



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:56 PM GMT

PDB ID : 1MRO  
Title : METHYL-COENZYME M REDUCTASE  
Authors : Ermler, U.; Grabarse, W.  
Deposited on : 1997-10-01  
Resolution : 1.16 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](mailto: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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

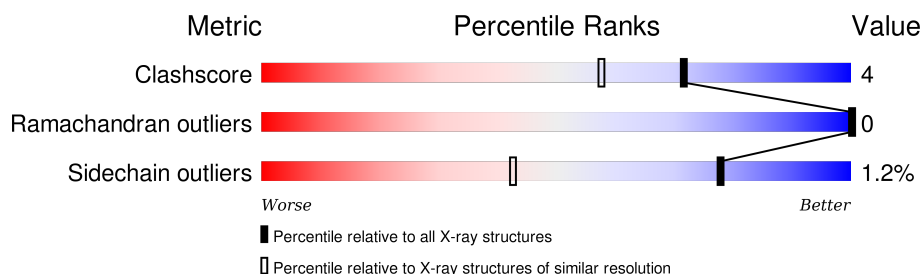
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.16 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))
Clashscore	102246	1109 (1.20-1.12)
Ramachandran outliers	100387	1058 (1.20-1.12)
Sidechain outliers	100360	1058 (1.20-1.12)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	548	
1	D	548	
2	B	442	
2	E	442	
3	C	247	
3	F	247	

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
6	F43	A	700	X	-	-	-
6	F43	D	800	X	-	-	-
7	TP7	A	9000	X	-	-	-
7	TP7	A	9500	X	-	-	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 21217 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 METHYL-COENZYME M REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	19	15	0
			4293	2717	717	839	20			
1	D	548	Total	C	N	O	S	16	13	0
			4290	2718	716	836	20			

- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	17	13	0
			3352	2123	553	655	21			
2	E	442	Total	C	N	O	S	10	7	0
			3328	2104	552	652	20			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	36	6	0
			2021	1253	358	399	11			
3	F	247	Total	C	N	O	S	34	3	0
			2013	1247	357	398	11			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

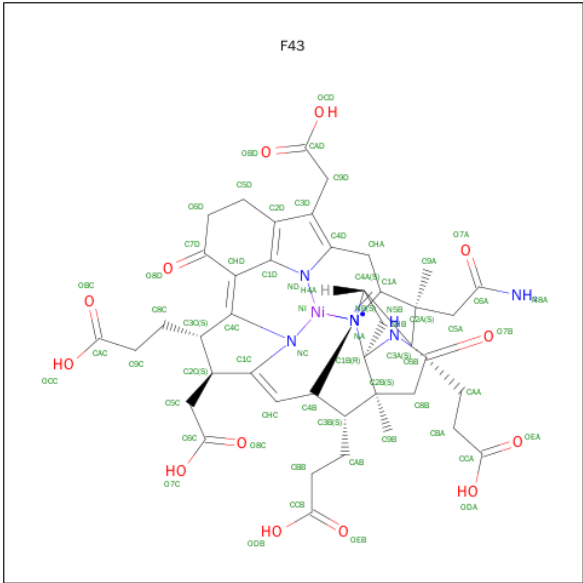
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Na	0	0
			1	1		

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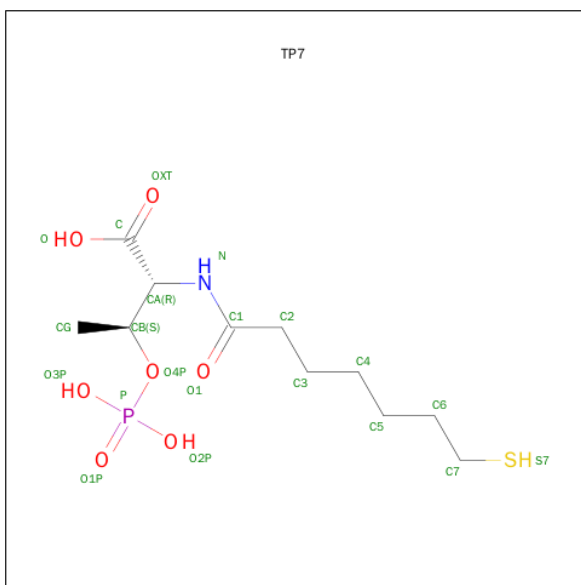
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Na	0	0
			1	1		

- Molecule 6 is FACTOR 430 (three-letter code: F43) (formula: C<sub>42</sub>H<sub>49</sub>N<sub>6</sub>NiO<sub>13</sub>).



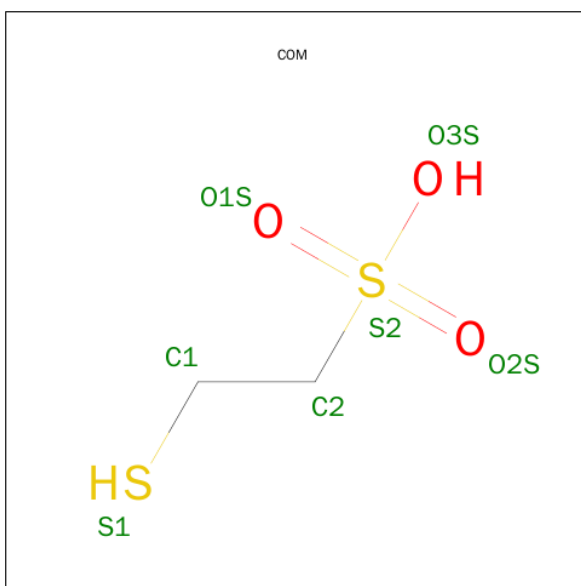
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
6	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 7 is COENZYME B (three-letter code: TP7) (formula: C<sub>11</sub>H<sub>22</sub>NO<sub>7</sub>PS).



