Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:28 AM GMT

PDB ID	:	3M32
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	:	1.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
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:

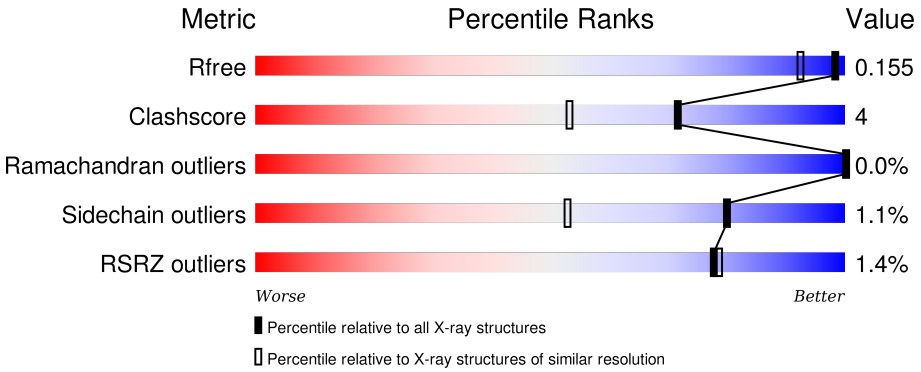
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.35 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.



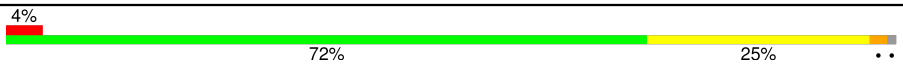
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2199 (1.40-1.32)
Clashscore	102246	2337 (1.40-1.32)
Ramachandran outliers	100387	2280 (1.40-1.32)
Sidechain outliers	100360	2279 (1.40-1.32)
RSRZ outliers	91569	2199 (1.40-1.32)

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	83% 15%
1	D	549	% 83% 15%
2	B	442	82% 16%
2	E	442	% 84% 15%
3	C	248	5% 80% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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
10	EDO	F	1	-	-	-	X
4	MG	C	250	-	-	-	X
5	TP7	A	553[A]	X	-	-	-
5	TP7	D	553[A]	X	-	-	-
6	F43	A	1	X	-	-	-
6	F43	D	552	X	-	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 22665 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	28	0
			4431	2801	735	874	21			
1	D	548	Total	C	N	O	S	0	22	0
			4380	2779	727	853	21			

- 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	24	0
			3462	2211	560	668	23			
2	E	442	Total	C	N	O	S	0	25	0
			3471	2216	564	668	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	0	10	0
			2056	1276	360	407	13			
3	F	246	Total	C	N	O	S	0	20	0
			2113	1309	372	418	14			

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

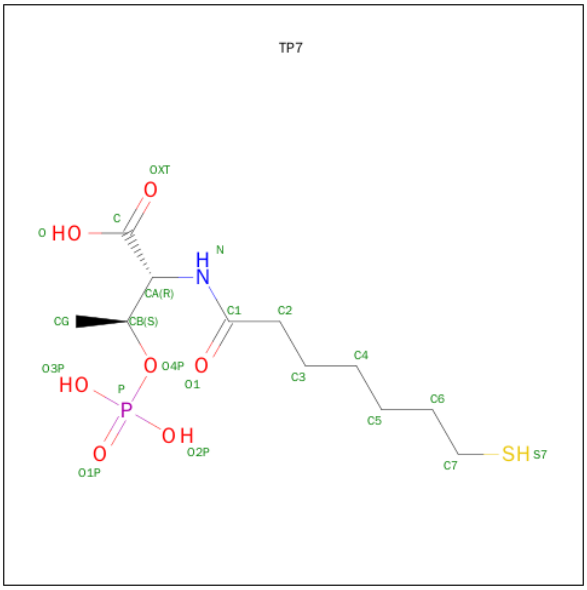
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		
4	E	1	Total	Mg	0	0
			1	1		
4	B	2	Total	Mg	0	1
			2	2		
4	C	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

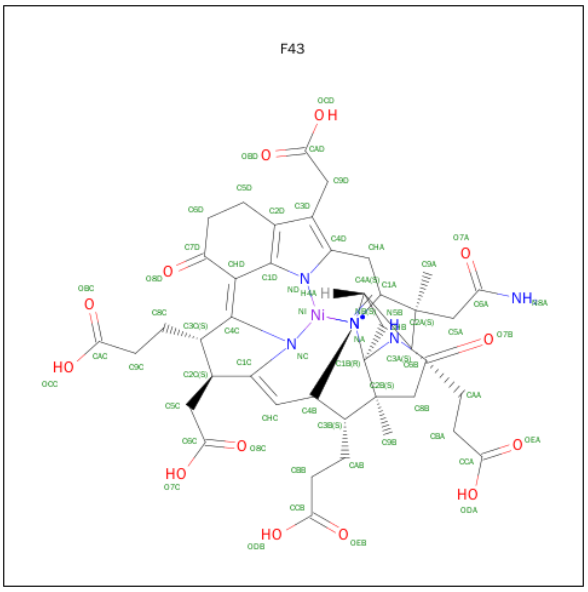
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	2
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is COENZYME B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



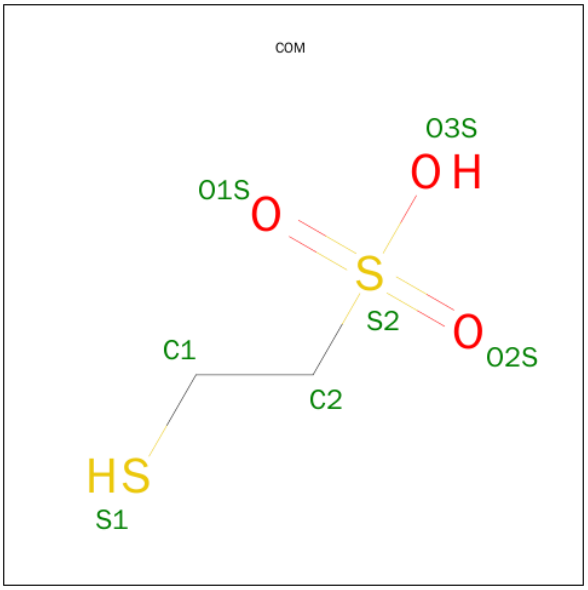
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P S 21 11 1 7 1 1	0	1
5	D	1	Total C N O P S 21 11 1 7 1 1	0	1

- Molecule 6 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{49}N_6NiO_{13}$).



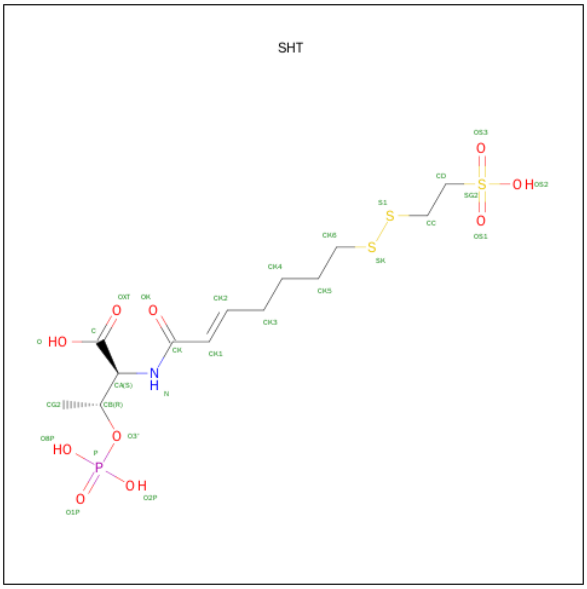
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
6	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

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



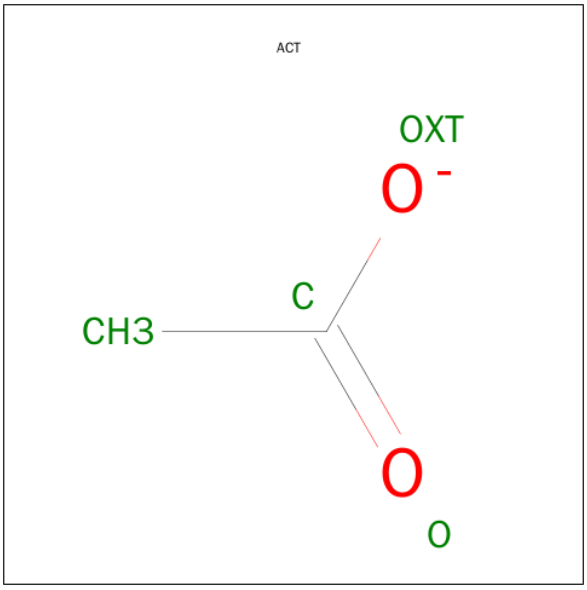
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	1
			7	2	3	2		
7	D	1	Total	C	O	S	0	1
			7	2	3	2		

- Molecule 8 is O-PHOSPHONO-N-{(2E)-7-[(2-SULFOETHYL)DITHIO]HEPT-2-ENOYL}-L-THREONINE (three-letter code: SHT) (formula: $C_{13}H_{24}NO_{10}PS_3$).



