



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:42 PM GMT

PDB ID : 3RN1
Title : Crystal Structure of the W199E-MauG/pre-MethylamineDehydrogenase Complex
Authors : Jensen, L.M.R.; Wilmot, C.M.
Deposited on : 2011-04-21
Resolution : 1.93 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

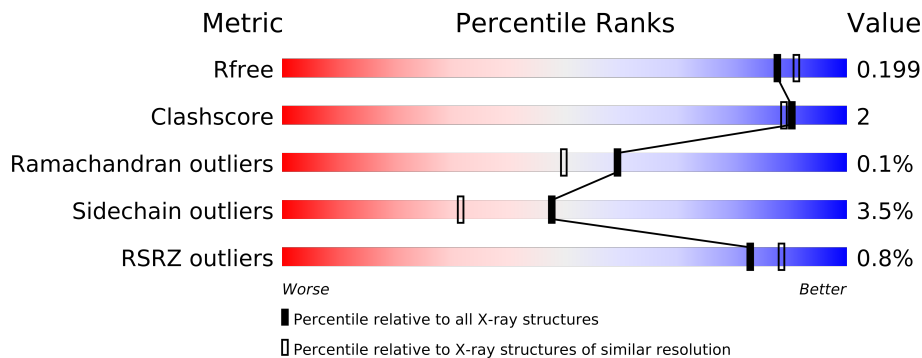
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.93 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}	66092	2024 (1.96-1.92)
Clashscore	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)
RSRZ outliers	66119	2024 (1.96-1.92)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	ACT	F	389	-	X
9	PG4	F	388	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14914 atoms, of which 0 are hydrogen and 0 are deuterium.

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	354	Total	C	N	O	S	0	1	0
			2735	1705	490	529	11			
1	B	355	Total	C	N	O	S	0	0	0
			2738	1706	490	531	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	GLU	TRP	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	199	GLU	TRP	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	2	0
			1021	630	179	198	14			
2	E	124	Total	C	N	O	S	0	1	0
			951	589	160	188	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	133	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	134	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	135	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	136	HIS	-	EXPRESSION TAG	UNP A1BBA0
C	137	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	132	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	133	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	134	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	135	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	136	HIS	-	EXPRESSION TAG	UNP A1BBA0
E	137	HIS	-	EXPRESSION TAG	UNP A1BBA0

- 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	2	0
			2932	1859	503	561	9			
3	F	376	Total	C	N	O	S	0	2	0
			2932	1859	503	561	9			

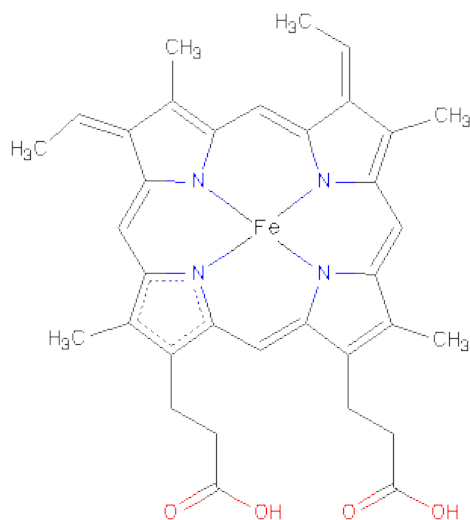
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

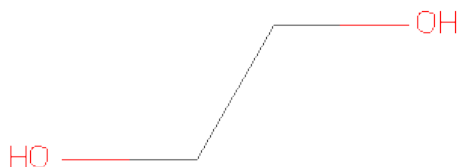
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	2	Total	Na	0	0
			2	2		

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



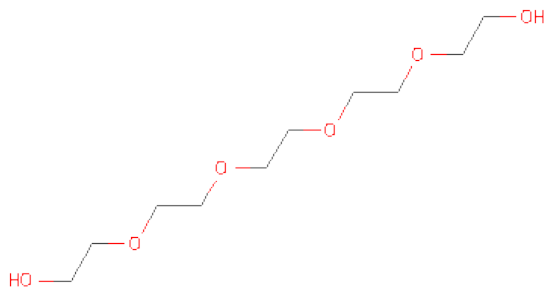
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



