Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:49 PM GMT

PDB ID	:	1HBM
Title	:	METHYL-COENZYME M REDUCTASE ENZYME PRODUCT COMPLEX
Authors	:	Ermler, U.; Grabarse, W.
Deposited on	:	2001-04-20
Resolution	:	1.80 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 (i) symbol.

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

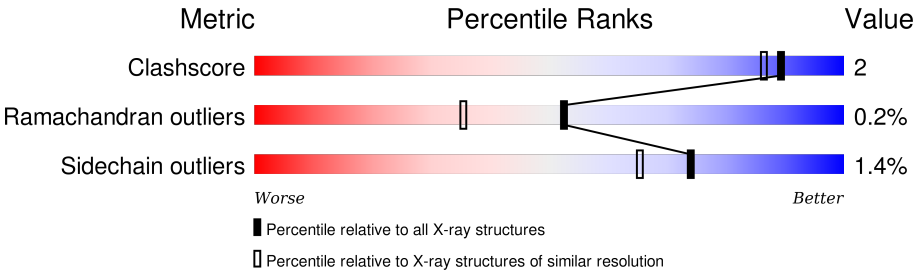
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	549	90% 9% •
1	D	549	92% 7% •
2	B	442	90% 9%
2	E	442	91% 7% •
3	C	248	91% 7% •
3	F	248	90% 7% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	F43	A	1550	X	-	-	-
4	F43	D	1550	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21641 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	23	13	0
			4291	2712	723	836	20			
1	D	548	Total	C	N	O	S	23	16	0
			4296	2717	721	838	20			

There are 10 discrepancies between the modelled and reference sequences:

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

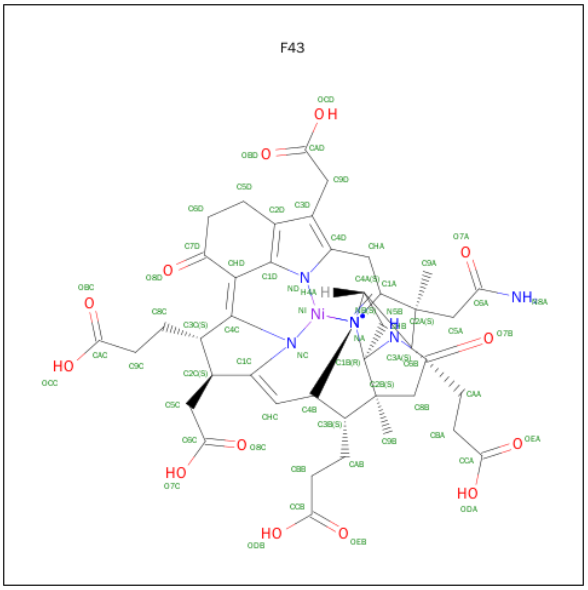
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	26	15	0
			3347	2115	557	653	22			
2	E	442	Total	C	N	O	S	41	12	0
			3339	2115	551	652	21			

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

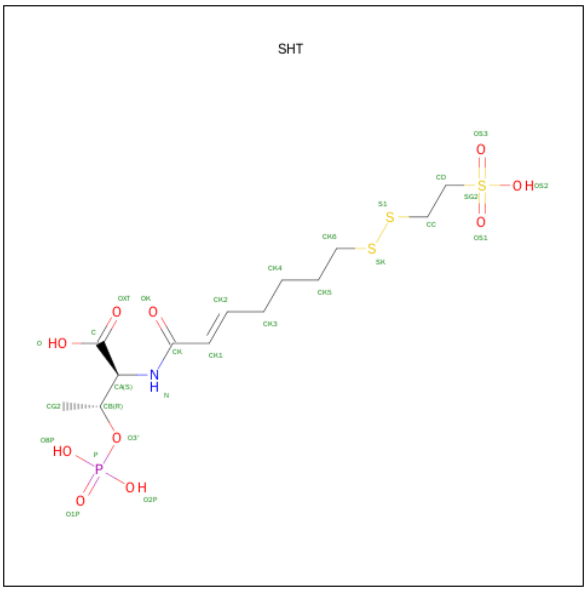
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	39	5	0
			2007	1242	355	398	12			
3	F	247	Total	C	N	O	S	44	5	0
			2006	1242	354	398	12			

- Molecule 4 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{49}N_6NiO_{13}$).



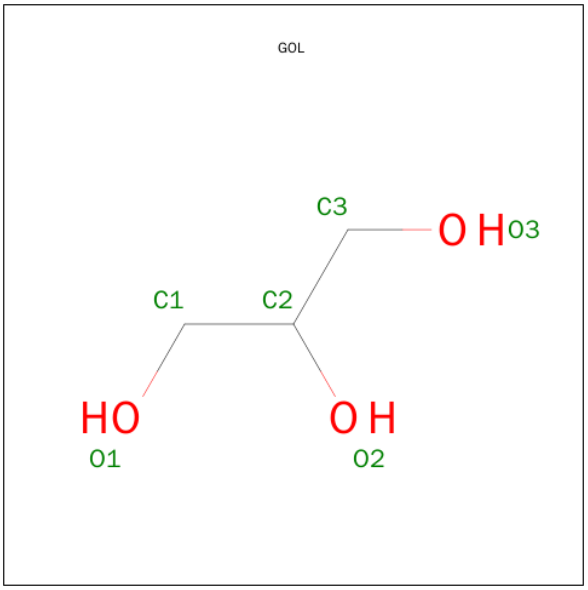
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
4	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 5 is 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
5	A	1	Total	C	N	O	P	S	0	0
			28	13	1	10	1	3		
5	D	1	Total	C	N	O	P	S	0	0
			28	13	1	10	1	3		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			6	3	3			
6	A	1	Total	C	O		0	0
			6	3	3			

