wwPDB X-ray Structure Validation Summary Report (i)

Jun 5, 2017 – 04:42 PM EDT

PDB ID	:	5N28
Title	:	METHYL-COENZYME M REDUCTASE III FROM METHANOTORRIS FORMICICUS MONOCLINIC FORM
Authors	:	Wagner, T.; Wegner, C.E.; Ermler, U.; Shima, S.
Deposited on	:	2017-02-07
Resolution	:	2.80 Å(reported)

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

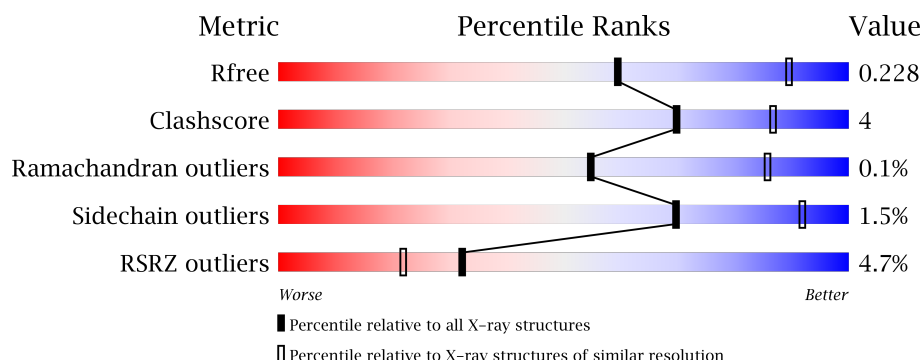|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

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 2.80 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	Percentile Ranks	Value
Rfree		0.228
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		1.5%
RSRZ outliers		4.7%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	552	3% — 86% — 13% •
1	D	552	7% — 87% — 12% •
2	B	444	.% — 93% — 7%
2	E	444	4% — 92% — 8%
3	C	260	2% — 87% — 12% •

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Mol	Chain	Length	Quality of chain
3	F	260	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19579 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total 4277	C 2721	N 718	O 816	S 22	0	0	0
1	D	547	Total 4268	C 2716	N 717	O 813	S 22	0	0	0

- Molecule 2 is a protein called Methyl-coenzyme M reductase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	443	Total 3324	C 2123	N 551	O 630	S 20	0	0	0
2	E	443	Total 3324	C 2123	N 551	O 630	S 20	0	0	0

- Molecule 3 is a protein called Methyl-coenzyme M reductase, gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	258	Total 2113	C 1331	N 376	O 396	S 10	0	0	0
3	F	252	Total 2064	C 1301	N 369	O 384	S 10	0	0	0

- Molecule 4 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).
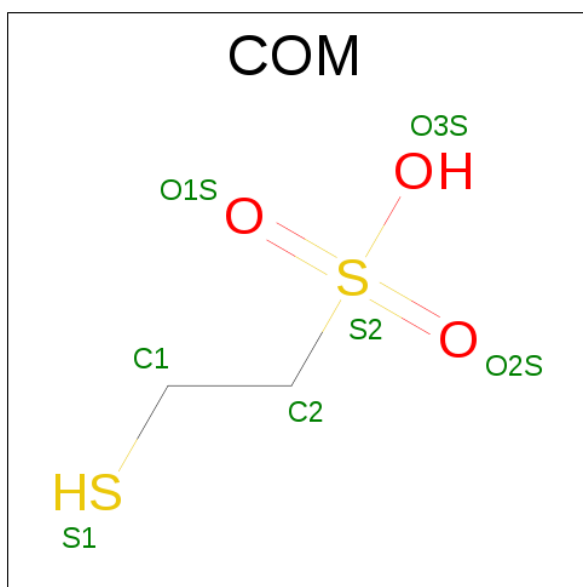
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			7	2	3	2		
4	D	1	Total	C	O	S	0	0
			7	2	3	2		

