	1.72	1.39
3	G	302	UMP	O4-C4	6.69	1.41	1.24
2	C	301	D16	C16-C15	6.74	1.72	1.39
2	F	301	D16	C16-C15	6.74	1.72	1.39
2	G	301	D16	C16-C15	6.76	1.73	1.39
2	H	301	D16	C16-C15	6.77	1.73	1.39
3	F	302	UMP	O4-C4	6.80	1.41	1.24
2	E	301	D16	C16-C15	6.86	1.73	1.39
3	H	302	UMP	O4-C4	6.88	1.41	1.24
3	F	302	UMP	C2-N3	6.89	1.51	1.38
3	D	302	UMP	C2-N3	7.02	1.52	1.38
2	D	301	D16	C7-C6	7.11	1.53	1.38
3	H	302	UMP	C2-N3	7.16	1.52	1.38
2	H	301	D16	C7-C6	7.20	1.53	1.38
3	A	302	UMP	C6-C5	7.24	1.53	1.38
2	B	302	D16	C7-C6	7.24	1.53	1.38
3	B	301	UMP	C2-N3	7.25	1.52	1.38
3	E	302	UMP	C6-C5	7.28	1.53	1.38
3	F	302	UMP	C6-C5	7.28	1.53	1.38
3	C	302	UMP	C6-C5	7.29	1.53	1.38
3	A	302	UMP	C2-N3	7.32	1.52	1.38
3	D	302	UMP	C6-C5	7.32	1.53	1.38
2	E	301	D16	C7-C6	7.36	1.54	1.38
2	B	302	D16	C8A-N1	7.39	1.50	1.37
2	G	301	D16	C7-C6	7.41	1.54	1.38
2	C	301	D16	C7-C6	7.44	1.54	1.38
3	G	302	UMP	C2-N3	7.46	1.52	1.38
3	B	301	UMP	C6-C5	7.46	1.54	1.38
3	G	302	UMP	C6-C5	7.47	1.54	1.38
3	H	302	UMP	C6-C5	7.48	1.54	1.38
3	C	302	UMP	C2-N3	7.48	1.53	1.38
2	A	301	D16	C7-C6	7.49	1.54	1.38
2	F	301	D16	C7-C6	7.68	1.54	1.38
2	A	301	D16	C8A-N1	7.72	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	UMP	C2-N3	7.83	1.53	1.38
2	E	301	D16	C8A-N1	7.98	1.51	1.37
2	F	301	D16	C8A-N1	8.19	1.51	1.37
2	D	301	D16	C8A-N1	8.30	1.51	1.37
2	C	301	D16	C8A-N1	8.46	1.51	1.37
2	D	301	D16	C5-C6	8.49	1.57	1.37
2	G	301	D16	C8A-N1	8.50	1.52	1.37
2	A	301	D16	C4-N3	8.61	1.48	1.33
2	H	301	D16	C8A-N1	8.64	1.52	1.37
2	C	301	D16	C4-N3	8.64	1.48	1.33
2	A	301	D16	C5-C6	8.68	1.58	1.37
2	C	301	D16	C5-C6	8.70	1.58	1.37
2	H	301	D16	C4-N3	8.75	1.48	1.33
2	F	301	D16	C5-C6	8.76	1.58	1.37
2	D	301	D16	C4-N3	8.77	1.48	1.33
2	H	301	D16	C5-C6	8.87	1.58	1.37
2	A	301	D16	C5-C4A	8.92	1.57	1.41
2	B	302	D16	C4-N3	9.01	1.49	1.33
2	G	301	D16	C5-C6	9.02	1.58	1.37
2	E	301	D16	C5-C6	9.03	1.59	1.37
2	F	301	D16	C4-N3	9.42	1.50	1.33
2	G	301	D16	C4-N3	9.52	1.50	1.33
2	B	302	D16	C5-C6	9.52	1.60	1.37
2	E	301	D16	C4-N3	9.59	1.50	1.33
2	D	301	D16	C5-C4A	9.67	1.59	1.41
2	E	301	D16	C5-C4A	9.76	1.59	1.41
2	G	301	D16	C5-C4A	9.78	1.59	1.41
2	D	301	D16	C8-C7	9.79	1.57	1.36
