



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:24 PM GMT

PDB ID : 4I52
Title : scMenB im complex with 1-hydroxy-2-naphthoyl-CoA
Authors : Song, H.G.; Sun, Y.R.; Li, J.; Li, Y.; Jiang, M.; Zhou, J.H.; Guo, Z.H.
Deposited on : 2012-11-28
Resolution : 2.35 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

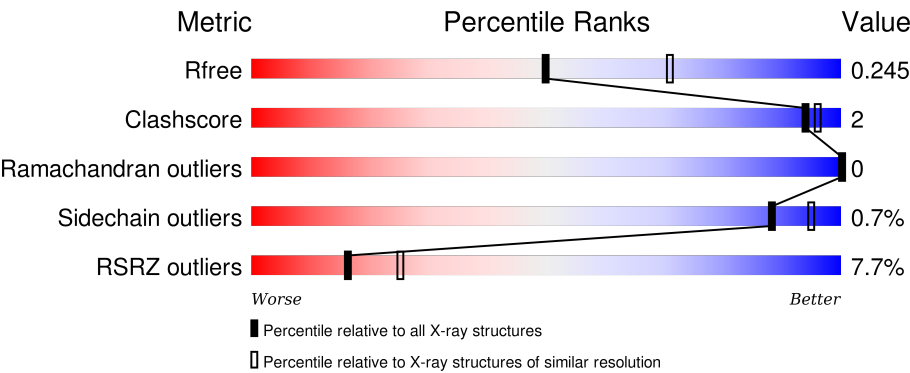
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



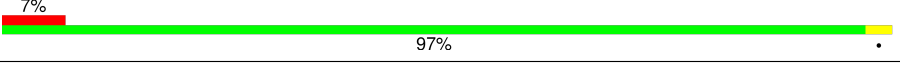
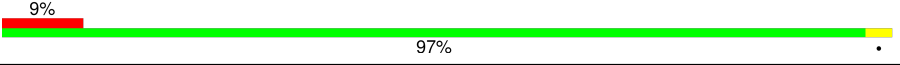
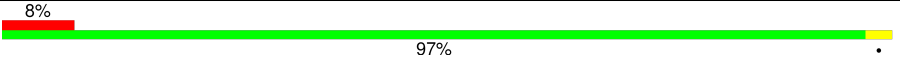
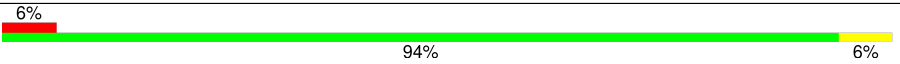
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	275	<div><div>11%</div><div>97%</div><div>.</div></div>
1	B	275	<div><div>9%</div><div>97%</div><div>.</div></div>
1	C	275	<div><div>9%</div><div>97%</div><div>.</div></div>
1	D	275	<div><div>5%</div><div>95%</div><div>5%</div></div>
1	E	275	<div><div>4%</div><div>97%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	F	275	
1	G	275	
1	H	275	
1	I	275	

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
3	CL	A	302	-	-	X	X
3	CL	B	302	-	-	-	X
3	CL	D	302	-	-	X	-
3	CL	H	302	-	-	X	-
3	CL	I	302	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19971 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 Naphthoate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2059	1308	357	383	11			
1	B	275	Total	C	N	O	S	0	0	0
			2094	1336	360	387	11			
1	C	274	Total	C	N	O	S	0	0	0
			2075	1318	357	390	10			
1	D	275	Total	C	N	O	S	0	0	0
			2100	1337	362	390	11			
1	E	274	Total	C	N	O	S	0	0	0
			2084	1326	363	385	10			
1	F	274	Total	C	N	O	S	0	0	0
			2096	1333	366	387	10			
1	G	275	Total	C	N	O	S	0	0	0
			2107	1340	370	386	11			
1	H	275	Total	C	N	O	S	0	0	0
			2118	1344	372	391	11			
1	I	275	Total	C	N	O	S	0	0	0
			2097	1335	365	386	11			

- Molecule 2 is 1-HYDROXY-2-NAPHTHOYL-COA (three-letter code: 1HA) (formula: C₃₂H₄₂N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			61	32	7	18	3	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		

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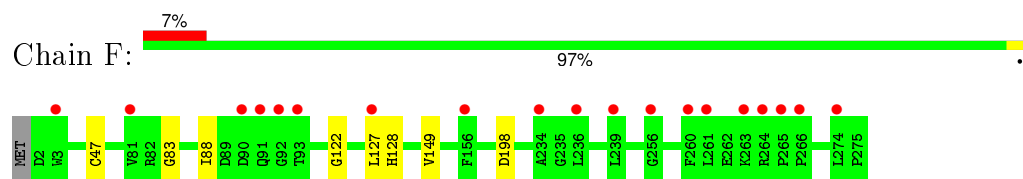
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0
3	I	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0

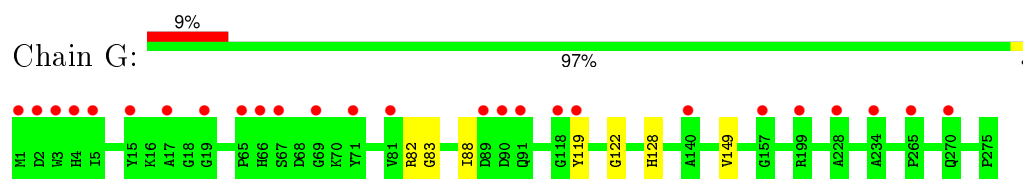
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total 43	O 43	0	0
4	B	53	Total 53	O 53	0	0
4	C	50	Total 50	O 50	0	0
4	D	82	Total 82	O 82	0	0
4	E	89	Total 89	O 89	0	0
4	F	75	Total 75	O 75	0	0
4	G	56	Total 56	O 56	0	0
4	H	73	Total 73	O 73	0	0
4	I	62	Total 62	O 62	0	0