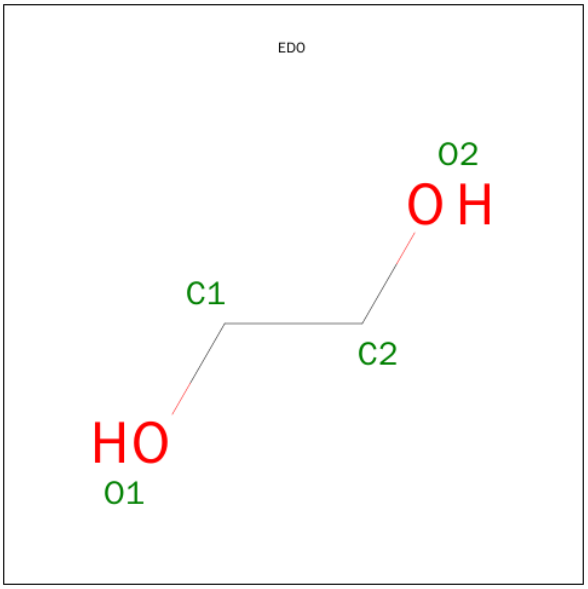
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			28	13	1	10	1	3		
8	D	1	Total	C	N	O	P	S	0	1
			28	13	1	10	1	3		

- 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 4 2 2	0	1

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

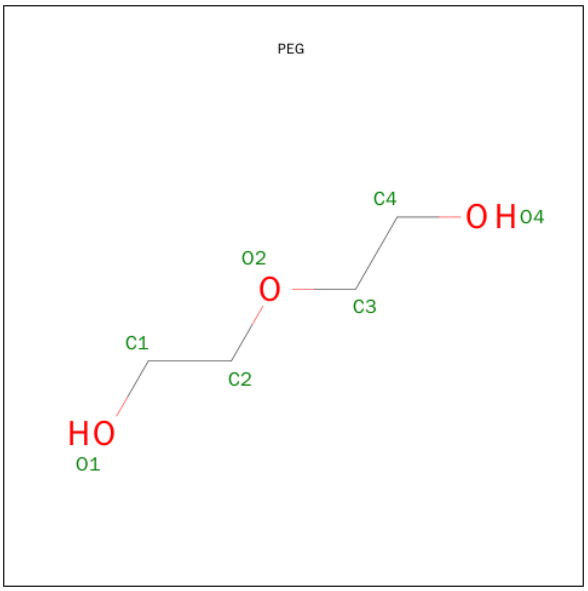


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0
10	F	1	Total C O 4 2 2	0	0
10	F	1	Total C O 4 2 2	0	0

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

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

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C O 7 4 3	0	0

- Molecule 13 is water.

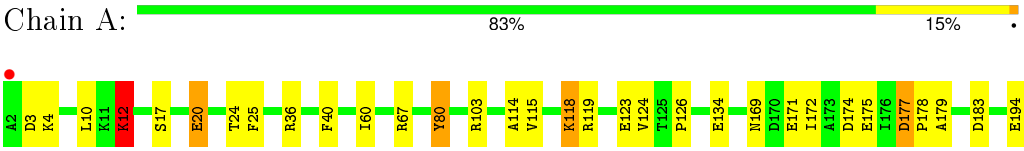
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	507	Total O 522 522	0	28
13	B	462	Total O 477 477	0	24
13	C	254	Total O 262 262	0	12
13	D	529	Total O 539 539	0	20
13	E	414	Total O 421 421	0	16
13	F	250	Total O 254 254	0	8

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.

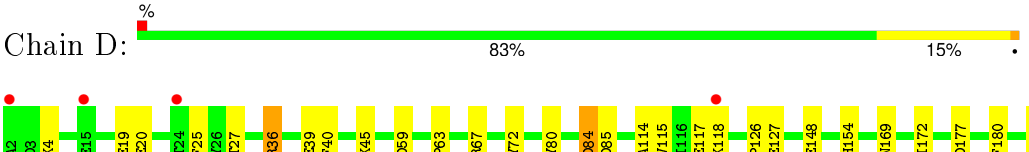
- Molecule 1: Methyl-coenzyme M reductase I subunit alpha

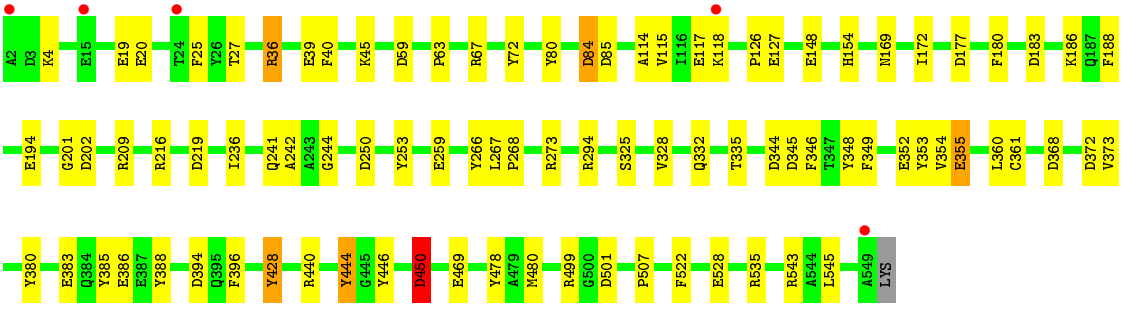
Chain A:



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

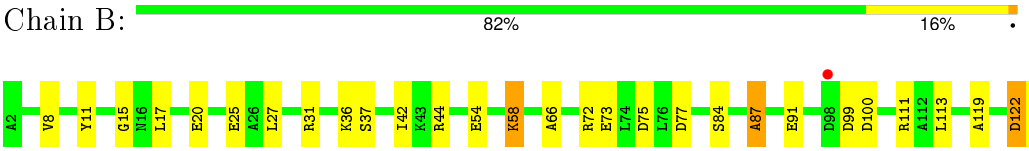
Chain D:





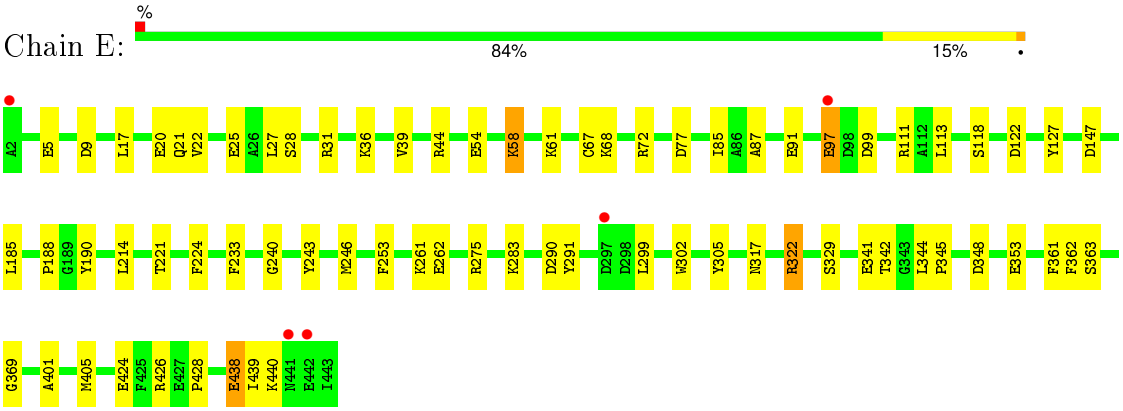
- Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain B:



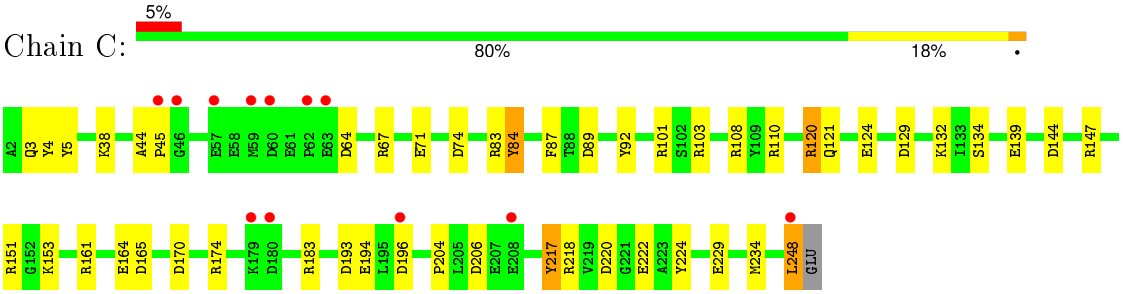
• Molecule 2: Methyl-coenzyme M reductase I subunit beta

Chain E:



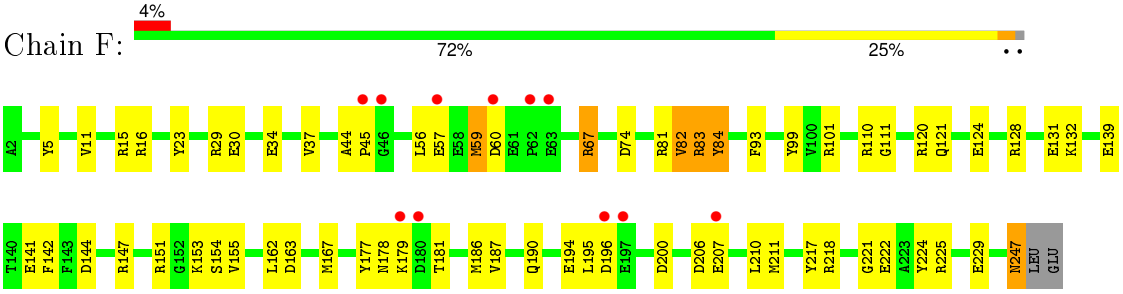
• Molecule 3: Methyl-coenzyme M reductase I subunit gamma

Chain C:



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

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	82.02Å 118.26Å 122.39Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	20.28 – 1.35 19.89 – 1.35	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.28-1.35) 92.4 (19.89-1.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.55 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.140 , 0.157 0.139 , 0.155	Depositor DCC
R_{free} test set	23829 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	10.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 51.7	EDS
Estimated twinning fraction	0.002 for -h,l,k 0.006 for -h,-l,-k 0.013 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 474725 reflections	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	22665	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: ZN, PEG, SHT, SMC, ACT, MG, F43, MGN, TP7, AGM, EDO, 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	1.58	28/4528 (0.6%)	1.45	44/6146 (0.7%)
1	D	1.62	29/4483 (0.6%)	1.52	55/6084 (0.9%)
2	B	1.58	27/3578 (0.8%)	1.49	37/4839 (0.8%)
2	E	1.65	28/3590 (0.8%)	1.41	25/4852 (0.5%)
3	C	1.80	20/2117 (0.9%)	1.63	29/2851 (1.0%)
3	F	1.84	31/2186 (1.4%)	1.68	40/2940 (1.4%)
All	All	1.65	163/20482 (0.8%)	1.51	230/27712 (0.8%)

