wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 10:28 AM GMT

PDB ID	:	3M2V
Title	:	Structural Insight into Methyl-Coenzyme M Reductase Chemistry using Coenzyme B Analogues
Authors	:	Cedervall, P.E.; Dey, M.; Ragsdale, S.W.; Wilmot, C.M.
Deposited on	:	2010-03-08
Resolution	:	1.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

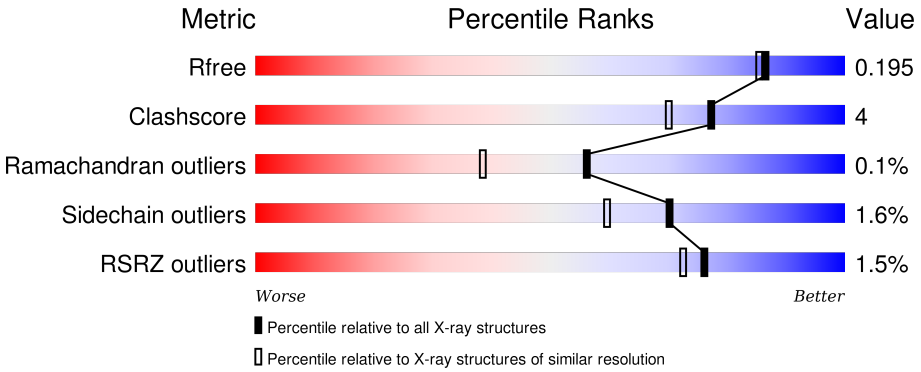
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	549	91% 8%
1	D	549	% 89% 10%
2	B	442	89% 9%
2	E	442	2% 91% 9%
3	C	248	3% 87% 12%

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Mol	Chain	Length	Quality of chain
3	F	248	6% 87% 11%

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
10	EDO	A	556	-	-	-	X
4	MG	C	250	-	-	-	X
4	MG	F	250	-	-	-	X
5	F43	A	1	X	-	-	-
5	F43	D	551	X	-	-	-
6	TP7	A	552[A]	X	-	-	-
6	TP7	D	1[A]	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21893 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	23	0
			4408	2785	731	871	21			
1	D	548	Total	C	N	O	S	0	19	0
			4359	2767	721	851	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	18	0
			3422	2177	559	664	22			
2	E	442	Total	C	N	O	S	0	19	0
			3431	2182	563	665	21			

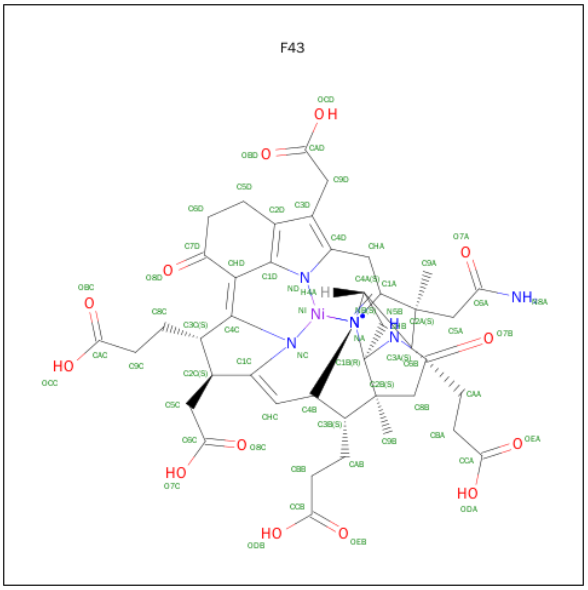
- Molecule 3 is a protein called Methyl-coenzyme M reductase I subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	248	Total	C	N	O	S	0	8	0
			2059	1273	362	412	12			
3	F	247	Total	C	N	O	S	0	11	0
			2071	1280	367	412	12			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

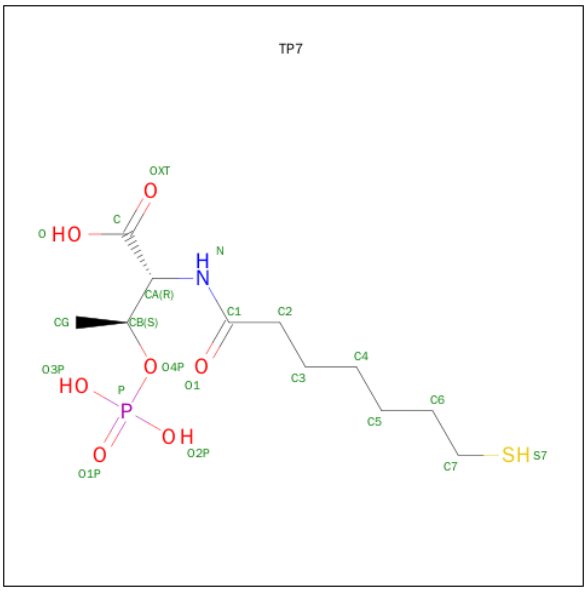
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{49}N_6NiO_{13}$).