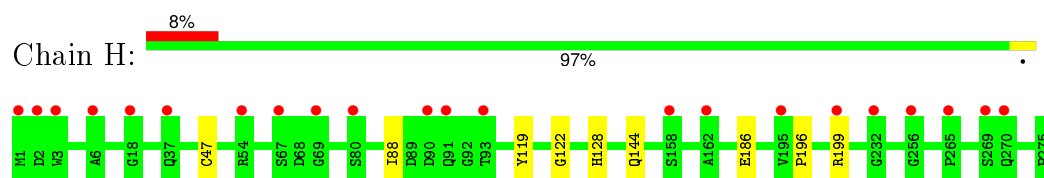
• Molecule 1: Naphthoate synthase



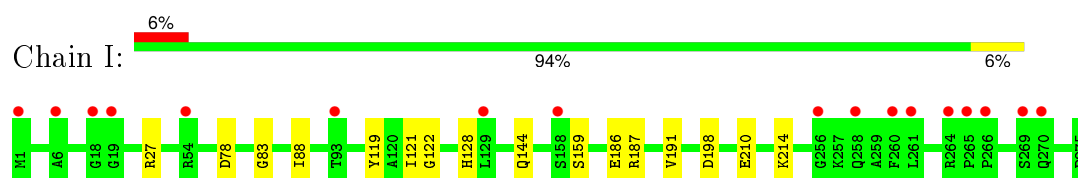
• Molecule 1: Naphthoate synthase



• Molecule 1: Naphthoate synthase



• Molecule 1: Naphthoate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.84Å 138.84Å 221.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 2.35 45.45 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.60-2.35) 99.8 (45.45-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.229 , 0.256 0.221 , 0.245	Depositor DCC
R_{free} test set	5146 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.5	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 102675 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19971	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.80 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7288e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 1HA, CL

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	0.34	0/2104	0.55	0/2854
1	B	0.32	0/2140	0.55	0/2896
1	C	0.33	0/2120	0.56	0/2874
1	D	0.35	0/2147	0.57	0/2907
1	E	0.34	0/2132	0.55	0/2889
1	F	0.34	0/2143	0.57	0/2901
1	G	0.33	0/2155	0.55	0/2917
1	H	0.34	0/2165	0.55	1/2928 (0.0%)
1	I	0.35	0/2143	0.58	1/2899 (0.0%)
All	All	0.34	0/19249	0.56	2/26065 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	88	ILE	CG1-CB-CG2	5.34	123.16	111.40
1	I	198	ASP	CB-CG-OD1	5.14	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2059	0	1976	4	0
1	B	2094	0	2048	7	0
1	C	2075	0	2002	7	0
1	D	2100	0	2042	12	0
1	E	2084	0	2014	4	0
1	F	2096	0	2041	6	0
1	G	2107	0	2061	5	0
1	H	2118	0	2074	7	0
1	I	2097	0	2051	15	0
2	A	61	0	37	2	0
2	B	61	0	36	2	0
2	C	61	0	36	0	0
2	D	61	0	35	4	0
2	E	61	0	36	2	0
2	F	61	0	37	1	0
2	G	61	0	36	3	0
2	H	61	0	37	1	0
2	I	61	0	37	2	0
3	A	1	0	0	2	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	1	0	0	2	0
3	E	1	0	0	1	0
3	F	1	0	0	1	0
3	G	1	0	0	1	0
3	H	1	0	0	2	0
3	I	1	0	0	2	0
4	A	43	0	0	0	0
4	B	53	0	0	2	0
4	C	50	0	0	0	0
4	D	82	0	0	2	0
4	E	89	0	0	0	0
4	F	75	0	0	1	0
4	G	56	0	0	0	0
4	H	73	0	0	2	0
4	I	62	0	0	3	0
All	All	19971	0	18636	70	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (70) 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:H:199:ARG:NH2	4:H:427:HOH:O	1.98	0.97
1:F:47:CYS:SG	4:F:451:HOH:O	2.37	0.82
1:D:106:ARG:NH1	1:D:160:TYR:CD1	2.48	0.81
1:C:125:HIS:CE1	1:C:142:PHE:HB3	2.18	0.78
1:I:210:GLU:O	1:I:214:LYS:HD3	1.85	0.76
1:C:31:ARG:NH2	1:C:70:LYS:HD2	2.01	0.76
1:C:31:ARG:HH22	1:C:70:LYS:HD2	1.58	0.69
1:F:198:ASP:OD2	1:H:186:GLU:OE1	2.13	0.67
1:H:119:TYR:CD1	2:H:301:1HA:H23	2.30	0.66
1:I:186:GLU:CA	1:I:191:VAL:HG22	2.26	0.66
1:I:187:ARG:NH2	4:I:447:HOH:O	2.28	0.65
1:E:119:TYR:CD1	2:E:301:1HA:H23	2.32	0.65
1:B:119:TYR:CD1	2:B:301:1HA:H23	2.33	0.63
1:D:106:ARG:NH1	1:D:160:TYR:CE1	2.67	0.62
1:G:119:TYR:CD1	2:G:301:1HA:H23	2.35	0.61
1:I:210:GLU:O	1:I:214:LYS:CD	2.48	0.61
1:I:122:GLY:HA2	3:I:302:CL:CL	2.39	0.60
1:I:186:GLU:HA	1:I:191:VAL:HG22	1.83	0.60
1:D:122:GLY:HA2	3:D:302:CL:CL	2.40	0.59
1:B:187:ARG:NH1	4:B:441:HOH:O	2.35	0.58
1:D:119:TYR:CD1	2:D:301:1HA:H23	2.38	0.58
1:B:183:GLN:HG2	4:B:413:HOH:O	2.04	0.58
1:H:196:PRO:HG2	1:H:199:ARG:CZ	2.34	0.57
1:C:125:HIS:HE1	1:C:142:PHE:HB3	1.67	0.57
1:H:122:GLY:HA2	3:H:302:CL:CL	2.42	0.57
1:C:31:ARG:NH2	1:C:70:LYS:CD	2.68	0.56
1:F:122:GLY:HA2	3:F:302:CL:CL	2.42	0.56
1:I:186:GLU:HB2	1:I:191:VAL:CG2	2.36	0.55
2:D:301:1HA:SBO	2:D:301:1HA:OAJ	2.66	0.54
1:I:214:LYS:NZ	4:I:438:HOH:O	2.40	0.53
1:I:119:TYR:CD1	2:I:301:1HA:H23	2.45	0.52
1:I:83:GLY:HA3	1:I:88:ILE:HD11	1.93	0.51
1:E:122:GLY:HA2	3:E:302:CL:CL	2.46	0.51
1:A:121:ILE:HG13	2:A:301:1HA:H20	1.92	0.51
1:I:186:GLU:N	1:I:191:VAL:HG22	2.26	0.51
1:G:83:GLY:HA3	1:G:88:ILE:HD11	1.93	0.50
1:C:83:GLY:HA3	1:C:88:ILE:HD11	1.93	0.50
1:B:83:GLY:HA3	1:B:88:ILE:HD11	1.93	0.50
1:E:83:GLY:HA3	1:E:88:ILE:HD11	1.93	0.50
1:F:83:GLY:HA3	1:F:88:ILE:HD11	1.93	0.49
1:G:149:VAL:HG21	2:G:301:1HA:H9	1.93	0.49
2:A:301:1HA:OAJ	2:A:301:1HA:SBO	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:GLY:HA3	1:D:88:ILE:HD11	1.94	0.48
1:I:27:ARG:NH2	1:I:78:ASP:OD2	2.42	0.48
1:B:121:ILE:HG13	2:B:301:1HA:H24	1.96	0.48
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.74	0.47
1:G:149:VAL:CG2	2:G:301:1HA:H9	2.43	0.47
1:B:97:ASN:O	1:B:97:ASN:OD1	2.33	0.46
1:D:1:MET:N	4:D:468:HOH:O	2.34	0.46
1:H:144:GLN:NE2	3:H:302:CL:CL	2.84	0.45
1:H:47:CYS:SG	4:H:441:HOH:O	2.61	0.45
1:I:144:GLN:NE2	3:I:302:CL:CL	2.86	0.45
1:E:4:HIS:CD2	1:E:16:LYS:O	2.70	0.44
1:A:146:GLY:N	3:A:302:CL:CL	2.87	0.44
1:G:122:GLY:HA2	3:G:302:CL:CL	2.55	0.44
1:D:27:ARG:NH2	1:D:78:ASP:OD2	2.43	0.44
1:F:127:LEU:HA	1:F:127:LEU:HD23	1.73	0.43
2:E:301:1HA:SBO	2:E:301:1HA:OAJ	2.72	0.43
1:D:183:GLN:NE2	4:D:474:HOH:O	2.52	0.43
1:B:122:GLY:HA2	3:B:302:CL:CL	2.56	0.43
1:D:106:ARG:NH1	1:D:160:TYR:CG	2.87	0.42
1:I:121:ILE:HG13	2:I:301:1HA:H20	2.01	0.42
1:A:122:GLY:HA2	3:A:302:CL:CL	2.56	0.42
1:F:149:VAL:HG21	2:F:301:1HA:H9	2.02	0.41
1:C:122:GLY:HA2	3:C:302:CL:CL	2.57	0.41
2:D:301:1HA:H36	2:D:301:1HA:O5'	2.21	0.41
1:D:144:GLN:NE2	3:D:302:CL:CL	2.87	0.40
1:D:149:VAL:O	1:D:149:VAL:HG22	2.21	0.40
1:D:149:VAL:HG11	2:D:301:1HA:H9	2.03	0.40
1:I:159:SER:HB3	4:I:457:HOH:O	2.20	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	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
1	B	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
1	C	272/275 (99%)	267 (98%)	5 (2%)	0	100	100
1	D	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
1	E	272/275 (99%)	267 (98%)	5 (2%)	0	100	100
1	F	272/275 (99%)	267 (98%)	5 (2%)	0	100	100
1	G	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
1	H	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
1	I	273/275 (99%)	268 (98%)	5 (2%)	0	100	100
All	All	2454/2475 (99%)	2409 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	200/218 (92%)	197 (98%)	3 (2%)	72	85
1	B	208/218 (95%)	207 (100%)	1 (0%)	92	97
1	C	205/218 (94%)	204 (100%)	1 (0%)	92	97
1	D	209/218 (96%)	208 (100%)	1 (0%)	92	97
1	E	206/218 (94%)	204 (99%)	2 (1%)	82	91
1	F	208/218 (95%)	207 (100%)	1 (0%)	92	97
1	G	211/218 (97%)	209 (99%)	2 (1%)	84	92
1	H	213/218 (98%)	212 (100%)	1 (0%)	92	97
1	I	208/218 (95%)	207 (100%)	1 (0%)	92	97
All	All	1868/1962 (95%)	1855 (99%)	13 (1%)	88	95