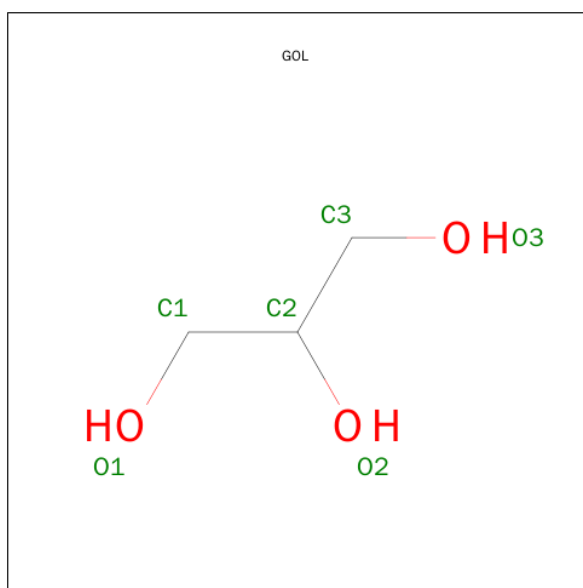
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0
7	A	1	Total 21	C 11	N 1	O 7	P 1	S 1	0	0

- Molecule 8 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula:  $\text{C}_2\text{H}_6\text{O}_3\text{S}_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	D	1	Total 7	C 2	O 3	S 2	0	0
8	A	1	Total 7	C 2	O 3	S 2	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		
9	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is water.

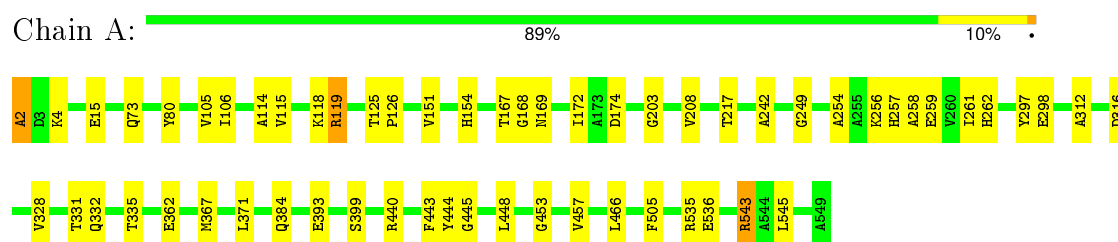
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	378	Total	O	0	0
			378	378		
10	B	306	Total	O	0	0
			306	306		
10	C	197	Total	O	0	0
			197	197		
10	D	367	Total	O	0	0
			367	367		
10	E	277	Total	O	0	0
			277	277		
10	F	188	Total	O	0	0
			188	188		

### 3 Residue-property plots

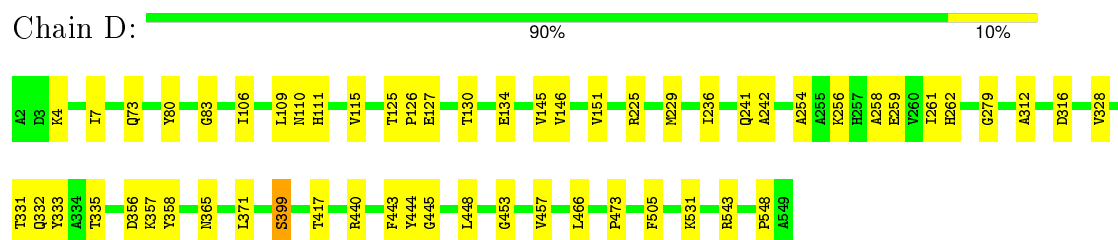
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

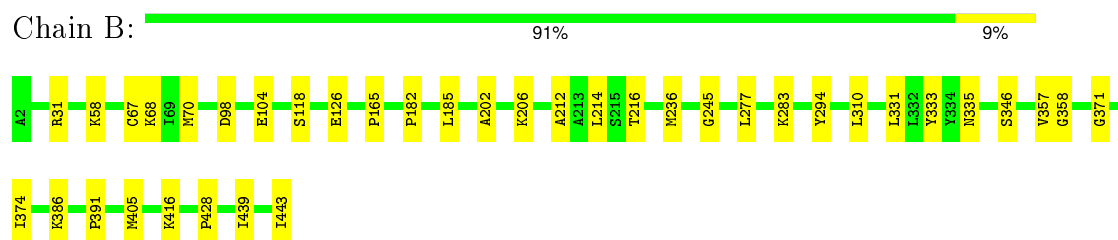
#### • Molecule 1: METHYL-COENZYME M REDUCTASE