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	1	0
1	D	1	0
3	C	0	2
All	All	2	2

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	124	GLU	CG-CD	9.37	1.66	1.51
1	A	352	GLU	CD-OE2	9.14	1.35	1.25
3	F	139	GLU	CD-OE2	8.46	1.34	1.25
2	E	341	GLU	CD-OE2	8.21	1.34	1.25
1	D	386	GLU	CD-OE1	7.83	1.34	1.25
3	C	124	GLU	CD-OE2	-7.75	1.17	1.25
3	F	124	GLU	CG-CD	7.65	1.63	1.51
2	B	54	GLU	CD-OE1	-7.20	1.17	1.25
2	B	278	GLU	CD-OE2	7.18	1.33	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	194	GLU	CD-OE2	7.00	1.33	1.25
2	E	243	TYR	CD2-CE2	6.77	1.49	1.39
1	D	19	GLU	CD-OE1	6.74	1.33	1.25
1	A	450	ASP	CA-CB	-6.65	1.39	1.53
2	B	353	GLU	CD-OE1	-6.48	1.18	1.25
2	B	426	ARG	CZ-NH2	6.47	1.41	1.33
1	A	171	GLU	CD-OE1	6.46	1.32	1.25
1	D	259	GLU	CG-CD	6.45	1.61	1.51
2	E	58	LYS	CB-CG	-6.44	1.35	1.52
1	A	123	GLU	CD-OE2	6.42	1.32	1.25
1	A	297	TYR	CB-CG	-6.42	1.42	1.51
2	E	58	LYS	CD-CE	6.41	1.67	1.51
2	E	118	SER	CA-CB	6.40	1.62	1.52
3	F	225	ARG	CZ-NH1	-6.35	1.24	1.33
3	F	218	ARG	CZ-NH1	6.30	1.41	1.33
1	D	355[A]	GLU	CB-CG	-6.29	1.40	1.52
1	D	355[B]	GLU	CB-CG	-6.29	1.40	1.52
2	E	341	GLU	CD-OE1	-6.22	1.18	1.25
3	F	30	GLU	CD-OE2	6.20	1.32	1.25
1	A	238	ALA	C-O	6.18	1.35	1.23
2	E	85	ILE	N-CA	6.17	1.58	1.46
3	C	139	GLU	CD-OE2	6.15	1.32	1.25
1	D	126	PRO	CA-C	-6.12	1.40	1.52
2	B	367	TYR	CG-CD1	6.10	1.47	1.39
3	F	155	VAL	CB-CG2	6.09	1.65	1.52
1	A	123	GLU	CG-CD	6.08	1.61	1.51
2	E	22	VAL	CB-CG2	6.06	1.65	1.52
2	B	278	GLU	CD-OE1	6.05	1.32	1.25
3	C	134	SER	CB-OG	5.96	1.50	1.42
2	E	353	GLU	CG-CD	5.93	1.60	1.51
2	B	322	ARG	CZ-NH1	5.92	1.40	1.33
2	B	8	VAL	CA-CB	5.92	1.67	1.54
3	F	229	GLU	CD-OE2	5.92	1.32	1.25
2	E	253	PHE	CD1-CE1	5.91	1.51	1.39
3	F	221	GLY	C-O	5.86	1.33	1.23
1	A	236	ILE	C-O	5.85	1.34	1.23
1	D	383	GLU	CB-CG	-5.85	1.41	1.52
3	C	3	GLN	CB-CG	-5.82	1.36	1.52
2	E	21	GLN	CG-CD	5.81	1.64	1.51
2	E	233[A]	PHE	CD1-CE1	5.79	1.50	1.39
2	E	233[B]	PHE	CD1-CE1	5.79	1.50	1.39
1	A	444	TYR	CE2-CZ	-5.78	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	239	TYR	CG-CD1	5.76	1.46	1.39
1	A	464	GLU	CD-OE2	-5.76	1.19	1.25
3	C	229	GLU	CD-OE1	-5.76	1.19	1.25
1	D	450	ASP	CA-CB	-5.74	1.41	1.53
3	F	139	GLU	CD-OE1	-5.74	1.19	1.25
2	E	25	GLU	CD-OE2	5.73	1.31	1.25
2	B	440	LYS	CE-NZ	5.71	1.63	1.49
3	C	218	ARG	CZ-NH1	5.70	1.40	1.33
1	D	385	TYR	CD1-CE1	5.67	1.47	1.39
2	B	87	ALA	CA-CB	5.66	1.64	1.52
2	B	186	GLU	CD-OE1	-5.66	1.19	1.25
3	C	92	TYR	CE1-CZ	5.65	1.45	1.38
2	E	302	TRP	CG-CD1	5.65	1.44	1.36
1	A	134	GLU	CD-OE1	5.65	1.31	1.25
2	E	353	GLU	CD-OE1	-5.64	1.19	1.25
1	D	72	TYR	CG-CD2	5.63	1.46	1.39
3	C	4	TYR	CE2-CZ	-5.63	1.31	1.38
3	F	142	PHE	CE2-CZ	5.62	1.48	1.37
2	B	240	GLY	N-CA	5.62	1.54	1.46
1	A	269	VAL	CA-CB	5.61	1.66	1.54
2	B	291	TYR	CD1-CE1	5.60	1.47	1.39
3	F	141	GLU	CD-OE2	-5.58	1.19	1.25
3	F	210	LEU	N-CA	5.57	1.57	1.46
1	D	373	VAL	CB-CG2	5.56	1.64	1.52
3	F	84	TYR	CD2-CE2	-5.56	1.31	1.39
3	C	153	LYS	CE-NZ	5.56	1.62	1.49
1	D	469	GLU	CD-OE1	-5.54	1.19	1.25
3	F	224	TYR	CE1-CZ	5.54	1.45	1.38
1	D	63	PRO	CA-CB	5.54	1.64	1.53
2	E	329	SER	CB-OG	5.54	1.49	1.42
3	C	71	GLU	CB-CG	5.53	1.62	1.52
3	F	93	PHE	CD2-CE2	5.53	1.50	1.39
3	C	183	ARG	CZ-NH1	5.52	1.40	1.33
2	E	28	SER	CB-OG	5.50	1.49	1.42
1	D	446	TYR	CD1-CE1	5.47	1.47	1.39
1	D	543	ARG	CG-CD	-5.46	1.38	1.51
1	D	127	GLU	N-CA	-5.46	1.35	1.46
2	B	11	TYR	CE2-CZ	-5.46	1.31	1.38
1	D	39	GLU	CD-OE2	-5.46	1.19	1.25
3	C	87	PHE	CE2-CZ	5.45	1.47	1.37
3	C	120	ARG	CZ-NH1	5.44	1.40	1.33
1	A	388	TYR	CG-CD1	5.43	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	190	TYR	CG-CD1	5.43	1.46	1.39
1	A	25	PHE	CG-CD2	5.42	1.46	1.38
1	A	487	GLU	CD-OE2	5.42	1.31	1.25
3	C	204	PRO	N-CA	5.41	1.56	1.47
2	B	302	TRP	CG-CD1	5.41	1.44	1.36
1	A	36	ARG	CG-CD	5.39	1.65	1.51
1	A	503	PHE	CG-CD1	5.39	1.46	1.38
2	E	54	GLU	CD-OE1	-5.39	1.19	1.25
3	F	11	VAL	CB-CG1	5.39	1.64	1.52
1	A	119	ARG	CB-CG	-5.38	1.38	1.52
2	E	240	GLY	N-CA	5.38	1.54	1.46
3	F	23	TYR	CG-CD2	5.38	1.46	1.39
3	F	177	TYR	CZ-OH	5.37	1.47	1.37
1	A	444	TYR	CZ-OH	5.36	1.47	1.37
1	A	292	SER	CB-OG	5.36	1.49	1.42
3	C	38	LYS	CE-NZ	5.35	1.62	1.49
3	C	222	GLU	CD-OE2	5.34	1.31	1.25
2	B	433	VAL	CB-CG1	5.32	1.64	1.52
1	D	80	TYR	CD1-CE1	5.32	1.47	1.39
1	D	244	GLY	C-O	5.32	1.32	1.23
1	D	201	GLY	N-CA	5.32	1.54	1.46
2	B	25	GLU	CD-OE1	-5.32	1.19	1.25
3	C	164	GLU	CG-CD	5.32	1.59	1.51
1	D	20	GLU	CG-CD	5.30	1.59	1.51
1	A	387	GLU	CD-OE1	5.30	1.31	1.25
3	C	193	ASP	CB-CG	5.29	1.62	1.51
2	B	428	PRO	CA-CB	5.29	1.64	1.53
1	D	543	ARG	CB-CG	5.28	1.66	1.52
2	E	302	TRP	CD2-CE2	5.28	1.47	1.41
2	E	54	GLU	CB-CG	5.25	1.62	1.52
3	F	217	TYR	CG-CD1	5.25	1.46	1.39
2	B	73	GLU	CD-OE2	5.25	1.31	1.25
3	F	190	GLN	N-CA	5.25	1.56	1.46
3	C	174	ARG	NE-CZ	5.24	1.39	1.33
2	B	427	GLU	CG-CD	5.23	1.59	1.51
3	F	154	SER	CB-OG	5.22	1.49	1.42
1	A	536	GLU	CB-CG	5.21	1.62	1.52
2	E	87	ALA	CA-CB	5.21	1.63	1.52
3	F	99	TYR	CD1-CE1	5.20	1.47	1.39
3	F	84	TYR	CG-CD1	5.19	1.46	1.39
1	D	148	GLU	CD-OE2	5.19	1.31	1.25
2	E	5	GLU	CB-CG	5.19	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	TRP	CG-CD1	5.17	1.44	1.36
1	D	428	TYR	CG-CD1	5.16	1.45	1.39
1	A	297	TYR	CG-CD2	5.15	1.45	1.39
1	A	80	TYR	CD1-CE1	5.15	1.47	1.39
1	A	385	TYR	CE2-CZ	-5.13	1.31	1.38
1	D	354	VAL	CA-CB	5.13	1.65	1.54
1	D	352	GLU	CG-CD	5.12	1.59	1.51
3	F	82	VAL	CB-CG1	5.12	1.63	1.52
2	B	84	SER	CB-OG	-5.11	1.35	1.42
1	D	528	GLU	CD-OE1	5.11	1.31	1.25
2	B	58	LYS	CB-CG	-5.10	1.38	1.52
2	B	284	VAL	C-O	5.09	1.33	1.23
2	E	401	ALA	C-O	5.09	1.33	1.23
2	E	97	GLU	CD-OE1	5.09	1.31	1.25
2	E	363	SER	CB-OG	5.08	1.48	1.42
3	F	229	GLU	CB-CG	5.08	1.61	1.52
2	B	417	GLU	CG-CD	-5.06	1.44	1.51
1	D	353	TYR	CE2-CZ	5.06	1.45	1.38
3	F	37	VAL	CB-CG2	-5.04	1.42	1.52
3	F	222	GLU	CB-CG	5.04	1.61	1.52
2	B	146	PHE	CE1-CZ	5.03	1.47	1.37
3	F	101	ARG	NE-CZ	5.03	1.39	1.33
1	A	124	VAL	CB-CG2	5.03	1.63	1.52
2	B	36	LYS	CE-NZ	5.03	1.61	1.49
1	D	380	TYR	CE2-CZ	5.02	1.45	1.38
2	B	417	GLU	CD-OE2	5.01	1.31	1.25
3	F	34	GLU	CG-CD	5.01	1.59	1.51
3	F	187	VAL	CB-CG1	5.01	1.63	1.52