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

- Molecule 6 is COENZYME B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



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

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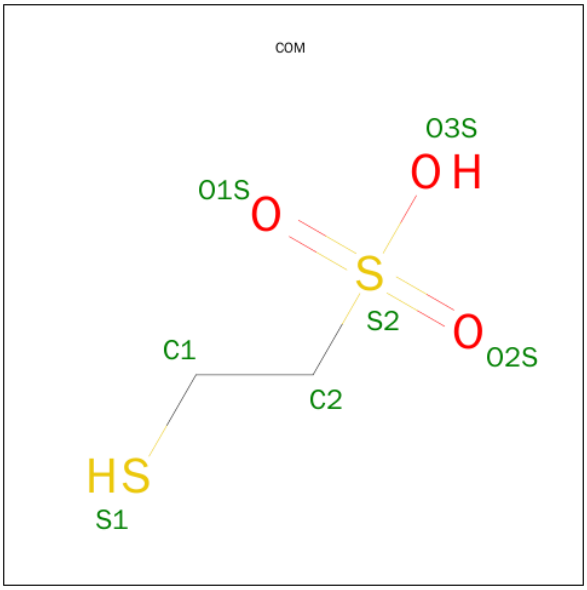
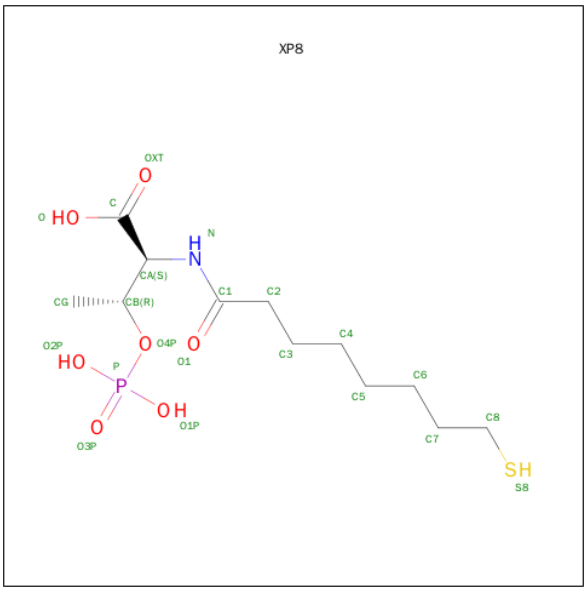
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	D	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		

- Molecule 7 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



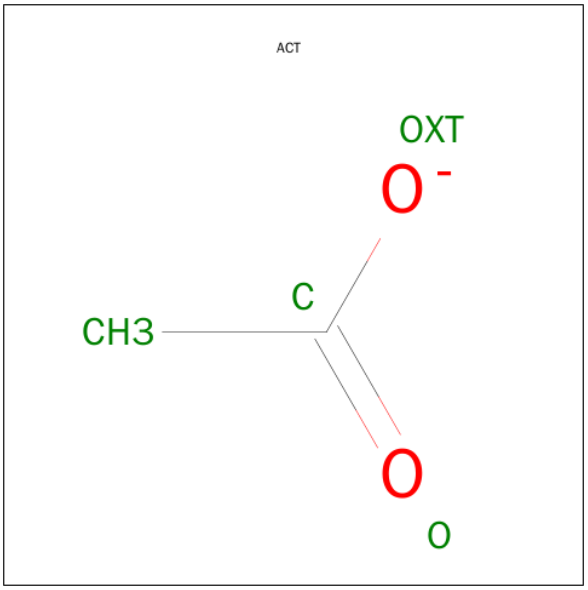
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			7	2	3	2		
7	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 8 is O-PHOSPHONO-N-(8-SULFANYLOCTANOYL)-L-THREONINE (three-letter code: XP8) (formula: $C_{12}H_{24}NO_7PS$).



