



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:49 PM GMT

PDB ID : 1HBU
Title : METHYL-COENZYME M REDUCTASE IN THE MCR-RED1-SILENT
STATE IN COMPLEX with COENZYME M
Authors : Ermler, U.; Grabarse, W.
Deposited on : 2001-04-20
Resolution : 1.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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) : **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

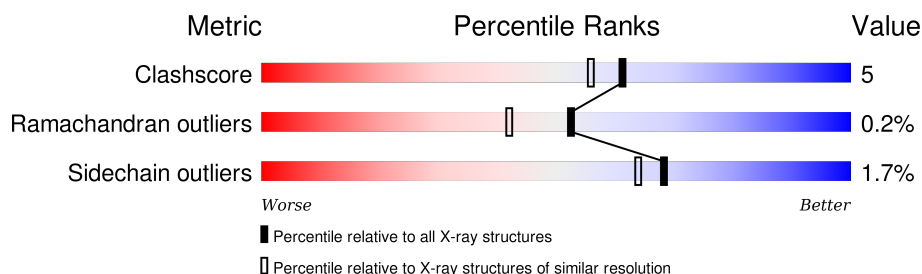
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	549	
1	D	549	
2	B	442	
2	E	442	
3	C	248	
3	F	248	

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	-	-	-
7	GOL	B	1444	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21674 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	C	N	O	S	24	10	0
			4285	2708	723	834	20			
1	D	548	Total	C	N	O	S	23	13	0
			4290	2710	721	839	20			

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

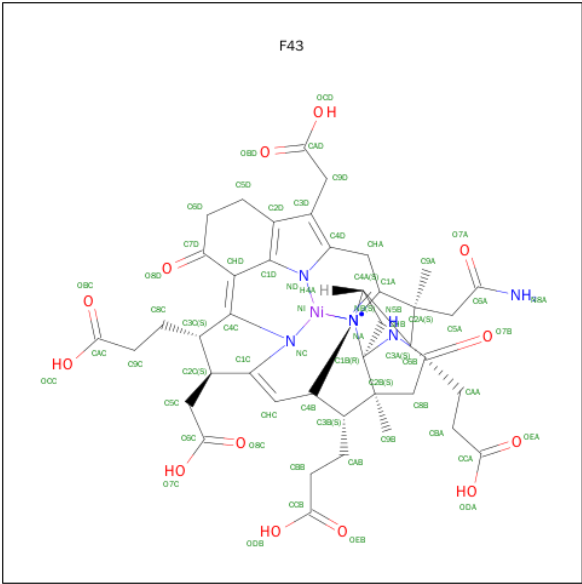
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	26	13	0
			3344	2113	556	654	21			
2	E	442	Total	C	N	O	S	41	11	0
			3333	2108	551	653	21			

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

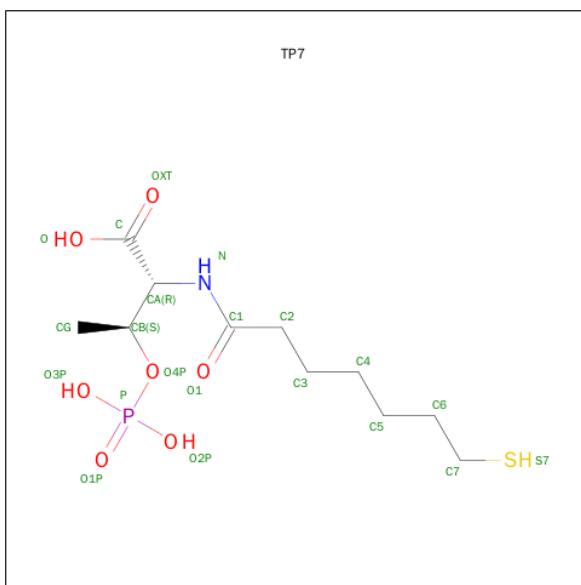
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	39	5	0
			2008	1242	355	399	12			
3	F	247	Total	C	N	O	S	45	5	0
			2007	1242	354	399	12			

- Molecule 4 is FACTOR 430 (three-letter code: F43) (formula: C₄₂H₄₉N₆NiO₁₃).