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	128	HIS
1	A	193	THR
1	B	128	HIS
1	C	128	HIS
1	D	128	HIS
1	E	82	ARG
1	E	128	HIS
1	F	128	HIS
1	G	82	ARG
1	G	128	HIS
1	H	128	HIS
1	I	128	HIS

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

Mol	Chain	Res	Type
1	B	97	ASN
1	C	125	HIS
1	C	144	GLN
1	D	183	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

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	1HA	A	301	-	55,65,65	1.79	11 (20%)	73,97,97	5.41	24 (32%)
2	1HA	B	301	-	55,65,65	1.83	12 (21%)	73,97,97	5.66	25 (34%)
2	1HA	C	301	-	55,65,65	1.90	13 (23%)	73,97,97	5.26	28 (38%)
2	1HA	D	301	-	55,65,65	1.72	11 (20%)	73,97,97	4.53	21 (28%)
2	1HA	E	301	-	55,65,65	1.79	12 (21%)	73,97,97	4.91	22 (30%)
2	1HA	F	301	-	55,65,65	1.80	12 (21%)	73,97,97	4.85	23 (31%)
2	1HA	G	301	-	55,65,65	1.86	11 (20%)	73,97,97	5.25	23 (31%)
2	1HA	H	301	-	55,65,65	1.83	10 (18%)	73,97,97	4.98	22 (30%)
2	1HA	I	301	-	55,65,65	1.73	11 (20%)	73,97,97	5.04	22 (30%)

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	1HA	A	301	-	-	0/50/71/71	0/5/5/5
2	1HA	B	301	-	-	0/50/71/71	0/5/5/5
2	1HA	C	301	-	-	0/50/71/71	0/5/5/5
2	1HA	D	301	-	-	0/50/71/71	0/5/5/5
2	1HA	E	301	-	-	0/50/71/71	0/5/5/5
2	1HA	F	301	-	-	0/50/71/71	0/5/5/5
2	1HA	G	301	-	-	0/50/71/71	0/5/5/5
2	1HA	H	301	-	-	0/50/71/71	0/5/5/5
2	1HA	I	301	-	-	0/50/71/71	0/5/5/5