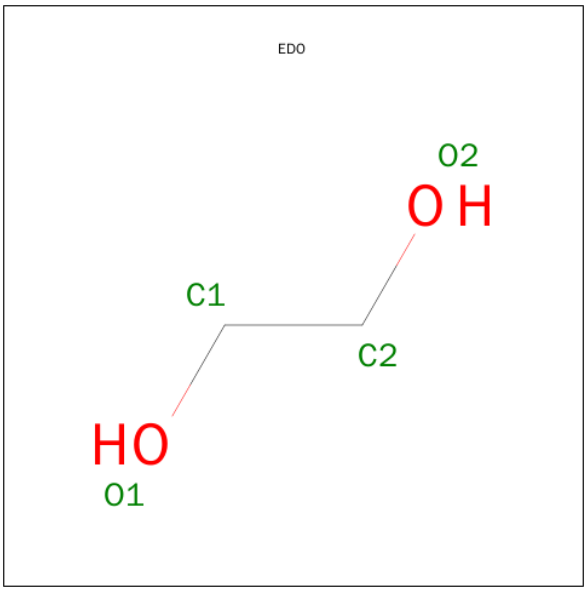
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			22	12	1	7	1	1		
8	D	1	Total	C	N	O	P	S	0	1
			22	12	1	7	1	1		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	O		0	1
			4	2	2			

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total Zn 1 1	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	427	Total O 435 435	0	15
12	B	345	Total O 349 349	0	5
12	C	200	Total O 201 201	0	8
12	D	415	Total O 421 421	0	9

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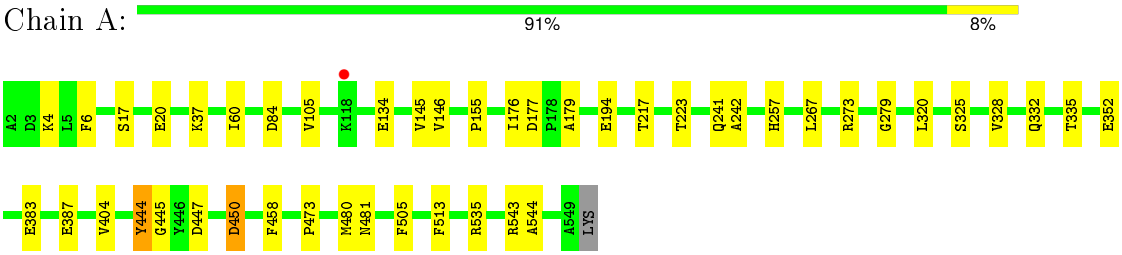
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	E	312	Total O 314 314	0	6
12	F	172	Total O 173 173	0	6

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 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.

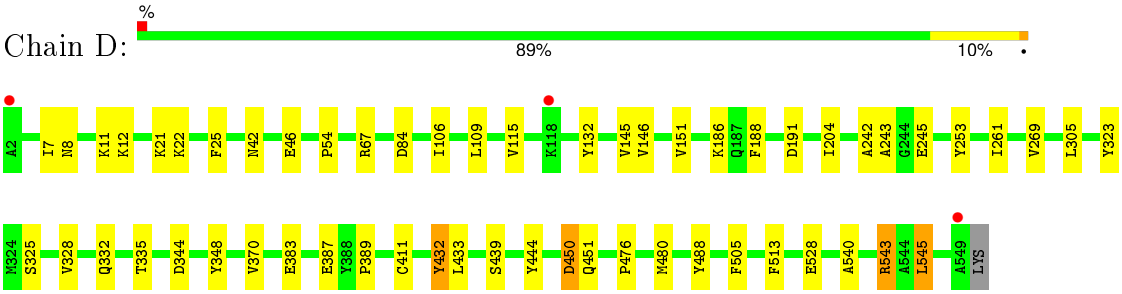
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

Chain A:



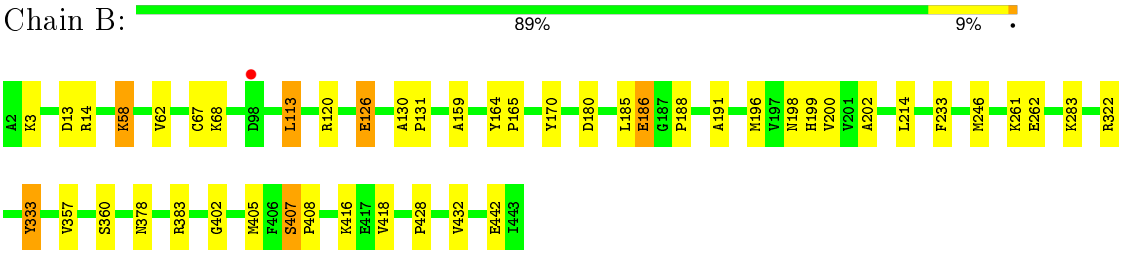
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

