



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:13 PM GMT

PDB ID : 3SJL
Title : Crystal Structure of the P107S-MauG/pre-Methylamine Dehydrogenase Complex
Authors : Jensen, L.M.R.; Wilmot, C.M.
Deposited on : 2011-06-21
Resolution : 1.63 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

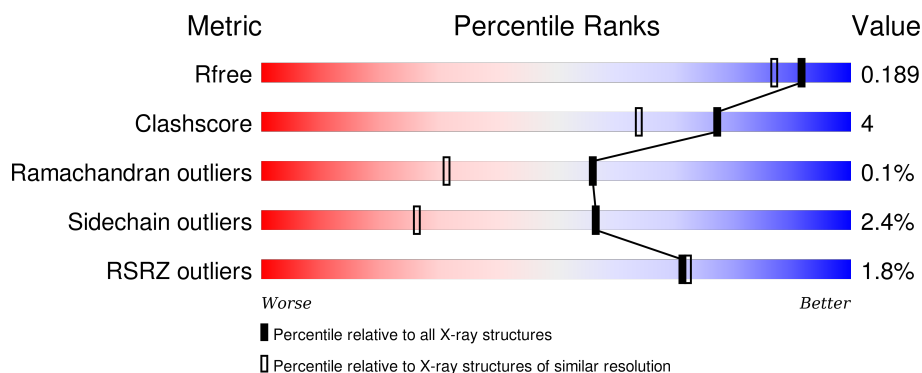
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1953 (1.66-1.62)
Clashscore	102246	2091 (1.66-1.62)
Ramachandran outliers	100387	2052 (1.66-1.62)
Sidechain outliers	100360	2052 (1.66-1.62)
RSRZ outliers	91569	1955 (1.66-1.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	
1	B	373	
2	C	137	
2	E	137	
3	D	386	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	386	<div> <div></div> <div>%</div> <div>84%</div> <div>13%</div> <div></div> </div>

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
5	NA	A	402	-	-	-	X
7	PEG	B	374	-	-	X	X
8	EDO	D	387	-	X	X	X
8	EDO	F	388	-	-	-	X
9	MES	F	387	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 15480 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 Methylamine utilization protein mauG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	6	0
			2659	1669	475	503	12			
1	B	343	Total	C	N	O	S	0	9	0
			2726	1705	495	514	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	SER	PRO	ENGINEERED MUTATION	UNP Q51658
A	368	HIS	-	EXPRESSION TAG	UNP Q51658
A	369	HIS	-	EXPRESSION TAG	UNP Q51658
A	370	HIS	-	EXPRESSION TAG	UNP Q51658
A	371	HIS	-	EXPRESSION TAG	UNP Q51658
A	372	HIS	-	EXPRESSION TAG	UNP Q51658
A	373	HIS	-	EXPRESSION TAG	UNP Q51658
B	107	SER	PRO	ENGINEERED MUTATION	UNP Q51658
B	368	HIS	-	EXPRESSION TAG	UNP Q51658
B	369	HIS	-	EXPRESSION TAG	UNP Q51658
B	370	HIS	-	EXPRESSION TAG	UNP Q51658
B	371	HIS	-	EXPRESSION TAG	UNP Q51658
B	372	HIS	-	EXPRESSION TAG	UNP Q51658
B	373	HIS	-	EXPRESSION TAG	UNP Q51658

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	131	Total	C	N	O	S	0	3	0
			1027	634	179	200	14			
2	E	125	Total	C	N	O	S	0	4	0
			978	610	162	192	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	EXPRESSION TAG	UNP P22619
C	133	HIS	-	EXPRESSION TAG	UNP P22619
C	134	HIS	-	EXPRESSION TAG	UNP P22619
C	135	HIS	-	EXPRESSION TAG	UNP P22619
C	136	HIS	-	EXPRESSION TAG	UNP P22619
C	137	HIS	-	EXPRESSION TAG	UNP P22619
E	132	HIS	-	EXPRESSION TAG	UNP P22619
E	133	HIS	-	EXPRESSION TAG	UNP P22619
E	134	HIS	-	EXPRESSION TAG	UNP P22619
E	135	HIS	-	EXPRESSION TAG	UNP P22619
E	136	HIS	-	EXPRESSION TAG	UNP P22619
E	137	HIS	-	EXPRESSION TAG	UNP P22619

- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	3	0
			2937	1865	502	562	8			
3	F	376	Total	C	N	O	S	0	7	0
			2964	1884	507	565	8			

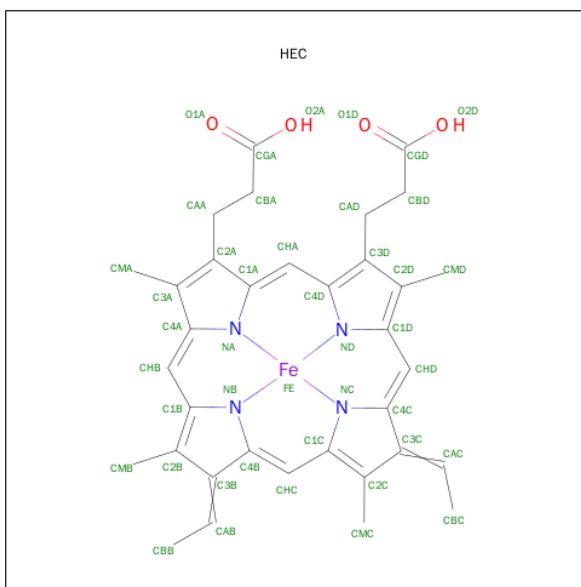
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