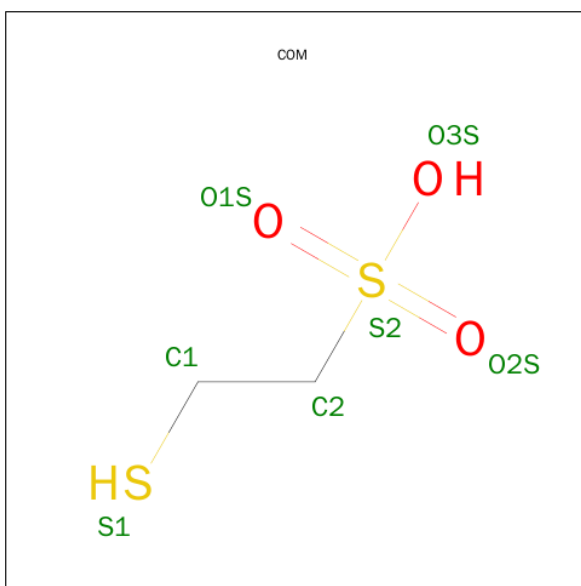
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
4	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 5 is COENZYME B (three-letter code: TP7) (formula: C₁₁H₂₂NO₇PS).



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

- Molecule 6 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
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	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total Mg 1 1	0	0
9	E	3	Total Mg 3 3	0	0
9	B	2	Total Mg 2 2	0	0
9	C	1	Total Mg 1 1	0	0
9	A	5	Total Mg 5 5	0	0
9	F	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	2	Total Na 2 2	0	0
10	A	4	Total Na 4 4	0	0
10	D	3	Total Na 3 3	0	0

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

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	444	Total O 444 444	0	27

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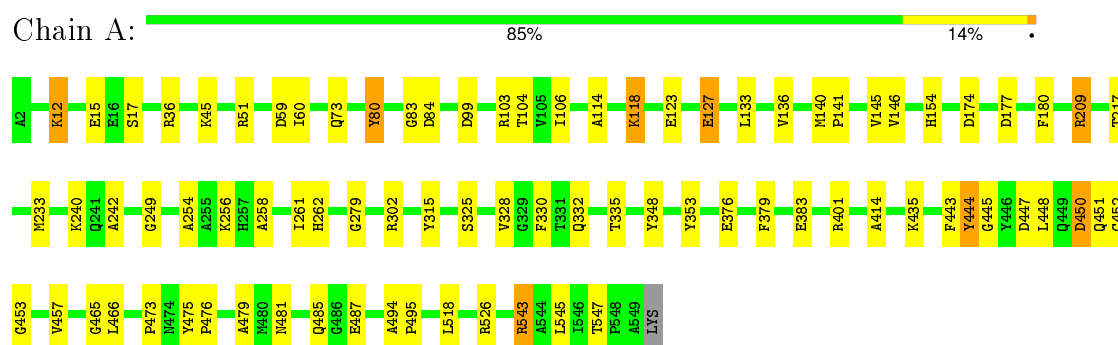
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	385	Total 385	O 385	0	23
12	C	254	Total 254	O 254	0	23
12	D	440	Total 440	O 440	0	32
12	E	360	Total 360	O 360	0	23
12	F	253	Total 253	O 253	0	13

3 Residue-property plots

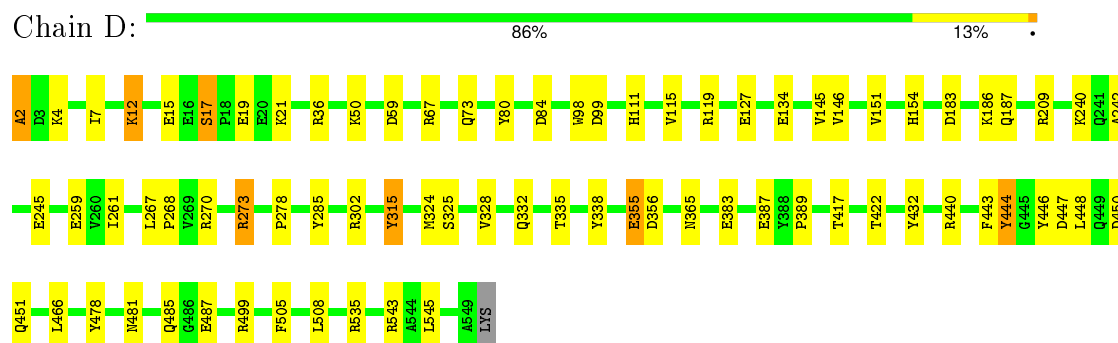
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