Chain D:



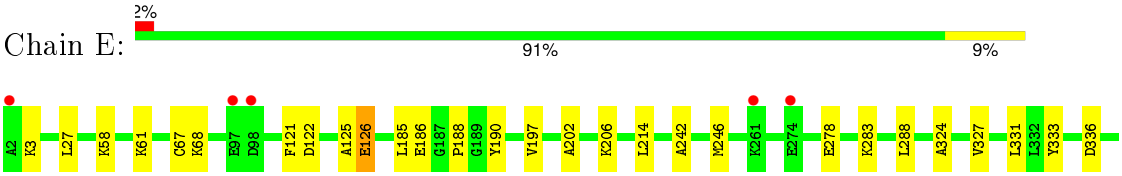
- Molecule 2: Methyl-coenzyme M reductase I subunit beta

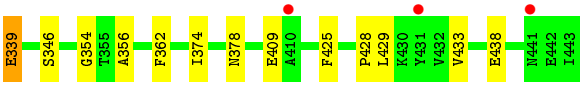
Chain B:



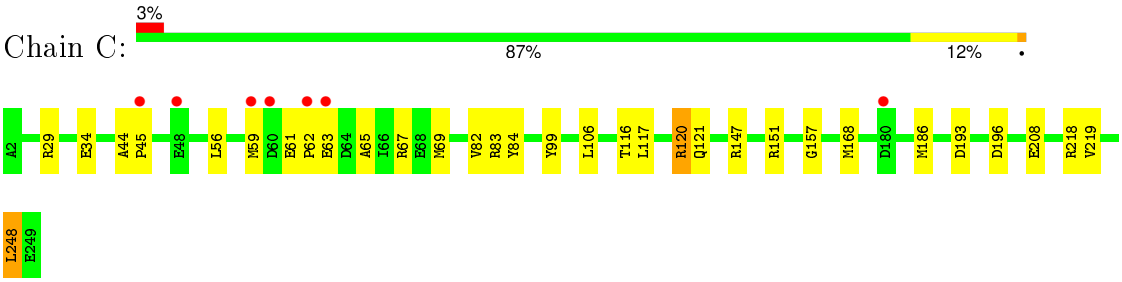
- Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain E:

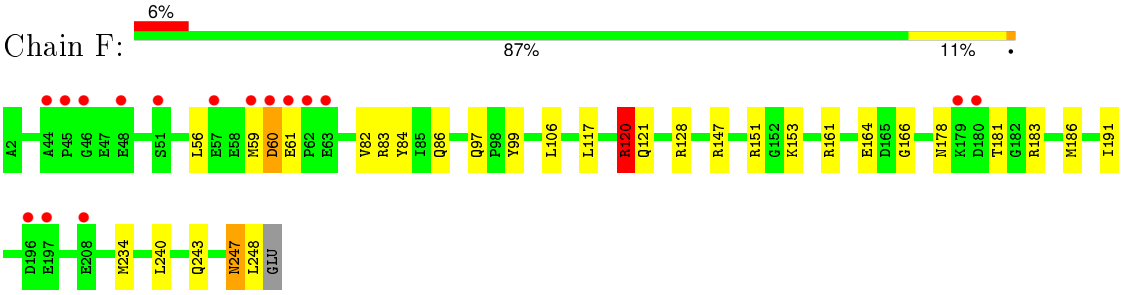




• Molecule 3: Methyl-coenzyme M reductase I subunit gamma



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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.02Å 118.26Å 122.39Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	19.93 – 1.80 19.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.93-1.80) 98.1 (19.93-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.150 , 0.195 0.150 , 0.195	Depositor DCC
R_{free} test set	10624 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	15.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.0	EDS
Estimated twinning fraction	0.000 for -h,l,k 0.010 for -h,-l,-k 0.017 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 211752 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21893	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XP8, ZN, COM, ACT, MG, F43, MGN, TP7, AGM, EDO, GL3, SMC, 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	1.39	7/4492 (0.2%)	1.02	3/6099 (0.0%)
1	D	1.44	14/4459 (0.3%)	1.06	5/6052 (0.1%)
2	B	1.34	7/3527 (0.2%)	1.01	4/4770 (0.1%)
2	E	1.28	7/3524 (0.2%)	0.99	2/4766 (0.0%)
3	C	1.23	3/2111 (0.1%)	1.05	7/2841 (0.2%)
3	F	1.19	3/2120 (0.1%)	1.03	3/2854 (0.1%)
All	All	1.34	41/20233 (0.2%)	1.03	24/27382 (0.1%)