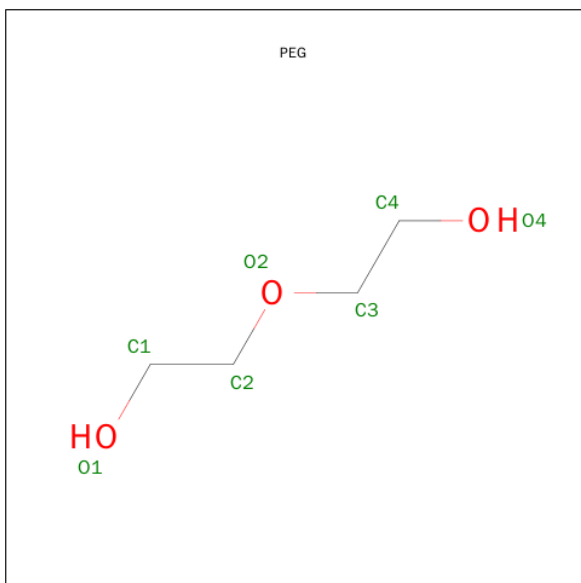
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



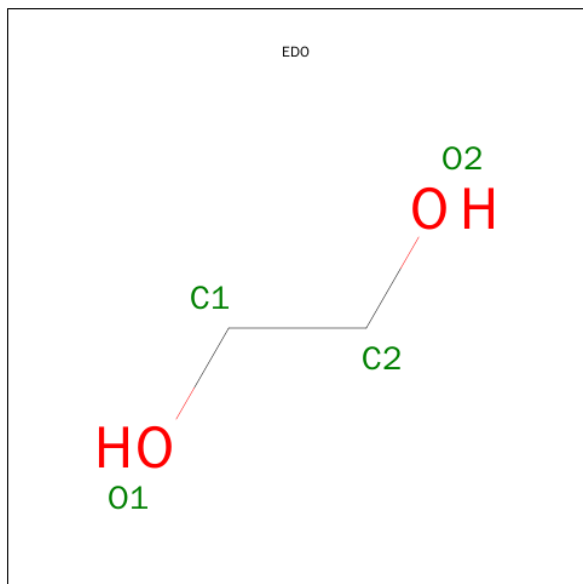
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



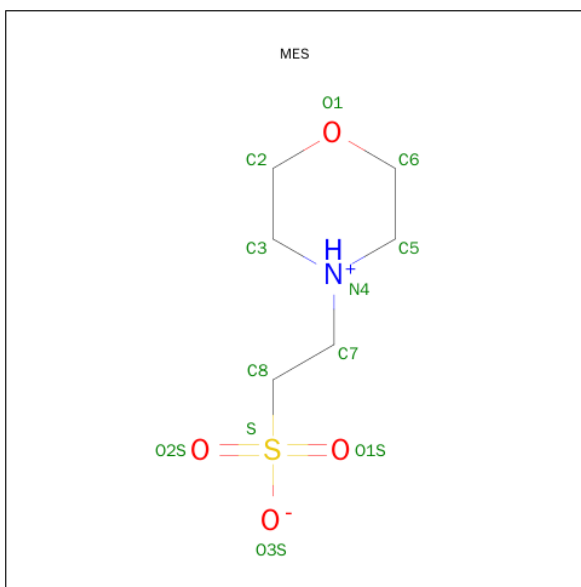
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

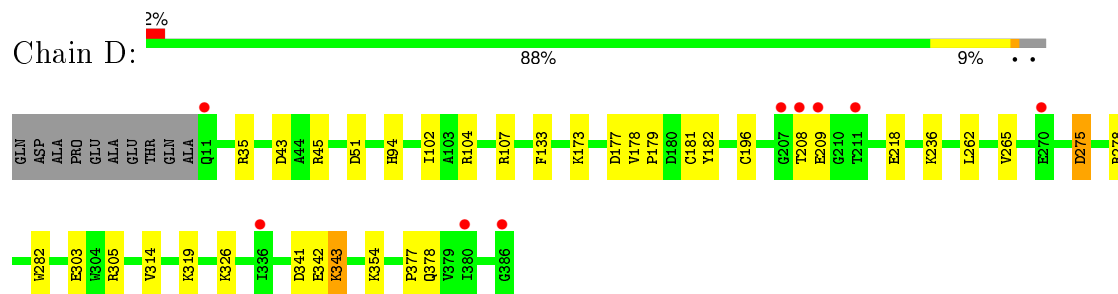


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

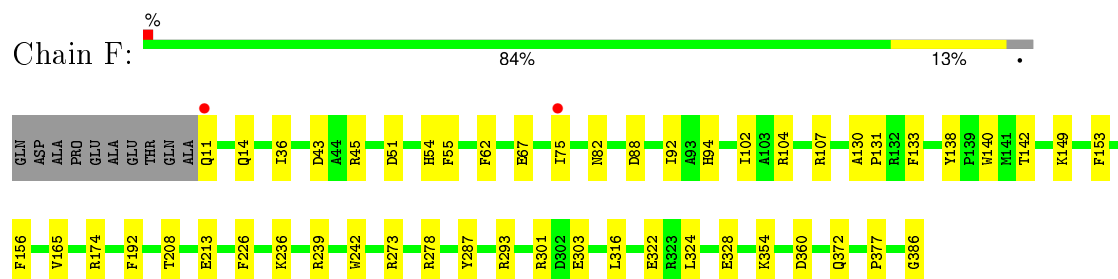
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	400	Total	O	0	0
			400	400		
10	B	383	Total	O	0	0
			383	383		
10	C	127	Total	O	0	0
			127	127		
10	D	385	Total	O	0	0
			385	385		
10	E	137	Total	O	0	0
			137	137		
10	F	534	Total	O	0	0
			534	534		