2	H	301	D16	C8-C7	9.80	1.57	1.36
2	B	302	D16	C8-C7	9.82	1.57	1.36
2	A	301	D16	C2-N1	9.88	1.52	1.34
2	H	301	D16	C5-C4A	9.89	1.59	1.41
2	C	301	D16	C5-C4A	9.95	1.59	1.41
2	D	301	D16	C8-C8A	9.97	1.59	1.41
2	B	302	D16	C8-C8A	9.98	1.59	1.41
2	F	301	D16	C5-C4A	10.00	1.59	1.41
2	B	302	D16	C2-N1	10.03	1.52	1.34
2	H	301	D16	C2-N1	10.09	1.52	1.34
2	A	301	D16	C8-C7	10.11	1.58	1.36
2	A	301	D16	C2-N3	10.12	1.52	1.34
2	G	301	D16	C8-C7	10.14	1.58	1.36
2	F	301	D16	C8-C7	10.21	1.58	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	D16	C8-C8A	10.21	1.60	1.41
2	E	301	D16	C2-N3	10.23	1.52	1.34
2	G	301	D16	C2-N1	10.25	1.52	1.34
2	G	301	D16	C8-C8A	10.32	1.60	1.41
2	D	301	D16	C2-N3	10.33	1.53	1.34
2	C	301	D16	C2-N1	10.35	1.53	1.34
2	E	301	D16	C8-C7	10.36	1.58	1.36
3	B	301	UMP	C4-N3	10.38	1.51	1.33
2	F	301	D16	C8-C8A	10.39	1.60	1.41
2	F	301	D16	C2-N1	10.43	1.53	1.34
2	E	301	D16	C2-N1	10.44	1.53	1.34
2	E	301	D16	C8-C8A	10.45	1.60	1.41
2	C	301	D16	C8-C7	10.46	1.58	1.36
2	H	301	D16	C8-C8A	10.53	1.60	1.41
2	C	301	D16	C8-C8A	10.54	1.60	1.41
2	B	302	D16	C5-C4A	10.57	1.61	1.41
2	H	301	D16	C2-N3	10.61	1.53	1.34
2	D	301	D16	C2-N1	10.63	1.53	1.34
3	D	302	UMP	C4-N3	10.72	1.52	1.33
2	G	301	D16	C2-N3	10.78	1.53	1.34
2	C	301	D16	C2-N3	10.81	1.53	1.34
3	F	302	UMP	C4-N3	10.88	1.52	1.33
3	H	302	UMP	C4-N3	10.95	1.52	1.33
3	C	302	UMP	C4-N3	10.98	1.52	1.33
2	F	301	D16	C2-N3	10.99	1.54	1.34
3	A	302	UMP	C4-N3	11.08	1.53	1.33
3	G	302	UMP	C4-N3	11.10	1.53	1.33
3	E	302	UMP	C4-N3	11.10	1.53	1.33
2	B	302	D16	C2-N3	11.45	1.55	1.34
3	D	302	UMP	C6-N1	11.86	1.51	1.35
3	A	302	UMP	C6-N1	11.95	1.52	1.35
3	H	302	UMP	C6-N1	12.02	1.52	1.35
3	C	302	UMP	C6-N1	12.03	1.52	1.35
3	E	302	UMP	C6-N1	12.12	1.52	1.35
3	F	302	UMP	C6-N1	12.17	1.52	1.35
3	G	302	UMP	C6-N1	12.23	1.52	1.35
3	B	301	UMP	C6-N1	12.41	1.52	1.35

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	D16	C4A-C4-N3	-7.64	119.06	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	D16	C4A-C8A-N1	-7.25	119.54	123.67
2	A	301	D16	C4A-C8A-N1	-7.10	119.62	123.67
2	F	301	D16	C4A-C8A-N1	-7.06	119.64	123.67
2	C	301	D16	C4A-C4-N3	-7.02	119.50	124.45