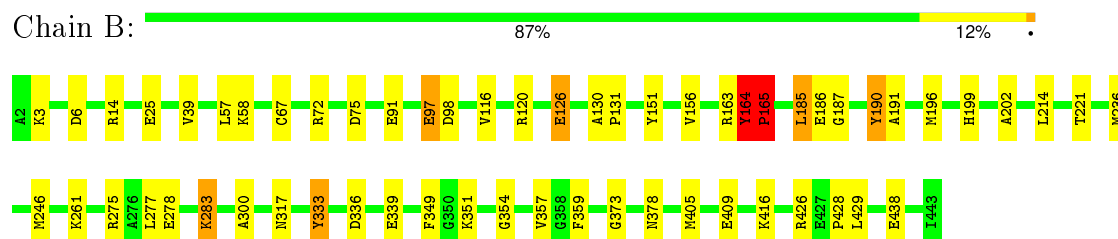
• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT



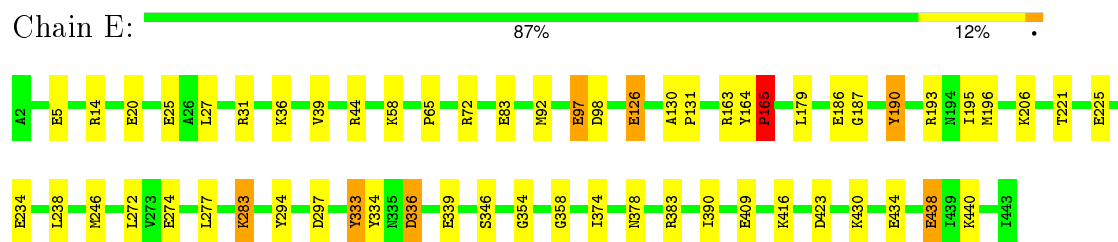
• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT



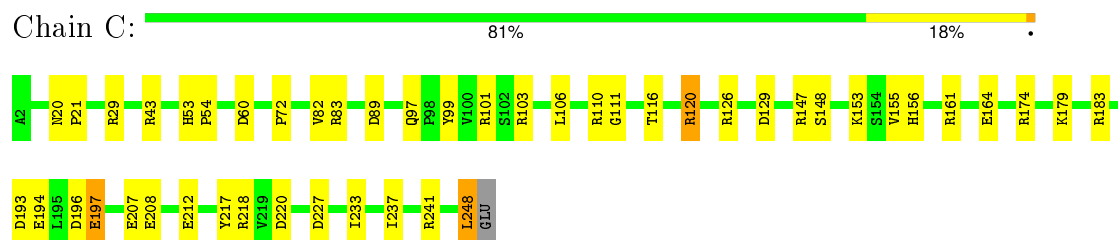
• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT



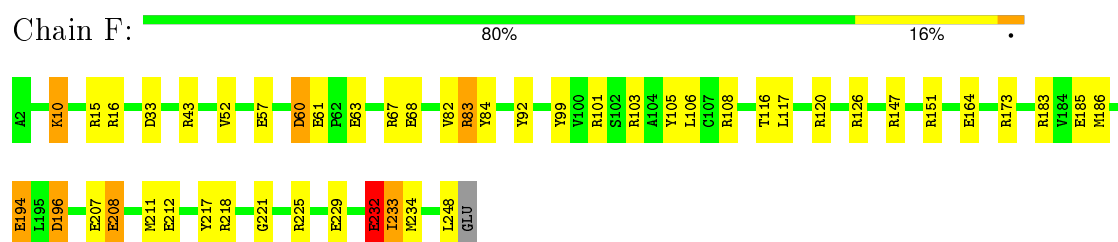
• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT



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



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



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, α , β , γ	81.10 Å 116.50 Å 121.80 Å 90.00° 91.80° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	94.3 (10.00-1.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.211	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21674	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	1.04	6/4390 (0.1%)	1.25	22/5956 (0.4%)
1	D	1.15	8/4411 (0.2%)	1.37	44/5984 (0.7%)
2	B	1.00	6/3476 (0.2%)	1.27	28/4703 (0.6%)
2	E	2.03	8/3447 (0.2%)	1.30	29/4666 (0.6%)
3	C	1.43	4/2073 (0.2%)	1.37	32/2790 (1.1%)
3	F	2.38	11/2071 (0.5%)	1.58	45/2789 (1.6%)
All	All	1.49	43/19868 (0.2%)	1.34	200/26888 (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	3
2	B	0	2
2	E	0	3
3	C	0	1
All	All	0	10