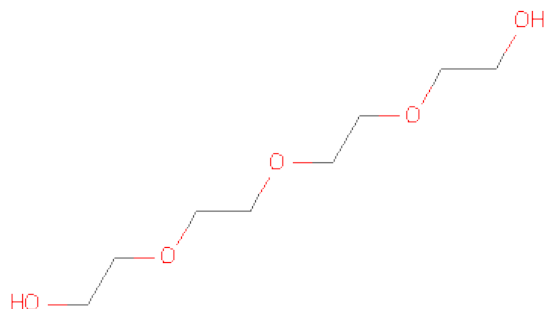
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



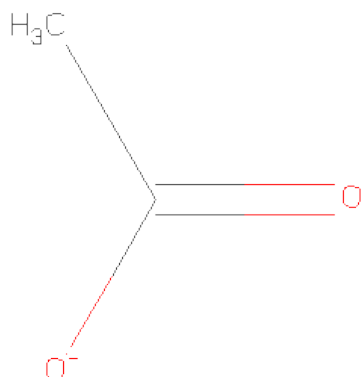
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			16	10	6		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

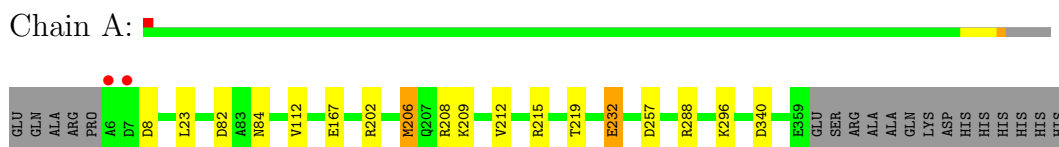
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	285	Total	O	0	0
			285	285		
11	B	277	Total	O	0	0
			277	277		
11	C	98	Total	O	0	0
			98	98		
11	D	280	Total	O	0	0
			280	280		
11	E	101	Total	O	0	0
			101	101		
11	F	349	Total	O	0	0
			349	349		

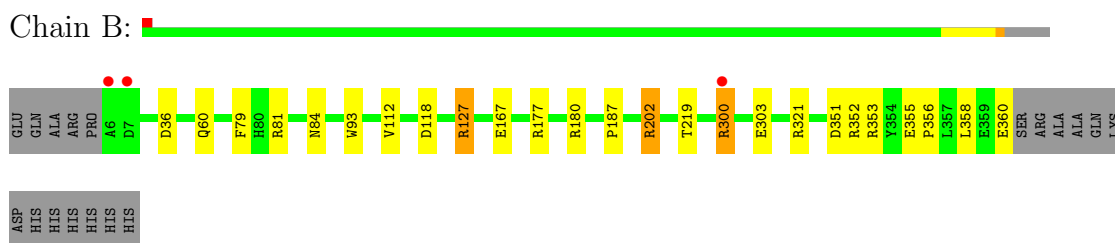
3 Residue-property plots

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: Methylamine utilization protein MauG



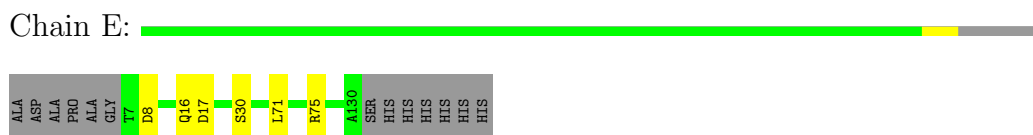
- Molecule 1: Methylamine utilization protein MauG



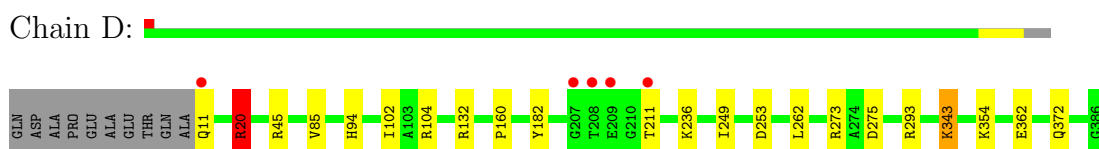
- Molecule 2: Methylamine dehydrogenase light chain