● Molecule 3: Methylamine dehydrogenase heavy chain



● Molecule 3: Methylamine dehydrogenase heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.61Å 89.00Å 104.81Å 67.05° 79.51° 79.72°	Depositor
Resolution (Å)	29.39 – 1.63 29.39 – 1.63	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.39-1.63) 82.8 (29.39-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.142 , 0.180 0.161 , 0.189	Depositor DCC
R_{free} test set	10468 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 208545 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15480	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 0AF, NA, CA, EDO, MES, HEC, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.39	13/2738 (0.5%)	1.30	23/3712 (0.6%)
1	B	1.31	7/2812 (0.2%)	1.19	15/3808 (0.4%)
2	C	1.37	1/1050 (0.1%)	1.17	6/1430 (0.4%)
2	E	1.33	2/1001 (0.2%)	1.20	3/1368 (0.2%)
3	D	1.24	3/3023 (0.1%)	1.13	9/4120 (0.2%)
3	F	1.44	13/3062 (0.4%)	1.25	20/4170 (0.5%)
All	All	1.35	39/13686 (0.3%)	1.21	76/18608 (0.4%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	213	GLU	CD-OE1	9.55	1.36	1.25
1	A	112	VAL	CB-CG2	-7.53	1.37	1.52
1	B	162	TYR	CD2-CE2	6.98	1.49	1.39
1	A	93	TRP	CE3-CZ3	6.93	1.50	1.38
3	F	213	GLU	CG-CD	6.71	1.62	1.51
1	A	167	GLU	CB-CG	-6.64	1.39	1.52
1	B	221	PHE	CD2-CE2	6.39	1.52	1.39
2	E	25	TYR	CE2-CZ	6.30	1.46	1.38
3	D	303	GLU	CD-OE2	-6.14	1.18	1.25
2	C	30	SER	CB-OG	6.07	1.50	1.42
3	F	287	TYR	CE1-CZ	6.06	1.46	1.38
3	F	55	PHE	CD2-CE2	6.00	1.51	1.39
1	A	81	ARG	CZ-NH2	5.93	1.40	1.33
1	B	167	GLU	CD-OE2	5.91	1.32	1.25
1	A	338	ARG	CZ-NH1	5.86	1.40	1.33
1	A	39[A]	ARG	CZ-NH2	5.85	1.40	1.33
1	A	39[B]	ARG	CZ-NH2	5.85	1.40	1.33
1	B	171	PHE	CE2-CZ	5.68	1.48	1.37
3	D	303	GLU	CB-CG	-5.62	1.41	1.52
1	B	79	PHE	CE2-CZ	5.59	1.48	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	PHE	CE2-CZ	5.57	1.48	1.37
3	F	140	TRP	CZ3-CH2	5.46	1.48	1.40
3	F	303	GLU	CG-CD	5.45	1.60	1.51
3	F	62	PHE	CE1-CZ	5.43	1.47	1.37
1	A	136	PHE	CE2-CZ	5.41	1.47	1.37
3	F	322	GLU	CG-CD	5.39	1.60	1.51
2	E	75	ARG	CZ-NH1	5.39	1.40	1.33
1	B	223	TYR	CG-CD2	5.30	1.46	1.39
3	F	239	ARG	CG-CD	5.30	1.65	1.51
3	F	165	VAL	CB-CG1	5.29	1.64	1.52
1	A	270	ARG	CZ-NH1	5.28	1.40	1.33
1	A	297	TYR	CE2-CZ	5.24	1.45	1.38
1	A	359	GLU	CG-CD	5.21	1.59	1.51
1	A	18	PHE	CD2-CE2	5.19	1.49	1.39
3	F	192	PHE	CD2-CE2	5.18	1.49	1.39
3	D	133	PHE	CE1-CZ	5.16	1.47	1.37
3	F	156	PHE	CD1-CE1	5.10	1.49	1.39
1	A	222	GLU	CD-OE1	5.07	1.31	1.25
3	F	242	TRP	CZ3-CH2	5.00	1.48	1.40