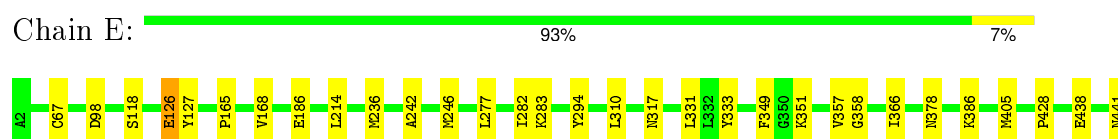
#### • Molecule 1: METHYL-COENZYME M REDUCTASE



#### • Molecule 2: METHYL-COENZYME M REDUCTASE



#### • Molecule 2: METHYL-COENZYME M REDUCTASE



E442  
I443

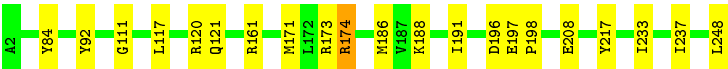
● Molecule 3: METHYL-COENZYME M REDUCTASE

Chain C: 91% 8%



● Molecule 3: METHYL-COENZYME M REDUCTASE

Chain F: 91% 8%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.72Å 116.88Å 122.58Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	30.00 – 1.16	Depositor
% Data completeness (in resolution range)	92.8 (30.00-1.16)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.197 , 0.207	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21217	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AGM, ZN, NA, MGN, F43, TP7, SMC, GL3, COM, MHS

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	0.36	2/4426 (0.0%)	0.58	6/6006 (0.1%)
1	D	0.32	0/4412	0.48	1/5988 (0.0%)
2	B	0.28	0/3462	0.46	0/4687
2	E	0.29	0/3413	0.45	0/4622
3	C	0.43	2/2083 (0.1%)	0.64	5/2804 (0.2%)
3	F	0.31	0/2061	0.56	4/2775 (0.1%)
All	All	0.33	4/19857 (0.0%)	0.52	16/26882 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	1
2	B	0	1
2	E	0	1
3	C	0	2
3	F	0	2
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	161	ARG	NE-CZ	-11.34	1.18	1.33
1	A	2	ALA	N-CA	-7.25	1.31	1.46
3	C	161	ARG	CZ-NH1	6.02	1.40	1.33
1	A	2	ALA	CA-C	-5.03	1.39	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	161	ARG	NE-CZ-NH2	16.42	128.51	120.30
1	A	2	ALA	O-C-N	-15.83	97.37	122.70
1	A	2	ALA	CA-C-O	13.59	148.65	120.10
3	C	161	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	D	440	ARG	NE-CZ-NH2	7.47	124.03	120.30
3	C	174	ARG	NE-CZ-NH2	7.44	124.02	120.30
3	F	174	ARG	NE-CZ-NH2	7.41	124.00	120.30
3	F	173	ARG	NE-CZ-NH2	7.40	124.00	120.30
3	C	173	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	A	119	ARG	NE-CZ-NH2	7.14	123.87	120.30
1	A	535	ARG	NE-CZ-NH2	6.95	123.78	120.30
3	F	161	ARG	NE-CZ-NH2	6.46	123.53	120.30
3	F	171	MET	CG-SD-CE	6.17	110.08	100.20
1	A	440	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	2	ALA	CB-CA-C	-5.31	102.13	110.10
3	C	161	ARG	CB-CG-CD	5.06	124.76	111.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ALA	Mainchain
1	A	257	MHS	Mainchain
1	A	399	SER	Mainchain
2	B	333	TYR	Sidechain
3	C	161	ARG	Sidechain
3	C	217	TYR	Sidechain
1	D	399	SER	Mainchain
2	E	333	TYR	Sidechain
3	F	217	TYR	Sidechain
3	F	92	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4293	0	4081	43	0
1	D	4290	0	4087	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3352	0	3352	41	0
2	E	3328	0	3319	26	0
3	C	2021	0	1958	16	0
3	F	2013	0	1947	9	0
4	A	1	0	0	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
6	A	62	0	43	2	0
6	D	62	0	43	2	0
7	A	42	0	38	1	0
8	A	7	0	5	1	0
8	D	7	0	5	1	0
9	A	12	0	16	3	0
9	D	12	0	16	3	0
10	A	378	0	0	7	2
10	B	306	0	0	11	1
10	C	197	0	0	6	1
10	D	367	0	0	14	2
10	E	277	0	0	1	0
10	F	188	0	0	0	0
All	All	21217	0	18910	164	3

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 4.