- Molecule 2: Methylamine dehydrogenase light chain

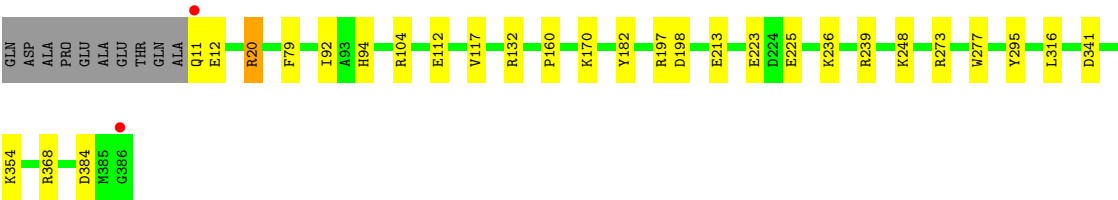


- Molecule 3: Methylamine dehydrogenase heavy chain



- 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	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	43.46 – 1.93 43.46 – 1.93	Depositor EDS
% Data completeness (in resolution range)	96.8 (43.46-1.93) 96.9 (43.46-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.00 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.144 , 0.192 0.150 , 0.199	Depositor DCC
R_{free} test set	6302 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 22.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 126581 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14914	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, ACT, EDO, 1PE, PG4, 0AF, HEC

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	1.11	2/2800 (0.1%)	0.96	5/3798 (0.1%)
1	B	1.07	3/2800 (0.1%)	0.98	12/3798 (0.3%)
2	C	1.06	0/1041	0.91	1/1418 (0.1%)
2	E	1.19	1/963 (0.1%)	0.98	4/1315 (0.3%)
3	D	1.10	1/3015 (0.0%)	0.95	5/4108 (0.1%)
3	F	1.20	3/3015 (0.1%)	0.99	8/4108 (0.2%)
All	All	1.12	10/13634 (0.1%)	0.97	35/18545 (0.2%)

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
2	C	1	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	75	ARG	CG-CD	-6.44	1.35	1.51
3	F	79	PHE	CE1-CZ	6.01	1.48	1.37
3	F	277	TRP	CZ3-CH2	5.57	1.49	1.40
1	B	79	PHE	CE1-CZ	5.55	1.48	1.37
1	A	232	GLU	CB-CG	-5.30	1.42	1.52
1	B	303	GLU	CD-OE1	5.27	1.31	1.25
1	B	93	TRP	CB-CG	5.14	1.59	1.50
1	A	212	VAL	CB-CG2	5.11	1.63	1.52
3	D	85	VAL	CB-CG2	5.04	1.63	1.52
3	F	213	GLU	CD-OE1	5.02	1.31	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ARG	NE-CZ-NH1	-12.20	114.20	120.30
1	A	208	ARG	NE-CZ-NH2	-10.22	115.19	120.30
3	D	20	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	208	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	B	180	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	B	127	ARG	NE-CZ-NH2	-7.59	116.50	120.30
2	E	75	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	B	202	ARG	NE-CZ-NH2	7.48	124.04	120.30
2	C	8	ASP	CB-CG-OD1	6.75	124.38	118.30
3	F	198	ASP	CB-CG-OD1	6.68	124.31	118.30
3	F	273	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	206	MET	CG-SD-CE	-6.57	89.69	100.20
1	B	118	ASP	CB-CG-OD1	6.52	124.17	118.30
3	D	20	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	177	ARG	NE-CZ-NH1	6.13	123.36	120.30
3	F	239	ARG	NE-CZ-NH2	-6.07	117.27	120.30
3	F	104	ARG	CG-CD-NE	-5.97	99.26	111.80
3	F	341	ASP	CB-CG-OD1	5.78	123.50	118.30
2	E	75	ARG	CA-CB-CG	-5.72	100.81	113.40
3	D	273	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	B	36	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	36	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	257	ASP	CB-CG-OD2	-5.42	113.42	118.30
3	D	132	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	202	ARG	CG-CD-NE	-5.36	100.55	111.80
1	B	127	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	E	8	ASP	CB-CG-OD1	5.31	123.08	118.30
3	F	170	LYS	CD-CE-NZ	-5.28	99.55	111.70
1	A	82	ASP	CB-CG-OD2	5.20	122.98	118.30
3	F	20	ARG	CG-CD-NE	-5.20	100.88	111.80
3	F	132	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	180	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	E	8	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	B	351	ASP	CB-CG-OD1	5.06	122.86	118.30
3	D	253	ASP	CB-CG-OD1	5.06	122.85	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	57	0AF	CA