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39[A]	ARG	NE-CZ-NH1	-14.86	112.87	120.30
1	A	39[B]	ARG	NE-CZ-NH1	-14.86	112.87	120.30
1	A	177	ARG	NE-CZ-NH1	9.70	125.15	120.30
3	D	104	ARG	NE-CZ-NH2	-9.50	115.55	120.30
3	F	278	ARG	NE-CZ-NH2	-9.33	115.63	120.30
3	D	305	ARG	NE-CZ-NH2	-8.95	115.83	120.30
3	F	88	ASP	CB-CG-OD1	8.81	126.23	118.30
3	F	301	ARG	NE-CZ-NH2	-8.72	115.94	120.30
3	F	104	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	39[A]	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	A	39[B]	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	B	64	ASP	CB-CG-OD2	8.18	125.66	118.30
3	F	278	ARG	NE-CZ-NH1	8.09	124.34	120.30
3	F	104	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	82	ASP	CB-CG-OD2	7.48	125.03	118.30
1	A	5	PRO	N-CA-CB	7.24	111.98	103.30
1	A	81	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	B	263[A]	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	B	263[B]	ARG	NE-CZ-NH1	-7.12	116.74	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	LEU	CB-CG-CD2	7.12	123.10	111.00
1	B	357	LEU	CB-CG-CD1	7.12	123.10	111.00
1	A	64	ASP	N-CA-CB	-6.90	98.19	110.60
2	E	75	ARG	NE-CZ-NH1	-6.85	116.87	120.30
3	D	35	ARG	NE-CZ-NH2	-6.60	117.00	120.30
3	F	133	PHE	CB-CG-CD2	-6.41	116.31	120.80
1	A	180	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	E	24	ASP	CB-CG-OD1	6.30	123.97	118.30
3	D	278	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	327	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	B	180	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	A	96	ARG	NE-CZ-NH1	-6.13	117.23	120.30
3	F	226	PHE	CB-CG-CD1	-6.12	116.51	120.80
1	A	263	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	150	ARG	NE-CZ-NH1	6.05	123.33	120.30
2	C	75	ARG	CD-NE-CZ	6.04	132.06	123.60
2	E	25	TYR	CZ-CE2-CD2	-6.03	114.38	119.80
1	A	82	ASP	CB-CG-OD1	-6.01	112.89	118.30
3	D	173	LYS	CD-CE-NZ	-5.92	98.10	111.70
1	A	180	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	B	338	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	C	10	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	C	80	TYR	CB-CG-CD2	-5.86	117.48	121.00
2	C	75	ARG	NE-CZ-NH1	5.77	123.19	120.30
3	D	35	ARG	NE-CZ-NH1	5.76	123.18	120.30
3	F	153	PHE	CB-CG-CD2	5.67	124.77	120.80
1	B	84	ASN	CB-CA-C	-5.67	99.07	110.40
3	F	45	ARG	CA-CB-CG	-5.66	100.94	113.40
1	A	215	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	64	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	C	119	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	A	75	LEU	CA-CB-CG	-5.56	102.51	115.30
3	D	107	ARG	NE-CZ-NH2	-5.48	117.56	120.30
3	F	107	ARG	NE-CZ-NH2	-5.47	117.56	120.30
3	F	138	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	109	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	B	86	LYS	CD-CE-NZ	-5.39	99.29	111.70
1	A	64	ASP	CB-CG-OD1	5.34	123.10	118.30
3	F	301	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	88	LYS	CD-CE-NZ	-5.33	99.45	111.70
3	F	324	LEU	CB-CG-CD1	-5.30	101.98	111.00
1	B	300	ARG	NE-CZ-NH1	-5.30	117.65	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	43	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	349	LEU	CB-CG-CD1	-5.21	102.14	111.00
3	F	67	GLU	OE1-CD-OE2	-5.21	117.05	123.30
2	C	8	ASP	CB-CG-OD1	5.20	122.98	118.30
3	F	43	ASP	CB-CG-OD1	5.20	122.98	118.30
3	F	360[A]	ASP	CB-CG-OD1	5.17	122.95	118.30
3	F	360[B]	ASP	CB-CG-OD1	5.17	122.95	118.30
3	D	275	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	B	252	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	321[A]	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	321[B]	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	327	GLU	CG-CD-OE1	5.10	128.50	118.30
3	F	149	LYS	CD-CE-NZ	-5.05	100.08	111.70
3	F	328	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	B	88	LYS	CD-CE-NZ	-5.02	100.16	111.70

There are no chirality outliers.

There are no planarity outliers.