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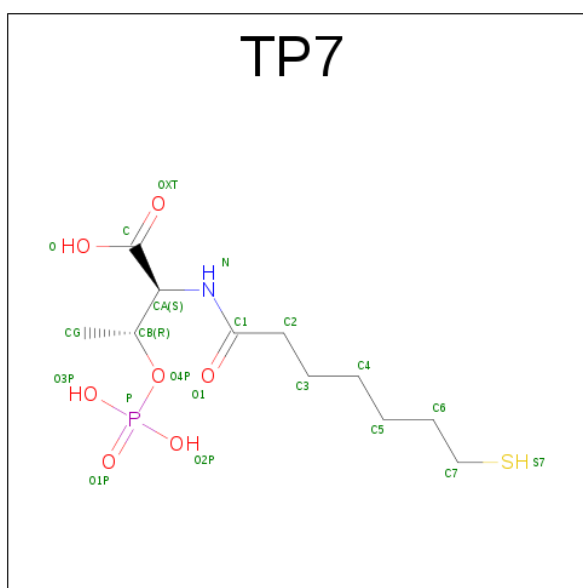
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

• Molecule 6 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).
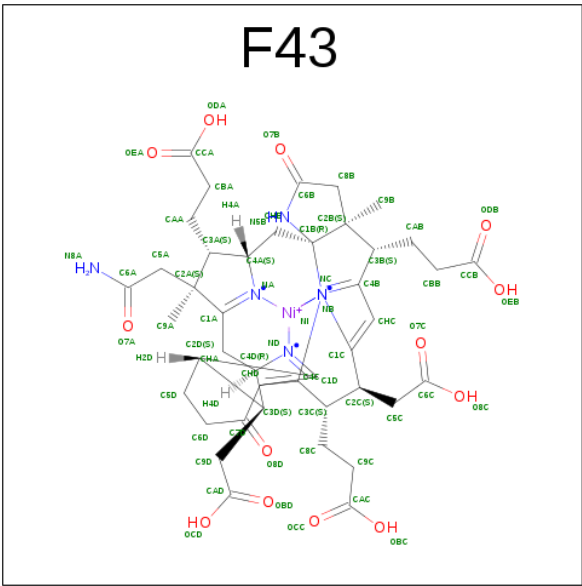
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 62	C 42	N 6	Ni 1	O 13	0	0
6	D	1	Total 62	C 42	N 6	Ni 1	O 13	0	0

• Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	K 1	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	9	Total 9	O 9	0	0
8	B	9	Total 9	O 9	0	0
8	C	3	Total 3	O 3	0	0
8	D	5	Total 5	O 5	0	0
8	E	2	Total 2	O 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Methyl-coenzyme M reductase subunit alpha
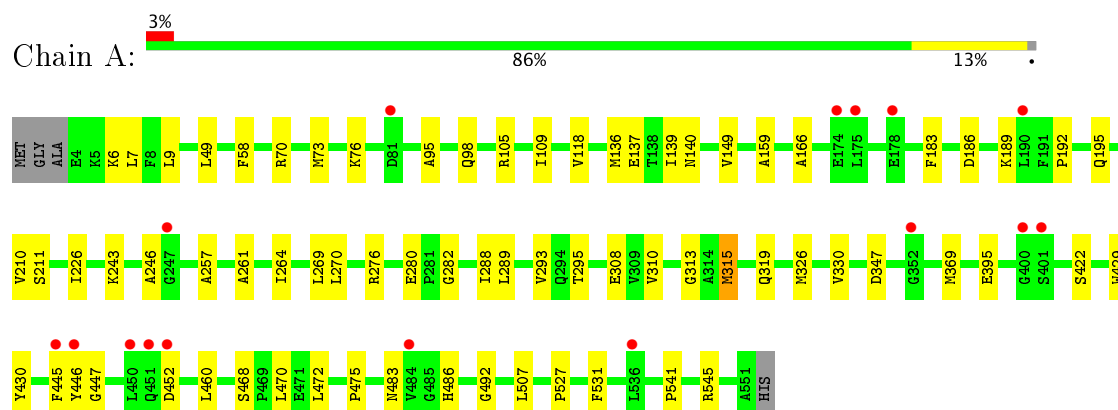
• Molecule 1: Methyl-coenzyme M reductase subunit alpha
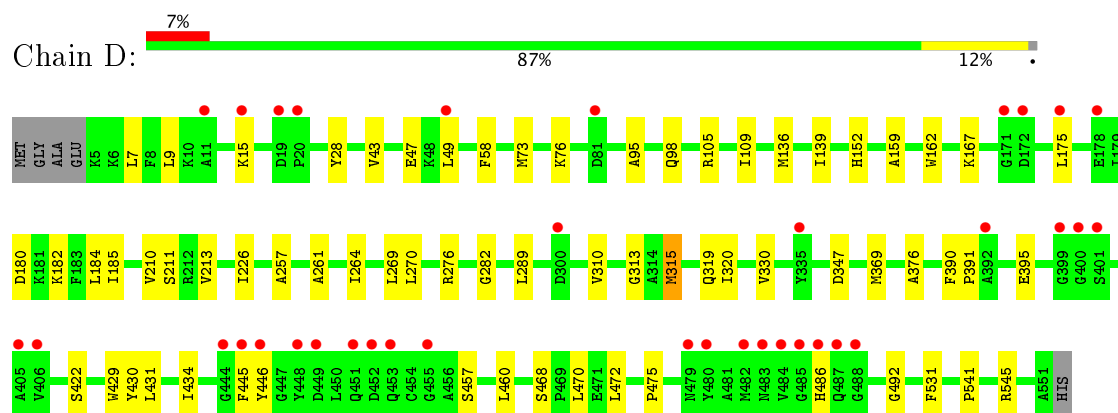
• Molecule 2: Methyl-coenzyme M reductase, beta subunit