2	D	301	D16	C4A-C8A-N1	-7.01	119.67	123.67
2	F	301	D16	C4A-C4-N3	-6.78	119.67	124.45
2	G	301	D16	C4A-C4-N3	-6.53	119.85	124.45
2	G	301	D16	C4A-C8A-N1	-6.53	119.95	123.67
2	H	301	D16	C4A-C8A-N1	-6.29	120.08	123.67
2	B	302	D16	C4A-C4-N3	-6.20	120.08	124.45
2	F	301	D16	C6-C9-N10	-6.12	104.97	113.00
2	E	301	D16	C4A-C4-N3	-6.09	120.16	124.45
2	C	301	D16	C4A-C8A-N1	-6.08	120.20	123.67
2	D	301	D16	C6-C9-N10	-5.84	105.34	113.00
2	H	301	D16	C4A-C4-N3	-5.79	120.37	124.45
2	B	302	D16	C4A-C8A-N1	-5.72	120.41	123.67
2	D	301	D16	C4A-C4-N3	-5.67	120.45	124.45
2	G	301	D16	C6-C9-N10	-5.54	105.73	113.00
2	A	301	D16	C6-C9-N10	-5.06	106.36	113.00
2	H	301	D16	C6-C9-N10	-4.10	107.63	113.00
2	A	301	D16	CB-CA-CT	-3.37	107.39	112.28
2	E	301	D16	C6-C9-N10	-3.30	108.67	113.00
2	B	302	D16	N1-C2-N3	-3.10	119.33	125.60
2	B	302	D16	C6-C9-N10	-3.05	109.00	113.00
2	B	302	D16	CB-CA-CT	-3.00	107.93	112.28
2	H	301	D16	CB-CA-CT	-2.97	107.97	112.28
2	H	301	D16	N1-C2-N3	-2.95	119.63	125.60
2	F	301	D16	CB-CA-CT	-2.89	108.09	112.28
2	D	301	D16	N1-C2-N3	-2.85	119.83	125.60
2	H	301	D16	CB-CA-N	-2.83	105.92	110.22
2	G	301	D16	CB-CA-CT	-2.77	108.27	112.28
2	F	301	D16	N1-C2-N3	-2.61	120.32	125.60
2	E	301	D16	N1-C2-N3	-2.57	120.40	125.60
2	G	301	D16	N1-C2-N3	-2.55	120.44	125.60
2	C	301	D16	N1-C2-N3	-2.55	120.45	125.60
3	D	302	UMP	O4'-C1'-N1	-2.47	103.62	107.78
2	A	301	D16	CB-CA-N	-2.45	106.50	110.22
2	H	301	D16	O-C-N	-2.28	118.29	122.46
2	C	301	D16	C5-C4A-C4	-2.25	118.66	122.09
2	D	301	D16	CB-CA-N	-2.22	106.85	110.22
2	A	301	D16	C6-C5-C4A	-2.20	119.02	122.60
2	C	301	D16	CG-CB-CA	-2.19	108.82	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	D16	N1-C2-N3	-2.18	121.19	125.60
2	F	301	D16	C6-C5-C4A	-2.12	119.15	122.60
2	D	301	D16	CP1-N10-C14	-2.10	115.69	119.86
2	F	301	D16	C5-C4A-C4	-2.08	118.92	122.09
2	D	301	D16	CB-CA-CT	-2.08	109.27	112.28
2	C	301	D16	C6-C5-C4A	-2.07	119.23	122.60
2	E	301	D16	O-C-N	-2.00	118.80	122.46
2	F	301	D16	CM2-C2-N3	2.01	120.49	117.20
2	H	301	D16	CP1-N10-C9	2.03	119.69	114.18
2	D	301	D16	CP1-N10-C9	2.04	119.72	114.18
2	H	301	D16	CM2-C2-N1	2.06	120.58	117.22