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	2659	0	2566	15	0
1	B	2726	0	2635	24	0
2	C	1027	0	916	15	0
2	E	978	0	890	13	0
3	D	2937	0	2832	12	0
3	F	2964	0	2874	19	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	86	0	60	3	0
6	B	86	0	60	1	0
7	A	7	0	10	0	0
7	B	14	0	20	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	4	0	6	1	0
8	D	4	0	6	6	0
8	F	4	0	6	1	0
9	F	12	0	12	0	0
10	A	400	0	0	3	0
10	B	383	0	0	8	0
10	C	127	0	0	5	0
10	D	385	0	0	5	0
10	E	137	0	0	5	0
10	F	534	0	0	5	0
All	All	15480	0	12893	97	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 (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASP:OD1	7:B:374:PEG:H11	1.50	1.09
3:F:372[B]:GLN:NE2	10:F:1487:HOH:O	1.87	1.08
3:F:372[A]:GLN:OE1	10:F:2086:HOH:O	1.73	1.04
1:B:64:ASP:HB2	10:B:423:HOH:O	1.58	1.03
8:F:388:EDO:H12	10:F:1692:HOH:O	1.63	0.96
1:B:208[B]:ARG:NH1	10:B:1695:HOH:O	2.05	0.88
1:B:102[B]:GLN:HG2	10:B:1580:HOH:O	1.76	0.83
1:B:48:LYS:HE2	1:B:285[A]:THR:HG22	1.59	0.83
2:E:127[A]:VAL:HG12	10:E:1704:HOH:O	1.80	0.81
1:B:102[B]:GLN:HE21	1:B:106:GLN:HE21	1.34	0.74
10:B:1896:HOH:O	2:E:127[A]:VAL:HG11	1.87	0.74
1:A:245[A]:VAL:HG13	1:A:247:HIS:NE2	2.03	0.74
8:D:387:EDO:H11	10:D:1241:HOH:O	1.91	0.70
3:D:236:LYS:NZ	10:D:976:HOH:O	2.23	0.70
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.57	0.68
1:B:320[A]:ALA:O	1:B:323:LEU:CD2	2.41	0.68
1:B:48:LYS:HE2	1:B:285[A]:THR:CG2	2.24	0.67
2:C:86:CYS:H	3:F:372[A]:GLN:HE22	1.44	0.66
1:A:86:LYS:HD3	10:A:516:HOH:O	1.96	0.66
3:F:236[B]:LYS:NZ	3:F:386:GLY:O	2.20	0.64
10:C:1671:HOH:O	3:F:36[A]:ILE:HD11	1.96	0.63
1:B:153:ASP:OD1	7:B:374:PEG:C1	2.39	0.61
10:A:1700:HOH:O	2:C:134:HIS:HD2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:177[A]:ASP:OD2	10:D:1216:HOH:O	2.16	0.59
1:B:152:PHE:HE2	7:B:374:PEG:H32	1.66	0.59
3:D:342:GLU:HA	10:D:1697:HOH:O	2.02	0.58
10:C:457:HOH:O	8:D:387:EDO:H12	2.04	0.58
2:C:101[B]:GLU:HG2	2:C:102:PHE:CD2	2.39	0.57
10:E:1503:HOH:O	3:F:54:HIS:HD2	1.86	0.57
2:C:46:CYS:HB2	3:F:36[B]:ILE:HD13	1.87	0.57
2:C:93:GLY:O	2:C:134:HIS:HE1	1.89	0.56
1:A:232:GLU:O	1:A:236:GLU:HG3	2.04	0.56
10:B:1896:HOH:O	2:E:127[A]:VAL:CG1	2.50	0.56
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.53	0.56
1:B:320[A]:ALA:O	1:B:323:LEU:HD23	2.05	0.55
1:A:197:ILE:CD1	2:C:71:LEU:HD13	2.36	0.55
1:B:215:ARG:HH12	8:B:376:EDO:H11	1.72	0.54
3:F:54:HIS:HE1	10:F:618:HOH:O	1.90	0.54
1:A:323[B]:LEU:HD12	10:A:1525:HOH:O	2.08	0.54
1:A:245[A]:VAL:CG1	1:A:247:HIS:NE2	2.70	0.54
1:B:358:LEU:O	7:B:375:PEG:H22	2.08	0.54
1:A:197:ILE:HD12	2:C:71:LEU:HD13	1.89	0.53
1:B:197:ILE:O	1:B:202:ARG:HD2	2.09	0.53
2:E:101[B]:GLU:HG2	2:E:102:PHE:CD2	2.46	0.51
10:C:1499:HOH:O	3:F:36[A]:ILE:CD1	2.59	0.50
2:C:75:ARG:HD3	10:C:960:HOH:O	2.12	0.50
1:B:299:SER:HB2	1:B:333:MET:HG3	1.94	0.50
1:B:102[B]:GLN:HE21	1:B:106:GLN:NE2	2.07	0.49
3:F:51:ASP:HA	3:F:377:PRO:HA	1.96	0.48
1:B:29:GLN:NE2	10:B:1945:HOH:O	2.36	0.47
