WORLDWIDE PDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:49 PM GMT

PDB ID	:	1HBN
Title	:	METHYL-COENZYME M REDUCTASE
Authors	:	Ermler, U.; Grabarse, W.
Deposited on	:	2001-04-20
Resolution	:	1.16 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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.
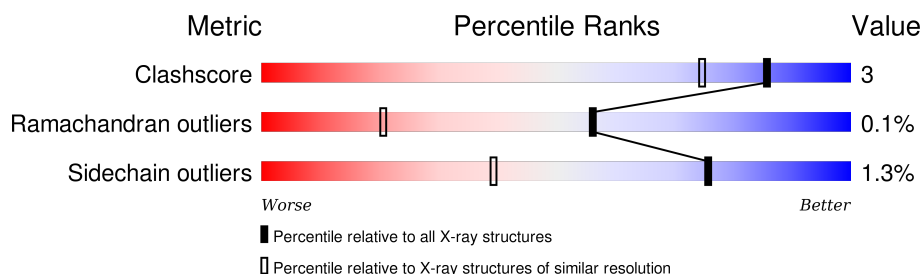
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1109 (1.20-1.12)
Ramachandran outliers	100387	1058 (1.20-1.12)
Sidechain outliers	100360	1058 (1.20-1.12)

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 >=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 <=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	549	90% 8% •
1	D	549	90% 9% •
2	B	442	89% 10% •
2	E	442	91% 8% •
3	C	248	88% 10% •
3	F	248	89% 9% •

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
4	F43	A	1550	X		-	-
4	F43	D	1550	X		-	-
5	TP7	A	1551	X		-	-
5	TP7	D	1551	X		-	-

2   Entry composition ⓘ

There are 12 unique types of molecules in this entry. The entry contains 21962 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 I ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total 4292	C 2712	N 723	O 837	S 20	23	13	0
1	D	548	Total 4297	C 2717	N 721	O 839	S 20	23	16	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	MHS	HIS	MODIFIED RESIDUE	UNP P11558
A	271	AGM	ARG	MODIFIED RESIDUE	UNP P11558
A	400	MGN	GLN	MODIFIED RESIDUE	UNP P11558
A	445	GL3	GLY	MODIFIED RESIDUE	UNP P11558
A	452	SMC	CYS	MODIFIED RESIDUE	UNP P11558
D	257	MHS	HIS	MODIFIED RESIDUE	UNP P11558
D	271	AGM	ARG	MODIFIED RESIDUE	UNP P11558
D	400	MGN	GLN	MODIFIED RESIDUE	UNP P11558
D	445	GL3	GLY	MODIFIED RESIDUE	UNP P11558
D	452	SMC	CYS	MODIFIED RESIDUE	UNP P11558

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total 3348	C 2115	N 557	O 654	S 22	26	15	0
2	E	442	Total 3340	C 2115	N 551	O 653	S 21	41	12	0

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE I GAMMA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total 2008	C 1242	N 355	O 399	S 12	39	5	0
3	F	247	Total 2007	C 1242	N 354	O 399	S 12	45	5	0

• Molecule 4 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{49}N_6NiO_{13}$).
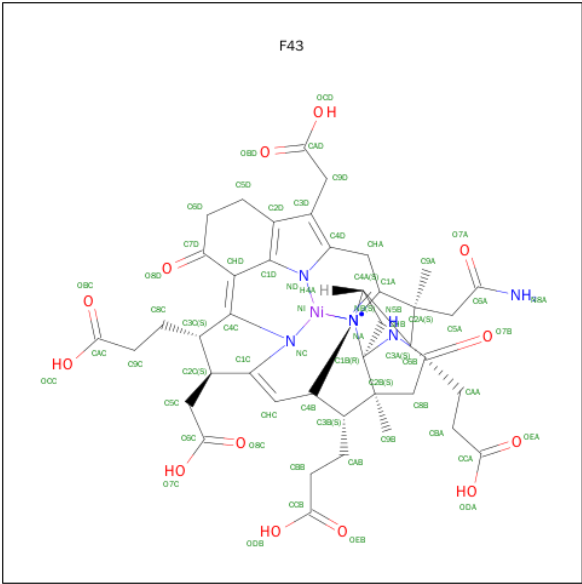
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 62	C 42	N 6	Ni 1	O 13	0	0
4	D	1	Total 62	C 42	N 6	Ni 1	O 13	0	0