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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	4	Total Mg 4 4	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	427	Total O 427 427	0	0
11	B	369	Total O 369 369	0	1
11	C	257	Total O 257 257	0	0
11	D	438	Total O 438 438	0	1
11	E	353	Total O 353 353	0	0
11	F	248	Total O 248 248	0	1

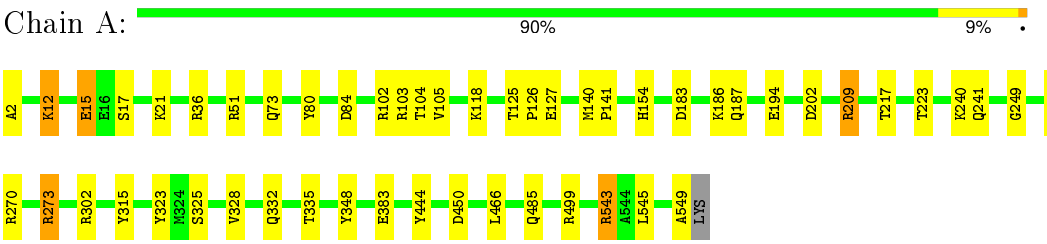
3 Residue-property plots (i)

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.

Note EDS was not executed.

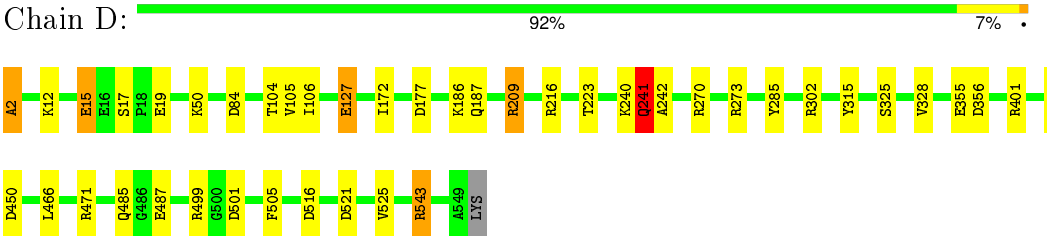
• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT

Chain A:



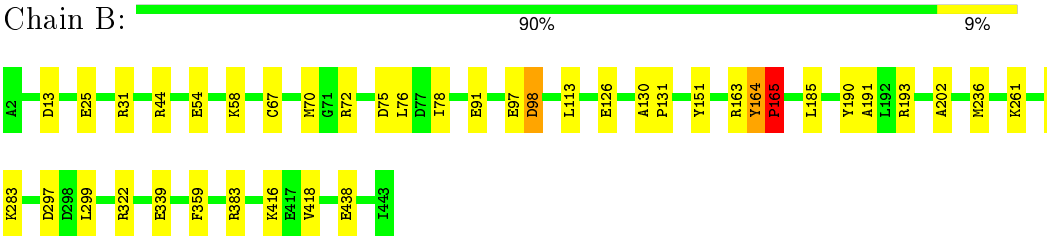
• Molecule 1: METHYL-COENZYME M REDUCTASE I ALPHA SUBUNIT

Chain D:



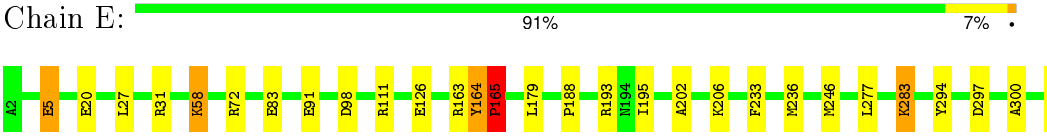
• Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain B:



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

Chain E:



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

Chain C:

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

Chain F:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.00Å 118.30Å 122.80Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	91.8 (10.00-1.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.164 , 0.193	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21641	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, SHT, CL, NA, AGM, F43, MGN, MG, 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	0.77	5/4411 (0.1%)	1.13	23/5986 (0.4%)
1	D	1.12	6/4432 (0.1%)	1.20	30/6015 (0.5%)
2	B	0.82	5/3492 (0.1%)	1.30	31/4724 (0.7%)
2	E	1.54	8/3458 (0.2%)	1.28	26/4682 (0.6%)
3	C	1.16	8/2072 (0.4%)	1.29	19/2790 (0.7%)
3	F	0.82	9/2070 (0.4%)	1.37	14/2789 (0.5%)
All	All	1.07	41/19935 (0.2%)	1.25	143/26986 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	3
2	B	0	2
2	E	0	2
3	C	0	1
All	All	0	9

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	438	GLU	CG-CD	53.14	2.31	1.51
1	D	355	GLU	CG-CD	45.45	2.20	1.51
2	E	91[A]	GLU	CG-CD	38.62	2.09	1.51
2	E	91[B]	GLU	CG-CD	38.62	2.09	1.51
2	E	83	GLU	CG-CD	30.66	1.98	1.51
1	D	240	LYS	CE-NZ	-29.87	0.74	1.49
2	B	438	GLU	CG-CD	-27.40	1.10	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	127	GLU	CG-CD	-25.84	1.13	1.51
3	C	164	GLU	CG-CD	23.72	1.87	1.51
1	A	240	LYS	CE-NZ	-19.99	0.99	1.49
3	C	212	GLU	CG-CD	-19.92	1.22	1.51
1	A	15	GLU	CB-CG	19.67	1.89	1.52
3	C	197	GLU	CG-CD	-17.40	1.25	1.51
3	F	208	GLU	CB-CG	-15.43	1.22	1.52
3	C	179	LYS	CD-CE	15.41	1.89	1.51
3	C	63	GLU	CB-CG	-15.28	1.23	1.52
1	D	50	LYS	CD-CE	14.21	1.86	1.51
3	C	57	GLU	CB-CG	14.02	1.78	1.52
2	E	5	GLU	CG-CD	-13.87	1.31	1.51
2	E	58	LYS	CG-CD	13.25	1.97	1.52
1	A	12	LYS	CG-CD	-12.89	1.08	1.52
2	B	261	LYS	CG-CD	-11.22	1.14	1.52
3	F	196	ASP	CB-CG	-10.95	1.28	1.51
2	B	98	ASP	CB-CG	-10.75	1.29	1.51
2	B	97	GLU	CB-CG	-10.58	1.32	1.52
2	B	91	GLU	CG-CD	-10.37	1.36	1.51
3	F	164	GLU	CG-CD	10.18	1.67	1.51
1	A	127	GLU	CG-CD	9.31	1.66	1.51
2	E	297	ASP	CB-CG	-9.25	1.32	1.51
3	C	24	GLU	CB-CG	9.17	1.69	1.52
3	F	212	GLU	CB-CG	-8.82	1.35	1.52
1	D	15	GLU	CB-CG	-8.43	1.36	1.52
3	C	208	GLU	CB-CG	-8.39	1.36	1.52
3	F	63	GLU	CB-CG	-8.37	1.36	1.52
2	E	20	GLU	CB-CG	-7.96	1.37	1.52
1	A	21	LYS	CD-CE	7.77	1.70	1.51
3	F	57	GLU	CG-CD	-6.86	1.41	1.51
3	F	10	LYS	CG-CD	-6.63	1.29	1.52
3	F	132	LYS	CG-CD	6.52	1.74	1.52
1	D	186	LYS	CD-CE	6.27	1.67	1.51
3	F	164	GLU	CB-CG	-5.65	1.41	1.52