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	1HA	O2'-C2'	-3.23	1.35	1.43
2	E	301	1HA	OAK-CBZ	-3.15	1.35	1.42
2	E	301	1HA	O2'-C2'	-3.10	1.35	1.43
2	G	301	1HA	O2'-C2'	-3.09	1.35	1.43
2	F	301	1HA	OAK-CBZ	-3.05	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	1HA	O2'-C2'	-3.02	1.35	1.43
2	D	301	1HA	O2'-C2'	-3.01	1.35	1.43
2	C	301	1HA	OAK-CBZ	-2.97	1.36	1.42
2	B	301	1HA	OAK-CBZ	-2.95	1.36	1.42
2	I	301	1HA	O2'-C2'	-2.94	1.35	1.43
2	B	301	1HA	O2'-C2'	-2.92	1.36	1.43
2	C	301	1HA	O2'-C2'	-2.91	1.36	1.43
2	C	301	1HA	C2'-C3'	-2.82	1.46	1.53
2	D	301	1HA	OAK-CBZ	-2.81	1.36	1.42
2	H	301	1HA	C2'-C3'	-2.80	1.46	1.53
2	A	301	1HA	C2'-C3'	-2.79	1.46	1.53
2	G	301	1HA	OAK-CBZ	-2.70	1.36	1.42
2	D	301	1HA	C2'-C3'	-2.68	1.47	1.53
2	H	301	1HA	OAK-CBZ	-2.68	1.36	1.42
2	E	301	1HA	C2'-C3'	-2.63	1.47	1.53
2	G	301	1HA	C2'-C3'	-2.63	1.47	1.53
2	I	301	1HA	C2'-C3'	-2.57	1.47	1.53
2	F	301	1HA	O2'-C2'	-2.55	1.36	1.43
2	A	301	1HA	OAK-CBZ	-2.52	1.37	1.42
2	B	301	1HA	C2'-C3'	-2.45	1.47	1.53
2	I	301	1HA	OAK-CBZ	-2.39	1.37	1.42
2	F	301	1HA	C2'-C3'	-2.23	1.48	1.53
2	I	301	1HA	PCI-OAI	-2.20	1.43	1.51
2	B	301	1HA	PCI-OAI	-2.12	1.43	1.51
2	D	301	1HA	PCI-OAI	-2.11	1.43	1.51
2	H	301	1HA	PCI-OAI	-2.09	1.43	1.51
2	F	301	1HA	PCI-OAI	-2.08	1.43	1.51
2	A	301	1HA	PCI-OAI	-2.07	1.43	1.51
2	E	301	1HA	PCI-OAI	-2.05	1.43	1.51
2	F	301	1HA	CAB-CCF	2.07	1.58	1.53
2	C	301	1HA	CBU-CBT	2.07	1.42	1.39
2	A	301	1HA	CAZ-CBB	2.09	1.58	1.51
2	B	301	1HA	CAZ-CBB	2.11	1.58	1.51
2	F	301	1HA	CAZ-CBB	2.12	1.58	1.51
2	G	301	1HA	CAZ-CBB	2.13	1.58	1.51
2	C	301	1HA	CAZ-CBB	2.15	1.58	1.51
2	E	301	1HA	CBR-SBO	2.16	1.81	1.76
2	I	301	1HA	CBR-SBO	2.17	1.81	1.76
2	E	301	1HA	CAB-CCF	2.21	1.58	1.53
2	B	301	1HA	CAB-CCF	2.24	1.58	1.53
2	B	301	1HA	CBR-SBO	2.25	1.81	1.76
2	C	301	1HA	CBB-CBP	2.28	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	1HA	CAB-CCF	2.30	1.58	1.53
2	E	301	1HA	CBU-CBT	2.31	1.42	1.39
2	G	301	1HA	CAB-CCF	2.37	1.58	1.53
2	G	301	1HA	CBR-SBO	2.39	1.81	1.76
2	D	301	1HA	CBR-SBO	2.44	1.81	1.76
2	H	301	1HA	CAB-CCF	2.47	1.59	1.53
2	C	301	1HA	CBR-SBO	2.50	1.81	1.76
2	D	301	1HA	CAB-CCF	2.52	1.59	1.53
2	B	301	1HA	CBU-CBR	2.55	1.53	1.50
2	A	301	1HA	CAB-CCF	2.57	1.59	1.53
2	I	301	1HA	CAB-CCF	2.61	1.59	1.53
2	H	301	1HA	C6-N6	2.63	1.43	1.34
2	I	301	1HA	CBU-CBR	2.74	1.53	1.50
2	D	301	1HA	CAA-CCF	2.77	1.59	1.53
2	A	301	1HA	CAA-CCF	2.78	1.59	1.53
2	I	301	1HA	C6-N6	2.80	1.43	1.34
2	F	301	1HA	C6-N6	2.81	1.43	1.34
2	I	301	1HA	CAA-CCF	2.82	1.59	1.53
2	C	301	1HA	C6-N6	2.83	1.43	1.34
2	A	301	1HA	C6-N6	2.85	1.43	1.34
2	B	301	1HA	C6-N6	2.86	1.43	1.34
2	H	301	1HA	CBU-CBR	2.87	1.53	1.50
2	D	301	1HA	C6-N6	2.87	1.43	1.34
2	F	301	1HA	CBR-SBO	2.90	1.82	1.76
2	G	301	1HA	C6-N6	2.90	1.43	1.34
2	E	301	1HA	C6-N6	2.91	1.43	1.34
2	F	301	1HA	CAA-CCF	2.93	1.60	1.53
2	H	301	1HA	CAA-CCF	2.95	1.60	1.53
2	C	301	1HA	CAA-CCF	2.96	1.60	1.53
2	D	301	1HA	CBU-CBR	2.96	1.53	1.50
2	A	301	1HA	CBU-CBR	2.97	1.53	1.50
2	G	301	1HA	CAA-CCF	3.09	1.60	1.53
2	E	301	1HA	CAA-CCF	3.09	1.60	1.53
2	E	301	1HA	CBU-CBR	3.10	1.54	1.50
2	G	301	1HA	CBU-CBR	3.14	1.54	1.50
2	B	301	1HA	CAA-CCF	3.26	1.60	1.53
2	F	301	1HA	CBU-CBR	3.42	1.54	1.50
2	C	301	1HA	CBU-CBR	3.57	1.54	1.50
2	D	301	1HA	CBP-NBH	4.42	1.44	1.33
2	I	301	1HA	CBP-NBH	4.74	1.44	1.33
2	F	301	1HA	CBP-NBH	5.02	1.45	1.33
2	A	301	1HA	CBP-NBH	5.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	1HA	CBP-NBH	5.15	1.45	1.33
2	B	301	1HA	CBP-NBH	5.42	1.46	1.33
2	C	301	1HA	CBP-NBH	5.43	1.46	1.33
2	G	301	1HA	CBP-NBH	5.51	1.46	1.33
2	H	301	1HA	CBP-NBH	5.53	1.46	1.33
2	D	301	1HA	CBQ-NBI	5.97	1.46	1.33
2	E	301	1HA	CBQ-NBI	6.35	1.46	1.33
2	I	301	1HA	CBQ-NBI	6.38	1.47	1.33
2	F	301	1HA	CBQ-NBI	6.56	1.47	1.33
2	H	301	1HA	CBQ-NBI	6.79	1.47	1.33
2	A	301	1HA	CBQ-NBI	6.86	1.48	1.33
2	B	301	1HA	CBQ-NBI	7.00	1.48	1.33
2	G	301	1HA	CBQ-NBI	7.07	1.48	1.33
2	C	301	1HA	CBQ-NBI	7.19	1.48	1.33