• Molecule 5 is COENZYME B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).
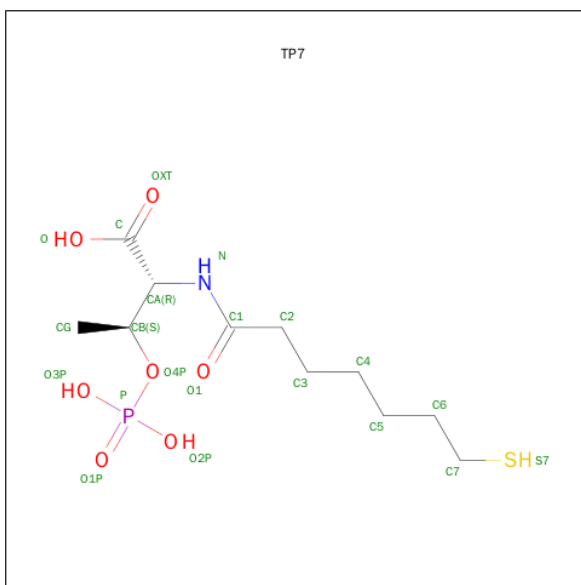
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 6 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).
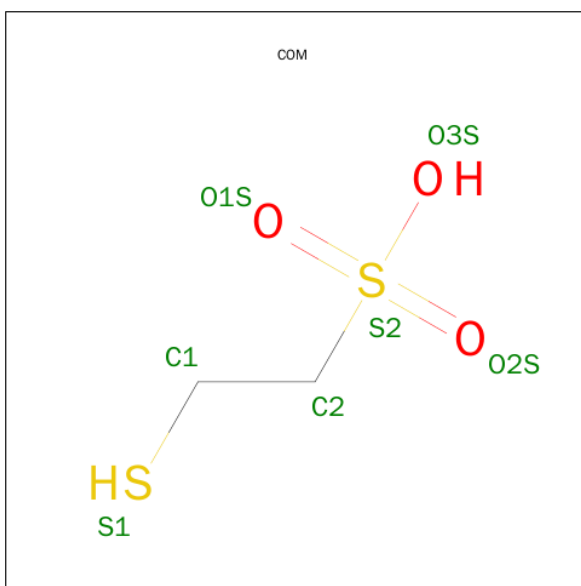
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			7	2	3	2		
6	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	C	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	E	1	Total 6	C 3	O 3	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total 2	Mg 2	0	0
9	E	5	Total 5	Mg 5	0	0
9	B	2	Total 2	Mg 2	0	0
9	C	2	Total 2	Mg 2	0	0
9	A	5	Total 5	Mg 5	0	0
9	F	2	Total 2	Mg 2	0	0

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	2	Total 2	Na 2	0	0
10	A	5	Total 5	Na 5	0	0
10	D	3	Total 3	Na 3	0	0

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total 1	Cl 1	0	0
11	E	1	Total 1	Cl 1	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	489	Total 489	O 489	0	29

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	423	Total 423	O 423	0	31
12	C	294	Total 294	O 294	0	25
12	D	510	Total 510	O 510	0	37
12	E	402	Total 402	O 402	0	33
12	F	275	Total 275	O 275	0	15

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 I ALPHA SUBUNIT
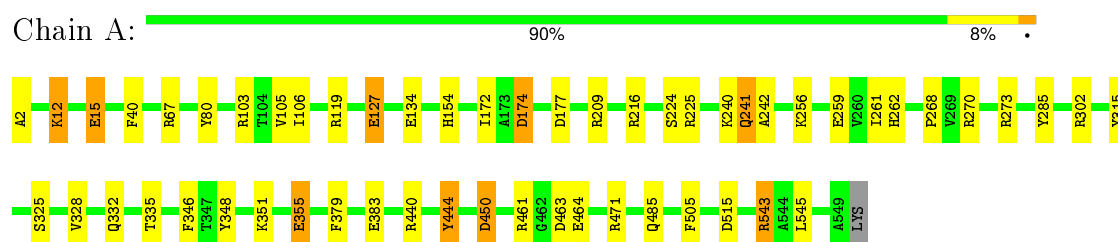
- Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT
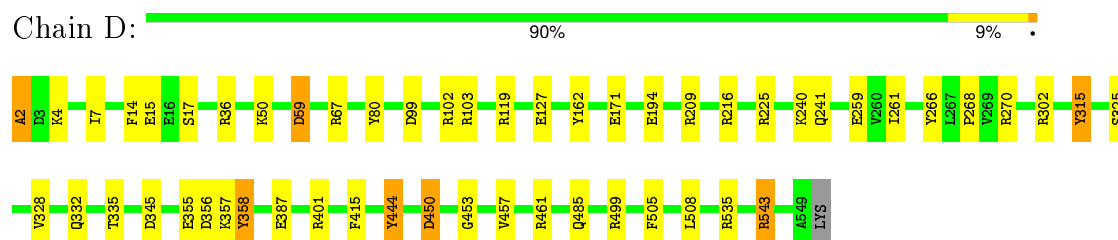
- Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

- Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT
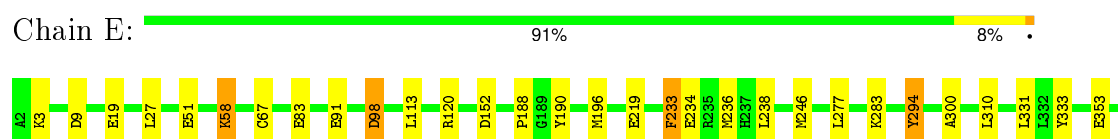
I374 F388 E409 V418 D423 E424 F425 R426 L429 V432 E438 I439 K440 I443

● Molecule 3: METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT

Chain C:

88%   10%   •

A2 R16 Y23 D33 E34 D35 R43 D60 E61 P62 E63 R103 A104 Y105 R120 E124 R128 R147 S148 R151 G152 K153 E164 K179 D193 D196 E197 E208 E212 D220 R225 E229 N247 L248 GLU

● Molecule 3: METHYL-COENZYME M REDUCTASE I GAMMA SUBUNIT

Chain F:

89%   9%   •

A2 K10 Y23 V52 E63 R67 R81 Y84 R103 A104 Y105 R120 E124 R128 K132 R151 R161 E164 R174 E185 M186 E194 L195 D196 E207 E208 R225 R236 L248 GLU
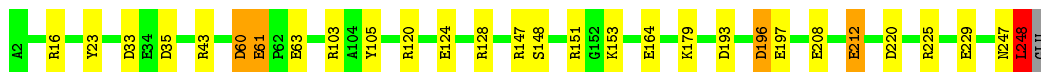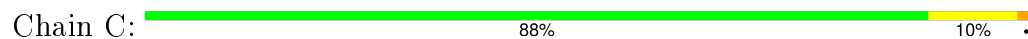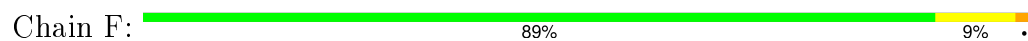
4 Data and refinement statistics (i)

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, α, β, γ	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)	93.1 (30.00-1.16)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.124 , 0.190	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21962	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, CL, ZN, NA, AGM, F43, MGN, 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	0.78	3/4412 (0.1%)	1.25	45/5986 (0.8%)
1	D	0.93	7/4433 (0.2%)	1.23	44/6015 (0.7%)
2	B	0.76	3/3493 (0.1%)	1.22	31/4724 (0.7%)
2	E	1.65	6/3459 (0.2%)	1.19	20/4682 (0.4%)
3	C	0.98	8/2073 (0.4%)	1.47	31/2790 (1.1%)
3	F	0.78	7/2071 (0.3%)	1.37	25/2789 (0.9%)
All	All	1.03	34/19941 (0.2%)	1.27	196/26986 (0.7%)

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	1
1	D	0	1
2	B	0	1
2	E	0	1
3	C	0	1
All	All	0	5

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	438	GLU	CG-CD	83.79	2.77	1.51
2	E	83	GLU	CG-CD	28.40	1.94	1.51
1	D	355	GLU	CG-CD	26.78	1.92	1.51
1	D	127	GLU	CG-CD	-25.44	1.13	1.51
3	C	179	LYS	CD-CE	16.63	1.92	1.51