All (164) 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)
3:C:153[B]:LYS:NZ	3:C:153[B]:LYS:CE	1.68	1.55
1:D:371[B]:LEU:CD2	1:D:371[B]:LEU:CG	1.89	1.50
2:E:236[B]:MET:CG	2:E:236[B]:MET:SD	2.08	1.40
2:E:277[B]:LEU:HD23	2:E:282:ILE:HG13	1.20	1.16
2:B:104[B]:GLU:HG3	10:B:7481:HOH:O	1.45	1.13
3:C:148[B]:SER:OG	10:C:7423:HOH:O	1.78	1.01
10:A:7706:HOH:O	2:B:236[B]:MET:CE	2.16	0.93
2:B:104[B]:GLU:CG	10:B:7481:HOH:O	2.05	0.93
10:A:7706:HOH:O	2:B:236[B]:MET:HE1	1.69	0.92
2:E:277[B]:LEU:HD23	2:E:282:ILE:CG1	2.01	0.91
2:B:104[B]:GLU:CD	10:B:7481:HOH:O	2.08	0.90
1:D:356:ASP:HB3	10:D:8697:HOH:O	1.71	0.90
1:A:256:LYS:O	9:A:804:GOL:H31	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LYS:O	9:D:806:GOL:H31	1.72	0.89
1:A:167[B]:THR:HG23	1:A:203:GLY:O	1.75	0.86
1:A:256:LYS:O	9:A:804:GOL:C3	2.26	0.83
2:B:212:ALA:O	2:B:216[B]:THR:HG23	1.79	0.82
3:C:153[B]:LYS:NZ	3:C:153[B]:LYS:CD	2.43	0.80
1:D:256:LYS:O	9:D:806:GOL:C3	2.30	0.80
2:E:277[B]:LEU:CD2	2:E:282:ILE:HG13	2.09	0.79
2:B:206[A]:LYS:NZ	10:B:8261:HOH:O	2.13	0.79
1:D:111:HIS:N	10:D:7761:HOH:O	2.16	0.79
2:B:70[B]:MET:SD	10:D:7163:HOH:O	2.42	0.77
2:B:277[B]:LEU:HD21	2:B:294:TYR:HE2	1.53	0.73
1:A:262:HIS:HD2	10:A:7101:HOH:O	1.72	0.73
1:A:172:ILE:HD12	10:A:8234:HOH:O	1.90	0.71
1:D:110:ASN:N	10:D:7761:HOH:O	2.22	0.70
2:B:104[B]:GLU:OE2	10:B:7481:HOH:O	2.09	0.69
1:A:167[B]:THR:HG22	1:A:169:ASN:H	1.58	0.68
2:E:277[B]:LEU:HD21	2:E:294:TYR:CE1	2.30	0.67
2:B:277[B]:LEU:HD21	2:B:294:TYR:CE2	2.32	0.64
2:B:31[B]:ARG:NH1	10:B:8232:HOH:O	2.30	0.64
1:D:125:THR:HB	1:D:126:PRO:HD2	1.80	0.64
10:A:7706:HOH:O	2:B:236[B]:MET:HE2	1.90	0.63
1:A:125:THR:HB	1:A:126:PRO:HD2	1.82	0.61
1:D:262:HIS:HD2	10:D:7428:HOH:O	1.84	0.61
1:D:371[B]:LEU:HB2	1:D:371[B]:LEU:CD2	2.30	0.60
3:C:148[A]:SER:HB2	10:C:7423:HOH:O	1.99	0.60
6:A:700:F43:H9A1	1:D:328:VAL:HB	1.85	0.58
1:A:328:VAL:HB	6:D:800:F43:H9A1	1.85	0.58
1:D:371[B]:LEU:CD1	1:D:371[B]:LEU:CD2	2.81	0.57
1:D:130:THR:HG22	1:D:134[B]:GLU:OE2	2.05	0.56
1:A:536:GLU:HA	1:D:548:PRO:HG3	1.89	0.55
1:D:236:ILE:HA	1:D:241[B]:GLN:NE2	2.21	0.55
1:D:357:LYS:HD2	10:D:7389:HOH:O	2.07	0.54
1:A:73:GLN:HB2	1:A:80:TYR:CE2	2.43	0.53
2:B:405:MET:HG3	1:D:115:VAL:HG22	1.90	0.53
1:D:254:ALA:HA	1:D:258:ALA:HB3	1.91	0.53
2:E:236[B]:MET:CG	2:E:236[B]:MET:CE	2.86	0.52
1:A:254:ALA:HA	1:A:258:ALA:HB3	1.90	0.52
1:D:531:LYS:HD2	10:D:7456:HOH:O	2.10	0.52
3:C:95:PRO:HD2	10:C:7423:HOH:O	2.10	0.52
2:B:216[B]:THR:CG2	2:B:391:PRO:HB3	2.40	0.52
3:C:64:ASP:HB3	3:C:67:ARG:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:8231:HOH:O	2:E:168:VAL:HG13	2.10	0.51
2:B:214:LEU:HB2	2:B:428:PRO:HG3	1.93	0.51
2:B:310:LEU:HD11	2:B:331:LEU:HD23	1.93	0.50
3:C:62:PRO:HA	10:C:7392:HOH:O	2.11	0.50
1:A:256:LYS:O	9:A:804:GOL:H32	2.10	0.49
3:C:86:GLN:OE1	3:C:120[A]:ARG:HD2	2.12	0.49
1:D:110:ASN:C	10:D:7761:HOH:O	2.48	0.49
2:E:214:LEU:HB2	2:E:428:PRO:HG3	1.94	0.49
10:B:7814:HOH:O	3:C:248:LEU:HD12	2.12	0.49
2:B:58:LYS:HG3	10:B:7961:HOH:O	2.13	0.48
2:B:202:ALA:HB1	2:B:416:LYS:HB2	1.96	0.48
1:A:115:VAL:HG22	2:E:405:MET:HG3	1.95	0.48
1:D:445:GL3:HA2	2:E:357:VAL:HG12	1.95	0.48
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.49	0.48
2:B:216[B]:THR:HG22	2:B:391:PRO:CB	2.44	0.48
2:B:68:LYS:HE3	10:B:7103:HOH:O	2.12	0.48
1:D:453:GLY:O	1:D:457:VAL:HG23	2.14	0.48
2:B:216[B]:THR:HG21	2:B:245:GLY:CA	2.42	0.48
10:D:7113:HOH:O	2:E:351:LYS:HE3	2.13	0.48
1:D:106:ILE:HB	1:D:261:ILE:HB	1.96	0.47
1:D:262:HIS:CD2	10:D:7428:HOH:O	2.64	0.47
1:D:443:PHE:HB2	8:D:9700:COM:O1S	2.14	0.47