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	196	ASP	CB-CG-OD2	29.36	144.72	118.30
2	B	98	ASP	CB-CG-OD2	27.17	142.76	118.30
3	F	196	ASP	CB-CG-OD1	-25.80	95.08	118.30
2	B	98	ASP	CB-CG-OD1	-25.10	95.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	60	ASP	CB-CG-OD1	-22.84	97.74	118.30
2	E	91[A]	GLU	CG-CD-OE2	-22.52	73.26	118.30
2	E	91[B]	GLU	CG-CD-OE2	-22.52	73.26	118.30
2	B	98	ASP	CA-CB-CG	-18.23	73.29	113.40
2	E	438	GLU	CB-CG-CD	-13.93	76.59	114.20
1	D	127	GLU	CB-CG-CD	13.45	150.52	114.20
1	A	12	LYS	CB-CG-CD	11.94	142.63	111.60
2	B	97	GLU	CB-CG-CD	-11.63	82.79	114.20
2	E	91[A]	GLU	CB-CG-CD	-11.56	82.99	114.20
2	E	91[B]	GLU	CB-CG-CD	-11.56	82.99	114.20
1	D	127	GLU	CG-CD-OE2	-10.75	96.81	118.30
3	F	60	ASP	CB-CG-OD2	10.56	127.80	118.30
2	E	91[A]	GLU	CG-CD-OE1	10.44	139.18	118.30
2	E	91[B]	GLU	CG-CD-OE1	10.44	139.18	118.30
2	E	297	ASP	CB-CG-OD1	-10.39	108.95	118.30
3	C	126	ARG	NE-CZ-NH1	-10.01	115.30	120.30
3	F	60	ASP	CB-CG-OD1	-10.00	109.30	118.30
2	E	72	ARG	NE-CZ-NH2	9.95	125.27	120.30
1	D	2	ALA	CB-CA-C	-9.74	95.50	110.10
2	B	322	ARG	NE-CZ-NH2	9.73	125.17	120.30
1	D	401	ARG	NE-CZ-NH2	9.55	125.08	120.30
1	A	240	LYS	CD-CE-NZ	9.38	133.27	111.70
2	B	165	PRO	CA-N-CD	-9.35	98.41	111.50
2	E	83	GLU	CB-CG-CD	-9.33	89.01	114.20
1	D	355	GLU	CB-CG-CD	-9.29	89.11	114.20
1	D	270	ARG	NE-CZ-NH2	9.27	124.94	120.30
1	D	209[A]	ARG	CD-NE-CZ	9.08	136.31	123.60
1	D	209[B]	ARG	CD-NE-CZ	9.08	136.31	123.60
2	E	58	LYS	CB-CG-CD	-8.96	88.30	111.60
3	C	120	ARG	NE-CZ-NH1	8.81	124.70	120.30
2	B	165	PRO	N-CA-CB	8.79	113.85	103.30
2	E	165	PRO	N-CA-CB	8.79	113.85	103.30
1	A	127	GLU	CB-CG-CD	-8.58	91.03	114.20
3	C	164	GLU	CB-CG-CD	-8.47	91.32	114.20
2	E	165	PRO	CA-N-CD	-8.39	99.75	111.50
1	A	543	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	D	499	ARG	NE-CZ-NH1	-8.18	116.21	120.30
2	B	97	GLU	CA-CB-CG	-8.15	95.47	113.40
1	D	444	TYR	CB-CG-CD1	-8.06	116.16	121.00
3	C	220	ASP	CB-CG-OD2	8.03	125.52	118.30
2	E	163	ARG	NE-CZ-NH1	-8.02	116.29	120.30
2	E	5	GLU	CG-CD-OE2	-7.95	102.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	127	GLU	CG-CD-OE1	7.91	134.12	118.30
2	E	5	GLU	CG-CD-OE1	7.87	134.05	118.30
2	E	193	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	D	2	ALA	CA-C-O	-7.87	103.57	120.10
2	E	297	ASP	CB-CG-OD2	7.58	125.12	118.30
1	D	499	ARG	NE-CZ-NH2	7.46	124.03	120.30
2	B	275	ARG	NE-CZ-NH2	7.27	123.93	120.30
2	B	297	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	103	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	102	ARG	NE-CZ-NH2	7.09	123.84	120.30
3	C	101	ARG	NE-CZ-NH1	-7.08	116.76	120.30
3	F	61	GLU	CA-CB-CG	7.00	128.79	113.40
2	B	193	ARG	NE-CZ-NH1	-6.93	116.83	120.30
3	C	126	ARG	NE-CZ-NH2	6.86	123.73	120.30
3	C	101	ARG	NE-CZ-NH2	6.85	123.73	120.30
3	C	183	ARG	CD-NE-CZ	6.81	133.13	123.60
2	B	193	ARG	NE-CZ-NH2	6.74	123.67	120.30
3	C	179	LYS	CG-CD-CE	-6.71	91.76	111.90
2	E	283	LYS	CG-CD-CE	6.71	132.02	111.90
2	B	322	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	A	36	ARG	CD-NE-CZ	6.64	132.89	123.60
1	D	273	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	D	543	ARG	NE-CZ-NH2	6.63	123.62	120.30
3	C	57	GLU	CB-CG-CD	-6.61	96.36	114.20
1	A	543	ARG	NE-CZ-NH1	-6.59	117.01	120.30
2	B	91	GLU	CG-CD-OE2	-6.54	105.23	118.30
3	C	197	GLU	CB-CG-CD	6.52	131.81	114.20
1	D	177	ASP	CB-CG-OD2	6.49	124.14	118.30
2	B	13	ASP	CB-CG-OD2	6.48	124.13	118.30