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	147	ARG	NE-CZ-NH1	16.68	128.64	120.30
2	B	44	ARG	NE-CZ-NH1	15.62	128.11	120.30
3	F	147	ARG	NE-CZ-NH1	14.07	127.33	120.30
1	D	499	ARG	NE-CZ-NH2	-13.57	113.52	120.30
2	B	44	ARG	NE-CZ-NH2	-12.99	113.80	120.30
3	F	206	ASP	CB-CG-OD1	12.62	129.66	118.30
3	F	144	ASP	CB-CG-OD2	10.59	127.83	118.30
2	B	31	ARG	NE-CZ-NH1	10.02	125.31	120.30
2	E	44	ARG	NE-CZ-NH1	9.58	125.09	120.30
2	E	44	ARG	NE-CZ-NH2	-9.54	115.53	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	101	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	D	440	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	B	72	ARG	NE-CZ-NH2	-9.20	115.70	120.30
2	E	353	GLU	OE1-CD-OE2	9.15	134.28	123.30
1	A	103	ARG	NE-CZ-NH2	-8.87	115.87	120.30
3	F	225	ARG	NE-CZ-NH2	-8.79	115.91	120.30
2	B	31	ARG	NE-CZ-NH2	-8.74	115.93	120.30
2	B	336	ASP	CB-CG-OD2	-8.69	110.48	118.30
3	C	144	ASP	CB-CG-OD2	8.54	125.99	118.30
2	E	111	ARG	NE-CZ-NH1	8.39	124.50	120.30
3	F	144	ASP	CB-CG-OD1	-8.23	110.89	118.30
3	C	83	ARG	NE-CZ-NH2	-8.20	116.20	120.30
3	F	196	ASP	CB-CG-OD1	8.11	125.60	118.30
3	C	147	ARG	NE-CZ-NH2	-8.02	116.29	120.30
3	F	218	ARG	NE-CZ-NH2	7.86	124.23	120.30
3	C	124	GLU	OE1-CD-OE2	7.66	132.49	123.30
3	C	161	ARG	NE-CZ-NH1	7.65	124.12	120.30
2	B	423	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	A	543	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	D	40	PHE	CB-CG-CD2	-7.46	115.58	120.80
1	A	521	ASP	CB-CG-OD1	7.41	124.97	118.30
1	D	444	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	D	368	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	D	385	TYR	CD1-CE1-CZ	-7.32	113.21	119.80
1	D	216	ARG	NE-CZ-NH1	7.32	123.96	120.30
3	C	161	ARG	NE-CZ-NH2	-7.30	116.65	120.30
3	F	59	MET	CG-SD-CE	-7.18	88.71	100.20
1	D	522	PHE	CB-CG-CD1	-7.18	115.78	120.80
3	F	15	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	A	209	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	450	ASP	CB-CA-C	7.00	124.39	110.40
1	D	344	ASP	CB-CG-OD1	-6.92	112.07	118.30
2	E	275	ARG	NE-CZ-NH2	-6.92	116.84	120.30
3	F	177	TYR	O-C-N	6.92	133.76	122.70
1	D	440	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	B	77	ASP	CB-CG-OD2	-6.87	112.12	118.30
3	F	147	ARG	NE-CZ-NH2	-6.87	116.86	120.30
2	E	426	ARG	NE-CZ-NH1	6.85	123.73	120.30
3	C	84	TYR	CB-CG-CD2	-6.85	116.89	121.00
3	C	144	ASP	CB-CG-OD1	-6.84	112.15	118.30
3	F	5	TYR	CB-CG-CD1	-6.83	116.90	121.00
1	A	209	ARG	NE-CZ-NH1	6.75	123.68	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	386	GLU	OE1-CD-OE2	-6.64	115.33	123.30
1	A	368	ASP	CB-CG-OD2	-6.53	112.42	118.30
2	E	147	ASP	CB-CG-OD1	6.52	124.17	118.30
2	E	322[A]	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	E	322[B]	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	B	193	ARG	NE-CZ-NH1	6.50	123.55	120.30
2	B	163	ARG	NE-CZ-NH2	-6.46	117.07	120.30
3	C	224	TYR	CB-CG-CD1	6.45	124.87	121.00
1	D	368	ASP	CB-CG-OD1	6.44	124.10	118.30
1	D	535	ARG	NE-CZ-NH1	-6.42	117.09	120.30
3	F	229	GLU	OE1-CD-OE2	-6.38	115.64	123.30
3	F	29	ARG	NE-CZ-NH1	6.36	123.48	120.30
3	F	128	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	D	346	PHE	CB-CG-CD2	-6.32	116.38	120.80
2	B	426	ARG	NE-CZ-NH1	6.31	123.45	120.30
3	F	222	GLU	OE1-CD-OE2	-6.29	115.75	123.30
3	C	151	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	E	122	ASP	CB-CG-OD1	6.25	123.92	118.30
1	D	202	ASP	CB-CG-OD1	6.23	123.91	118.30
2	B	152	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	529	PHE	CB-CG-CD2	-6.19	116.47	120.80
1	A	415	PHE	CB-CG-CD2	-6.18	116.47	120.80
1	D	294	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	D	67	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	E	185	LEU	CB-CG-CD1	6.15	121.45	111.00
3	F	16	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	501	ASP	CB-CG-OD1	6.13	123.81	118.30
3	F	101	ARG	NE-CZ-NH2	-6.13	117.24	120.30
2	E	348	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	40	PHE	CB-CG-CD2	-6.05	116.56	120.80
1	D	499	ARG	NH1-CZ-NH2	6.04	126.05	119.40
1	D	59	ASP	CB-CG-OD1	6.00	123.70	118.30
3	F	163	ASP	CB-CG-OD1	6.00	123.70	118.30
1	D	84	ASP	CB-CG-OD2	6.00	123.70	118.30
1	D	385	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	D	346	PHE	CB-CG-CD1	5.96	124.97	120.80
3	C	108	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	E	31	ARG	NE-CZ-NH1	5.94	123.27	120.30
3	F	110	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	A	447	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	294	ARG	NE-CZ-NH1	-5.92	117.34	120.30
2	E	9	ASP	CB-CG-OD2	-5.91	112.98	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	388	TYR	CB-CG-CD1	-5.90	117.46	121.00
1	A	225	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	270	ARG	NE-CZ-NH1	5.87	123.23	120.30
3	C	217	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	20	GLU	OE1-CD-OE2	5.85	130.32	123.30
3	C	165	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	D	209	ARG	NE-CZ-NH1	5.84	123.22	120.30
3	F	131	GLU	OE1-CD-OE2	5.82	130.29	123.30
2	B	127	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	D	450	ASP	CB-CA-C	5.80	121.99	110.40
3	C	174	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	E	72	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	D	372	ASP	CB-CG-OD2	5.79	123.51	118.30
2	B	336	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	401	ARG	NE-CZ-NH2	5.76	123.18	120.30
2	E	243	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	A	250	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	80	TYR	CD1-CE1-CZ	-5.73	114.64	119.80
1	D	388	TYR	CD1-CE1-CZ	-5.71	114.66	119.80
1	A	471	ARG	NE-CZ-NH2	-5.71	117.45	120.30
3	F	83	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	D	478	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	D	180	PHE	CA-C-N	5.68	129.70	117.20
2	E	77	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	458	PHE	CB-CG-CD2	-5.67	116.83	120.80
2	B	400	ASP	CB-CG-OD1	-5.66	113.21	118.30
3	C	196	ASP	CB-CG-OD1	5.66	123.39	118.30
3	F	74	ASP	CB-CG-OD2	-5.63	113.23	118.30
2	E	291	TYR	CD1-CE1-CZ	-5.62	114.75	119.80
1	D	478	TYR	CB-CG-CD1	5.59	124.36	121.00
1	D	444	TYR	CB-CG-CD1	5.59	124.35	121.00
3	F	120	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	219	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	345	ASP	CB-CG-OD1	-5.57	113.28	118.30
2	B	152	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	119	ARG	NE-CZ-NH2	-5.55	117.52	120.30
3	F	224	TYR	CZ-CE2-CD2	5.55	124.79	119.80
3	C	120	ARG	NE-CZ-NH1	5.55	123.07	120.30
3	C	103	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	67	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	505	PHE	CB-CG-CD2	-5.53	116.93	120.80
3	F	167	MET	O-C-N	5.51	131.52	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	253	TYR	CZ-CE2-CD2	-5.51	114.84	119.80
2	E	290	ASP	CB-CG-OD1	-5.50	113.35	118.30
2	B	305	TYR	CG-CD2-CE2	-5.50	116.90	121.30
2	E	361	PHE	CB-CG-CD2	-5.49	116.96	120.80
3	C	87	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	D	396	PHE	CZ-CE2-CD2	-5.49	113.52	120.10
3	C	129	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	238	ALA	CA-C-N	5.43	129.15	117.20
2	B	185	LEU	CB-CG-CD1	5.42	120.21	111.00
1	D	428	TYR	CB-CG-CD2	5.41	124.25	121.00
1	A	436	GLU	OE1-CD-OE2	-5.41	116.81	123.30
1	A	450	ASP	N-CA-CB	5.40	120.33	110.60
1	D	148	GLU	OE1-CD-OE2	-5.40	116.82	123.30
3	C	89	ASP	CB-CG-OD1	5.39	123.16	118.30
1	D	528	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	D	450	ASP	N-CA-CB	5.38	120.29	110.60
2	E	224	PHE	CB-CG-CD2	-5.38	117.03	120.80
3	F	16	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	B	99	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	10	LEU	O-C-N	5.37	131.29	122.70
3	C	217	TYR	CB-CG-CD2	5.36	124.21	121.00
2	B	75	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	A	478	TYR	CZ-CE2-CD2	-5.35	114.98	119.80
1	A	183	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	219	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	250	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	A	67	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	302	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	E	99	ASP	CB-CG-OD1	5.32	123.08	118.30
3	C	220	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	4	LYS	CA-CB-CG	5.31	125.08	113.40
3	F	162	LEU	CB-CG-CD2	5.30	120.02	111.00
3	F	110	ARG	CD-NE-CZ	5.30	131.02	123.60
3	F	81	ARG	NE-CZ-NH2	5.30	122.95	120.30
3	F	217	TYR	CB-CG-CD2	5.30	124.18	121.00
1	D	428	TYR	CB-CG-CD1	-5.29	117.83	121.00
2	B	333	TYR	CG-CD2-CE2	-5.29	117.07	121.30
2	B	291	TYR	CD1-CE1-CZ	-5.27	115.06	119.80
2	B	279	ASP	CB-CG-OD1	5.26	123.04	118.30
3	F	151	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	B	100	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	D	444	TYR	CD1-CE1-CZ	-5.24	115.09	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	478	TYR	CD1-CE1-CZ	-5.24	115.09	119.80
1	D	177	ASP	CB-CG-OD1	5.23	123.00	118.30
3	C	170	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	225	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	B	429	LEU	CB-CG-CD2	-5.20	102.16	111.00
3	C	110	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	12[A]	LYS	CD-CE-NZ	5.20	123.65	111.70
1	A	12[B]	LYS	CD-CE-NZ	5.20	123.65	111.70
2	B	224	PHE	CB-CG-CD2	-5.20	117.16	120.80
2	B	305	TYR	CD1-CE1-CZ	-5.19	115.13	119.80
1	A	333	TYR	CZ-CE2-CD2	-5.17	115.14	119.80
3	F	29	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	177[A]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	177[B]	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	353	TYR	CZ-CE2-CD2	-5.16	115.15	119.80
3	F	151	ARG	CG-CD-NE	-5.16	100.96	111.80
1	A	348	TYR	CB-CG-CD2	-5.16	117.90	121.00
3	F	56	LEU	CB-CG-CD1	-5.15	102.24	111.00
2	E	58	LYS	CD-CE-NZ	5.15	123.54	111.70
1	D	349	PHE	O-C-N	-5.13	114.48	123.20
1	A	3	ASP	CB-CG-OD2	-5.13	113.69	118.30
3	F	141	GLU	CG-CD-OE1	-5.12	108.06	118.30
2	B	111	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	466	LEU	CB-CG-CD2	5.12	119.70	111.00
2	B	423	ASP	CB-CG-OD1	5.11	122.89	118.30
3	C	206	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	394	ASP	CB-CG-OD1	5.10	122.89	118.30