2:E:130:ALA:O	2:E:131:SER:HB2	2.14	0.46
3:D:378:GLN:HE22	8:D:387:EDO:C1	2.29	0.46
2:C:21:GLN:HE22	3:F:14:GLN:NE2	2.14	0.46
3:F:82:ASN:HB3	3:F:142:THR:HB	1.98	0.46
8:D:387:EDO:C1	10:D:1241:HOH:O	2.56	0.45
2:C:23:CYS:CB	2:C:88[B]:CYS:SG	3.04	0.45
1:B:62:HIS:N	10:B:2097:HOH:O	2.48	0.45
1:B:102[B]:GLN:NE2	1:B:106:GLN:HE21	2.09	0.45
3:F:273[A]:ARG:HG2	10:F:509:HOH:O	2.17	0.45
1:B:120:ALA:HA	1:B:148:PRO:HB3	1.99	0.45
3:F:75[B]:ILE:HD11	3:F:92:ILE:HD11	1.99	0.45
2:E:73:ALA:HB2	2:E:127[A]:VAL:HG21	1.99	0.44
1:A:299:SER:HB2	1:A:333:MET:HG3	1.98	0.44
2:C:57:0AF:CE3	2:C:108:TRP:CD1	3.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:ARG:HD2	10:B:1867:HOH:O	2.17	0.44
3:D:314:VAL:HG12	3:D:326:LYS:HG3	1.99	0.44
6:B:500:HEC:HMC1	6:B:500:HEC:HBC3	2.00	0.44
3:D:282:TRP:CH2	8:D:387:EDO:H22	2.52	0.43
1:A:272:VAL:HG21	6:A:600:HEC:HMA3	2.00	0.43
2:C:23:CYS:HB3	2:C:88[B]:CYS:SG	2.57	0.43
10:C:457:HOH:O	8:D:387:EDO:C1	2.62	0.43
3:F:174:ARG:HD2	3:F:208:THR:O	2.18	0.42
1:A:113:GLU:HG2	6:A:500:HEC:C4C	2.49	0.42
1:A:245[A]:VAL:HG23	1:A:318:GLU:HG2	2.01	0.42
3:F:75[B]:ILE:CD1	3:F:92:ILE:HD11	2.49	0.42
1:B:105:GLY:HA3	7:B:374:PEG:H32	2.02	0.42
3:D:178:VAL:HB	3:D:179:PRO:CD	2.49	0.42
2:E:13[B]:TRP:HD1	10:E:1442:HOH:O	2.02	0.42
2:E:23:CYS:SG	2:E:88[B]:CYS:SG	3.18	0.42
1:B:64:ASP:OD1	1:B:235:ARG:NE	2.41	0.42
2:C:86:CYS:H	3:F:372[A]:GLN:NE2	2.16	0.41
2:E:13[B]:TRP:HB3	10:E:1442:HOH:O	2.20	0.41
3:D:181:CYS:C	3:D:182:TYR:CD1	2.94	0.41
3:D:45:ARG:NH2	3:D:343:LYS:O	2.53	0.41
3:D:181:CYS:HA	3:D:196:CYS:HA	2.02	0.41
1:A:21:PRO:HA	1:A:29:GLN:O	2.20	0.41
2:C:23:CYS:SG	2:C:88[B]:CYS:SG	3.19	0.41
1:A:64:ASP:HB2	1:A:240:LEU:HD12	2.02	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.95	0.40
3:D:341:ASP:OD1	3:D:341:ASP:N	2.53	0.40
6:A:500:HEC:HMC1	6:A:500:HEC:HBC3	2.03	0.40
3:D:51:ASP:HA	3:D:377:PRO:HA	2.03	0.40
2:E:57:0AF:CE3	2:E:108:TRP:CD1	3.05	0.40
1:A:359:GLU:OE1	1:A:359:GLU:HA	2.21	0.40
2:E:23:CYS:CB	2:E:88[B]:CYS:SG	3.09	0.40
2:E:99:ARG:NH1	10:E:1882:HOH:O	2.27	0.40
3:F:130:ALA:N	3:F:131:PRO:HD3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	340/373 (91%)	331 (97%)	9 (3%)	0	100	100
1	B	348/373 (93%)	336 (97%)	12 (3%)	0	100	100
2	C	131/137 (96%)	126 (96%)	5 (4%)	0	100	100
2	E	126/137 (92%)	124 (98%)	2 (2%)	0	100	100
3	D	377/386 (98%)	366 (97%)	10 (3%)	1 (0%)	46	23
3	F	381/386 (99%)	370 (97%)	10 (3%)	1 (0%)	46	23
All	All	1703/1792 (95%)	1653 (97%)	48 (3%)	2 (0%)	56	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	102	ILE
3	F	102	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/292 (93%)	266 (98%)	5 (2%)	66	41
1	B	277/292 (95%)	269 (97%)	8 (3%)	50	18
2	C	113/112 (101%)	111 (98%)	2 (2%)	66	41
2	E	108/112 (96%)	105 (97%)	3 (3%)	51	20
3	D	307/311 (99%)	297 (97%)	10 (3%)	45	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	311/311 (100%)	306 (98%)	5 (2%)	70	46
All	All	1387/1430 (97%)	1354 (98%)	33 (2%)	57	26