2	B	297	ASP	CB-CG-OD2	-6.47	112.47	118.30
3	F	248	LEU	N-CA-C	-6.47	93.54	111.00
2	B	91	GLU	CB-CG-CD	-6.44	96.82	114.20
3	F	217	TYR	CA-CB-CG	6.43	125.62	113.40
3	C	120	ARG	CD-NE-CZ	6.39	132.55	123.60
1	D	241	GLN	CA-CB-CG	6.35	127.37	113.40
1	D	2	ALA	N-CA-C	6.34	128.12	111.00
1	D	444	TYR	CB-CG-CD2	6.32	124.79	121.00
1	D	216	ARG	NE-CZ-NH1	-6.32	117.14	120.30
2	B	164	TYR	CA-C-O	-6.31	106.84	120.10
2	B	163	ARG	NE-CZ-NH1	-6.27	117.17	120.30
2	B	91	GLU	CG-CD-OE1	6.21	130.71	118.30
1	A	183	ASP	CB-CG-OD1	6.17	123.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	194	GLU	CB-CG-CD	-6.08	97.78	114.20
2	B	72	ARG	NE-CZ-NH1	-6.05	117.28	120.30
3	C	105	TYR	CB-CG-CD2	6.05	124.63	121.00
1	D	302[A]	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	D	302[B]	ARG	NE-CZ-NH2	5.87	123.23	120.30
3	F	241	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	487	GLU	OE1-CD-OE2	-5.80	116.34	123.30
1	D	285	TYR	CB-CG-CD1	-5.75	117.55	121.00
2	E	297	ASP	CA-CB-CG	-5.71	100.83	113.40
1	A	12	LYS	CG-CD-CE	5.71	129.02	111.90
2	B	44	ARG	NE-CZ-NH2	5.70	123.15	120.30
3	C	164	GLU	CG-CD-OE1	-5.70	106.90	118.30
3	F	126	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	273	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	A	499	ARG	NE-CZ-NH2	5.53	123.06	120.30
3	C	60	ASP	OD1-CG-OD2	5.50	133.76	123.30
1	D	521	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	440	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	323	TYR	CB-CG-CD2	-5.48	117.71	121.00
3	C	147	ARG	NE-CZ-NH2	5.48	123.04	120.30
2	E	111	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	E	164	TYR	CA-C-O	-5.46	108.63	120.10
3	F	57	GLU	CB-CG-CD	5.45	128.90	114.20
1	A	51	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	302	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	D	209[A]	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	D	209[B]	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	549	ALA	CA-C-O	-5.37	108.82	120.10
3	F	33	ASP	CB-CG-OD2	5.36	123.12	118.30
2	B	278	GLU	CG-CD-OE2	-5.33	107.64	118.30
1	D	240	LYS	CD-CE-NZ	5.32	123.93	111.70
3	F	174	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	471	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	E	31	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	209[A]	ARG	CD-NE-CZ	5.29	131.01	123.60
1	A	209[B]	ARG	CD-NE-CZ	5.29	131.01	123.60
2	B	383	ARG	NE-CZ-NH1	-5.29	117.65	120.30
2	B	359	PHE	CB-CG-CD2	5.23	124.46	120.80
3	F	194	GLU	CB-CG-CD	5.20	128.23	114.20
1	A	118	LYS	CD-CE-NZ	5.19	123.65	111.70
2	B	278	GLU	CG-CD-OE1	5.19	128.68	118.30
2	B	322	ARG	CD-NE-CZ	5.18	130.85	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	217	TYR	CA-CB-CG	5.18	123.24	113.40
2	E	322	ARG	CD-NE-CZ	5.17	130.84	123.60
2	E	165	PRO	N-CD-CG	5.16	110.94	103.20
2	B	151	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	202	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	270	ARG	NE-CZ-NH2	5.09	122.85	120.30
3	F	61	GLU	CB-CG-CD	5.08	127.93	114.20
2	B	261	LYS	CB-CG-CD	5.06	124.76	111.60
2	E	72	ARG	CD-NE-CZ	5.05	130.67	123.60
2	B	31[A]	ARG	NE-CZ-NH1	-5.04	117.78	120.30
2	B	31[B]	ARG	NE-CZ-NH1	-5.04	117.78	120.30
3	C	164	GLU	CG-CD-OE2	5.04	128.39	118.30
1	A	84	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	GLN	Peptide
2	B	164	TYR	Mainchain,Peptide
3	C	60	ASP	Sidechain
1	D	127	GLU	Sidechain
1	D	2	ALA	Mainchain
1	D	241	GLN	Peptide
2	E	164	TYR	Mainchain,Peptide