1:D:4:LYS:HB2	1:D:7:ILE:HG12	1.96	0.47
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.49	0.47
1:D:332:GLN:HA	1:D:335:THR:OG1	2.15	0.47
1:D:331:THR:O	1:D:335:THR:HG23	2.15	0.47
1:A:367[B]:MET:HE3	1:A:371:LEU:HG	1.97	0.47
2:B:182:PRO:O	2:B:185[B]:LEU:HG	2.15	0.47
2:B:216[B]:THR:HG22	2:B:391:PRO:HB3	1.96	0.46
1:D:236:ILE:N	1:D:241[B]:GLN:HE22	2.13	0.46
1:A:249:GLY:HA3	10:E:8180:HOH:O	2.16	0.46
6:A:700:F43:O7B	2:E:366:ILE:HG12	2.16	0.46
1:D:357:LYS:HD3	1:D:358:TYR:CE2	2.51	0.46
2:B:67:CYS:HB3	1:D:505:PHE:CE1	2.51	0.46
1:A:4[B]:LYS:NZ	1:A:384:GLN:OE1	2.49	0.46
1:A:298[B]:GLU:HA	1:A:298[B]:GLU:OE1	2.12	0.46
1:A:297[B]:TYR:O	1:A:298[B]:GLU:OE1	2.33	0.46
1:A:466[A]:LEU:HD22	2:E:165:PRO:HD2	1.97	0.46
3:C:61:GLU:HG3	10:C:7281:HOH:O	2.16	0.46
1:A:453:GLY:O	1:A:457:VAL:HG23	2.16	0.46
1:A:262:HIS:CD2	10:A:7101:HOH:O	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167[B]:THR:HG22	1:A:168:GLY:N	2.31	0.45
1:D:73:GLN:HB2	1:D:80:TYR:CE2	2.51	0.45
1:D:109:LEU:C	10:D:7761:HOH:O	2.51	0.45
1:D:145:VAL:HG23	1:D:146:VAL:HG23	1.98	0.45
3:F:233:ILE:O	3:F:237[A]:ILE:HG12	2.17	0.45
2:B:371:GLY:O	2:B:374:ILE:HG13	2.16	0.45
1:A:362:GLU:HG3	10:A:7505:HOH:O	2.15	0.45
2:B:216[B]:THR:HG22	2:B:391:PRO:CG	2.47	0.44
1:A:445:GL3:HA2	2:B:357:VAL:HG12	2.00	0.44
1:D:259[B]:GLU:OE1	10:D:7761:HOH:O	2.17	0.44
2:B:31[B]:ARG:NH1	2:B:31[B]:ARG:HG3	2.32	0.44
1:D:333:TYR:HE1	1:D:399:SER:HB2	1.83	0.44
1:A:105[A]:VAL:HG23	1:A:208:VAL:HB	1.99	0.44
1:A:151:VAL:HG11	1:D:83:GLY:HA3	2.00	0.44
2:B:335:ASN:OD1	2:B:346:SER:HB2	2.17	0.43
1:D:110:ASN:CA	10:D:7761:HOH:O	2.63	0.43
1:A:505:PHE:CE1	2:E:67:CYS:HB3	2.54	0.43
2:B:216[B]:THR:HG21	2:B:245:GLY:HA3	2.00	0.43
2:B:236[A]:MET:HB2	3:C:248:LEU:HD13	2.01	0.43
1:A:254:ALA:O	1:A:259[B]:GLU:HG2	2.18	0.43
1:A:312:ALA:O	1:A:316:ASP:HB2	2.18	0.43
2:E:310:LEU:HD11	2:E:331:LEU:HD23	1.99	0.43
7:A:9500:TP7:H72C	7:A:9500:TP7:H42C	1.79	0.43
1:A:393:GLU:HG3	3:C:160:LEU:HG	2.00	0.43
2:B:165:PRO:HD2	1:D:466[A]:LEU:HD22	2.01	0.42
3:C:233:ILE:O	3:C:237[A]:ILE:HG12	2.19	0.42
1:D:312:ALA:O	1:D:316:ASP:HB2	2.19	0.42
2:E:242:ALA:O	2:E:246:MET:HB2	2.18	0.42
1:A:114:ALA:O	1:A:118:LYS:HB2	2.18	0.42
1:A:242:ALA:HB2	3:F:84:TYR:CZ	2.54	0.42
1:D:225:ARG:O	1:D:229:MET:HG2	2.19	0.42
2:B:386:LYS:HD3	2:B:386:LYS:HA	1.82	0.42
1:A:332:GLN:HA	1:A:335:THR:OG1	2.20	0.42
1:A:217:THR:HG23	10:D:7609:HOH:O	2.20	0.42
2:E:186:GLU:HG3	2:E:378:ASN:O	2.20	0.42
2:B:31[B]:ARG:HG3	2:B:31[B]:ARG:HH11	1.85	0.41
3:C:95:PRO:HA	3:C:214:THR:HA	2.02	0.41
1:A:154:HIS:CE1	1:A:545:LEU:HD21	2.54	0.41
2:B:439:ILE:HD12	2:B:443:ILE:HD11	2.01	0.41
2:E:317:ASN:O	3:F:111:GLY:HA2	2.21	0.41
3:F:117:LEU:HB2	3:F:120[B]:ARG:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:800:F43:H3C	6:D:800:F43:O8D	2.19	0.41
2:E:386:LYS:HA	2:E:386:LYS:HD3	1.81	0.41
1:D:256:LYS:O	9:D:806:GOL:H32	2.16	0.41
1:A:331:THR:O	1:A:335:THR:HG23	2.20	0.41
3:F:191:ILE:HA	3:F:191:ILE:HD12	1.95	0.41
3:F:174:ARG:HG2	3:F:188:LYS:HB2	2.03	0.41
1:A:443:PHE:HB2	8:A:9800:COM:O1S	2.21	0.41
3:F:197:GLU:HA	3:F:198:PRO:HD3	1.97	0.41
1:A:106:ILE:HB	1:A:261:ILE:HB	2.03	0.41
1:D:448:LEU:HD12	2:E:358:GLY:HA3	2.03	0.40
2:E:349:PHE:HZ	3:F:248:LEU:HD21	1.85	0.40
1:D:365:ASN:HD22	1:D:417:THR:HB	1.86	0.40
1:D:279:GLY:HA2	1:D:473:PRO:HB2	2.03	0.40
1:A:448:LEU:HD12	2:B:358:GLY:HA3	2.03	0.40
2:B:31[B]:ARG:NH2	10:B:8637:HOH:O	2.46	0.40
1:A:328:VAL:HG13	1:D:151:VAL:O	2.21	0.40
2:E:126:GLU:HB2	2:E:127:TYR:H	1.72	0.40
3:C:100:VAL:HG13	10:C:8259:HOH:O	2.21	0.40