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	84	ASN
1	A	202	ARG
1	A	219	THR
1	A	357	LEU
1	B	84	ASN
1	B	167	GLU
1	B	184	LYS
1	B	190	GLU
1	B	235	ARG
1	B	296	LYS
1	B	357	LEU
1	B	360	GLU
2	C	7	THR
2	C	29	CYS
3	D	94	HIS
3	D	208	THR
3	D	209	GLU
3	D	218	GLU
3	D	262	LEU
3	D	265	VAL
3	D	275	ASP
3	D	319	LYS
3	D	343	LYS
3	D	354	LYS
2	E	7	THR
2	E	71	LEU
2	E	131	SER
3	F	11	GLN
3	F	94	HIS
3	F	293	ARG
3	F	316	LEU
3	F	354	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	B	16	GLN
1	B	91	GLN
1	B	106	GLN
1	B	210	GLN
2	C	134	HIS
3	D	14	GLN
3	D	30	GLN
3	F	14	GLN
3	F	54	HIS
3	F	300	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 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$
2	0AF	C	57	2	13,16,17	1.49	3 (23%)	10,22,24	1.78	2 (20%)
2	0AF	E	57	2	13,16,17	2.11	4 (30%)	10,22,24	1.64	3 (30%)

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
2	0AF	C	57	2	-	0/3/6/8	0/2/2/2
2	0AF	E	57	2	-	0/3/6/8	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CZ2-CE2	-3.69	1.37	1.42
2	C	57	0AF	CB-CA	-3.43	1.46	1.53
2	C	57	0AF	CZ2-CE2	-2.52	1.39	1.42
2	C	57	0AF	CZ3-CE3	2.31	1.42	1.36
2	E	57	0AF	CB-CG	2.69	1.59	1.51
2	E	57	0AF	CZ3-CH2	2.77	1.44	1.38
2	E	57	0AF	CH2-CZ2	3.43	1.44	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	0AF	O-C-CA	-3.68	115.90	125.49
2	E	57	0AF	O-C-CA	-3.15	117.28	125.49
2	C	57	0AF	CB-CG-CD1	-2.77	124.54	127.97
2	E	57	0AF	CE3-CZ3-CH2	-2.38	117.01	120.96
2	E	57	0AF	CE3-CD2-CE2	2.48	122.14	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	57	0AF	1	0
2	E	57	0AF	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	$\# Z > 2$
7	PEG	A	374	-	6,6,6	0.83	0	5,5,5	1.25	1 (20%)
6	HEC	A	500	1	24,50,50	1.61	6 (25%)	19,82,82	3.23	7 (36%)
6	HEC	A	600	1	24,50,50	1.35	3 (12%)	19,82,82	3.56	10 (52%)
7	PEG	B	374	-	6,6,6	1.26	1 (16%)	5,5,5	1.27	0
7	PEG	B	375	-	6,6,6	0.77	0	5,5,5	0.97	0
8	EDO	B	376	-	3,3,3	0.52	0	2,2,2	0.78	0
6	HEC	B	500	1	24,50,50	1.75	6 (25%)	19,82,82	2.95	6 (31%)
6	HEC	B	600	1	24,50,50	1.18	3 (12%)	19,82,82	3.22	8 (42%)
8	EDO	D	387	-	3,3,3	2.07	2 (66%)	2,2,2	3.13	2 (100%)
9	MES	F	387	-	11,12,12	0.84	0	14,16,16	2.91	4 (28%)
8	EDO	F	388	-	3,3,3	0.97	0	2,2,2	0.29	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
7	PEG	A	374	-	-	0/4/4/4	0/0/0/0
6	HEC	A	500	1	-	0/6/54/54	0/0/8/8
6	HEC	A	600	1	-	0/6/54/54	0/0/8/8
7	PEG	B	374	-	-	0/4/4/4	0/0/0/0
7	PEG	B	375	-	-	0/4/4/4	0/0/0/0
8	EDO	B	376	-	-	0/1/1/1	0/0/0/0
6	HEC	B	500	1	-	0/6/54/54	0/0/8/8
6	HEC	B	600	1	-	0/6/54/54	0/0/8/8
8	EDO	D	387	-	-	0/1/1/1	0/0/0/0
9	MES	F	387	-	-	0/6/14/14	0/1/1/1
8	EDO	F	388	-	-	0/1/1/1	0/0/0/0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	500	HEC	C3C-C2C	-3.91	1.36	1.40
6	B	500	HEC	C3B-C2B	-3.61	1.37	1.40
6	A	500	HEC	C4B-NB	-2.82	1.32	1.36
6	B	500	HEC	C4B-NB	-2.70	1.33	1.36
6	B	600	HEC	C3B-C2B	-2.68	1.38	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	500	HEC	CAD-C3D	-2.30	1.48	1.52
6	A	500	HEC	C1A-NA	-2.24	1.33	1.36
6	B	600	HEC	C1D-CHD	2.08	1.45	1.39
6	A	600	HEC	C3B-C4B	2.16	1.47	1.42
6	B	600	HEC	C4D-CHA	2.20	1.45	1.39
6	B	500	HEC	C3C-C4C	2.25	1.47	1.42
8	D	387	EDO	O1-C1	2.25	1.54	1.42
8	D	387	EDO	O2-C2	2.27	1.54	1.42
6	B	500	HEC	C1D-CHD	2.28	1.46	1.39
6	B	500	HEC	C1C-CHC	2.35	1.46	1.39
7	B	374	PEG	O4-C4	2.40	1.54	1.42
6	A	500	HEC	C1B-CHB	2.47	1.46	1.39
6	A	500	HEC	C3B-C4B	2.79	1.49	1.42
6	A	600	HEC	CBB-CAB	2.79	1.61	1.49
6	A	600	HEC	C1D-CHD	2.94	1.47	1.39
6	A	500	HEC	C1C-CHC	3.21	1.48	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	HEC	CBB-CAB-C3B	-10.58	103.84	127.35
6	A	500	HEC	CBB-CAB-C3B	-8.90	107.58	127.35
6	B	600	HEC	CBB-CAB-C3B	-8.49	108.49	127.35
6	B	500	HEC	CBB-CAB-C3B	-8.06	109.44	127.35
6	A	500	HEC	CBC-CAC-C3C	-7.10	111.57	127.35