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	4291	0	4093	19	0
1	D	4296	0	4108	17	0
2	B	3347	0	3331	25	0
2	E	3339	0	3325	22	0
3	C	2007	0	1937	9	0
3	F	2006	0	1937	8	0
4	A	62	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	62	0	43	1	0
5	A	28	0	21	0	0
5	D	28	0	21	0	0
6	A	24	0	31	5	0
6	B	6	0	8	3	0
6	C	6	0	8	0	0
6	D	24	0	31	1	0
6	E	6	0	8	2	0
7	A	4	0	0	0	0
7	B	2	0	0	0	0
7	D	3	0	0	0	0
8	B	1	0	0	0	0
8	E	1	0	0	0	0
9	C	1	0	0	0	0
9	F	4	0	0	0	0
10	D	1	0	0	0	0
11	A	427	0	0	5	0
11	B	369	0	0	4	0
11	C	257	0	0	2	0
11	D	438	0	0	4	0
11	E	353	0	0	3	0
11	F	248	0	0	0	0
All	All	21641	0	18945	91	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 2.

All (91) 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:236[C]:MET:SD	2:B:236[C]:MET:CE	2.04	1.45
2:B:185[B]:LEU:HD21	2:B:191:ALA:HA	1.62	0.80
2:E:349:PHE:HZ	3:F:248:LEU:HD21	1.57	0.70
2:E:246[A]:MET:CE	2:E:429:LEU:HD12	2.21	0.69
2:B:58[A]:LYS:HE3	2:B:75:ASP:OD1	1.94	0.68
2:B:185[B]:LEU:HD21	2:B:191:ALA:CA	2.25	0.67
2:B:113[A]:LEU:HD13	2:B:418:VAL:HG13	1.77	0.66
11:B:2201:HOH:O	2:E:188:PRO:HD3	1.96	0.66
2:B:236[A]:MET:HB2	3:C:248:LEU:CD1	2.28	0.64
2:B:25:GLU:OE1	6:B:1444:GOL:H32	1.98	0.63
2:B:236[B]:MET:HB2	3:C:248:LEU:CD1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1554:GOL:H12	11:A:2392:HOH:O	2.00	0.61
2:E:349:PHE:CZ	3:F:248:LEU:HD21	2.36	0.61
2:E:246[A]:MET:HE1	2:E:429:LEU:HD12	1.85	0.58
2:E:236[B]:MET:SD	3:F:248:LEU:HD11	2.44	0.57
2:B:185[B]:LEU:CD2	2:B:191:ALA:HA	2.32	0.57
2:B:339:GLU:HB3	3:C:237[A]:ILE:HD13	1.85	0.57
1:A:383[B]:GLU:HG3	11:A:2325:HOH:O	2.04	0.57
1:D:328:VAL:HB	4:D:1550:F43:H9A1	1.86	0.56
2:B:70[B]:MET:HE2	1:D:501:ASP:HB3	1.87	0.56
1:A:73:GLN:HB2	1:A:80:TYR:CE2	2.40	0.56
1:D:172[A]:ILE:HD13	11:D:2119:HOH:O	2.04	0.56
2:E:233[B]:PHE:HD2	2:E:236[B]:MET:HE2	1.71	0.56
2:E:246[A]:MET:HE3	2:E:429:LEU:HD12	1.86	0.56
1:D:315:TYR:HB3	1:D:485:GLN:HE21	1.70	0.55
2:B:202:ALA:HB1	2:B:416:LYS:HB2	1.88	0.55
2:E:233[B]:PHE:CD2	2:E:236[B]:MET:HE2	2.41	0.55
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.47	0.54
1:A:328:VAL:HB	4:A:1550:F43:H9A1	1.87	0.54
1:A:315:TYR:HB3	1:A:485:GLN:HE21	1.72	0.54
1:A:154:HIS:CE1	1:A:545:LEU:HD21	2.42	0.54
1:A:256:LYS:O	6:A:1552:GOL:H31	2.08	0.53
2:E:233[B]:PHE:CD2	2:E:236[B]:MET:CE	2.92	0.53
2:E:246[A]:MET:HE3	2:E:429:LEU:CD1	2.39	0.53
2:B:113[A]:LEU:HD13	2:B:418:VAL:CG1	2.40	0.52
2:E:202:ALA:HB1	2:E:416:LYS:HB2	1.92	0.52
1:D:17:SER:OG	1:D:19:GLU:OE2	2.28	0.51
1:D:105[B]:VAL:HG22	1:D:223:THR:HG22	1.94	0.49
2:E:206[A]:LYS:NZ	2:E:400:ASP:O	2.42	0.49
1:D:104:THR:HG21	1:D:209[B]:ARG:HH21	1.78	0.49
1:A:104:THR:HG21	1:A:209[B]:ARG:HH21	1.78	0.48
1:D:187:GLN:HE21	1:D:187:GLN:HA	1.79	0.48
1:A:125:THR:HB	1:A:126:PRO:HD2	1.95	0.48
1:D:356:ASP:HB3	11:D:2313:HOH:O	2.13	0.47
2:B:299:LEU:HB2	3:C:248:LEU:HD23	1.96	0.47