• Molecule 2: Methyl-coenzyme M reductase, beta subunit

Chain E:

• Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain C:

• Molecule 3: Methyl-coenzyme M reductase, gamma subunit

Chain F:
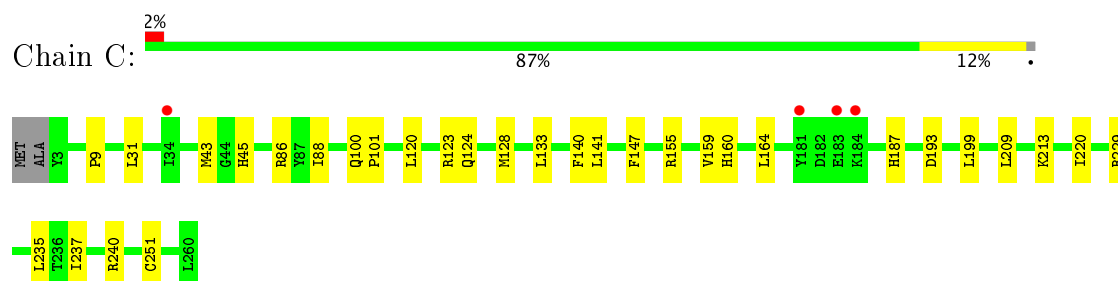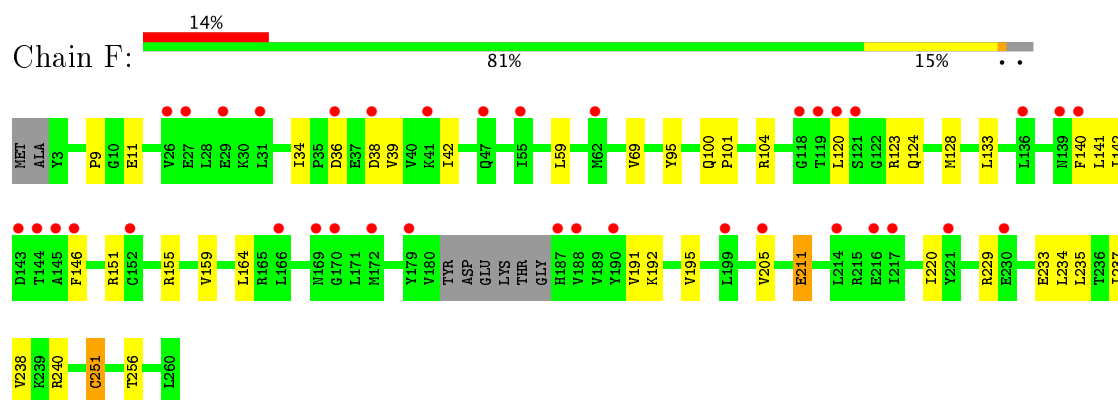
4   Data and refinement statistics (i)