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	1HA	CBU-CBR-SBO	-19.63	92.46	115.22
2	B	301	1HA	CBU-CBR-SBO	-18.88	93.33	115.22
2	I	301	1HA	CBU-CBR-SBO	-17.12	95.37	115.22
2	G	301	1HA	CBU-CBR-SBO	-17.09	95.40	115.22
2	C	301	1HA	CBU-CBR-SBO	-16.69	95.87	115.22
2	H	301	1HA	CBU-CBR-SBO	-15.68	97.04	115.22
2	E	301	1HA	CBU-CBR-SBO	-14.72	98.15	115.22
2	F	301	1HA	CBU-CBR-SBO	-14.70	98.17	115.22
2	I	301	1HA	N3-C2-N1	-13.08	118.88	128.89
2	C	301	1HA	N3-C2-N1	-12.67	119.19	128.89
2	F	301	1HA	N3-C2-N1	-12.57	119.27	128.89
2	G	301	1HA	N3-C2-N1	-12.55	119.28	128.89
2	E	301	1HA	N3-C2-N1	-12.55	119.28	128.89
2	B	301	1HA	N3-C2-N1	-12.47	119.35	128.89
2	A	301	1HA	N3-C2-N1	-12.32	119.46	128.89
2	D	301	1HA	N3-C2-N1	-11.97	119.73	128.89
2	H	301	1HA	N3-C2-N1	-11.81	119.85	128.89
2	D	301	1HA	CBU-CBR-SBO	-11.05	102.40	115.22
2	C	301	1HA	CAB-CCF-CBD	-10.08	95.43	108.50
2	B	301	1HA	CAB-CCF-CBD	-9.57	96.10	108.50
2	G	301	1HA	CAB-CCF-CBD	-9.46	96.24	108.50
2	E	301	1HA	CAB-CCF-CBD	-9.02	96.81	108.50
2	B	301	1HA	CAA-CCF-CAB	-8.61	91.99	109.28
2	I	301	1HA	CAB-CCF-CBD	-8.37	97.65	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	1HA	CAA-CCF-CBZ	-8.19	94.39	109.34
2	H	301	1HA	CAB-CCF-CBD	-8.14	97.94	108.50
2	A	301	1HA	CAA-CCF-CAB	-8.08	93.05	109.28
2	A	301	1HA	CAB-CCF-CBD	-8.06	98.05	108.50
2	G	301	1HA	CAA-CCF-CAB	-7.79	93.63	109.28
2	I	301	1HA	CAA-CCF-CAB	-7.55	94.12	109.28
2	H	301	1HA	CAA-CCF-CAB	-7.54	94.14	109.28
2	A	301	1HA	CAA-CCF-CBZ	-7.50	95.66	109.34
2	F	301	1HA	CAB-CCF-CBD	-7.44	98.86	108.50
2	F	301	1HA	CAA-CCF-CBZ	-7.28	96.06	109.34
2	E	301	1HA	CAA-CCF-CAB	-7.26	94.70	109.28
2	C	301	1HA	CAA-CCF-CAB	-7.14	94.94	109.28
2	D	301	1HA	CAA-CCF-CAB	-7.10	95.02	109.28
2	B	301	1HA	CAA-CCF-CBZ	-6.95	96.66	109.34
2	F	301	1HA	CAA-CCF-CAB	-6.74	95.74	109.28
2	D	301	1HA	CAA-CCF-CBZ	-6.74	97.05	109.34
2	D	301	1HA	CAB-CCF-CBD	-6.38	100.24	108.50
2	H	301	1HA	CAA-CCF-CBZ	-6.28	97.89	109.34
2	I	301	1HA	CAA-CCF-CBZ	-6.19	98.04	109.34
2	G	301	1HA	CAA-CCF-CBZ	-5.85	98.67	109.34
2	E	301	1HA	CAA-CCF-CBZ	-5.61	99.10	109.34
2	E	301	1HA	CAT-CBU-CBR	-4.66	109.55	119.88
2	E	301	1HA	OAD-CBP-CBB	-4.21	114.73	121.98
2	D	301	1HA	PCH-OBN-PCI	-4.15	121.07	132.73
2	I	301	1HA	PCH-OBN-PCI	-4.09	121.25	132.73
2	G	301	1HA	OAD-CBP-CBB	-4.08	114.94	121.98
2	E	301	1HA	PCH-OBN-PCI	-3.97	121.58	132.73
2	I	301	1HA	CAT-CBU-CBR	-3.87	111.30	119.88
2	C	301	1HA	CAT-CBU-CBR	-3.80	111.46	119.88
2	H	301	1HA	CAT-CBU-CBR	-3.73	111.62	119.88
2	B	301	1HA	OAD-CBP-CBB	-3.70	115.59	121.98
2	D	301	1HA	CAT-CBU-CBR	-3.70	111.69	119.88
2	G	301	1HA	PCH-OBN-PCI	-3.69	122.37	132.73
2	A	301	1HA	PCH-OBN-PCI	-3.62	122.56	132.73
2	A	301	1HA	OAD-CBP-CBB	-3.60	115.77	121.98
2	I	301	1HA	OAD-CBP-CBB	-3.57	115.82	121.98
2	F	301	1HA	CAT-CBU-CBR	-3.48	112.17	119.88
2	D	301	1HA	OAD-CBP-CBB	-3.47	115.99	121.98
2	H	301	1HA	OAD-CBP-CBB	-3.47	115.99	121.98
2	F	301	1HA	OAD-CBP-CBB	-3.44	116.06	121.98
2	G	301	1HA	CAT-CBU-CBR	-3.36	112.44	119.88
2	F	301	1HA	C4-C5-N7	-3.26	106.48	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	1HA	PCH-OBN-PCI	-3.18	123.81	132.73
2	E	301	1HA	C4-C5-N7	-3.05	106.67	109.48
2	H	301	1HA	C4-C5-N7	-3.02	106.70	109.48
2	C	301	1HA	OAD-CBP-CBB	-2.93	116.92	121.98
2	B	301	1HA	CAT-CBU-CBR	-2.91	113.42	119.88
2	B	301	1HA	PCH-OBN-PCI	-2.89	124.60	132.73
2	A	301	1HA	OAK-CBZ-CBQ	-2.82	103.91	110.38
2	C	301	1HA	OAK-CBZ-CBQ	-2.73	104.11	110.38
2	D	301	1HA	C4-C5-N7	-2.73	106.97	109.48
2	A	301	1HA	CAT-CBU-CBR	-2.72	113.85	119.88
2	C	301	1HA	C4-C5-N7	-2.59	107.10	109.48
2	G	301	1HA	C4-C5-N7	-2.54	107.14	109.48
2	D	301	1HA	C4'-O4'-C1'	-2.53	106.93	109.72