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	62	VAL	CB-CG1	6.38	1.66	1.52
1	D	370	VAL	CB-CG1	6.15	1.65	1.52
1	D	25	PHE	CD1-CE1	5.96	1.51	1.39
1	D	411	CYS	CB-SG	5.92	1.92	1.82
1	A	458	PHE	CE1-CZ	5.85	1.48	1.37

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	122	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	D	488	TYR	CB-CG-CD2	-5.99	117.41	121.00
3	C	147	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	450	ASP	N-CA-CB	5.65	120.78	110.60
3	F	161	ARG	NE-CZ-NH1	5.56	123.08	120.30

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	4408	0	4185	29	0
1	D	4359	0	4196	37	0
2	B	3422	0	3450	36	0
2	E	3431	0	3455	21	0
3	C	2059	0	1985	21	0
3	F	2071	0	2003	27	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
5	A	62	0	43	2	0
5	D	62	0	43	3	0
6	A	21	0	19	3	0
6	D	21	0	19	1	0
7	A	7	0	5	1	0
7	D	7	0	5	0	0
8	A	22	0	21	1	0
8	D	22	0	21	1	0
9	A	4	0	3	0	0
10	A	8	0	12	0	0
10	D	8	0	12	3	0
11	D	1	0	0	0	0
12	A	435	0	0	3	0
12	B	349	0	0	3	0
12	C	201	0	0	3	0
12	D	421	0	0	8	0
12	E	314	0	0	3	0
12	F	173	0	0	4	0
All	All	21893	0	19477	146	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 146 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:196[A]:MET:CE	2:B:198:ASN:HB2	1.71	1.18
1:D:432:TYR:HB2	3:F:234[B]:MET:HE3	1.18	1.16
2:B:196[A]:MET:HE1	2:B:198:ASN:HB2	1.38	1.02
1:D:432:TYR:CB	3:F:234[B]:MET:HE3	1.90	1.02
2:B:196[A]:MET:HE3	2:B:198:ASN:HB2	1.45	0.94

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	564/549 (103%)	543 (96%)	20 (4%)	1 (0%)	52	35
1	D	560/549 (102%)	543 (97%)	16 (3%)	1 (0%)	52	35
2	B	459/442 (104%)	448 (98%)	10 (2%)	1 (0%)	52	35
2	E	459/442 (104%)	449 (98%)	10 (2%)	0	100	100
3	C	254/248 (102%)	243 (96%)	11 (4%)	0	100	100
3	F	256/248 (103%)	246 (96%)	10 (4%)	0	100	100
All	All	2552/2478 (103%)	2472 (97%)	77 (3%)	3 (0%)	56	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	325	SER
1	A	325	SER
2	B	402	GLY

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	456/434 (105%)	452 (99%)	4 (1%)	84	80
1	D	452/434 (104%)	444 (98%)	8 (2%)	66	54
2	B	360/341 (106%)	355 (99%)	5 (1%)	74	65
2	E	360/341 (106%)	354 (98%)	6 (2%)	68	57
3	C	224/216 (104%)	220 (98%)	4 (2%)	66	54
3	F	225/216 (104%)	219 (97%)	6 (3%)	52	36
All	All	2077/1982 (105%)	2044 (98%)	33 (2%)	70	59