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	438	GLU	CG-CD	90.76	2.88	1.51
3	F	207	GLU	CG-CD	53.45	2.32	1.51
1	A	127	GLU	CG-CD	49.49	2.26	1.51
3	F	164	GLU	CB-CG	45.51	2.38	1.52
3	F	194	GLU	CB-CG	42.64	2.33	1.52

The worst 5 of 200 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	438	GLU	CB-CG-CD	-22.34	53.90	114.20
3	F	10	LYS	CB-CG-CD	17.37	156.75	111.60
3	F	232	GLU	O-C-N	16.81	149.60	122.70
1	D	15	GLU	CA-CB-CG	16.76	150.27	113.40
3	F	196	ASP	CB-CG-OD1	15.76	132.48	118.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	547	THR	Mainchain
2	B	164	TYR	Mainchain,Peptide
3	C	197	GLU	Sidechain
1	D	2	ALA	Mainchain,Peptide
1	D	355	GLU	Sidechain

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	4285	0	4085	52	0
1	D	4290	0	4091	40	0
2	B	3344	0	3329	62	0
2	E	3333	0	3320	34	0
3	C	2008	0	1937	23	0
3	F	2007	0	1937	23	0
4	A	62	0	43	4	0
4	D	62	0	43	2	0
5	A	21	0	19	4	0
5	D	21	0	19	6	0
6	A	7	0	4	3	0
6	D	7	0	5	1	0
7	A	24	0	31	5	0
7	B	6	0	8	6	0
7	C	6	0	8	0	0
7	D	24	0	31	1	0
7	E	6	0	8	1	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	1	0	0	0	0
9	D	1	0	0	0	0
9	E	3	0	0	0	0
9	F	1	0	0	0	0
10	A	4	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	444	0	0	5	0
12	B	385	0	0	6	0
12	C	254	0	0	2	0
12	D	440	0	0	7	0
12	E	360	0	0	6	0
12	F	253	0	0	5	0
All	All	21674	0	18918	209	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 5.

The worst 5 of 209 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:185[B]:LEU:HD22	2:B:190:TYR:CB	1.26	1.62
2:B:185[B]:LEU:CD2	2:B:190:TYR:CB	2.02	1.36
2:B:236[B]:MET:CE	2:B:236[B]:MET:SD	2.14	1.36
2:B:185[B]:LEU:HD21	2:B:190:TYR:C	1.48	1.33
3:F:232:GLU:CA	12:F:2241:HOH:O	1.75	1.27

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	551/549 (100%)	532 (97%)	18 (3%)	1 (0%)	52	42
1	D	554/549 (101%)	530 (96%)	23 (4%)	1 (0%)	52	42
2	B	454/442 (103%)	441 (97%)	12 (3%)	1 (0%)	52	42
2	E	451/442 (102%)	438 (97%)	12 (3%)	1 (0%)	52	42
3	C	250/248 (101%)	242 (97%)	8 (3%)	0	100	100
3	F	250/248 (101%)	240 (96%)	9 (4%)	1 (0%)	39	27
All	All	2510/2478 (101%)	2423 (96%)	82 (3%)	5 (0%)	52	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	165	PRO
2	B	165	PRO
3	F	232	GLU
1	A	325	SER
1	D	325	SER

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	443/434 (102%)	436 (98%)	7 (2%)	70	66
1	D	446/434 (103%)	440 (99%)	6 (1%)	76	73
2	B	355/341 (104%)	350 (99%)	5 (1%)	74	71
2	E	352/341 (103%)	347 (99%)	5 (1%)	74	71
3	C	220/216 (102%)	214 (97%)	6 (3%)	52	43
3	F	220/216 (102%)	213 (97%)	7 (3%)	46	35
All	All	2036/1982 (103%)	2000 (98%)	36 (2%)	68	61

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	196	ASP
1	D	84	ASP
3	F	196	ASP
1	D	12	LYS
1	D	444	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	187	GLN
3	F	235	GLN
1	D	485	GLN
1	D	111	HIS
1	D	365	ASN