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2735	0	0	2	0
1	B	2738	0	0	4	0
2	C	1021	0	0	5	0
2	E	951	0	0	1	0
3	D	2932	0	0	7	0
3	F	2932	0	0	10	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	0	0	0
6	B	86	0	0	0	0
7	B	4	0	6	0	0
8	F	16	0	22	0	0
9	F	13	0	18	1	0
10	F	4	0	3	0	0
11	A	285	0	0	1	0
11	B	277	0	0	3	0
11	C	98	0	0	2	0
11	D	280	0	0	3	0
11	E	101	0	0	0	0
11	F	349	0	0	5	0
All	All	14914	0	49	28	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (28) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:372[B]:GLN:NE2	11:D:1225:HOH:O	1.77	1.15
2:C:127:VAL:CG2	2:C:127:VAL:O	2.34	0.75
3:D:20:ARG:NH2	2:E:17:ASP:O	2.28	0.66
2:C:129:LYS:O	2:C:130:ALA:CB	2.47	0.62
1:A:215:ARG:N	11:A:755:HOH:O	2.33	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:12:GLU:OE2	3:F:20:ARG:NH1	2.33	0.60
3:D:104:ARG:NE	11:D:948:HOH:O	2.39	0.55
3:F:197:ARG:NE	11:F:1100:HOH:O	2.41	0.53
3:D:236:LYS:NZ	11:D:959:HOH:O	2.42	0.51
3:F:236:LYS:NZ	3:F:384:ASP:O	2.43	0.51
2:C:135:HIS:CE1	11:C:696:HOH:O	2.66	0.48
9:F:388:PG4:H12	11:F:1039:HOH:O	2.14	0.48
2:C:57:0AF:CE3	2:C:108:TRP:CD1	2.97	0.47
1:A:288:ARG:NH1	1:A:340:ASP:OD1	2.49	0.46
3:F:248:LYS:CE	11:F:949:HOH:O	2.64	0.46
3:D:45:ARG:NH2	3:D:343:LYS:O	2.49	0.45
1:B:353:ARG:NE	11:B:1263:HOH:O	2.50	0.44
1:B:300:ARG:NH1	11:B:699:HOH:O	2.51	0.43
1:B:355:GLU:N	1:B:356:PRO:CD	2.82	0.43
2:C:135:HIS:CD2	11:C:348:HOH:O	2.72	0.41
1:B:127:ARG:NH1	11:B:1342:HOH:O	2.53	0.41
3:D:104:ARG:NH2	3:F:112:GLU:OE2	2.54	0.41
3:F:248:LYS:NZ	11:F:949:HOH:O	2.54	0.41
3:F:225:GLU:OE2	3:F:248:LYS:NZ	2.53	0.41
3:F:368:ARG:NH2	11:F:1097:HOH:O	2.54	0.40
3:F:295:TYR:CD1	3:F:295:TYR:N	2.90	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	353/373 (95%)	344 (98%)	9 (2%)	0	100	100
1	B	353/373 (95%)	345 (98%)	8 (2%)	0	100	100
2	C	130/137 (95%)	125 (96%)	4 (3%)	1 (1%)	27	12
2	E	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
3	D	376/386 (97%)	364 (97%)	11 (3%)	1 (0%)	50	37
3	F	376/386 (97%)	363 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1710/1792 (95%)	1660 (97%)	48 (3%)	2 (0%)	59 50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	130	ALA
3	D	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	277/292 (95%)	266 (96%)	11 (4%)	42 26
1	B	277/292 (95%)	264 (95%)	13 (5%)	36 18
2	C	112/112 (100%)	111 (99%)	1 (1%)	87 86
2	E	104/112 (93%)	101 (97%)	3 (3%)	55 40
3	D	306/311 (98%)	294 (96%)	12 (4%)	43 26
3	F	306/311 (98%)	298 (97%)	8 (3%)	59 45
All	All	1382/1430 (97%)	1334 (96%)	48 (4%)	48 31

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	23	LEU
1	A	84	ASN
1	A	112	VAL
1	A	167	GLU
1	A	202	ARG
1	A	206	MET
1	A	209	LYS
1	A	219	THR
1	A	232	GLU
1	A	296	LYS
1	B	60	GLN