2	B	233[A]	PHE	CD1-CE1-CZ	-5.09	113.99	120.10
2	B	233[B]	PHE	CD1-CE1-CZ	-5.09	113.99	120.10
2	B	290	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	D	188	PHE	CB-CG-CD2	-5.09	117.24	120.80
3	F	195	LEU	CB-CG-CD1	-5.08	102.36	111.00
2	B	15	GLY	O-C-N	5.08	130.84	122.70
3	F	141	GLU	OE1-CD-OE2	5.08	129.40	123.30
2	E	127	TYR	CZ-CE2-CD2	-5.08	115.23	119.80
1	A	356	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	A	535	ARG	NE-CZ-NH1	-5.07	117.77	120.30
2	B	291	TYR	CB-CG-CD1	-5.07	117.96	121.00
3	C	5	TYR	CZ-CE2-CD2	-5.06	115.24	119.80
1	D	183	ASP	CB-CG-OD1	5.06	122.85	118.30
2	B	353	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	D	266	TYR	CD1-CE1-CZ	-5.05	115.25	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	74	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	345	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	A	238	ALA	CA-C-O	-5.02	109.56	120.10
2	E	305	TYR	CD1-CE1-CZ	-5.02	115.28	119.80
3	C	74	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	333	TYR	CG-CD2-CE2	5.01	125.31	121.30
3	F	30	GLU	CG-CD-OE1	5.01	128.31	118.30
2	B	122[A]	ASP	CB-CG-OD1	5.00	122.81	118.30
2	B	122[B]	ASP	CB-CG-OD1	5.00	122.81	118.30
1	D	183	ASP	CB-CG-OD2	-5.00	113.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	450	ASP	CA
1	D	450	ASP	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	120	ARG	Sidechain
3	C	217	TYR	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	4431	0	4224	47	0
1	D	4380	0	4219	29	0
2	B	3462	0	3517	40	0
2	E	3471	0	3532	33	0
3	C	2056	0	2000	23	0
3	F	2113	0	2065	21	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	21	0	19	0	0
5	D	21	0	19	0	0
6	A	62	0	43	2	0
6	D	62	0	43	1	0
7	A	7	0	4	0	0
7	D	7	0	5	1	0
8	A	28	0	21	0	0
8	D	28	0	21	1	0
9	A	4	0	3	0	0
10	A	4	0	6	0	0
10	B	4	0	6	0	0
10	D	4	0	6	1	0
10	F	8	0	12	0	0
11	A	1	0	0	0	0
12	C	7	0	10	0	0
13	A	522	0	0	12	0
13	B	477	0	0	14	0
13	C	262	0	0	4	0
13	D	539	0	0	8	0
13	E	421	0	0	11	0
13	F	254	0	0	10	0
All	All	22665	0	19775	172	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.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:207[B]:GLU:HG3	13:F:3759:HOH:O	1.39	1.23
2:E:91[B]:GLU:HG2	13:E:3974:HOH:O	1.64	0.97
1:D:545[A]:LEU:HD12	13:D:2591:HOH:O	1.66	0.93
1:A:433:LEU:HD23	3:C:234[B]:MET:SD	2.08	0.93
1:A:433:LEU:CD2	3:C:234[B]:MET:SD	2.60	0.88
1:A:429:LEU:HD12	3:C:234[B]:MET:HE3	1.55	0.88
1:D:36[A]:ARG:HD3	1:D:85:ASP:OD1	1.76	0.86
2:E:438[A]:GLU:OE1	2:E:439:ILE:HG23	1.77	0.83
2:B:196[B]:MET:CE	13:B:3731:HOH:O	2.25	0.83
1:D:545[A]:LEU:CD1	13:D:2591:HOH:O	2.23	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67[B]:ARG:HG3	3:C:67[B]:ARG:HH11	1.44	0.81
3:C:67[B]:ARG:CG	3:C:67[B]:ARG:HH11	1.95	0.80
3:F:67[A]:ARG:HH11	3:F:67[A]:ARG:HG2	1.48	0.79
13:A:3768:HOH:O	1:D:545[A]:LEU:HD11	1.82	0.79
1:A:24[A]:THR:HG23	13:A:3803:HOH:O	1.84	0.77
2:B:196[B]:MET:CE	13:B:574:HOH:O	2.31	0.77
2:E:27:LEU:HD22	2:E:246[B]:MET:CE	2.16	0.75
1:A:429:LEU:HD12	3:C:234[B]:MET:CE	2.17	0.75
1:A:24[A]:THR:CG2	13:A:3803:HOH:O	2.35	0.73
2:E:261[A]:LYS:HG2	13:F:3664:HOH:O	1.88	0.73
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.70	0.73
2:B:196[B]:MET:HE3	13:B:574:HOH:O	1.88	0.72
2:B:27:LEU:HD22	2:B:246[B]:MET:CE	2.21	0.70
1:A:178[A]:PRO:HD3	13:A:1631:HOH:O	1.94	0.67
2:E:17:LEU:HD21	2:E:20[A]:GLU:HG3	1.77	0.67
2:B:299:LEU:HD23	2:B:349[A]:PHE:CE1	2.30	0.65
2:B:196[B]:MET:SD	13:B:3731:HOH:O	2.54	0.64
1:D:194[B]:GLU:HG2	13:D:3701:HOH:O	1.97	0.64
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	2.28	0.64
2:E:322[A]:ARG:CZ	3:F:67[A]:ARG:HD2	2.27	0.63
13:B:2205:HOH:O	2:E:188:PRO:HD3	1.98	0.63
1:D:268:PRO:HB3	13:E:1668:HOH:O	1.99	0.62
2:B:27:LEU:HD22	2:B:246[B]:MET:HE1	1.80	0.62
3:C:67[B]:ARG:NH1	3:C:67[B]:ARG:HB2	2.15	0.61
2:E:322[A]:ARG:NH1	3:F:67[A]:ARG:HD2	2.15	0.61
2:E:61[B]:LYS:CE	13:E:2444:HOH:O	2.49	0.61
1:A:429:LEU:CD1	3:C:234[B]:MET:CE	2.79	0.60
2:E:342:THR:OG1	2:E:344[B]:LEU:HB2	2.02	0.60
2:E:261[B]:LYS:O	2:E:261[B]:LYS:HD2	2.01	0.60
2:E:261[B]:LYS:HG3	2:E:262:GLU:HG3	1.82	0.60
1:A:241[B]:GLN:HA	13:F:4106:HOH:O	2.01	0.59
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.43	0.59
1:A:241[A]:GLN:HA	13:F:4106:HOH:O	2.02	0.59
1:A:114:ALA:O	1:A:118:LYS:HD3	2.02	0.59
2:B:196[B]:MET:HE1	13:B:3731:HOH:O	1.92	0.58
1:A:432:TYR:HB2	3:C:234[B]:MET:HE3	1.85	0.58
1:A:60:ILE:HD12	13:D:3878:HOH:O	2.04	0.58
1:A:169[A]:ASN:ND2	1:A:172:ILE:HD12	2.18	0.57
2:E:27:LEU:CD2	2:E:246[B]:MET:CE	2.82	0.57
3:C:67[B]:ARG:NH1	3:C:67[B]:ARG:CB	2.68	0.57
3:F:83:ARG:NH2	13:F:4106:HOH:O	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:CB	2.18	0.56
1:D:114:ALA:O	1:D:118:LYS:HD3	2.06	0.56
2:B:261[A]:LYS:HG3	13:B:4130:HOH:O	2.06	0.56
3:F:57:GLU:HG2	13:F:939:HOH:O	2.06	0.56
1:A:241[B]:GLN:HB3	1:A:242:ALA:O	2.06	0.56
1:D:169[A]:ASN:CG	1:D:172:ILE:HG12	2.25	0.56
3:F:132[A]:LYS:HD2	13:F:1990:HOH:O	2.05	0.56
2:B:257:LYS:NZ	13:B:3430:HOH:O	2.38	0.55
1:D:360:LEU:O	1:D:361[A]:CYS:HB2	2.07	0.55
2:E:299:LEU:HD22	13:E:2973:HOH:O	2.07	0.55
2:B:27:LEU:CD2	2:B:246[B]:MET:HE1	2.38	0.54
1:A:360:LEU:O	1:A:361[B]:CYS:HB2	2.06	0.54
3:F:44:ALA:HB1	3:F:45:PRO:HD2	1.90	0.54
2:B:322:ARG:NH1	3:C:67[A]:ARG:HD3	2.23	0.54
3:C:194[B]:GLU:HG3	13:C:1318:HOH:O	2.08	0.54
2:B:119:ALA:HA	2:B:122[B]:ASP:OD2	2.06	0.53
1:A:17[A]:SER:OG	1:A:20:GLU:HG3	2.09	0.53
1:A:545:LEU:HD11	13:D:1948[B]:HOH:O	2.08	0.53
1:D:169[A]:ASN:OD1	1:D:172:ILE:HG12	2.09	0.53
1:A:383[A]:GLU:HG3	13:A:2606:HOH:O	2.09	0.53
1:A:4[A]:LYS:NZ	13:A:2253:HOH:O	2.42	0.52
2:B:58:LYS:HE2	13:B:3633:HOH:O	2.09	0.52
2:B:299:LEU:HD23	2:B:349[A]:PHE:HE1	1.71	0.52
2:B:233[B]:PHE:CE1	3:C:248:LEU:HG	2.44	0.52
1:A:174[A]:ASP:HB2	13:A:1937:HOH:O	2.10	0.51
1:A:194[B]:GLU:HG2	13:A:2095:HOH:O	2.11	0.50
1:A:328:VAL:HB	6:D:552:F43:H9A1	1.92	0.50
1:A:433:LEU:HD21	3:C:234[B]:MET:SD	2.48	0.50
3:F:67[A]:ARG:HH11	3:F:67[A]:ARG:CG	2.20	0.50
1:A:24[B]:THR:HG23	13:A:677:HOH:O	2.11	0.50
1:A:268:PRO:HG3	13:A:4030:HOH:O	2.11	0.50
2:E:344[A]:LEU:HB3	2:E:345:PRO:HD2	1.93	0.49
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.47	0.49
2:B:199:HIS:CE1	2:B:415[B]:ILE:HD12	2.47	0.49
3:F:200[A]:ASP:HB2	13:F:1920:HOH:O	2.11	0.49
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.47	0.49
1:A:169[A]:ASN:ND2	1:A:172:ILE:CD1	2.76	0.49
2:E:424[B]:GLU:HG3	13:E:3642:HOH:O	2.12	0.49
1:A:432:TYR:HB2	3:C:234[B]:MET:CE	2.43	0.49
1:A:126:PRO:HB2	1:A:175[A]:GLU:HG2	1.94	0.49
3:F:178[B]:ASN:HB3	3:F:181[B]:THR:OG1	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:GLU:HB2	1:D:118:LYS:HD2	1.95	0.48
2:B:261[A]:LYS:HE3	13:B:4130:HOH:O	2.14	0.48
2:B:188:PRO:HD3	13:E:1304:HOH:O	2.12	0.48
2:B:299:LEU:HD23	2:B:349[A]:PHE:CZ	2.48	0.48
3:F:67[A]:ARG:NH1	3:F:67[A]:ARG:HG2	2.25	0.47
1:D:236:ILE:HA	1:D:241[A]:GLN:HB2	1.96	0.47
1:D:154:HIS:CE1	1:D:545[A]:LEU:HD21	2.49	0.47
2:B:246[A]:MET:CE	2:B:429:LEU:HD12	2.45	0.47
2:E:299:LEU:CD2	13:E:2973:HOH:O	2.62	0.47
1:D:169[A]:ASN:CG	1:D:172:ILE:CG1	2.83	0.47
2:B:113[A]:LEU:HD13	2:B:418:VAL:HG13	1.97	0.46
2:E:61[B]:LYS:HE2	13:E:2444:HOH:O	2.14	0.46
3:F:153[A]:LYS:NZ	13:F:1186:HOH:O	2.27	0.46
1:A:332:GLN:HA	1:A:335:THR:OG1	2.15	0.46
2:E:317:ASN:O	3:F:111:GLY:HA2	2.16	0.46
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:HB2	1.75	0.46
1:D:480:MET:O	8:D:555[B]:SHT:HK61	2.16	0.46
1:D:332:GLN:HA	1:D:335:THR:OG1	2.16	0.46
3:C:64[B]:ASP:HB2	13:C:3620:HOH:O	2.15	0.45
2:E:39:VAL:HG21	2:E:221:THR:HG21	1.98	0.45
3:F:67[A]:ARG:NH1	3:F:67[A]:ARG:CG	2.80	0.45
2:B:196[B]:MET:CE	13:B:1152:HOH:O	2.64	0.45
1:D:36[A]:ARG:HG2	1:D:84:ASP:HB2	1.98	0.45
2:B:37:SER:OG	2:B:424[B]:GLU:OE1	2.21	0.45
1:A:115:VAL:HG22	2:E:405[A]:MET:HG3	1.99	0.45
1:A:12[A]:LYS:HE2	1:A:80:TYR:CZ	2.52	0.45
1:A:177[B]:ASP:C	1:A:179:ALA:N	2.69	0.44
3:C:44:ALA:HB1	3:C:45:PRO:HD2	1.98	0.44
1:A:178[A]:PRO:HD2	13:A:1652:HOH:O	2.18	0.44
3:F:82:VAL:O	3:F:83:ARG:HD2	2.16	0.44
3:C:132:LYS:HE3	13:C:4098:HOH:O	2.18	0.44
2:B:87:ALA:O	2:B:91[B]:GLU:HG3	2.17	0.44
1:D:545[A]:LEU:HD11	13:D:2591:HOH:O	2.07	0.44
2:E:113[B]:LEU:HD23	2:E:113[B]:LEU:C	2.39	0.43
2:B:299:LEU:HD21	13:C:1043:HOH:O	2.17	0.43
1:A:60:ILE:CD1	13:D:3878:HOH:O	2.65	0.43
1:A:169[A]:ASN:HD22	1:A:172:ILE:HD12	1.82	0.43
2:B:42[A]:ILE:HG13	2:B:425:PHE:CE1	2.54	0.43
6:A:1:F43:H9A1	1:D:328:VAL:HB	2.01	0.43
3:C:67[B]:ARG:CG	3:C:67[B]:ARG:NH1	2.64	0.43
2:B:27:LEU:CD2	2:B:246[B]:MET:CE	2.92	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LEU:HD12	1:D:273:ARG:HB2	2.01	0.42
1:A:429:LEU:CD1	3:C:234[B]:MET:HE1	2.48	0.42
1:A:12[A]:LYS:HE2	1:A:80:TYR:CE1	2.54	0.42
2:B:17:LEU:HD21	2:B:20[A]:GLU:HG3	2.01	0.42
3:F:207[B]:GLU:CG	13:F:3759:HOH:O	2.24	0.42
2:E:61[B]:LYS:HE2	2:E:68[B]:LYS:HE3	2.01	0.42
2:B:424[A]:GLU:HG3	13:B:3930:HOH:O	2.19	0.42
2:E:20[B]:GLU:HG2	13:E:768:HOH:O	2.19	0.42
2:E:61[B]:LYS:HE3	13:E:2370:HOH:O	2.20	0.42
1:A:505:PHE:CE1	2:E:67:CYS:HB3	2.54	0.42
2:B:246[B]:MET:HB3	2:B:246[B]:MET:HE3	1.66	0.42
1:A:279:GLY:HA2	1:A:473:PRO:HB2	2.01	0.42
1:D:241[A]:GLN:HB3	1:D:242:ALA:O	2.20	0.42
2:E:61[A]:LYS:HB3	2:E:61[A]:LYS:HE3	1.95	0.42
2:E:214:LEU:HB2	2:E:428:PRO:HG3	2.02	0.42
1:A:12[A]:LYS:HG2	1:A:80:TYR:CD2	2.55	0.42
1:D:45[A]:LYS:HE2	1:D:45[A]:LYS:HB3	1.78	0.42
1:D:348:TYR:CZ	10:D:556:EDO:H11	2.55	0.41
1:A:172:ILE:HD12	13:A:3660:HOH:O	2.20	0.41
1:A:126:PRO:CB	1:A:175[A]:GLU:HG2	2.51	0.41
2:B:123[B]:VAL:HG12	2:E:36:LYS:HA	2.01	0.41
1:D:25:PHE:O	1:D:27:THR:HG23	2.21	0.41
2:B:405[A]:MET:HG3	1:D:115:VAL:HG22	2.02	0.41
3:F:59:MET:O	3:F:60:ASP:C	2.57	0.41
2:B:362:PHE:O	2:B:369:GLY:HA3	2.20	0.41
2:B:119:ALA:O	2:B:122[B]:ASP:HB2	2.21	0.41
1:A:445:GL3:HA2	2:B:357:VAL:HG12	2.02	0.41
2:B:122[B]:ASP:HB2	13:B:1261:HOH:O	2.20	0.41
3:F:247:ASN:HD22	3:F:247:ASN:C	2.24	0.41
1:A:453:GLY:O	1:A:457:VAL:HG23	2.21	0.41
6:A:1:F43:C1C	7:D:554[A]:COM:H12	2.51	0.40
2:B:183:GLN:HG2	13:E:1668:HOH:O	2.19	0.40
1:D:355[B]:GLU:HG2	13:D:1824:HOH:O	2.21	0.40
1:D:428:TYR:HD1	1:D:450:ASP:HB3	1.86	0.40
2:B:261[A]:LYS:CE	13:B:4130:HOH:O	2.70	0.40
2:B:66:ALA:O	1:D:507:PRO:HD2	2.22	0.40
2:E:362:PHE:O	2:E:369:GLY:HA3	2.21	0.40