2:B:185[B]:LEU:HD22	2:B:190:TYR:C	2.35	0.47
1:A:348:TYR:HB3	6:A:1555:GOL:H31	1.97	0.47
2:E:336[B]:ASP:OD1	3:F:103:ARG:NE	2.42	0.46
6:B:1444:GOL:H31	11:B:2369:HOH:O	2.15	0.46
2:B:236[A]:MET:HB2	3:C:248:LEU:HD11	1.98	0.46
2:B:130:ALA:HB3	2:B:131:PRO:CD	2.46	0.45
2:B:70[B]:MET:HE2	1:D:501:ASP:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:GLU:HA	2:B:78:ILE:HD12	1.99	0.45
2:E:179[B]:LEU:CD1	2:E:195:ILE:HD11	2.46	0.45
1:A:2:ALA:HB3	11:A:2002:HOH:O	2.16	0.45
1:A:105[B]:VAL:HG13	1:A:223:THR:CG2	2.47	0.45
6:E:1444:GOL:H31	11:E:2353:HOH:O	2.15	0.45
3:C:212:GLU:HG3	11:C:2219:HOH:O	2.16	0.45
1:D:525[B]:VAL:HG13	11:D:2396:HOH:O	2.16	0.45
1:A:348:TYR:CB	6:A:1555:GOL:H31	2.47	0.45
2:E:277[B]:LEU:HD21	2:E:294:TYR:CE2	2.52	0.45
3:F:117:LEU:HD13	3:F:120:ARG:HG3	1.99	0.44
1:D:516:ASP:HA	6:D:1554:GOL:H32	2.00	0.44
3:F:117:LEU:HD22	3:F:120:ARG:HD3	1.99	0.44
1:A:466[B]:LEU:HD12	2:E:165:PRO:HD2	2.00	0.43
2:B:67:CYS:HB3	1:D:505:PHE:CE1	2.52	0.43
2:E:58:LYS:HG3	11:E:2098:HOH:O	2.18	0.43
1:A:140:MET:HB3	1:A:141:PRO:HD3	2.01	0.43
6:A:1555:GOL:H11	11:A:2008:HOH:O	2.17	0.43
2:B:130:ALA:HB3	2:B:131:PRO:HD3	2.01	0.43
2:B:236[B]:MET:HG3	3:C:248:LEU:HD11	2.00	0.42
1:A:217:THR:HG23	11:D:2140:HOH:O	2.20	0.42
2:B:58[A]:LYS:NZ	2:B:76:LEU:O	2.53	0.42
1:A:186:LYS:NZ	1:A:187:GLN:OE1	2.53	0.42
2:E:430:LYS:O	2:E:434:GLU:HG3	2.20	0.42
2:B:165:PRO:HD2	1:D:466[A]:LEU:HD22	2.02	0.41
6:E:1444:GOL:C3	11:E:2353:HOH:O	2.68	0.41
1:A:332:GLN:HA	1:A:335:THR:OG1	2.18	0.41
1:A:249:GLY:HA3	11:A:2239:HOH:O	2.19	0.41
3:C:99:TYR:CD2	3:C:116:THR:HG21	2.56	0.41
1:A:267:LEU:HD12	1:A:273:ARG:HB2	2.03	0.41
3:C:179:LYS:HG3	11:C:2185:HOH:O	2.19	0.41
2:E:424:GLU:H	2:E:424:GLU:CD	2.24	0.40
1:D:187:GLN:NE2	1:D:187:GLN:HA	2.36	0.40
3:F:211:MET:HE1	3:F:221:GLY:HA2	2.03	0.40
1:D:241:GLN:HB3	1:D:242:ALA:O	2.20	0.40
2:E:300:ALA:HB2	3:F:248:LEU:HD13	2.03	0.40
6:B:1444:GOL:C3	11:B:2369:HOH:O	2.68	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	554/549 (101%)	537 (97%)	16 (3%)	1 (0%)	52 35
1	D	557/549 (102%)	535 (96%)	21 (4%)	1 (0%)	52 35
2	B	456/442 (103%)	447 (98%)	8 (2%)	1 (0%)	52 35
2	E	452/442 (102%)	443 (98%)	8 (2%)	1 (0%)	52 35
3	C	250/248 (101%)	243 (97%)	7 (3%)	0	100 100
3	F	250/248 (101%)	245 (98%)	5 (2%)	0	100 100
All	All	2519/2478 (102%)	2450 (97%)	65 (3%)	4 (0%)	52 35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	165	PRO
2	E	165	PRO
1	A	325	SER
1	D	325	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	446/434 (103%)	440 (99%)	6 (1%)	76 68
1	D	449/434 (104%)	443 (99%)	6 (1%)	76 68
2	B	357/341 (105%)	354 (99%)	3 (1%)	86 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	353/341 (104%)	348 (99%)	5 (1%)	74 65
3	C	220/216 (102%)	218 (99%)	2 (1%)	84 80
3	F	220/216 (102%)	215 (98%)	5 (2%)	58 42
All	All	2045/1982 (103%)	2018 (99%)	27 (1%)	74 68