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	1.73	1 (12%)	7,14,16	1.63	3 (42%)
1	AGM	A	271	1	7,11,12	0.83	0	5,13,15	1.71	2 (40%)
1	MGN	A	400	1	6,9,10	1.09	1 (16%)	6,12,14	2.39	1 (16%)
1	GL3	A	445	1	3,3,4	2.74	1 (33%)	2,2,4	2.05	1 (50%)
1	SMC	A	452	1	5,6,7	1.43	1 (20%)	2,6,8	1.09	0
1	MHS	D	257	1	8,11,12	1.67	1 (12%)	7,14,16	0.95	0
1	AGM	D	271	1	7,11,12	0.60	0	5,13,15	1.27	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MGN	D	400	1	6,9,10	1.04	0	6,12,14	2.31	1 (16%)
1	GL3	D	445	1	3,3,4	2.69	1 (33%)	2,2,4	1.62	1 (50%)
1	SMC	D	452	1	5,6,7	0.75	0	2,6,8	1.86	1 (50%)

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	A	445	GL3	C-S	-4.69	1.64	1.80
1	D	445	GL3	C-S	-4.52	1.65	1.80
1	A	452	SMC	CB-SG	-2.90	1.77	1.80
1	A	400	MGN	CB1-CA	2.25	1.57	1.55
1	D	257	MHS	CM-ND1	4.12	1.56	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	400	MGN	CB2-CA-CB1	-4.92	102.20	110.92
1	A	400	MGN	CB2-CA-CB1	-4.90	102.24	110.92
1	A	271	AGM	CE2-CD-NE1	-3.00	106.36	112.05
1	D	271	AGM	CE2-CD-NE1	-2.41	107.47	112.05
1	A	257	MHS	O-C-CA	-2.41	119.21	125.49

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	A	452	SMC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 25 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			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	F43	A	1550	1,6	42,71,71	3.80	21 (50%)	35,118,118	2.58	14 (40%)
5	TP7	A	1551	-	16,20,20	2.13	5 (31%)	16,26,26	2.06	4 (25%)
6	COM	A	1552	4	5,6,6	1.16	1 (20%)	5,8,8	2.20	1 (20%)
7	GOL	A	1553	10	5,5,5	0.73	0	5,5,5	1.19	0
7	GOL	A	1554	-	5,5,5	0.68	0	5,5,5	0.92	0
7	GOL	A	1555	-	5,5,5	0.83	0	5,5,5	0.84	0
7	GOL	A	1556	-	5,5,5	0.68	0	5,5,5	0.85	0
7	GOL	B	1444	-	5,5,5	0.87	0	5,5,5	1.24	0
7	GOL	C	1249	-	5,5,5	0.69	0	5,5,5	0.46	0
4	F43	D	1550	1,6	42,71,71	4.17	21 (50%)	35,118,118	2.29	15 (42%)
5	TP7	D	1551	-	16,20,20	2.07	4 (25%)	16,26,26	2.02	5 (31%)
6	COM	D	1552	4	5,6,6	1.29	1 (20%)	5,8,8	1.41	1 (20%)
7	GOL	D	1553	-	5,5,5	0.96	0	5,5,5	0.75	0
7	GOL	D	1554	10	5,5,5	0.58	0	5,5,5	1.16	0
7	GOL	D	1555	-	5,5,5	0.74	0	5,5,5	0.66	0
7	GOL	D	1556	-	5,5,5	0.78	0	5,5,5	0.79	0
7	GOL	E	1444	-	5,5,5	0.68	0	5,5,5	0.80	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 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1550	F43	C4B-NB	-14.86	1.26	1.49
4	A	1550	F43	C4B-NB	-12.87	1.29	1.49
4	A	1550	F43	C4A-NA	-5.53	1.39	1.49
5	A	1551	TP7	C2-C1	-5.51	1.40	1.51
4	D	1550	F43	C4A-NA	-5.28	1.40	1.49

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1550	F43	C9D-C3D-C4D	-7.07	115.10	127.01
4	A	1550	F43	C9D-C3D-C4D	-5.36	117.99	127.01
4	D	1550	F43	O8D-C7D-C6D	-4.50	112.59	120.76
5	A	1551	TP7	C-CA-N	-3.79	105.91	113.51
4	A	1550	F43	O8D-C7D-CHD	-3.68	118.36	122.56

All (4) chirality outliers are listed below:

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

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1550	F43	4	0
5	A	1551	TP7	4	0
6	A	1552	COM	3	0
7	A	1553	GOL	1	0
7	A	1555	GOL	1	0
7	A	1556	GOL	3	0
7	B	1444	GOL	6	0
4	D	1550	F43	2	0
5	D	1551	TP7	6	0
6	D	1552	COM	1	0
7	D	1556	GOL	1	0
7	E	1444	GOL	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.