2	H	301	1HA	PCH-OBN-PCI	-2.50	125.69	132.73
2	B	301	1HA	C4-C5-N7	-2.47	107.20	109.48
2	F	301	1HA	OAD-CBP-NBH	-2.46	118.06	122.94
2	D	301	1HA	OAD-CBP-NBH	-2.45	118.07	122.94
2	I	301	1HA	C4-C5-N7	-2.40	107.27	109.48
2	A	301	1HA	C4-C5-N7	-2.38	107.29	109.48
2	B	301	1HA	OAE-CBQ-NBI	-2.37	118.33	123.08
2	F	301	1HA	OAK-CBZ-CBQ	-2.33	105.04	110.38
2	C	301	1HA	PCH-OBN-PCI	-2.23	126.46	132.73
2	G	301	1HA	C4'-O4'-C1'	-2.23	107.27	109.72
2	C	301	1HA	OAD-CBP-NBH	-2.22	118.54	122.94
2	A	301	1HA	OAD-CBP-NBH	-2.18	118.60	122.94
2	B	301	1HA	C4'-O4'-C1'	-2.14	107.37	109.72
2	B	301	1HA	OAD-CBP-NBH	-2.10	118.77	122.94
2	E	301	1HA	C4'-O4'-C1'	-2.02	107.50	109.72
2	E	301	1HA	OAK-CBZ-CBQ	-2.01	105.76	110.38
2	C	301	1HA	C4'-O4'-C1'	-2.01	107.51	109.72
2	H	301	1HA	O4'-C1'-N9	2.00	112.29	108.10
2	C	301	1HA	CAY-CBA-SBO	2.03	116.80	111.36
2	I	301	1HA	O5'-C5'-C4'	2.04	116.64	109.12
2	C	301	1HA	CBT-CBW-CBV	2.05	120.97	118.57
2	E	301	1HA	CBT-CBW-CBV	2.05	120.97	118.57
2	F	301	1HA	C2-N1-C6	2.05	122.44	118.77
2	A	301	1HA	C2-N1-C6	2.07	122.46	118.77
2	H	301	1HA	C2-N1-C6	2.09	122.50	118.77
2	H	301	1HA	CBA-CAY-NBH	2.10	116.55	112.36
2	H	301	1HA	OBN-PCI-OBK	2.13	108.59	102.94
2	I	301	1HA	OBN-PCH-O5'	2.15	108.64	102.94
2	I	301	1HA	CBT-CBW-CBV	2.17	121.11	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	1HA	C2-N1-C6	2.24	122.77	118.77
2	D	301	1HA	C2-N1-C6	2.24	122.78	118.77
2	I	301	1HA	C2-N1-C6	2.27	122.83	118.77
2	F	301	1HA	CBZ-CBQ-NBI	2.28	121.51	116.47
2	G	301	1HA	CBZ-CBQ-NBI	2.30	121.56	116.47
2	I	301	1HA	OBN-PCI-OBK	2.31	109.06	102.94
2	A	301	1HA	CBZ-CBQ-NBI	2.32	121.61	116.47
2	C	301	1HA	CAZ-CBB-CBP	2.32	116.13	112.31
2	C	301	1HA	C2-N1-C6	2.34	122.95	118.77
2	C	301	1HA	O5'-C5'-C4'	2.36	117.83	109.12
2	F	301	1HA	CBA-CAY-NBH	2.38	117.11	112.36
2	E	301	1HA	C2-N1-C6	2.38	123.02	118.77
2	G	301	1HA	OBN-PCI-OBK	2.41	109.33	102.94
2	H	301	1HA	CBZ-CBQ-NBI	2.45	121.89	116.47
2	B	301	1HA	CBB-CAZ-NBI	2.46	117.29	111.88
2	G	301	1HA	C2-N1-C6	2.47	123.18	118.77
2	C	301	1HA	CBA-CAY-NBH	2.58	117.52	112.36
2	B	301	1HA	CBT-CBU-CBR	2.58	127.25	121.01
2	C	301	1HA	O4'-C1'-N9	2.61	113.55	108.10
2	C	301	1HA	CBZ-CBQ-NBI	2.61	122.25	116.47
2	F	301	1HA	OBK-CBD-CCF	2.66	114.82	110.55
2	H	301	1HA	CBA-SBO-CBR	2.66	102.98	99.59
2	A	301	1HA	CBT-CBU-CBR	2.68	127.48	121.01
2	A	301	1HA	CBB-CAZ-NBI	2.72	117.86	111.88
2	G	301	1HA	CAY-CBA-SBO	2.72	118.66	111.36
2	E	301	1HA	OBN-PCI-OBK	2.77	110.29	102.94
2	D	301	1HA	CBA-CAY-NBH	2.78	117.91	112.36
2	F	301	1HA	CBA-SBO-CBR	2.81	103.16	99.59
2	D	301	1HA	OBN-PCI-OBK	2.81	110.40	102.94
2	B	301	1HA	CBA-CAY-NBH	2.84	118.03	112.36
2	A	301	1HA	OBN-PCI-OBK	2.94	110.73	102.94
2	B	301	1HA	CBZ-CBQ-NBI	2.97	123.04	116.47
2	B	301	1HA	OBN-PCI-OBK	2.97	110.81	102.94
2	A	301	1HA	CBA-CAY-NBH	3.02	118.39	112.36
2	D	301	1HA	OAF-CBR-CBU	3.11	128.27	123.28
2	F	301	1HA	OBN-PCI-OBK	3.14	111.27	102.94
2	G	301	1HA	CBT-CBU-CBR	3.31	129.01	121.01
2	E	301	1HA	CBA-CAY-NBH	3.44	119.23	112.36
2	H	301	1HA	CBT-CBU-CBR	3.50	129.45	121.01
2	I	301	1HA	CBA-CAY-NBH	3.53	119.42	112.36
2	C	301	1HA	CBA-SBO-CBR	3.55	104.10	99.59
2	B	301	1HA	CBA-SBO-CBR	3.60	104.17	99.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	1HA	CBA-CAY-NBH	3.61	119.58	112.36
2	I	301	1HA	CBT-CBU-CBR	3.62	129.75	121.01
2	F	301	1HA	CBT-CBU-CBR	3.75	130.07	121.01
2	D	301	1HA	CBT-CBU-CBR	3.79	130.17	121.01
2	C	301	1HA	CBT-CBU-CBR	3.91	130.45	121.01
2	H	301	1HA	CBB-CBP-NBH	3.98	123.37	116.46
2	A	301	1HA	CBA-SBO-CBR	4.29	105.05	99.59
2	G	301	1HA	CBA-SBO-CBR	4.31	105.07	99.59
2	E	301	1HA	CBT-CBU-CBR	4.53	131.95	121.01
2	E	301	1HA	CBB-CBP-NBH	4.57	124.40	116.46