The worst 5 of 196 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	60	ASP	CB-CG-OD1	-22.90	97.69	118.30
2	E	438	GLU	CB-CG-CD	-20.86	57.87	114.20
3	F	196	ASP	CB-CG-OD2	18.44	134.90	118.30
2	B	98	ASP	CA-CB-CG	-16.64	76.78	113.40
3	C	120	ARG	NE-CZ-NH2	-15.87	112.36	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	GLN	Peptide
2	B	333	TYR	Sidechain
3	C	60	ASP	Sidechain
1	D	2	ALA	Mainchain
2	E	333	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	4292	0	4093	24	0
1	D	4297	0	4108	16	1
2	B	3348	0	3331	31	0
2	E	3340	0	3325	28	0
3	C	2008	0	1937	9	0
3	F	2007	0	1937	3	0
4	A	62	0	43	1	0
4	D	62	0	43	1	0
5	A	21	0	19	0	0
5	D	21	0	19	0	0
6	A	7	0	5	0	0
6	D	7	0	5	0	0
7	A	24	0	31	7	0
7	B	6	0	7	1	0
7	C	6	0	8	0	0
7	D	24	0	31	2	0
7	E	6	0	8	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	5	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	2	0	0	0	0
9	E	5	0	0	0	0
9	F	2	0	0	0	0
10	A	5	0	0	0	0
10	B	2	0	0	0	0
10	D	3	0	0	0	0
11	B	1	0	0	0	0
11	E	1	0	0	0	0
12	A	489	0	0	10	0
12	B	423	0	0	10	0
12	C	294	0	0	3	0
12	D	510	0	0	6	0
12	E	402	0	0	6	0
12	F	275	0	0	0	0
All	All	21962	0	18950	106	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 106 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21[B]:GLN:OE1	12:B:2048[B]:HOH:O	1.58	1.20
2:E:196[B]:MET:HE1	2:E:374:ILE:HG22	1.39	1.01
2:B:236[B]:MET:CE	2:B:236[B]:MET:SD	2.53	0.97
2:B:236[B]:MET:HB2	3:C:248:LEU:HD11	1.51	0.92
2:B:236[A]:MET:HB2	3:C:248:LEU:HD11	1.53	0.91

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:ASP:OD2	1:D:357:LYS:NZ[2_644]	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	554/549 (101%)	535 (97%)	18 (3%)	1 (0%)	52	20
1	D	557/549 (102%)	539 (97%)	17 (3%)	1 (0%)	52	20
2	B	456/442 (103%)	447 (98%)	9 (2%)	0	100	100
2	E	452/442 (102%)	445 (98%)	7 (2%)	0	100	100
3	C	250/248 (101%)	245 (98%)	5 (2%)	0	100	100
3	F	250/248 (101%)	242 (97%)	8 (3%)	0	100	100
All	All	2519/2478 (102%)	2453 (97%)	64 (2%)	2 (0%)	56	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	SER
1	D	325	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/434 (103%)	440 (99%)	6 (1%)	76	39
1	D	449/434 (104%)	445 (99%)	4 (1%)	84	55
2	B	357/341 (105%)	353 (99%)	4 (1%)	80	47
2	E	353/341 (104%)	350 (99%)	3 (1%)	86	59
3	C	220/216 (102%)	216 (98%)	4 (2%)	66	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	220/216 (102%)	215 (98%)	5 (2%)	58	17
All	All	2045/1982 (103%)	2019 (99%)	26 (1%)	76	39

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	148[B]	SER
1	D	17	SER
3	F	196	ASP
3	C	196	ASP
3	C	248	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	187	GLN
2	E	40	GLN
1	D	365	ASN
1	D	42	ASN
1	D	485	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)

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	1.67	1 (12%)	7,14,16	1.65	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	AGM	A	271	1	7,11,12	0.98	1 (14%)	5,13,15	1.37	1 (20%)
1	MGN	A	400	1	6,9,10	0.74	0	6,12,14	0.82	0
1	GL3	A	445	1	3,3,4	2.02	1 (33%)	2,2,4	0.72	0
1	SMC	A	452	1	5,6,7	0.61	0	2,6,8	1.94	1 (50%)
1	MHS	D	257	1	8,11,12	1.53	1 (12%)	7,14,16	2.16	3 (42%)
1	AGM	D	271	1	7,11,12	0.96	0	5,13,15	1.34	1 (20%)
1	MGN	D	400	1	6,9,10	1.27	1 (16%)	6,12,14	0.76	0
1	GL3	D	445	1	3,3,4	2.55	1 (33%)	2,2,4	0.96	0
1	SMC	D	452	1	5,6,7	1.06	0	2,6,8	1.30	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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	GL3	C-S	-4.41	1.65	1.80
1	A	445	GL3	C-S	-3.46	1.68	1.80
1	D	400	MGN	CB1-CA	-2.48	1.52	1.55
1	A	271	AGM	CB-CA	-2.05	1.51	1.53
1	D	257	MHS	CM-ND1	3.29	1.54	1.47