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	84	ASP
1	D	476	PRO
3	F	121	GLN
1	D	186	LYS
1	D	444	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	111	HIS
3	F	247	ASN
2	E	318	GLN
2	B	318	GLN
3	F	121	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	2.48	2 (25%)	7,14,16	4.40	6 (85%)
1	AGM	A	271	1	7,11,12	0.91	0	5,13,15	2.76	3 (60%)
1	MGN	A	400	1	6,9,10	2.14	1 (16%)	6,12,14	1.75	1 (16%)
1	GL3	A	445	1	3,3,4	3.08	1 (33%)	2,2,4	1.39	0
1	SMC	A	452	1	5,6,7	1.32	1 (20%)	2,6,8	1.90	1 (50%)
1	MHS	D	257	1	8,11,12	2.50	1 (12%)	7,14,16	4.05	5 (71%)
1	AGM	D	271	1	7,11,12	1.91	2 (28%)	5,13,15	2.31	2 (40%)
1	MGN	D	400	1	6,9,10	1.71	1 (16%)	6,12,14	1.69	1 (16%)
1	GL3	D	445	1	3,3,4	3.46	1 (33%)	2,2,4	1.24	0
1	SMC	D	452	1	5,6,7	1.14	1 (20%)	2,6,8	2.46	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 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	GL3	C-S	-5.84	1.60	1.80
1	A	445	GL3	C-S	-5.31	1.62	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	400	MGN	CB1-CA	-3.47	1.51	1.55
1	A	452	SMC	CB-SG	-2.46	1.78	1.80
1	D	452	SMC	CB-SG	2.22	1.83	1.80

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	MHS	NE2-CE1-ND1	-9.55	99.36	112.28
1	D	257	MHS	NE2-CE1-ND1	-9.00	100.11	112.28
1	A	400	MGN	CB1-CG-CD	-3.74	103.62	111.17
1	A	257	MHS	O-C-CA	-3.69	115.88	125.49
1	A	271	AGM	CE2-CD-NE1	-3.61	105.21	112.05

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	257	MHS	1	0
1	A	445	GL3	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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	$\#\|Z\|>2$
5	F43	A	1	1,7	42,71,71	3.01	10 (23%)	35,118,118	2.12	9 (25%)
6	TP7	A	552[A]	-	16,20,20	0.75	0	16,26,26	1.25	1 (6%)
7	COM	A	553	5	5,6,6	1.83	2 (40%)	5,8,8	4.77	3 (60%)
8	XP8	A	554[B]	-	17,21,21	0.69	0	17,27,27	1.22	1 (5%)
9	ACT	A	555[A]	4	1,3,3	2.61	1 (100%)	0,3,3	0.00	-
10	EDO	A	556	-	3,3,3	0.87	0	2,2,2	0.51	0
10	EDO	A	557	-	3,3,3	0.48	0	2,2,2	0.44	0
6	TP7	D	1[A]	-	16,20,20	0.73	0	16,26,26	1.07	0
5	F43	D	551	1,7	42,71,71	3.34	9 (21%)	35,118,118	2.48	8 (22%)
7	COM	D	552	5	5,6,6	2.11	1 (20%)	5,8,8	4.37	4 (80%)
8	XP8	D	553[B]	-	17,21,21	0.62	0	17,27,27	0.90	1 (5%)
10	EDO	D	554	-	3,3,3	0.37	0	2,2,2	0.32	0
10	EDO	D	555	-	3,3,3	0.53	0	2,2,2	0.56	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
5	F43	A	1	1,7	1/1/25/27	0/18/165/165	0/0/10/10
6	TP7	A	552[A]	-	1/1/5/6	0/20/24/24	0/0/0/0
7	COM	A	553	5	-	0/4/4/4	0/0/0/0
8	XP8	A	554[B]	-	-	0/21/25/25	0/0/0/0
9	ACT	A	555[A]	4	-	0/0/0/0	0/0/0/0
10	EDO	A	556	-	-	0/1/1/1	0/0/0/0
10	EDO	A	557	-	-	0/1/1/1	0/0/0/0
6	TP7	D	1[A]	-	1/1/5/6	0/20/24/24	0/0/0/0
5	F43	D	551	1,7	1/1/25/27	0/18/165/165	0/0/10/10
7	COM	D	552	5	-	0/4/4/4	0/0/0/0
8	XP8	D	553[B]	-	-	0/21/25/25	0/0/0/0
10	EDO	D	554	-	-	0/1/1/1	0/0/0/0
10	EDO	D	555	-	-	0/1/1/1	0/0/0/0

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	F43	C4B-NB	-13.05	1.29	1.49
5	D	551	F43	C4B-NB	-12.08	1.31	1.49
5	D	551	F43	C1D-ND	-2.61	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	F43	C2A-C1A	2.06	1.54	1.51
7	A	553	COM	O2S-S2	2.09	1.51	1.45