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

Mol	Chain	Res	Type
1	A	12	LYS
1	A	15	GLU
1	A	17	SER
1	A	444	TYR
1	A	450	ASP
1	A	543	ARG
2	B	98	ASP
2	B	126	GLU
2	B	283	LYS
3	C	196	ASP
3	C	248	LEU
1	D	12	LYS
1	D	15	GLU
1	D	84	ASP
1	D	444	TYR
1	D	450	ASP
1	D	543	ARG
2	E	5	GLU
2	E	98	ASP
2	E	126	GLU
2	E	283	LYS
2	E	438	GLU
3	F	10	LYS
3	F	61	GLU
3	F	186	MET
3	F	194	GLU
3	F	208	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	HIS

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Mol	Chain	Res	Type
1	A	485	GLN
1	D	111	HIS
1	D	187	GLN
1	D	365	ASN
1	D	485	GLN
2	E	40	GLN

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	1.79	1 (12%)	7,14,16	1.24	1 (14%)
1	AGM	A	271	1	7,11,12	0.79	0	5,13,15	1.60	1 (20%)
1	MGN	A	400	1	6,9,10	0.40	0	6,12,14	2.16	1 (16%)
1	GL3	A	445	1	3,3,4	2.31	1 (33%)	2,2,4	1.59	1 (50%)
1	SMC	A	452	1	5,6,7	0.64	0	2,6,8	0.82	0
1	MHS	D	257	1	8,11,12	1.81	1 (12%)	7,14,16	1.24	0
1	AGM	D	271	1	7,11,12	0.54	0	5,13,15	1.20	0
1	MGN	D	400	1	6,9,10	0.86	0	6,12,14	2.15	1 (16%)
1	GL3	D	445	1	3,3,4	2.67	1 (33%)	2,2,4	1.79	1 (50%)
1	SMC	D	452	1	5,6,7	0.70	0	2,6,8	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MHS	A	257	1	-	0/4/6/8	0/1/1/1
1	AGM	A	271	1	-	0/7/11/13	0/0/0/0
1	MGN	A	400	1	-	0/6/9/12	0/0/0/0
1	GL3	A	445	1	-	0/1/1/2	0/0/0/0
1	SMC	A	452	1	-	0/3/5/7	0/0/0/0
1	MHS	D	257	1	-	0/4/6/8	0/1/1/1
1	AGM	D	271	1	-	0/7/11/13	0/0/0/0
1	MGN	D	400	1	-	0/6/9/12	0/0/0/0
1	GL3	D	445	1	-	0/1/1/2	0/0/0/0
1	SMC	D	452	1	-	0/3/5/7	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	GL3	C-S	-4.53	1.65	1.80
1	A	445	GL3	C-S	-3.92	1.67	1.80
1	D	257	MHS	CM-ND1	4.29	1.57	1.47
1	A	257	MHS	CM-ND1	4.80	1.58	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	400	MGN	CB2-CA-CB1	-4.93	102.18	110.92
1	D	400	MGN	CB2-CA-CB1	-4.48	102.99	110.92
1	A	271	AGM	CE2-CD-NE1	-2.85	106.64	112.05
1	A	257	MHS	O-C-CA	-2.03	120.19	125.49
1	A	445	GL3	CA-C-S	2.24	120.26	112.79
1	D	445	GL3	CA-C-S	2.53	121.22	112.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 17 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	$\#\|Z\| > 2$
4	F43	A	1550	1,5	42,71,71	4.00	22 (52%)	35,118,118	2.89	12 (34%)
5	SHT	A	1551	4	22,27,27	2.15	6 (27%)	24,36,36	1.83	6 (25%)
6	GOL	A	1552	7	5,5,5	0.67	0	5,5,5	1.40	1 (20%)
6	GOL	A	1553	-	5,5,5	0.60	0	5,5,5	0.97	0
6	GOL	A	1554	-	5,5,5	0.76	0	5,5,5	0.75	0
6	GOL	A	1555	-	5,5,5	0.78	0	5,5,5	0.72	0
6	GOL	B	1444	-	5,5,5	0.86	0	5,5,5	1.25	0
6	GOL	C	1249	-	5,5,5	0.64	0	5,5,5	0.49	0
4	F43	D	1550	1,5	42,71,71	4.06	21 (50%)	35,118,118	2.72	14 (40%)
5	SHT	D	1551	4	22,27,27	2.21	8 (36%)	24,36,36	1.50	4 (16%)
6	GOL	D	1552	-	5,5,5	0.79	0	5,5,5	0.30	0
6	GOL	D	1553	7	5,5,5	0.71	0	5,5,5	0.80	0
6	GOL	D	1554	-	5,5,5	0.75	0	5,5,5	0.89	0
6	GOL	D	1555	-	5,5,5	0.72	0	5,5,5	0.84	0
6	GOL	E	1444	-	5,5,5	0.89	0	5,5,5	1.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	F43	A	1550	1,5	1/1/25/27	0/18/165/165	0/0/10/10
5	SHT	A	1551	4	-	0/27/31/31	0/0/0/0
6	GOL	A	1552	7	-	0/4/4/4	0/0/0/0
6	GOL	A	1553	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1554	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1555	-	-	0/4/4/4	0/0/0/0
6	GOL	B	1444	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1249	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	F43	D	1550	1,5	1/1/25/27	0/18/165/165	0/0/10/10
5	SHT	D	1551	4	-	0/27/31/31	0/0/0/0
6	GOL	D	1552	-	-	0/4/4/4	0/0/0/0
6	GOL	D	1553	7	-	0/4/4/4	0/0/0/0
6	GOL	D	1554	-	-	0/4/4/4	0/0/0/0
6	GOL	D	1555	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1444	-	-	0/4/4/4	0/0/0/0