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MHS	NE2-CE1-ND1	-3.68	107.30	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	MHS	O-C-CA	-2.87	118.01	125.49
1	D	271	AGM	CE2-CD-NE1	-2.83	106.67	112.05
1	A	452	SMC	O-C-CA	-2.67	118.52	125.49
1	D	257	MHS	O-C-CA	-2.30	119.50	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 31 are monoatomic - leaving 17 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 Counts	Bond lengths RMSZ	Bond lengths #$|Z| > 2$	Bond angles Counts	Bond angles RMSZ	Bond angles #$|Z| > 2$
4	F43	A	1550	1,6	42,71,71	3.38	14 (33%)	35,118,118	1.65	4 (11%)
5	TP7	A	1551	-	16,20,20	1.47	2 (12%)	16,26,26	1.39	3 (18%)
6	COM	A	1552	4	5,6,6	0.88	0	5,8,8	1.68	1 (20%)
7	GOL	A	1553	10	5,5,5	0.41	0	5,5,5	1.90	2 (40%)
7	GOL	A	1554	-	5,5,5	0.68	0	5,5,5	1.23	1 (20%)
7	GOL	A	1555	-	5,5,5	0.95	0	5,5,5	0.97	0
7	GOL	A	1556	-	5,5,5	1.10	0	5,5,5	0.93	0
7	GOL	B	1444	-	5,5,5	1.24	1 (20%)	5,5,5	1.21	0
7	GOL	C	1249	-	5,5,5	0.55	0	5,5,5	0.30	0
4	F43	D	1550	1,6	42,71,71	3.44	13 (30%)	35,118,118	1.75	6 (17%)
5	TP7	D	1551	-	16,20,20	1.62	2 (12%)	16,26,26	1.29	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	COM	D	1552	4	5,6,6	0.96	1 (20%)	5,8,8	0.49	0
7	GOL	D	1553	-	5,5,5	0.87	0	5,5,5	0.91	0
7	GOL	D	1554	10	5,5,5	0.67	0	5,5,5	0.59	0
7	GOL	D	1555	-	5,5,5	0.73	0	5,5,5	0.97	0
7	GOL	D	1556	-	5,5,5	1.11	1 (20%)	5,5,5	1.59	2 (40%)
7	GOL	E	1444	-	5,5,5	0.90	0	5,5,5	0.83	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
4	F43	A	1550	1,6	1/1/25/27	0/18/165/165	0/0/10/10
5	TP7	A	1551	-	1/1/5/6	0/20/24/24	0/0/0/0
6	COM	A	1552	4	-	0/4/4/4	0/0/0/0
7	GOL	A	1553	10	-	0/4/4/4	0/0/0/0
7	GOL	A	1554	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1555	-	-	0/4/4/4	0/0/0/0
7	GOL	A	1556	-	-	0/4/4/4	0/0/0/0
7	GOL	B	1444	-	-	0/4/4/4	0/0/0/0
7	GOL	C	1249	-	-	0/4/4/4	0/0/0/0
4	F43	D	1550	1,6	1/1/25/27	0/18/165/165	0/0/10/10
5	TP7	D	1551	-	1/1/5/6	0/20/24/24	0/0/0/0
6	COM	D	1552	4	-	0/4/4/4	0/0/0/0
7	GOL	D	1553	-	-	0/4/4/4	0/0/0/0
7	GOL	D	1554	10	-	0/4/4/4	0/0/0/0
7	GOL	D	1555	-	-	0/4/4/4	0/0/0/0
7	GOL	D	1556	-	-	0/4/4/4	0/0/0/0
7	GOL	E	1444	-	-	0/4/4/4	0/0/0/0

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1550	F43	C4B-NB	-14.36	1.27	1.49
4	A	1550	F43	C4B-NB	-13.51	1.28	1.49
5	D	1551	TP7	C2-C1	-4.70	1.42	1.51
5	A	1551	TP7	C2-C1	-4.29	1.43	1.51
4	A	1550	F43	C4A-NA	-3.56	1.43	1.49

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1550	F43	C9D-C3D-C4D	-7.28	114.74	127.01
4	A	1550	F43	C9D-C3D-C4D	-6.59	115.91	127.01
5	A	1551	TP7	O1-C1-N	-3.51	117.05	123.01
6	A	1552	COM	O1S-S2-C2	-3.32	104.07	106.91
7	A	1553	GOL	O3-C3-C2	-3.24	94.49	110.18

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	1551	TP7	C1
4	A	1550	F43	C4B
5	A	1551	TP7	C1
4	D	1550	F43	C4B

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1550	F43	1	0
7	A	1553	GOL	2	0
7	A	1554	GOL	1	0
7	A	1555	GOL	1	0
7	A	1556	GOL	3	0
7	B	1444	GOL	1	0
4	D	1550	F43	1	0
7	D	1556	GOL	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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