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	551	F43	C9D-C3D-C4D	-11.20	108.15	127.01
5	A	1	F43	C9D-C3D-C4D	-9.02	111.81	127.01
5	A	1	F43	O7B-C6B-C8B	-3.78	121.83	126.90
5	D	551	F43	O8D-C7D-C6D	-3.69	114.05	120.76
7	A	553	COM	O3S-S2-O2S	-3.29	103.96	111.61

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	D	1[A]	TP7	C1
6	A	552[A]	TP7	C1
5	D	551	F43	C4B
5	A	1	F43	C4B

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	F43	2	0
6	A	552[A]	TP7	3	0
7	A	553	COM	1	0
8	A	554[B]	XP8	1	0
6	D	1[A]	TP7	1	0
5	D	551	F43	3	0
8	D	553[B]	XP8	1	0
10	D	554	EDO	2	0
10	D	555	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	543/549 (98%)	-0.76	1 (0%)	95	93	6, 11, 24, 39	0
1	D	543/549 (98%)	-0.74	3 (0%)	90	88	6, 11, 24, 40	0
2	B	442/442 (100%)	-0.54	1 (0%)	95	93	8, 16, 27, 43	0
2	E	442/442 (100%)	-0.32	8 (1%)	71	67	8, 19, 37, 53	0
3	C	248/248 (100%)	-0.38	7 (2%)	56	51	9, 18, 37, 58	0
3	F	247/248 (99%)	-0.10	16 (6%)	22	18	11, 22, 41, 63	0
All	All	2465/2478 (99%)	-0.53	36 (1%)	76	72	6, 15, 31, 63	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	62	PRO	5.4
3	C	60	ASP	4.8
3	F	60	ASP	4.5
3	C	45	PRO	4.3
1	D	549	ALA	4.2

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

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, 95^{th} 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	GL3	A	445	4/5	0.99	0.06	-	6,6,7,10	0
1	MGN	A	400	10/11	0.98	0.05	-	6,6,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	AGM	A	271	12/13	0.98	0.06	-	7,9,10,11	0
1	AGM	D	271	12/13	0.98	0.07	-	7,9,11,13	0
1	MGN	D	400	10/11	0.99	0.04	-	7,9,10,12	0
1	SMC	D	452	7/8	0.98	0.06	-	9,10,13,16	0
1	MHS	D	257	11/12	0.96	0.08	-	15,18,20,21	0
1	GL3	D	445	4/5	1.00	0.04	-	7,8,9,10	0
1	SMC	A	452	7/8	0.98	0.06	-	7,8,11,12	0
1	MHS	A	257	11/12	0.96	0.06	-	15,18,21,22	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, 95^{th} 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
10	EDO	A	556	4/4	0.86	0.17	4.20	31,31,31,34	0
4	MG	F	250	1/1	0.96	0.13	2.69	28,28,28,28	0
4	MG	C	250	1/1	0.97	0.12	2.56	32,32,32,32	0
8	XP8	A	554[B]	22/22	0.97	0.09	1.92	11,14,18,18	22
8	XP8	D	553[B]	22/22	0.96	0.09	1.77	12,14,17,19	22
6	TP7	A	552[A]	21/21	0.97	0.08	1.41	10,14,16,17	21
6	TP7	D	1[A]	21/21	0.97	0.09	1.28	12,14,17,19	21
9	ACT	A	555[A]	4/4	0.96	0.10	-0.23	21,21,21,22	4
7	COM	D	552	7/7	0.99	0.07	-0.30	14,16,18,22	0
10	EDO	D	554	4/4	0.89	0.10	-0.35	33,38,38,38	0
7	COM	A	553	7/7	0.99	0.06	-0.46	12,15,17,20	0
5	F43	A	1	62/62	0.99	0.05	-0.63	5,9,14,19	0
5	F43	D	551	62/62	0.99	0.05	-0.64	3,8,12,16	0
11	ZN	D	556	1/1	1.00	0.03	-2.60	14,14,14,14	1
4	MG	A	551	1/1	0.94	0.18	-	22,22,22,22	1
10	EDO	D	555	4/4	0.81	0.14	-	39,43,43,45	0
4	MG	B	1	1/1	0.89	0.12	-	41,41,41,41	0
10	EDO	A	557	4/4	0.81	0.13	-	40,42,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	MG	B	444	1/1	0.91	0.10	-	30,30,30,30	1

6.5 Other polymers (i)

There are no such residues in this entry.