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Mol	Chain	Res	Type
1	B	81	ARG
1	B	84	ASN
1	B	112	VAL
1	B	167	GLU
1	B	187	PRO
1	B	202	ARG
1	B	219	THR
1	B	300	ARG
1	B	321	ARG
1	B	352	ARG
1	B	358	LEU
1	B	360	GLU
2	C	7	THR
3	D	11	GLN
3	D	20	ARG
3	D	94	HIS
3	D	160	PRO
3	D	211	THR
3	D	249	ILE
3	D	262	LEU
3	D	275	ASP
3	D	293	ARG
3	D	343	LYS
3	D	354	LYS
3	D	362	GLU
2	E	16	GLN
2	E	30	SER
2	E	71	LEU
3	F	11	GLN
3	F	92	ILE
3	F	94	HIS
3	F	117	VAL
3	F	160	PRO
3	F	223	GLU
3	F	316	LEU
3	F	354	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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	16,16,17	5.59	5 (31%)	19,22,24	2.31	7 (36%)
2	0AF	E	57	2	16,16,17	4.06	5 (31%)	19,22,24	2.48	5 (26%)

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	1/1/1/2	0/4/6/8	0/0/2/2
2	0AF	E	57	2	-	0/4/6/8	0/0/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	0AF	O-C	21.57	1.26	1.11
2	E	57	0AF	O-C	15.03	1.21	1.11
2	E	57	0AF	CB-CG	3.33	1.56	1.51
2	E	57	0AF	CZ3-CE3	3.08	1.43	1.36
2	C	57	0AF	CZ3-CE3	2.96	1.43	1.36
2	C	57	0AF	CB-CG	2.36	1.55	1.51
2	C	57	0AF	CD1-CG	2.29	1.41	1.37
2	E	57	0AF	CD2-CE2	-2.20	1.37	1.41
2	C	57	0AF	CD2-CE2	-2.14	1.37	1.41
2	E	57	0AF	CH2-CZ2	2.11	1.42	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	0AF	CH2-CZ2-CE2	7.12	124.12	118.40
2	C	57	0AF	CG-CB-CA	-5.61	100.00	114.16
2	E	57	0AF	CG-CB-CA	-4.57	102.64	114.16
2	C	57	0AF	CH2-CZ2-CE2	4.44	121.97	118.40
2	C	57	0AF	CB-CA-N	3.49	128.27	112.03
2	E	57	0AF	CB-CA-N	3.24	127.12	112.03
2	C	57	0AF	C-CA-N	-3.07	110.76	113.83
2	E	57	0AF	CZ3-CH2-CZ2	-2.94	116.54	120.34
2	E	57	0AF	C-CA-N	-2.93	110.90	113.83
2	C	57	0AF	CB-CG-CD1	-2.44	123.94	128.12
2	C	57	0AF	CD1-NE1-CE2	2.42	111.90	107.66
2	C	57	0AF	CE3-CZ3-CH2	-2.32	116.99	120.92

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	57	0AF	CA

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	HEC	A	500	1	50,50,50	3.29	20 (40%)	56,82,82	3.34	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEC	A	600	1	50,50,50	2.94	25 (50%)	56,82,82	3.67	28 (50%)
7	EDO	B	374	-	3,3,3	0.64	0	2,2,2	0.32	0
6	HEC	B	500	1	50,50,50	3.11	20 (40%)	56,82,82	3.35	32 (57%)
6	HEC	B	600	1	50,50,50	2.71	20 (40%)	56,82,82	3.53	26 (46%)
8	1PE	F	387	-	15,15,15	0.60	0	14,14,14	0.53	0
9	PG4	F	388	-	12,12,12	0.55	0	11,11,11	0.48	0
10	ACT	F	389	-	1,3,3	0.62	0	0,3,3	0.00	-

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	HEC	A	500	1	-	0/10/54/54	0/0/8/8
6	HEC	A	600	1	-	0/10/54/54	0/0/8/8
7	EDO	B	374	-	-	0/1/1/1	0/0/0/0
6	HEC	B	500	1	-	0/10/54/54	0/0/8/8
6	HEC	B	600	1	-	0/10/54/54	0/0/8/8
8	1PE	F	387	-	-	0/13/13/13	0/0/0/0
9	PG4	F	388	-	-	0/10/10/10	0/0/0/0
10	ACT	F	389	-	-	0/0/0/0	0/0/0/0