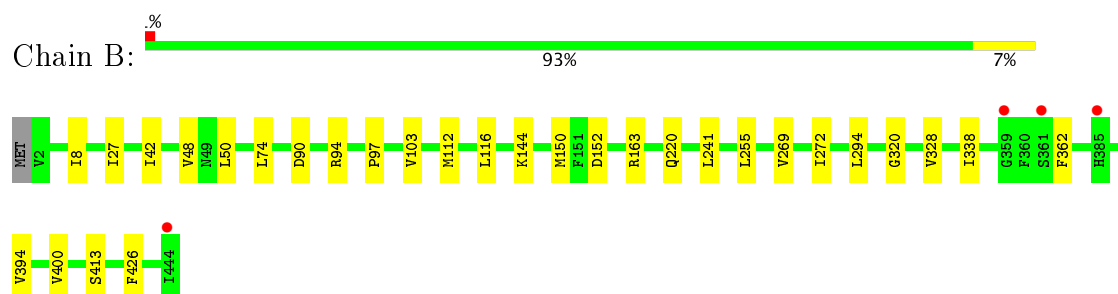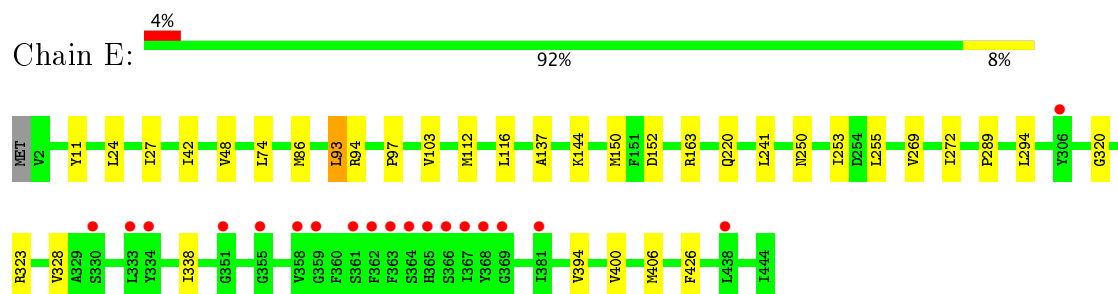| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.68Å 81.16Å 154.95Å 90.00° 107.80° 90.00°	Depositor
Resolution (Å)	48.43 – 2.80 48.43 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.43-2.80) 99.9 (48.43-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.78 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.193 , 0.204 0.215 , 0.228	Depositor DCC
R_{free} test set	3016 reflections (5.23%)	DCC
Wilson B-factor (Å^2)	72.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.4	EDS
L-test for twinning[2]	$<|L|> = 0.46, <L^2> = 0.29$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19579	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: AGM, K, F43, MGN, TP7, TRX, 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	0.41	0/4319	0.62	0/5844
1	D	0.41	0/4310	0.62	0/5832
2	B	0.43	0/3382	0.62	0/4590
2	E	0.42	0/3382	0.62	0/4590
3	C	0.41	0/2161	0.64	0/2919
3	F	0.43	0/2110	0.64	0/2849
All	All	0.42	0/19664	0.63	0/26624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	4277	0	4140	55	0
1	D	4268	0	4134	44	0
2	B	3324	0	3372	18	0
2	E	3324	0	3372	23	0
3	C	2113	0	2073	18	0
3	F	2064	0	2030	30	0
4	A	7	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	7	0	6	1	0
5	A	42	0	38	1	0
6	A	62	0	43	2	0
6	D	62	0	43	1	0
7	A	1	0	0	0	0
8	A	9	0	0	0	0
8	B	9	0	0	0	0
8	C	3	0	0	0	0
8	D	5	0	0	0	0
8	E	2	0	0	0	0
All	All	19579	0	19257	162	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 4.