2	G	301	D16	CP1-N10-C9	2.10	119.88	114.18
2	C	301	D16	C4-C4A-C8A	2.26	120.45	118.51
2	D	301	D16	O-C-C11	2.27	125.98	121.13
2	C	301	D16	C5-C4A-C8A	2.33	120.89	118.16
2	F	301	D16	CP1-N10-C9	2.38	120.62	114.18
2	A	301	D16	C4-C4A-C8A	2.50	120.65	118.51
2	F	301	D16	C4-C4A-C8A	2.59	120.73	118.51
2	D	301	D16	CM2-C2-N1	2.71	121.65	117.22
2	B	302	D16	CM2-C2-N3	2.92	121.99	117.20
2	B	302	D16	CA-N-C	3.01	126.27	122.15
3	A	302	UMP	C4-N3-C2	4.98	118.41	114.13
3	C	302	UMP	C4-N3-C2	5.76	119.08	114.13
3	G	302	UMP	C4-N3-C2	6.36	119.59	114.13
3	H	302	UMP	C4-N3-C2	6.98	120.12	114.13
3	E	302	UMP	C4-N3-C2	6.98	120.12	114.13
3	D	302	UMP	C4-N3-C2	7.18	120.30	114.13
3	B	301	UMP	C4-N3-C2	7.44	120.52	114.13
3	F	302	UMP	C4-N3-C2	7.57	120.64	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	D16	7	0
3	A	302	UMP	2	0
3	B	301	UMP	2	0
2	B	302	D16	6	0
2	C	301	D16	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	UMP	1	0
2	D	301	D16	15	0
3	D	302	UMP	1	0
2	E	301	D16	7	0
3	E	302	UMP	1	0
2	F	301	D16	10	0
3	F	302	UMP	3	0
2	G	301	D16	9	0
3	G	302	UMP	4	0
2	H	301	D16	15	0
3	H	302	UMP	2	0

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, 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	261/263 (99%)	0.33	2 (0%) 86 89	31, 43, 69, 92	0
1	B	261/263 (99%)	0.26	1 (0%) 92 95	30, 47, 74, 97	0
1	C	261/263 (99%)	0.73	24 (9%) 10 13	35, 69, 104, 143	0
1	D	263/263 (100%)	0.49	7 (2%) 55 62	29, 44, 69, 103	0
1	E	260/263 (98%)	0.24	5 (1%) 67 73	34, 55, 82, 119	0
1	F	261/263 (99%)	0.36	7 (2%) 55 62	33, 55, 81, 114	0
1	G	260/263 (98%)	0.53	20 (7%) 14 19	39, 62, 119, 174	0
1	H	259/263 (98%)	0.68	24 (9%) 9 13	39, 62, 95, 133	0
All	All	2086/2104 (99%)	0.45	90 (4%) 36 43	29, 54, 91, 174	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	262	ALA	9.1
1	C	72	LEU	8.4
1	G	106	GLY	8.1
1	F	1	MET	6.4
1	C	90	LEU	5.9
1	H	149	PHE	5.9
1	H	148	ALA	5.4
1	D	263	VAL	5.2
1	C	107	GLU	4.7
1	H	104	PRO	4.7
1	C	77	VAL	4.6
1	C	80	TRP	4.0
1	D	261	VAL	3.8
1	H	192	ALA	3.7
1	G	72	LEU	3.6
1	H	101	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	136	GLY	3.5
1	E	20	ASP	3.4
1	C	22	THR	3.4
1	F	19	SER	3.3