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1550	F43	C4B-NB	-14.39	1.27	1.49
4	A	1550	F43	C4B-NB	-14.15	1.27	1.49
4	D	1550	F43	C4A-NA	-5.52	1.39	1.49
4	A	1550	F43	C4A-NA	-5.25	1.40	1.49
4	D	1550	F43	C9B-C2B	-3.76	1.46	1.54
4	A	1550	F43	C9B-C2B	-3.01	1.47	1.54
4	D	1550	F43	C1D-ND	-2.61	1.31	1.36
4	D	1550	F43	C5D-C2D	-2.51	1.47	1.51
4	A	1550	F43	C1D-ND	-2.49	1.31	1.36
4	D	1550	F43	C9D-C3D	-2.17	1.47	1.52
5	D	1551	SHT	CK6-SK	-2.15	1.71	1.82
4	A	1550	F43	C9D-C3D	-2.14	1.47	1.52
4	A	1550	F43	C5D-C2D	-2.04	1.48	1.51
5	D	1551	SHT	P-O1P	2.05	1.57	1.51
4	A	1550	F43	NI-ND	2.06	2.05	1.92
4	A	1550	F43	C9A-C2A	2.06	1.58	1.54
4	A	1550	F43	CAB-C3B	2.13	1.58	1.53
5	A	1551	SHT	P-O1P	2.15	1.58	1.51
4	D	1550	F43	C9A-C2A	2.19	1.58	1.54
5	A	1551	SHT	OS3-SG2	2.23	1.52	1.45
5	D	1551	SHT	CK1-CK	2.27	1.52	1.48
4	D	1550	F43	NI-ND	2.27	2.06	1.92
4	A	1550	F43	C2A-C3A	2.34	1.59	1.54
4	A	1550	F43	CHD-C7D	2.36	1.51	1.46
4	D	1550	F43	CAB-C3B	2.45	1.59	1.53
4	D	1550	F43	CHD-C7D	2.49	1.52	1.46
4	A	1550	F43	C1B-N5B	2.65	1.51	1.45
5	D	1551	SHT	OS3-SG2	2.70	1.53	1.45
4	D	1550	F43	C1B-N5B	2.85	1.51	1.45
5	A	1551	SHT	OS1-SG2	2.91	1.54	1.45
5	D	1551	SHT	OS2-SG2	2.93	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1551	SHT	OS1-SG2	2.95	1.54	1.45
4	A	1550	F43	CAA-C3A	3.24	1.60	1.53
4	D	1550	F43	CAA-C3A	3.26	1.60	1.53
4	A	1550	F43	C1C-NC	3.29	1.44	1.37
4	D	1550	F43	CHB-C4A	3.34	1.57	1.52
5	A	1551	SHT	OS2-SG2	3.43	1.55	1.46
4	A	1550	F43	CHB-C4A	3.86	1.58	1.52
4	D	1550	F43	NI-NC	4.16	2.08	1.90
5	A	1551	SHT	OK-CK	4.21	1.32	1.24
4	D	1550	F43	C1C-NC	4.41	1.46	1.37
5	D	1551	SHT	OK-CK	4.62	1.33	1.24
4	A	1550	F43	C1D-C2D	4.71	1.53	1.40
4	A	1550	F43	C2B-C3B	4.72	1.62	1.54
4	A	1550	F43	C6D-C7D	5.08	1.58	1.50
4	A	1550	F43	NI-NC	5.13	2.12	1.90
4	D	1550	F43	C2B-C3B	5.27	1.63	1.54
4	D	1550	F43	C6D-C7D	5.53	1.58	1.50
4	D	1550	F43	C1D-C2D	5.68	1.55	1.40
5	A	1551	SHT	CK1-CK2	6.07	1.48	1.31
5	D	1551	SHT	CK1-CK2	6.27	1.49	1.31
4	A	1550	F43	C3D-C2D	7.78	1.56	1.39
4	D	1550	F43	C3D-C2D	7.82	1.56	1.39
4	D	1550	F43	C2A-C1A	8.01	1.62	1.51
4	A	1550	F43	C2A-C1A	8.44	1.62	1.51
4	D	1550	F43	C4D-C3D	9.73	1.50	1.37
4	A	1550	F43	C4D-C3D	10.34	1.51	1.37

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1550	F43	O7B-C6B-C8B	-6.44	118.28	126.90
4	A	1550	F43	C9D-C3D-C4D	-6.32	116.37	127.01
4	D	1550	F43	C9D-C3D-C4D	-5.57	117.63	127.01
4	D	1550	F43	O8D-C7D-C6D	-4.91	111.84	120.76
4	A	1550	F43	O8D-C7D-C6D	-4.81	112.02	120.76
4	A	1550	F43	O7B-C6B-C8B	-4.49	120.89	126.90
4	D	1550	F43	CBB-CAB-C3B	-3.61	106.04	113.98
5	D	1551	SHT	C-CA-N	-3.04	107.42	113.51
5	A	1551	SHT	C-CA-N	-2.94	107.62	113.51
5	A	1551	SHT	OK-CK-CK1	-2.82	117.57	123.01
4	D	1550	F43	O7A-C6A-N8A	-2.76	114.55	122.46
4	A	1550	F43	CBB-CAB-C3B	-2.72	108.00	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1550	F43	C9B-C2B-C8B	-2.57	103.19	110.17
4	D	1550	F43	O7B-C6B-N5B	-2.56	120.74	124.71
5	D	1551	SHT	CK3-CK2-CK1	-2.46	121.28	126.16
6	A	1552	GOL	C3-C2-C1	-2.41	101.68	111.12
5	D	1551	SHT	OK-CK-CK1	-2.36	118.47	123.01
4	A	1550	F43	C8C-C3C-C4C	-2.21	104.67	112.47
5	A	1551	SHT	OS2-SG2-OS1	-2.20	106.50	111.61
4	A	1550	F43	O7A-C6A-C5A	-2.17	114.97	122.02
4	A	1550	F43	C2A-C3A-C4A	-2.02	99.00	102.38
5	A	1551	SHT	CB-CA-N	2.12	115.78	111.69
4	D	1550	F43	C3C-C4C-CHD	2.12	127.82	124.26
5	D	1551	SHT	O8P-P-O1P	2.22	117.72	110.58
4	D	1550	F43	C5A-C6A-N8A	2.41	124.95	116.58
5	A	1551	SHT	CK1-CK-N	2.61	119.87	114.12
4	A	1550	F43	C3C-C4C-CHD	2.75	128.86	124.26
4	D	1550	F43	C3A-C4A-NA	2.90	106.95	102.27
4	D	1550	F43	C3B-C4B-NB	3.94	118.35	106.03
4	A	1550	F43	C1C-NC-C4C	4.47	112.70	107.93
4	A	1550	F43	C3B-C4B-NB	4.53	120.18	106.03
5	A	1551	SHT	OS3-SG2-CD	4.74	110.95	106.91
4	D	1550	F43	C4A-NA-C1A	4.77	112.99	108.21
4	D	1550	F43	O8D-C7D-CHD	4.88	128.13	122.56
4	D	1550	F43	C9B-C2B-C3B	5.15	121.96	111.81
4	A	1550	F43	C9B-C2B-C3B	5.57	122.81	111.81
4	A	1550	F43	C4A-NA-C1A	8.83	117.07	108.21

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	1550	F43	C4B
4	A	1550	F43	C4B

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1550	F43	1	0
6	A	1552	GOL	1	0
6	A	1554	GOL	1	0
6	A	1555	GOL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1444	GOL	3	0
4	D	1550	F43	1	0
6	D	1554	GOL	1	0
6	E	1444	GOL	2	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

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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