2	C	301	1HA	CBB-CBP-NBH	4.65	124.54	116.46
2	D	301	1HA	OAF-CBR-SBO	4.66	128.31	122.37
2	H	301	1HA	OAF-CBR-CBU	4.78	130.95	123.28
2	I	301	1HA	CBB-CBP-NBH	4.88	124.94	116.46
2	G	301	1HA	CBB-CBP-NBH	5.09	125.30	116.46
2	F	301	1HA	OAF-CBR-CBU	5.26	131.72	123.28
2	B	301	1HA	CBB-CBP-NBH	5.27	125.61	116.46
2	A	301	1HA	CBB-CBP-NBH	5.27	125.62	116.46
2	E	301	1HA	OAF-CBR-CBU	5.29	131.77	123.28
2	G	301	1HA	OAF-CBR-CBU	5.36	131.88	123.28
2	C	301	1HA	OBK-CBD-CCF	5.38	119.20	110.55
2	F	301	1HA	CBB-CBP-NBH	5.40	125.85	116.46
2	A	301	1HA	OBK-CBD-CCF	5.43	119.27	110.55
2	D	301	1HA	CBB-CBP-NBH	5.44	125.91	116.46
2	C	301	1HA	OAF-CBR-CBU	5.65	132.34	123.28
2	E	301	1HA	OAF-CBR-SBO	5.91	129.90	122.37
2	I	301	1HA	OAF-CBR-CBU	5.98	132.87	123.28
2	F	301	1HA	OAF-CBR-SBO	6.04	130.06	122.37
2	B	301	1HA	OAF-CBR-CBU	6.08	133.03	123.28
2	H	301	1HA	OBK-CBD-CCF	6.32	120.70	110.55
2	H	301	1HA	OAF-CBR-SBO	6.61	130.79	122.37
2	I	301	1HA	OBK-CBD-CCF	6.90	121.64	110.55
2	A	301	1HA	OAF-CBR-CBU	7.05	134.59	123.28
2	G	301	1HA	OBK-CBD-CCF	7.10	121.96	110.55
2	D	301	1HA	OBK-CBD-CCF	7.24	122.18	110.55
2	I	301	1HA	OAF-CBR-SBO	7.36	131.75	122.37
2	C	301	1HA	OAF-CBR-SBO	7.37	131.76	122.37
2	A	301	1HA	OAF-CBR-SBO	7.58	132.03	122.37
2	E	301	1HA	OBK-CBD-CCF	7.63	122.82	110.55
2	B	301	1HA	OBK-CBD-CCF	7.76	123.03	110.55
2	G	301	1HA	OAF-CBR-SBO	8.08	132.67	122.37
2	B	301	1HA	OAF-CBR-SBO	8.09	132.68	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	1HA	CAB-CCF-CBZ	11.96	131.18	109.34
2	D	301	1HA	CAB-CCF-CBZ	11.97	131.19	109.34
2	I	301	1HA	CAB-CCF-CBZ	12.32	131.83	109.34
2	H	301	1HA	CAB-CCF-CBZ	12.77	132.65	109.34
2	G	301	1HA	CAB-CCF-CBZ	13.66	134.28	109.34
2	B	301	1HA	CAB-CCF-CBZ	13.80	134.53	109.34
2	F	301	1HA	CAB-CCF-CBZ	14.10	135.08	109.34
2	C	301	1HA	CAB-CCF-CBZ	14.11	135.10	109.34
2	A	301	1HA	CAB-CCF-CBZ	15.47	137.58	109.34
2	D	301	1HA	CAA-CCF-CBD	26.46	142.81	108.50
2	F	301	1HA	CAA-CCF-CBD	27.38	144.00	108.50
2	I	301	1HA	CAA-CCF-CBD	27.68	144.39	108.50
2	E	301	1HA	CAA-CCF-CBD	27.79	144.53	108.50
2	H	301	1HA	CAA-CCF-CBD	29.15	146.29	108.50
2	G	301	1HA	CAA-CCF-CBD	29.28	146.46	108.50
2	C	301	1HA	CAA-CCF-CBD	29.41	146.63	108.50
2	A	301	1HA	CAA-CCF-CBD	29.53	146.79	108.50
2	B	301	1HA	CAA-CCF-CBD	33.09	151.39	108.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	1HA	2	0
2	B	301	1HA	2	0
2	D	301	1HA	4	0
2	E	301	1HA	2	0
2	F	301	1HA	1	0
2	G	301	1HA	3	0
2	H	301	1HA	1	0
2	I	301	1HA	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	275/275 (100%)	0.82	31 (11%)	7 12	21, 46, 68, 92	0
1	B	275/275 (100%)	0.58	26 (9%)	10 17	25, 44, 73, 99	0
1	C	274/275 (99%)	0.78	25 (9%)	11 18	29, 48, 83, 93	0
1	D	275/275 (100%)	0.47	13 (4%)	35 50	22, 34, 59, 76	0
1	E	274/275 (99%)	0.27	11 (4%)	42 56	23, 36, 58, 69	0
1	F	274/275 (99%)	0.55	19 (6%)	20 30	25, 40, 65, 100	0
1	G	275/275 (100%)	0.71	26 (9%)	10 17	26, 45, 68, 94	0
1	H	275/275 (100%)	0.38	22 (8%)	15 23	27, 38, 59, 80	0
1	I	275/275 (100%)	0.48	17 (6%)	24 36	25, 38, 63, 80	0
All	All	2472/2475 (99%)	0.56	190 (7%)	16 25	21, 41, 68, 100	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	GLY	7.6
1	C	93	THR	7.5
1	A	67	SER	7.5
1	B	67	SER	7.4
1	G	67	SER	6.4
1	A	3	TRP	6.1
1	C	92	GLY	6.0
1	G	3	TRP	6.0
1	A	70	LYS	5.8
1	C	90	ASP	5.7
1	A	90	ASP	5.5
1	C	91	GLN	5.5
1	A	275	PRO	5.5
1	C	256	GLY	5.2
1	B	197	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	69	GLY	5.1
1	A	1	MET	5.1
1	C	67	SER	5.1
1	B	90	ASP	5.0
1	G	265	PRO	4.9
1	F	261	LEU	4.7
1	F	90	ASP	4.6
1	G	90	ASP	4.6
1	I	269	SER	4.4
1	H	69	GLY	4.4
1	F	91	GLN	4.4
1	I	265	PRO	4.4
1	G	81	VAL	4.4
1	G	2	ASP	4.4
1	B	89	ASP	4.3
1	G	1	MET	4.1
1	B	1	MET	4.1