The worst 5 of 162 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:D:395:GLU:HG3	3:F:164:LEU:HD22	1.49	0.92
1:A:276:ARG:NH1	1:A:326:MET:HE1	1.86	0.90
1:A:70:ARG:HH21	1:A:395:GLU:HG2	1.40	0.87
1:A:276:ARG:HH12	1:A:326:MET:HE1	1.43	0.80
1:A:276:ARG:NH1	1:A:326:MET:CE	2.46	0.79

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	541/552 (98%)	513 (95%)	27 (5%)	1 (0%)	51	83
1	D	540/552 (98%)	515 (95%)	24 (4%)	1 (0%)	51	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	441/444 (99%)	428 (97%)	13 (3%)	0	100	100
2	E	441/444 (99%)	429 (97%)	12 (3%)	0	100	100
3	C	256/260 (98%)	247 (96%)	9 (4%)	0	100	100
3	F	248/260 (95%)	240 (97%)	8 (3%)	0	100	100
All	All	2467/2512 (98%)	2372 (96%)	93 (4%)	2 (0%)	55	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	SER
1	D	468	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	436/438 (100%)	428 (98%)	8 (2%)	64	90
1	D	435/438 (99%)	424 (98%)	11 (2%)	53	84
2	B	350/351 (100%)	347 (99%)	3 (1%)	82	95
2	E	350/351 (100%)	347 (99%)	3 (1%)	82	95
3	C	228/229 (100%)	226 (99%)	2 (1%)	82	95
3	F	223/229 (97%)	220 (99%)	3 (1%)	73	93
All	All	2022/2036 (99%)	1992 (98%)	30 (2%)	70	92

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	28	TYR
1	D	175	LEU
3	F	211	GLU
1	D	76	LYS
1	D	211	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
2	E	184	ASN
3	F	45	HIS

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 Counts	Bond lengths RMSZ	Bond lengths $\#|Z| > 2$	Bond angles Counts	Bond angles RMSZ	Bond angles $\#|Z| > 2$
1	MHS	A	260	1	9,11,12	1.09	1 (11%)	9,14,16	1.52	2 (22%)
1	AGM	A	274	1	11,11,12	0.84	1 (9%)	8,13,15	1.19	0
1	MGN	A	402	1	7,9,10	0.53	0	5,12,14	0.52	0
1	TRX	A	429	1	15,16,17	1.35	2 (13%)	15,22,24	1.43	4 (26%)
1	GL3	A	447	1	3,3,4	2.34	1 (33%)	1,2,4	0.03	0
1	MHS	D	260	1	9,11,12	1.06	1 (11%)	9,14,16	1.65	2 (22%)
1	AGM	D	274	1	11,11,12	0.92	1 (9%)	8,13,15	1.22	1 (12%)
1	MGN	D	402	1	7,9,10	0.54	0	5,12,14	0.46	0
1	TRX	D	429	1	15,16,17	1.27	2 (13%)	15,22,24	1.50	4 (26%)
1	GL3	D	447	1	3,3,4	2.22	1 (33%)	1,2,4	0.05	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	260	1	-	0/4/6/8	0/1/1/1
1	AGM	A	274	1	-	0/9/11/13	0/0/0/0
1	MGN	A	402	1	-	0/7/9/12	0/0/0/0
1	TRX	A	429	1	-	0/3/6/8	0/2/2/2
1	GL3	A	447	1	-	0/1/1/2	0/0/0/0
1	MHS	D	260	1	-	0/4/6/8	0/1/1/1
1	AGM	D	274	1	-	0/9/11/13	0/0/0/0
1	MGN	D	402	1	-	0/7/9/12	0/0/0/0
1	TRX	D	429	1	-	0/3/6/8	0/2/2/2
1	GL3	D	447	1	-	0/1/1/2	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	GL3	C-S	-4.05	1.67	1.80
1	D	447	GL3	C-S	-3.85	1.68	1.80
1	D	429	TRX	CD2-CE2	2.16	1.48	1.42
1	A	429	TRX	CD2-CE2	2.18	1.48	1.42
1	D	260	MHS	CA-C	2.29	1.53	1.50