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	569/549 (104%)	555 (98%)	14 (2%)	0	100	100
1	D	563/549 (103%)	544 (97%)	18 (3%)	1 (0%)	52	22
2	B	465/442 (105%)	457 (98%)	8 (2%)	0	100	100
2	E	466/442 (105%)	457 (98%)	9 (2%)	0	100	100
3	C	255/248 (103%)	247 (97%)	8 (3%)	0	100	100
3	F	264/248 (106%)	258 (98%)	6 (2%)	0	100	100
All	All	2582/2478 (104%)	2518 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	461/434 (106%)	455 (99%)	6 (1%)	76	45
1	D	455/434 (105%)	450 (99%)	5 (1%)	80	53
2	B	366/341 (107%)	365 (100%)	1 (0%)	94	83
2	E	367/341 (108%)	361 (98%)	6 (2%)	70	36
3	C	225/216 (104%)	223 (99%)	2 (1%)	84	61
3	F	233/216 (108%)	226 (97%)	7 (3%)	48	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2107/1982 (106%)	2080 (99%)	27 (1%)	80 45

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12[A]	LYS
1	A	12[B]	LYS
1	A	118	LYS
1	A	444	TYR
1	A	450	ASP
1	A	543	ARG
2	B	283	LYS
3	C	121	GLN
3	C	248	LEU
1	D	36[A]	ARG
1	D	36[B]	ARG
1	D	186	LYS
1	D	444	TYR
1	D	450	ASP
2	E	58	LYS
2	E	97	GLU
2	E	283	LYS
2	E	438[A]	GLU
2	E	438[B]	GLU
2	E	440	LYS
3	F	67[A]	ARG
3	F	67[B]	ARG
3	F	121	GLN
3	F	179[A]	LYS
3	F	179[B]	LYS
3	F	186	MET
3	F	247	ASN