1	C	66	HIS	4.0
1	C	258	GLN	4.0
1	B	88	ILE	4.0
1	F	263	LYS	4.0
1	D	265	PRO	3.9
1	A	270	GLN	3.9
1	B	91	GLN	3.9
1	H	270	GLN	3.9
1	C	84	GLU	3.9
1	H	256	GLY	3.9
1	G	71	TYR	3.9
1	G	91	GLN	3.8
1	H	91	GLN	3.8
1	F	260	PHE	3.8
1	G	65	PRO	3.8
1	B	68	ASP	3.8
1	C	266	PRO	3.8
1	C	81	VAL	3.8
1	H	1	MET	3.7
1	F	265	PRO	3.7
1	A	68	ASP	3.7
1	C	70	LYS	3.7
1	I	266	PRO	3.6
1	B	80	SER	3.6
1	B	70	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	15	TYR	3.5
1	H	54	ARG	3.4
1	E	80	SER	3.4
1	H	265	PRO	3.4
1	B	2	ASP	3.4
1	G	234	ALA	3.4
1	D	261	LEU	3.4
1	H	2	ASP	3.4
1	C	69	GLY	3.3
1	G	66	HIS	3.3
1	H	18	GLY	3.2
1	C	260	PHE	3.2
1	H	90	ASP	3.2
1	I	6	ALA	3.2
1	H	67	SER	3.1
1	E	236	LEU	3.1
1	C	71	TYR	3.1
1	I	270	GLN	3.1
1	G	4	HIS	3.1
1	H	199	ARG	3.1
1	H	93	THR	3.0
1	B	71	TYR	3.0
1	C	265	PRO	3.0
1	H	37	GLN	3.0
1	G	140	ALA	3.0
1	G	270	GLN	3.0
1	C	12	ILE	2.9
1	A	88	ILE	2.9
1	F	93	THR	2.8
1	B	30	LYS	2.8
1	B	66	HIS	2.8
1	D	2	ASP	2.7
1	D	1	MET	2.7
1	F	236	LEU	2.7
1	B	63	ALA	2.7
1	E	92	GLY	2.7
1	H	6	ALA	2.7
1	A	236	LEU	2.6
1	D	127	LEU	2.6
1	I	261	LEU	2.6
1	G	17	ALA	2.6
1	H	162	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	266	PRO	2.6
1	I	18	GLY	2.6
1	A	234	ALA	2.6
1	F	234	ALA	2.6
1	F	92	GLY	2.6
1	B	240	ALA	2.6
1	F	3	TRP	2.6
1	D	130	VAL	2.6
1	G	228	ALA	2.6
1	I	129	LEU	2.6
1	B	79	GLN	2.6
1	E	90	ASP	2.5
1	E	93	THR	2.5
1	F	127	LEU	2.5
1	B	228	ALA	2.5
1	B	10	ASP	2.5
1	F	274	LEU	2.5
1	I	256	GLY	2.5
1	A	66	HIS	2.5
1	D	126	VAL	2.5
1	D	40	PHE	2.5
1	C	63	ALA	2.5
1	F	239	LEU	2.5
1	E	5	ILE	2.5
1	D	228	ALA	2.4
1	G	69	GLY	2.4
1	C	80	SER	2.4
1	I	93	THR	2.4
1	I	264	ARG	2.4
1	E	225	ALA	2.4
1	D	258	GLN	2.4
1	A	84	GLU	2.4
1	C	228	ALA	2.4
1	B	5	ILE	2.4
1	A	141	ILE	2.3
1	C	14	TYR	2.3
1	G	119	TYR	2.3
1	G	199	ARG	2.3
1	A	228	ALA	2.3
1	D	162	ALA	2.3
1	H	232	GLY	2.3
1	A	5	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	199	ARG	2.3
1	G	157	GLY	2.3
1	C	30	LYS	2.3
1	B	261	LEU	2.3
1	I	1	MET	2.3
1	G	5	ILE	2.2
1	C	94	PRO	2.2
1	A	207	TRP	2.2
1	A	25	ILE	2.2
1	B	87	TYR	2.2
1	I	258	GLN	2.2
1	A	29	HIS	2.2
1	A	4	HIS	2.2
1	A	211	ILE	2.2
1	B	119	TYR	2.2
1	B	69	GLY	2.2
1	F	264	ARG	2.2
1	E	69	GLY	2.2
1	F	256	GLY	2.2
1	G	89	ASP	2.2
1	A	71	TYR	2.2
1	E	270	GLN	2.2
1	E	269	SER	2.2
1	F	81	VAL	2.1
1	A	91	GLN	2.1
1	F	156	PHE	2.1
1	H	158	SER	2.1
1	H	269	SER	2.1
1	E	228	ALA	2.1
1	G	118	GLY	2.1
1	A	265	PRO	2.1
1	H	80	SER	2.1
1	C	101	LEU	2.1
1	I	19	GLY	2.1
1	H	3	TRP	2.1
1	I	54	ARG	2.1
1	C	160	TYR	2.0
1	A	269	SER	2.0
1	D	80	SER	2.0
1	I	158	SER	2.0
1	B	141	ILE	2.0
1	A	235	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	103	ARG	2.0
1	G	19	GLY	2.0
1	I	260	PHE	2.0
1	A	232	GLY	2.0
1	H	195	VAL	2.0
1	A	6	ALA	2.0
1	A	239	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	CL	B	302	1/1	0.97	0.27	12.75	50,50,50,50	0
3	CL	A	302	1/1	0.92	0.20	4.29	54,54,54,54	0
2	1HA	C	301	61/61	0.71	0.30	1.07	61,77,100,100	0
2	1HA	G	301	61/61	0.85	0.23	0.53	49,61,68,69	0
2	1HA	B	301	61/61	0.81	0.22	0.32	62,68,80,82	0
2	1HA	H	301	61/61	0.90	0.15	0.12	37,47,58,59	0
2	1HA	A	301	61/61	0.87	0.19	0.10	49,62,81,83	0
2	1HA	E	301	61/61	0.92	0.16	0.08	37,44,54,55	0
2	1HA	F	301	61/61	0.92	0.15	-0.24	37,45,49,53	0
2	1HA	I	301	61/61	0.93	0.13	-0.51	34,44,53,59	0
3	CL	C	302	1/1	0.79	0.13	-0.65	89,89,89,89	0
2	1HA	D	301	61/61	0.93	0.13	-0.81	28,39,46,48	0
3	CL	H	302	1/1	0.94	0.10	-0.83	47,47,47,47	0
3	CL	I	302	1/1	0.98	0.06	-1.86	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	F	302	1/1	0.95	0.07	-1.98	45,45,45,45	0
3	CL	E	302	1/1	0.94	0.09	-2.59	54,54,54,54	0
3	CL	D	302	1/1	0.99	0.07	-2.85	39,39,39,39	0
3	CL	G	302	1/1	0.98	0.05	-3.05	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.