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	429	TRX	CZ3-CE3-CD2	-2.67	117.48	121.14
1	A	429	TRX	CZ3-CE3-CD2	-2.58	117.61	121.14
1	D	429	TRX	CZ2-CE2-CD2	-2.39	118.08	121.14
1	A	260	MHS	O-C-CA	-2.28	118.72	125.02
1	D	260	MHS	O-C-CA	-2.27	118.74	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	429	TRX	2	0
1	A	447	GL3	1	0
1	D	429	TRX	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	COM	A	601	-	6,6,6	1.42	2 (33%)	8,8,8	3.89	4 (50%)
5	TP7	A	602	-	16,20,20	0.45	0	18,26,26	0.89	0
5	TP7	A	603	-	16,20,20	0.47	0	18,26,26	0.94	1 (5%)
6	F43	A	604	1	47,71,71	2.24	6 (12%)	48,118,118	1.35	6 (12%)
6	F43	D	601	1	47,71,71	2.23	6 (12%)	48,118,118	1.32	5 (10%)
4	COM	D	602	-	6,6,6	1.33	1 (16%)	8,8,8	3.57	4 (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
4	COM	A	601	-	-	0/4/4/4	0/0/0/0
5	TP7	A	602	-	-	0/20/24/24	0/0/0/0
5	TP7	A	603	-	-	0/20/24/24	0/0/0/0
6	F43	A	604	1	-	0/18/185/185	0/0/10/10
6	F43	D	601	1	-	0/18/185/185	0/0/10/10
4	COM	D	602	-	-	0/4/4/4	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	601	F43	CHD-C1D	-6.03	1.35	1.43
6	A	604	F43	CHD-C1D	-5.99	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	601	F43	C4D-ND	-2.23	1.45	1.49
6	A	604	F43	C4D-ND	-2.16	1.45	1.49
4	D	602	COM	O1S-S2	2.09	1.51	1.45

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	COM	O2S-S2-O1S	-4.29	98.99	113.86
4	D	602	COM	O2S-S2-O1S	-3.51	101.68	113.86
6	A	604	F43	O7B-C6B-C8B	-3.40	122.46	126.83
6	D	601	F43	CAB-C3B-C2B	-3.26	112.92	119.03
6	A	604	F43	CAB-C3B-C2B	-3.17	113.11	119.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	COM	1	0
5	A	603	TP7	1	0
6	A	604	F43	2	0
6	D	601	F43	1	0
4	D	602	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	543/552 (98%)	0.11	16 (2%)	52	41	49, 86, 132, 150	0
1	D	542/552 (98%)	0.29	36 (6%)	19	11	52, 91, 141, 176	0
2	B	443/444 (99%)	-0.22	4 (0%)	84	79	44, 68, 102, 118	0
2	E	443/444 (99%)	-0.03	19 (4%)	36	26	55, 85, 122, 155	1 (0%)
3	C	258/260 (99%)	0.01	4 (1%)	72	65	58, 94, 127, 153	0
3	F	252/260 (96%)	0.81	37 (14%)	3	1	91, 142, 185, 208	0
All	All	2481/2512 (98%)	0.13	116 (4%)	32	22	44, 88, 150, 208	1 (0%)

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	205	VAL	6.2
3	F	139	ASN	5.9
3	F	190	TYR	5.0
3	F	143	ASP	4.5
1	D	445	PHE	4.2

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	AGM	A	274	12/13	0.97	0.26	-	47,48,51,51	0
1	MHS	D	260	11/12	0.93	0.16	-	62,66,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	MGN	D	402	10/11	0.93	0.36	-	92,93,96,97	0
1	MHS	A	260	11/12	0.97	0.08	-	65,65,71,71	0
1	MGN	A	402	10/11	0.97	0.20	-	68,69,72,72	0
1	AGM	D	274	12/13	0.96	0.26	-	52,53,56,57	0
1	TRX	A	429	15/16	0.98	0.20	-	55,56,63,63	0
1	GL3	A	447	4/5	0.96	0.31	-	59,60,60,61	0
1	GL3	D	447	4/5	0.97	0.52	-	82,83,84,85	0
1	TRX	D	429	15/16	0.92	0.25	-	75,76,84,84	0

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
5	TP7	A	603	21/21	0.96	0.28	0.16	64,71,76,77	0
5	TP7	A	602	21/21	0.94	0.33	-0.20	77,80,83,84	0
6	F43	A	604	62/62	0.95	0.26	-0.26	83,86,95,102	0
6	F43	D	601	62/62	0.97	0.21	-0.38	60,66,74,76	0
4	COM	D	602	7/7	0.95	0.36	-0.42	98,100,101,102	0
4	COM	A	601	7/7	0.97	0.22	-1.16	66,68,71,73	0
7	K	A	605	1/1	0.95	0.10	-2.27	72,72,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.