All (3) 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)
10:A:8708:HOH:O	10:D:8435:HOH:O[2_644]	1.87	0.33
10:A:8554:HOH:O	10:D:8672:HOH:O[2_645]	1.98	0.22
10:B:8702:HOH:O	10:C:8682:HOH:O[2_555]	2.19	0.01

## 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	556/548 (102%)	532 (96%)	24 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	554/548 (101%)	528 (95%)	26 (5%)	0	100	100
2	B	453/442 (102%)	449 (99%)	4 (1%)	0	100	100
2	E	447/442 (101%)	442 (99%)	5 (1%)	0	100	100
3	C	251/247 (102%)	245 (98%)	6 (2%)	0	100	100
3	F	248/247 (100%)	241 (97%)	7 (3%)	0	100	100
All	All	2509/2474 (101%)	2437 (97%)	72 (3%)	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	448/433 (104%)	442 (99%)	6 (1%)	76	39
1	D	446/433 (103%)	442 (99%)	4 (1%)	84	55
2	B	354/341 (104%)	351 (99%)	3 (1%)	86	59
2	E	348/341 (102%)	343 (99%)	5 (1%)	74	37
3	C	221/215 (103%)	218 (99%)	3 (1%)	74	37
3	F	218/215 (101%)	214 (98%)	4 (2%)	66	26
All	All	2035/1978 (103%)	2010 (99%)	25 (1%)	78	43

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	119	ARG
1	A	174	ASP
1	A	444	TYR
1	A	543[A]	ARG
1	A	543[B]	ARG
2	B	98	ASP
2	B	126	GLU

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Mol	Chain	Res	Type
2	B	283	LYS
3	C	121	GLN
3	C	196	ASP
3	C	248	LEU
1	D	127	GLU
1	D	444	TYR
1	D	543[A]	ARG
1	D	543[B]	ARG
2	E	98	ASP
2	E	126	GLU
2	E	283	LYS
2	E	438	GLU
2	E	441	ASN
3	F	121	GLN
3	F	186	MET
3	F	196	ASP
3	F	208	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	262	HIS
3	C	121	GLN
3	C	238	HIS
1	D	365	ASN
3	F	121	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	MHS	A	257	1	8,11,12	3.52	4 (50%)	7,14,16	2.54	4 (57%)
1	AGM	A	271	1	7,11,12	0.43	0	5,13,15	0.91	0
1	MGN	A	400	1	6,9,10	1.17	1 (16%)	6,12,14	1.95	1 (16%)
1	GL3	A	445	1	3,3,4	0.15	0	2,2,4	1.16	0
1	SMC	A	452	1	5,6,7	0.44	0	2,6,8	1.25	0
1	MHS	D	257	1	8,11,12	1.52	2 (25%)	7,14,16	1.71	2 (28%)
1	AGM	D	271	1	7,11,12	0.51	0	5,13,15	0.89	0
1	MGN	D	400	1	6,9,10	1.08	1 (16%)	6,12,14	1.87	1 (16%)
1	GL3	D	445	1	3,3,4	0.21	0	2,2,4	1.04	0
1	SMC	D	452	1	5,6,7	0.56	0	2,6,8	1.29	0