1	C	135	VAL	3.3
1	D	260	PRO	3.2
1	C	78	THR	3.2
1	H	114	ALA	3.2
1	A	105	SER	3.2
1	G	104	PRO	3.1
1	H	96	VAL	3.0
1	D	259	ALA	3.0
1	H	62	PHE	3.0
1	H	259	ALA	2.9
1	G	83	TRP	2.9
1	H	70	GLY	2.9
1	H	233	ALA	2.9
1	C	190	ALA	2.8
1	G	149	PHE	2.8
1	G	90	LEU	2.7
1	C	73	HIS	2.7
1	G	132	ALA	2.7
1	H	138	ILE	2.7
1	C	176	PHE	2.7
1	H	194	LEU	2.7
1	H	207	HIS	2.6
1	G	209	TYR	2.6
1	C	20	ASP	2.6
1	C	171	PHE	2.6
1	C	54	SER	2.6
1	H	103	ALA	2.6
1	F	124	ASP	2.5
1	G	136	GLY	2.5
1	G	103	ALA	2.5
1	G	135	VAL	2.5
1	G	194	LEU	2.5
1	G	192	ALA	2.4
1	G	208	ILE	2.4
1	F	122	ASP	2.4
1	E	149	PHE	2.4
1	D	88	GLY	2.4
1	C	108	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	122	ASP	2.4
1	C	104	PRO	2.4
1	A	149	PHE	2.4
1	F	22	THR	2.4
1	C	57	TYR	2.4
1	G	69	ILE	2.4
1	C	134	ASN	2.3
1	H	130	VAL	2.3
1	H	20	ASP	2.3
1	D	133	TRP	2.3
1	E	171	PHE	2.2
1	H	135	VAL	2.2
1	C	100	SER	2.2
1	G	63	LEU	2.2
1	C	103	ALA	2.2
1	G	101	TRP	2.2
1	G	70	GLY	2.2
1	H	133	TRP	2.2
1	H	127	ARG	2.2
1	C	66	ASP	2.2
1	B	211	ASN	2.1
1	H	121	THR	2.1
1	E	129	ILE	2.1
1	G	128	ILE	2.1
1	F	72	LEU	2.1
1	C	247	VAL	2.1
1	E	157	GLY	2.1
1	G	21	ARG	2.0
1	H	61	TRP	2.0
1	H	132	ALA	2.0
1	C	158	ARG	2.0
1	F	171	PHE	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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
3	UMP	A	302	20/20	0.94	0.22	3.66	40,48,57,66	0
2	D16	A	301	32/32	0.94	0.21	1.88	43,54,72,76	0
2	D16	E	301	32/32	0.90	0.22	1.68	54,78,110,111	0
3	UMP	F	302	20/20	0.95	0.23	1.63	47,60,66,66	0
3	UMP	D	302	20/20	0.97	0.20	1.29	38,50,63,76	0
3	UMP	B	301	20/20	0.93	0.21	1.27	48,64,68,85	0
2	D16	H	301	32/32	0.89	0.22	1.20	44,73,108,118	0
3	UMP	G	302	20/20	0.93	0.24	0.96	62,69,85,148	0
3	UMP	E	302	20/20	0.94	0.17	0.66	43,61,71,75	0
2	D16	B	302	32/32	0.91	0.20	0.55	44,64,96,98	0
2	D16	D	301	32/32	0.92	0.23	0.24	40,58,71,138	0
3	UMP	H	302	20/20	0.96	0.19	0.24	51,68,78,170	0
3	UMP	C	302	20/20	0.96	0.17	0.12	46,55,61,61	0
2	D16	F	301	32/32	0.90	0.20	-0.09	57,75,100,128	0
2	D16	G	301	32/32	0.92	0.18	-0.10	53,74,88,92	0
2	D16	C	301	32/32	0.91	0.19	-0.22	52,75,82,84	0

6.5 Other polymers

There are no such residues in this entry.