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

Mol	Chain	Res	Type
3	C	121	GLN
3	F	121	GLN
3	F	247	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	1.84	2 (25%)	7,14,16	3.85	3 (42%)
1	AGM	A	271	1	7,11,12	0.76	0	5,13,15	1.95	1 (20%)
1	MGN	A	400	1	6,9,10	1.25	1 (16%)	6,12,14	0.75	0
1	GL3	A	445	1	3,3,4	2.22	1 (33%)	2,2,4	1.08	0
1	SMC	A	452	1	5,6,7	1.07	0	2,6,8	1.24	0
1	MHS	D	257	1	8,11,12	1.43	1 (12%)	7,14,16	4.05	3 (42%)
1	AGM	D	271	1	7,11,12	0.90	0	5,13,15	1.86	2 (40%)
1	MGN	D	400	1	6,9,10	1.86	2 (33%)	6,12,14	0.88	0
1	GL3	D	445	1	3,3,4	2.19	1 (33%)	2,2,4	0.89	0
1	SMC	D	452	1	5,6,7	1.20	0	2,6,8	1.73	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GL3	D	445	1	-	0/1/1/2	0/0/0/0
1	SMC	D	452	1	-	0/3/5/7	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	GL3	C-S	-3.79	1.67	1.80
1	A	445	GL3	C-S	-3.48	1.68	1.80
1	D	400	MGN	CB1-CA	-3.22	1.51	1.55
1	A	257	MHS	CG-ND1	-2.24	1.33	1.38
1	D	400	MGN	O-C	2.39	1.27	1.20
1	A	400	MGN	CB1-CA	2.61	1.57	1.55
1	D	257	MHS	CE1-NE2	3.33	1.41	1.34
1	A	257	MHS	CE1-NE2	3.78	1.41	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	257	MHS	NE2-CE1-ND1	-8.61	100.64	112.28
1	A	257	MHS	NE2-CE1-ND1	-8.60	100.65	112.28
1	D	257	MHS	O-C-CA	-3.97	115.15	125.49
1	A	257	MHS	O-C-CA	-3.80	115.58	125.49
1	A	271	AGM	CE2-CD-NE1	-3.45	105.50	112.05
1	D	271	AGM	CE2-CD-NE1	-2.73	106.88	112.05
1	D	452	SMC	O-C-CA	-2.10	120.02	125.49
1	D	271	AGM	CE2-CD-CG	2.45	115.20	111.24
1	A	257	MHS	CD2-NE2-CE1	3.06	110.53	105.71
1	D	257	MHS	CD2-NE2-CE1	4.22	112.36	105.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	F43	A	1	1,8,7	42,71,71	3.05	10 (23%)	35,118,118	2.15	7 (20%)
5	TP7	A	553[A]	-	16,20,20	0.89	0	16,26,26	2.08	6 (37%)
7	COM	A	554[A]	6	5,6,6	0.96	0	5,8,8	2.50	1 (20%)
8	SHT	A	555[B]	6	22,27,27	1.89	2 (9%)	24,36,36	2.20	7 (29%)
9	ACT	A	556[B]	4	1,3,3	1.13	0	0,3,3	0.00	-
10	EDO	A	557	-	3,3,3	0.59	0	2,2,2	0.38	0
10	EDO	B	445	-	3,3,3	0.74	0	2,2,2	0.24	0
12	PEG	C	1	-	6,6,6	0.55	0	5,5,5	1.14	1 (20%)
6	F43	D	552	1,8,7	42,71,71	3.20	16 (38%)	35,118,118	2.15	7 (20%)
5	TP7	D	553[A]	-	16,20,20	1.01	1 (6%)	16,26,26	1.55	3 (18%)
7	COM	D	554[A]	6	5,6,6	1.70	1 (20%)	5,8,8	1.10	0
8	SHT	D	555[B]	6	22,27,27	2.00	2 (9%)	24,36,36	2.14	6 (25%)
10	EDO	D	556	-	3,3,3	0.36	0	2,2,2	0.42	0
10	EDO	F	1	-	3,3,3	0.58	0	2,2,2	0.58	0
10	EDO	F	251	-	3,3,3	0.68	0	2,2,2	0.46	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
6	F43	A	1	1,8,7	1/1/25/27	0/18/165/165	0/0/10/10
5	TP7	A	553[A]	-	1/1/5/6	0/20/24/24	0/0/0/0
7	COM	A	554[A]	6	-	0/4/4/4	0/0/0/0
8	SHT	A	555[B]	6	-	0/27/31/31	0/0/0/0
9	ACT	A	556[B]	4	-	0/0/0/0	0/0/0/0
10	EDO	A	557	-	-	0/1/1/1	0/0/0/0
10	EDO	B	445	-	-	0/1/1/1	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PEG	C	1	-	-	0/4/4/4	0/0/0/0
6	F43	D	552	1,8,7	1/1/25/27	0/18/165/165	0/0/10/10
5	TP7	D	553[A]	-	1/1/5/6	0/20/24/24	0/0/0/0
7	COM	D	554[A]	6	-	0/4/4/4	0/0/0/0
8	SHT	D	555[B]	6	-	0/27/31/31	0/0/0/0
10	EDO	D	556	-	-	0/1/1/1	0/0/0/0
10	EDO	F	1	-	-	0/1/1/1	0/0/0/0
10	EDO	F	251	-	-	0/1/1/1	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1	F43	C4B-NB	-12.23	1.30	1.49
6	D	552	F43	C4B-NB	-11.29	1.32	1.49
6	D	552	F43	C1D-ND	-5.28	1.26	1.36
6	D	552	F43	C6D-C7D	-3.81	1.45	1.50
6	D	552	F43	C1B-NB	-3.06	1.45	1.49
6	D	552	F43	C3C-C2C	-2.88	1.47	1.54
6	D	552	F43	C6B-N5B	-2.12	1.31	1.34
6	A	1	F43	C5C-C2C	-2.12	1.50	1.54
6	A	1	F43	C4A-NA	2.13	1.53	1.49
6	D	552	F43	C5C-C2C	2.17	1.57	1.54
6	D	552	F43	CAB-C3B	2.18	1.58	1.53
5	D	553[A]	TP7	C7-S7	2.18	1.88	1.80
8	A	555[B]	SHT	CG2-CB	2.22	1.57	1.51
6	A	1	F43	CHB-C4A	2.23	1.56	1.52
6	D	552	F43	NI-ND	2.32	2.07	1.92
6	A	1	F43	O8D-C7D	2.40	1.28	1.23
6	D	552	F43	C8C-C3C	2.64	1.59	1.54
6	D	552	F43	NI-NC	2.80	2.02	1.90
7	D	554[A]	COM	O3S-S2	2.85	1.53	1.46
6	D	552	F43	O8D-C7D	3.11	1.30	1.23
6	A	1	F43	C1D-C2D	3.11	1.49	1.40
6	A	1	F43	NI-NC	3.16	2.04	1.90
6	D	552	F43	C1C-NC	3.26	1.44	1.37
8	D	555[B]	SHT	OS3-SG2	3.78	1.57	1.45
6	A	1	F43	C5D-C2D	4.33	1.58	1.51
6	D	552	F43	C1D-C2D	4.34	1.52	1.40
6	A	1	F43	C3D-C2D	4.91	1.50	1.39
6	D	552	F43	C3D-C2D	6.76	1.54	1.39
8	A	555[B]	SHT	CK1-CK2	7.43	1.52	1.31
8	D	555[B]	SHT	CK1-CK2	7.73	1.53	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	552	F43	C4D-C3D	9.80	1.50	1.37
6	A	1	F43	C4D-C3D	11.11	1.52	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1	F43	C9D-C3D-C4D	-9.12	111.64	127.01
6	D	552	F43	C9D-C3D-C4D	-8.81	112.18	127.01
8	D	555[B]	SHT	CK3-CK2-CK1	-7.67	110.95	126.16
8	A	555[B]	SHT	CK3-CK2-CK1	-5.40	115.46	126.16
7	A	554[A]	COM	O1S-S2-C2	-5.24	102.43	106.91
5	A	553[A]	TP7	C-CA-N	-4.42	104.64	113.51
6	D	552	F43	C3C-C4C-CHD	-3.94	117.66	124.26
6	D	552	F43	O8D-C7D-CHD	-3.90	118.10	122.56
6	A	1	F43	C4A-NA-C1A	-3.31	104.89	108.21
6	D	552	F43	C5C-C2C-C1C	-3.05	105.71	113.63
5	A	553[A]	TP7	O4P-P-O1P	-2.83	100.04	107.11
8	A	555[B]	SHT	OS2-SG2-OS1	-2.83	105.03	111.61
5	D	553[A]	TP7	C-CA-N	-2.78	107.93	113.51
8	D	555[B]	SHT	OS1-SG2-OS3	-2.72	103.55	113.48
6	D	552	F43	O7B-C6B-N5B	-2.68	120.54	124.71
5	D	553[A]	TP7	O4P-P-O1P	-2.62	100.55	107.11
8	A	555[B]	SHT	OS1-SG2-CD	-2.54	104.74	106.91
6	A	1	F43	O8D-C7D-C6D	-2.43	116.34	120.76
8	A	555[B]	SHT	C-CA-N	-2.32	108.86	113.51
6	D	552	F43	C6D-C5D-C2D	-2.21	107.21	112.46
8	D	555[B]	SHT	CA-N-CK	-2.18	118.51	122.12
8	D	555[B]	SHT	OS2-SG2-OS1	-2.16	106.58	111.61
6	A	1	F43	C9B-C2B-C8B	-2.13	104.37	110.17
8	D	555[B]	SHT	O3'-P-O1P	-2.10	101.86	107.11
5	A	553[A]	TP7	O1-C1-N	-2.04	119.55	123.01
6	A	1	F43	C6D-C5D-C2D	-2.01	107.70	112.46
8	A	555[B]	SHT	O8P-P-O2P	2.03	115.12	107.38
12	C	1	PEG	C3-O2-C2	2.16	122.60	113.31
8	A	555[B]	SHT	CK1-CK-N	2.23	119.02	114.12
6	D	552	F43	C8B-C2B-C1B	2.25	106.26	102.05
5	A	553[A]	TP7	CA-N-C1	2.49	126.76	121.79
6	A	1	F43	C3B-C4B-NB	2.96	115.27	106.03
5	A	553[A]	TP7	C2-C1-N	3.01	120.75	115.83
8	D	555[B]	SHT	OS2-SG2-OS3	3.42	119.56	111.61
5	D	553[A]	TP7	CB-CA-N	3.69	118.81	111.69
6	A	1	F43	C9B-C2B-C3B	4.00	119.70	111.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	553[A]	TP7	CB-CA-N	4.14	119.68	111.69
8	A	555[B]	SHT	OS3-SG2-CD	6.78	112.69	106.91