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	MHS	A	257	1	-	0/4/6/8	0/1/1/1
1	AGM	A	271	1	-	0/7/11/13	0/0/0/0
1	MGN	A	400	1	-	0/6/9/12	0/0/0/0
1	GL3	A	445	1	-	0/1/1/2	0/0/0/0
1	SMC	A	452	1	-	0/3/5/7	0/0/0/0
1	MHS	D	257	1	-	0/4/6/8	0/1/1/1
1	AGM	D	271	1	-	0/7/11/13	0/0/0/0
1	MGN	D	400	1	-	0/6/9/12	0/0/0/0
1	GL3	D	445	1	-	0/1/1/2	0/0/0/0
1	SMC	D	452	1	-	0/3/5/7	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	MHS	CE1-NE2	-2.83	1.28	1.34
1	A	400	MGN	CB1-CA	-2.55	1.52	1.55
1	D	400	MGN	CB1-CA	-2.37	1.52	1.55
1	A	257	MHS	CD2-NE2	2.10	1.42	1.35
1	D	257	MHS	CD2-NE2	2.71	1.43	1.35
1	D	257	MHS	CB-CG	2.93	1.54	1.50
1	A	257	MHS	CB-CG	5.33	1.58	1.50
1	A	257	MHS	CM-ND1	7.18	1.63	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	400	MGN	CB2-CA-CB1	-4.48	102.98	110.92
1	D	400	MGN	CB2-CA-CB1	-4.21	103.45	110.92
1	A	257	MHS	O-C-CA	-3.97	115.14	125.49
1	A	257	MHS	CG-CD2-NE2	-3.58	101.77	108.71
1	D	257	MHS	O-C-CA	-2.07	120.10	125.49
1	A	257	MHS	NE2-CE1-ND1	-2.03	109.53	112.28
1	A	257	MHS	CD2-NE2-CE1	3.00	110.45	105.71
1	D	257	MHS	CM-ND1-CG	3.46	129.04	124.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	445	GL3	1	0
1	D	445	GL3	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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$
6	F43	A	700	1,8	42,71,71	4.10	20 (47%)	35,118,118	2.15	7 (20%)
9	GOL	A	804	-	5,5,5	0.77	0	5,5,5	0.79	0
9	GOL	A	807	-	5,5,5	0.79	0	5,5,5	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	TP7	A	9000	-	16,20,20	2.23	6 (37%)	16,26,26	1.50	2 (12%)
7	TP7	A	9500	-	16,20,20	2.35	5 (31%)	16,26,26	1.48	2 (12%)
8	COM	A	9800	6	5,6,6	1.47	1 (20%)	5,8,8	1.72	2 (40%)
6	F43	D	800	1,8	42,71,71	4.37	21 (50%)	35,118,118	2.50	11 (31%)
9	GOL	D	805	-	5,5,5	0.78	0	5,5,5	0.79	0
9	GOL	D	806	-	5,5,5	0.76	0	5,5,5	0.79	0
8	COM	D	9700	6	5,6,6	1.52	0	5,8,8	1.79	2 (40%)

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
6	F43	A	700	1,8	1/1/25/27	0/18/165/165	0/0/10/10
9	GOL	A	804	-	-	0/4/4/4	0/0/0/0
9	GOL	A	807	-	-	0/4/4/4	0/0/0/0
7	TP7	A	9000	-	1/1/5/6	0/20/24/24	0/0/0/0
7	TP7	A	9500	-	1/1/5/6	0/20/24/24	0/0/0/0
8	COM	A	9800	6	-	0/4/4/4	0/0/0/0
6	F43	D	800	1,8	1/1/25/27	0/18/165/165	0/0/10/10
9	GOL	D	805	-	-	0/4/4/4	0/0/0/0
9	GOL	D	806	-	-	0/4/4/4	0/0/0/0
8	COM	D	9700	6	-	0/4/4/4	0/0/0/0