6	B	600	HEC	CBC-CAC-C3C	-6.75	112.36	127.35
6	B	500	HEC	CBC-CAC-C3C	-6.34	113.25	127.35
6	A	600	HEC	CBD-CAD-C3D	-5.59	102.50	112.53
6	B	600	HEC	CBD-CAD-C3D	-4.90	103.75	112.53
9	F	387	MES	C2-C3-N4	-4.66	103.06	110.12
6	B	500	HEC	CBD-CAD-C3D	-4.37	104.69	112.53
6	A	600	HEC	CBC-CAC-C3C	-4.16	118.11	127.35
6	A	500	HEC	CAA-C2A-C1A	-4.16	122.49	127.01
6	A	600	HEC	C4C-C3C-C2C	-3.85	102.20	106.35
6	B	600	HEC	CBA-CAA-C2A	-3.77	105.78	112.53
6	A	500	HEC	CBD-CAD-C3D	-3.68	105.94	112.53
6	A	600	HEC	C4B-C3B-C2B	-3.11	102.99	106.35
6	A	600	HEC	CBA-CAA-C2A	-3.05	107.07	112.53
6	B	500	HEC	CMC-C2C-C1C	-3.00	123.40	128.36
6	B	500	HEC	CMB-C2B-C1B	-2.99	123.42	128.36
6	B	500	HEC	C4C-C3C-C2C	-2.76	103.37	106.35
6	B	600	HEC	CMC-C2C-C1C	-2.75	123.81	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	500	HEC	CMB-C2B-C1B	-2.69	123.92	128.36
6	A	600	HEC	CMB-C2B-C1B	-2.68	123.93	128.36
6	B	600	HEC	C4C-C3C-C2C	-2.47	103.68	106.35
6	A	600	HEC	CMD-C2D-C1D	-2.24	124.65	128.36
7	A	374	PEG	O2-C2-C1	-2.22	100.20	110.43
6	B	600	HEC	CAD-C3D-C2D	-2.05	123.16	129.00
6	A	500	HEC	CMD-C2D-C3D	2.26	129.96	125.24
6	A	500	HEC	CMA-C3A-C2A	2.68	130.84	125.24
9	F	387	MES	C7-N4-C5	2.76	118.33	111.27
6	A	600	HEC	CMA-C3A-C2A	2.77	131.02	125.24
8	D	387	EDO	O2-C2-C1	2.88	133.21	112.54
9	F	387	MES	O2S-S-C8	3.04	109.50	106.91
8	D	387	EDO	O1-C1-C2	3.35	136.56	112.54
6	B	600	HEC	CAD-C3D-C4D	3.45	130.75	127.01
6	A	600	HEC	CMD-C2D-C3D	3.78	133.15	125.24
9	F	387	MES	C5-N4-C3	8.31	126.91	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	500	HEC	2	0
6	A	600	HEC	1	0
7	B	374	PEG	4	0
7	B	375	PEG	1	0
8	B	376	EDO	1	0
6	B	500	HEC	1	0
8	D	387	EDO	6	0
8	F	388	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	338/373 (90%)	-0.14	9 (2%) 58 56	15, 21, 39, 61	0
1	B	343/373 (91%)	-0.21	6 (1%) 73 73	13, 21, 38, 61	0
2	C	130/137 (94%)	-0.18	3 (2%) 64 63	14, 19, 32, 49	0
2	E	124/137 (90%)	-0.31	1 (0%) 87 88	13, 17, 27, 55	0
3	D	376/386 (97%)	-0.11	9 (2%) 62 61	15, 26, 43, 66	0
3	F	376/386 (97%)	-0.31	2 (0%) 91 92	12, 17, 28, 53	0
All	All	1687/1792 (94%)	-0.20	30 (1%) 71 72	12, 20, 39, 66	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	PRO	10.9
1	B	49	ALA	6.1
1	A	359	GLU	5.5
3	D	208	THR	5.5
1	A	6	ALA	5.3
1	B	6	ALA	4.8
3	F	11	GLN	4.8
3	D	11	GLN	4.4
1	A	7	ASP	4.4
1	A	237	ALA	4.3
1	A	239	GLY	3.8
3	D	207	GLY	3.8
2	C	7	THR	3.6
1	B	62	HIS	3.1
1	B	7	ASP	3.1
3	D	270	GLU	3.0
1	B	48	LYS	3.0
3	D	380	ILE	2.9
3	D	386	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	360	GLU	2.8
3	D	336	ILE	2.7
3	F	75[A]	ILE	2.6
2	E	131	SER	2.4
1	A	63	GLY	2.3
1	A	242	ALA	2.3
3	D	211	THR	2.3
3	D	209	GLU	2.2
1	A	240	LEU	2.2
2	C	133	HIS	2.1
2	C	72	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	0AF	E	57	15/16	0.96	0.08	-	16,18,22,24	0
2	0AF	C	57	15/16	0.97	0.08	-	17,20,22,25	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	EDO	F	388	4/4	0.86	0.17	13.45	33,33,34,40	0
9	MES	F	387	12/12	0.97	0.12	4.71	23,39,44,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	PEG	B	374	7/7	0.79	0.21	3.70	24,37,45,47	0
5	NA	A	402	1/1	0.98	0.09	2.08	26,26,26,26	0
8	EDO	D	387	4/4	0.90	0.12	2.02	25,28,31,32	0
7	PEG	A	374	7/7	0.89	0.14	1.52	26,31,37,37	0
8	EDO	B	376	4/4	0.88	0.09	0.91	36,42,47,48	0
6	HEC	B	600	43/43	0.99	0.11	0.34	9,13,16,18	0
6	HEC	A	500	43/43	0.99	0.10	0.21	13,15,18,19	0
6	HEC	A	600	43/43	0.99	0.10	0.11	13,16,18,19	0
6	HEC	B	500	43/43	0.98	0.09	-0.12	12,16,19,22	0
4	CA	B	400	1/1	1.00	0.07	-1.17	16,16,16,16	0
5	NA	B	402	1/1	0.99	0.04	-1.41	24,24,24,24	0
4	CA	A	400	1/1	1.00	0.04	-2.35	19,19,19,19	0
5	NA	B	401	1/1	0.96	0.23	-	30,30,30,30	0
7	PEG	B	375	7/7	0.85	0.10	-	43,48,52,53	0
5	NA	A	401	1/1	0.95	0.14	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.