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	1	F43	C4B
6	D	552	F43	C4B
5	A	553[A]	TP7	C1
5	D	553[A]	TP7	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1	F43	2	0
6	D	552	F43	1	0
7	D	554[A]	COM	1	0
8	D	555[B]	SHT	1	0
10	D	556	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%)	-0.47	1 (0%)	95	94	6, 10, 21, 33	0
1	D	543/549 (98%)	-0.46	5 (0%)	85	86	6, 10, 20, 37	0
2	B	442/442 (100%)	-0.47	1 (0%)	95	94	7, 12, 21, 35	0
2	E	442/442 (100%)	-0.40	5 (1%)	82	83	7, 12, 23, 40	0
3	C	247/248 (99%)	-0.23	12 (4%)	33	33	9, 14, 32, 47	0
3	F	246/248 (99%)	-0.16	11 (4%)	37	37	8, 14, 30, 53	0
All	All	2463/2478 (99%)	-0.40	35 (1%)	78	78	6, 12, 23, 53	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	ASP	6.9
3	C	60	ASP	5.0
3	F	45	PRO	4.8
2	E	441	ASN	4.6
1	D	549	ALA	4.4
3	C	45	PRO	4.3
3	C	180	ASP	4.1
3	F	57	GLU	3.9
3	F	180[A]	ASP	3.6
2	B	98	ASP	3.4
3	C	62	PRO	3.3
2	E	2	ALA	3.1
1	A	2	ALA	2.9
3	F	63	GLU	2.9
3	C	208	GLU	2.8
3	C	46	GLY	2.8
3	F	46	GLY	2.7
2	E	97	GLU	2.6
3	C	63	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	297[A]	ASP	2.6
1	D	118	LYS	2.6
3	C	57	GLU	2.5
2	E	442	GLU	2.5
3	C	59	MET	2.5
1	D	2	ALA	2.5
3	C	179	LYS	2.4
3	F	62	PRO	2.4
3	C	248	LEU	2.3
3	F	196	ASP	2.3
1	D	24	THR	2.2
3	F	197	GLU	2.2
3	F	179[A]	LYS	2.1
1	D	15	GLU	2.1
3	F	207[A]	GLU	2.1
3	C	196	ASP	2.0

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, 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	MHS	A	257	11/12	0.97	0.05	-	8,10,14,17	0
1	AGM	A	271	12/13	0.98	0.05	-	6,6,7,8	0
1	SMC	A	452	7/8	0.99	0.05	-	7,7,9,10	0
1	MGN	D	400	10/11	0.98	0.05	-	6,8,8,8	0
1	GL3	A	445	4/5	0.99	0.06	-	6,7,7,8	0
1	GL3	D	445	4/5	0.99	0.06	-	6,6,7,7	0
1	MGN	A	400	10/11	0.98	0.05	-	7,8,9,10	0
1	MHS	D	257	11/12	0.98	0.05	-	9,10,12,16	0
1	SMC	D	452	7/8	0.99	0.05	-	7,8,9,11	0
1	AGM	D	271	12/13	0.97	0.07	-	6,7,7,8	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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	F	1	4/4	0.87	0.11	14.76	38,39,39,39	0
4	MG	C	250	1/1	0.98	0.10	4.86	17,17,17,17	0
4	MG	F	250	1/1	0.98	0.08	1.08	16,16,16,16	0
5	TP7	A	553[A]	21/21	0.98	0.06	0.42	5,7,7,8	21
7	COM	D	554[A]	7/7	0.98	0.06	0.27	6,9,10,10	7
8	SHT	A	555[B]	28/28	0.98	0.06	0.21	6,7,12,14	28
10	EDO	B	445	4/4	0.81	0.08	0.20	42,42,43,46	0
6	F43	A	1	62/62	0.99	0.05	-0.27	6,8,11,13	0
5	TP7	D	553[A]	21/21	0.99	0.05	-0.32	4,6,8,8	21
8	SHT	D	555[B]	28/28	0.99	0.05	-0.48	6,7,11,13	28
6	F43	D	552	62/62	0.99	0.05	-0.95	6,8,11,12	0
9	ACT	A	556[B]	4/4	0.98	0.06	-1.07	15,16,17,19	4
7	COM	A	554[A]	7/7	0.99	0.04	-1.72	8,9,12,12	7
11	ZN	A	558	1/1	1.00	0.03	-3.64	10,10,10,10	1
4	MG	E	444	1/1	0.98	0.20	-	22,22,22,22	0
4	MG	A	552[B]	1/1	0.99	0.17	-	14,14,14,14	1
4	MG	D	551	1/1	0.99	0.17	-	18,18,18,18	0
10	EDO	D	556	4/4	0.88	0.10	-	32,38,40,44	0
10	EDO	F	251	4/4	0.81	0.16	-	39,42,43,48	0
4	MG	B	1[B]	1/1	0.97	0.18	-	21,21,21,21	1
10	EDO	A	557	4/4	0.85	0.08	-	30,35,39,42	0
4	MG	A	551[A]	1/1	0.98	0.22	-	18,18,18,18	1
4	MG	B	444	1/1	0.97	0.15	-	23,23,23,23	0
4	MG	D	1	1/1	0.98	0.13	-	20,20,20,20	0
12	PEG	C	1	7/7	0.86	0.13	-	34,38,42,42	0

6.5 Other polymers

There are no such residues in this entry.