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	800	F43	C4B-NB	-19.67	1.19	1.49
6	A	700	F43	C4B-NB	-15.90	1.25	1.49
7	A	9500	TP7	C2-C1	-6.07	1.39	1.51
7	A	9000	TP7	C2-C1	-5.96	1.39	1.51
6	A	700	F43	C4A-NA	-5.34	1.40	1.49
7	A	9500	TP7	CB-CA	-4.41	1.45	1.54
6	D	800	F43	C9A-C2A	-4.03	1.47	1.54
6	A	700	F43	C9D-C3D	-3.27	1.44	1.52
6	A	700	F43	C9B-C2B	-3.21	1.47	1.54
7	A	9000	TP7	CB-CA	-3.21	1.48	1.54
6	D	800	F43	C1D-ND	-3.12	1.30	1.36
6	D	800	F43	C8B-C2B	-2.96	1.50	1.54
6	D	800	F43	C6B-N5B	-2.95	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	700	F43	C1D-ND	-2.85	1.30	1.36
6	D	800	F43	C4A-NA	-2.69	1.44	1.49
6	D	800	F43	C6D-C7D	-2.51	1.47	1.50
6	A	700	F43	C5D-C2D	-2.48	1.47	1.51
7	A	9500	TP7	CA-N	-2.42	1.41	1.46
7	A	9000	TP7	CA-N	-2.38	1.41	1.46
7	A	9000	TP7	P-O2P	-2.26	1.46	1.54
6	D	800	F43	C5D-C2D	-2.16	1.48	1.51
6	A	700	F43	C5A-C2A	-2.06	1.49	1.56
7	A	9000	TP7	P-O3P	-2.01	1.47	1.54
7	A	9500	TP7	P-O2P	-2.01	1.47	1.54
8	A	9800	COM	O3S-S2	2.02	1.51	1.46
6	A	700	F43	NI-ND	2.05	2.05	1.92
6	D	800	F43	C2A-C3A	2.18	1.59	1.54
6	D	800	F43	C3C-C2C	2.24	1.60	1.54
6	D	800	F43	CHD-C7D	2.77	1.52	1.46
6	A	700	F43	C1B-N5B	2.85	1.51	1.45
6	A	700	F43	CHD-C7D	2.87	1.53	1.46
6	D	800	F43	C1D-C2D	2.95	1.48	1.40
6	A	700	F43	CAA-C3A	2.97	1.60	1.53
6	A	700	F43	NI-NC	3.08	2.03	1.90
7	A	9500	TP7	C1-N	3.22	1.40	1.34
7	A	9000	TP7	C1-N	3.28	1.40	1.34
6	A	700	F43	CHB-C4A	3.68	1.58	1.52
6	D	800	F43	NI-NC	3.78	2.07	1.90
6	A	700	F43	C1C-NC	4.04	1.45	1.37
6	D	800	F43	CAA-C3A	4.42	1.63	1.53
6	D	800	F43	C1B-N5B	4.87	1.55	1.45
6	D	800	F43	C2B-C3B	4.95	1.63	1.54
6	A	700	F43	C6D-C7D	4.98	1.57	1.50
6	A	700	F43	C1D-C2D	5.17	1.54	1.40
6	D	800	F43	CAB-C3B	5.32	1.65	1.53
6	A	700	F43	C2B-C3B	5.65	1.64	1.54
6	D	800	F43	C4D-C3D	5.66	1.45	1.37
6	D	800	F43	C1B-NB	6.02	1.58	1.49
6	A	700	F43	C3D-C2D	6.79	1.54	1.39
6	D	800	F43	C3D-C2D	7.96	1.57	1.39
6	A	700	F43	C2A-C1A	8.13	1.62	1.51
6	D	800	F43	C2A-C1A	8.33	1.62	1.51
6	A	700	F43	C4D-C3D	9.73	1.50	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	800	F43	C9D-C3D-C4D	-6.49	116.08	127.01
6	A	700	F43	C9D-C3D-C4D	-6.46	116.13	127.01
6	D	800	F43	C3C-C4C-CHD	-5.05	115.79	124.26
6	A	700	F43	O8D-C7D-C6D	-4.12	113.27	120.76
6	D	800	F43	O8D-C7D-C6D	-3.65	114.14	120.76
7	A	9500	TP7	O1-C1-N	-3.39	117.25	123.01
7	A	9000	TP7	O1-C1-N	-3.34	117.34	123.01
6	D	800	F43	O8D-C7D-CHD	-2.87	119.28	122.56
6	D	800	F43	C8C-C3C-C2C	-2.44	106.21	113.29
6	D	800	F43	CBB-CAB-C3B	-2.09	109.38	113.98
6	A	700	F43	O8D-C7D-CHD	2.05	124.90	122.56
6	D	800	F43	C9A-C2A-C5A	2.24	114.32	110.78
8	A	9800	COM	O1S-S2-C2	2.28	108.85	106.91
8	D	9700	COM	O1S-S2-C2	2.39	108.94	106.91
6	A	700	F43	C3C-C4C-CHD	2.52	128.49	124.26
8	A	9800	COM	O2S-S2-C2	2.74	109.24	106.91
8	D	9700	COM	O2S-S2-C2	2.88	109.37	106.91
6	A	700	F43	C9B-C2B-C3B	3.03	117.79	111.81
7	A	9500	TP7	C4-C3-C2	3.04	124.45	113.29
7	A	9000	TP7	C4-C3-C2	3.07	124.56	113.29
6	D	800	F43	C9A-C2A-C3A	3.13	118.03	112.94
6	D	800	F43	C3A-C4A-NA	3.51	107.94	102.27
6	A	700	F43	C3B-C4B-NB	4.15	118.99	106.03
6	D	800	F43	C8B-C2B-C1B	4.53	110.52	102.05
6	A	700	F43	C4A-NA-C1A	6.09	114.31	108.21
6	D	800	F43	C3B-C4B-NB	6.96	127.75	106.03

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	800	F43	C4B
7	A	9500	TP7	C1
6	A	700	F43	C4B
7	A	9000	TP7	C1

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	700	F43	2	0
9	A	804	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	9500	TP7	1	0
8	A	9800	COM	1	0
6	D	800	F43	2	0
9	D	806	GOL	3	0
8	D	9700	COM	1	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.