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	500	HEC	C3B-CAB	9.12	1.54	1.35
6	B	600	HEC	C3B-CAB	8.97	1.53	1.35
6	B	500	HEC	C3B-CAB	8.38	1.52	1.35
6	A	500	HEC	C1D-C2D	8.27	1.50	1.40
6	A	600	HEC	C3C-CAC	8.01	1.51	1.35
6	A	500	HEC	C3C-CAC	7.86	1.51	1.35
6	B	500	HEC	C3C-CAC	7.68	1.51	1.35
6	A	500	HEC	C1B-C2B	7.53	1.49	1.40
6	B	600	HEC	C3C-CAC	7.49	1.50	1.35
6	B	500	HEC	C1D-C2D	7.40	1.49	1.40
6	A	600	HEC	C3B-CAB	7.31	1.50	1.35
6	B	500	HEC	C1C-C2C	6.65	1.48	1.40
6	A	500	HEC	C3B-C4B	6.55	1.49	1.41
6	A	500	HEC	C1C-C2C	6.18	1.47	1.40
6	B	500	HEC	C3C-C4C	5.94	1.49	1.41
6	A	600	HEC	C3B-C4B	5.76	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	HEC	C1B-C2B	5.71	1.47	1.40
6	B	600	HEC	C1C-C2C	5.54	1.47	1.40
6	B	500	HEC	C1B-C2B	5.49	1.47	1.40
6	B	500	HEC	C3B-C4B	5.29	1.48	1.41
6	A	600	HEC	C1C-C2C	5.22	1.46	1.40
6	B	600	HEC	C1D-C2D	4.65	1.46	1.40
6	B	600	HEC	C1B-C2B	4.59	1.45	1.40
6	A	500	HEC	C3C-C4C	4.48	1.47	1.41
6	A	600	HEC	C3C-C4C	4.38	1.47	1.41
6	A	600	HEC	C1D-C2D	4.26	1.45	1.40
6	B	500	HEC	C1A-CHA	3.96	1.50	1.38
6	A	500	HEC	FE-NA	3.87	2.09	1.92
6	A	500	HEC	C1D-CHD	3.84	1.50	1.39
6	A	600	HEC	C4C-NC	-3.82	1.31	1.37
6	B	600	HEC	C1A-NA	-3.77	1.31	1.37
6	B	500	HEC	FE-NB	3.72	2.08	1.92
6	A	500	HEC	C4D-C3D	3.71	1.49	1.43
6	A	500	HEC	FE-NB	3.68	2.08	1.92
6	B	500	HEC	FE-NC	3.65	2.08	1.92
6	A	600	HEC	FE-ND	3.61	2.08	1.92
6	A	600	HEC	C4A-NA	-3.57	1.32	1.37
6	B	500	HEC	C1C-CHC	3.54	1.49	1.39
6	A	500	HEC	FE-ND	3.53	2.07	1.92
6	A	600	HEC	C4B-NB	-3.51	1.32	1.37
6	A	600	HEC	FE-NA	3.51	2.07	1.92
6	B	500	HEC	C4D-C3D	3.51	1.49	1.43
6	B	600	HEC	FE-NA	3.45	2.07	1.92
6	B	500	HEC	FE-ND	3.29	2.06	1.92
6	B	600	HEC	C3B-C4B	3.27	1.45	1.41
6	A	600	HEC	FE-NC	3.25	2.06	1.92
6	A	500	HEC	FE-NC	3.24	2.06	1.92
6	A	600	HEC	C4B-CHC	3.23	1.48	1.38
6	B	500	HEC	C4C-CHD	3.12	1.48	1.38
6	B	600	HEC	C1A-CHA	3.09	1.47	1.38
6	A	500	HEC	C4C-CHD	3.08	1.47	1.38
6	B	600	HEC	C3C-C4C	3.00	1.45	1.41
6	B	600	HEC	C4B-NB	-3.00	1.32	1.37
6	A	500	HEC	C1C-CHC	3.00	1.48	1.39
6	A	500	HEC	C4A-CHB	2.94	1.47	1.38
6	B	600	HEC	C4A-NA	-2.94	1.32	1.37
6	B	500	HEC	C1B-CHB	2.92	1.47	1.39
6	B	500	HEC	FE-NA	2.92	2.04	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	500	HEC	C4B-CHC	2.92	1.47	1.38
6	A	500	HEC	C1A-CHA	2.91	1.47	1.38
6	A	600	HEC	C1D-CHD	2.91	1.47	1.39
6	B	600	HEC	C4C-NC	-2.91	1.32	1.37
6	A	600	HEC	FE-NB	2.88	2.04	1.92
6	A	600	HEC	C1C-CHC	2.85	1.47	1.39
6	B	600	HEC	C4B-CHC	2.76	1.46	1.38
6	B	600	HEC	C1D-CHD	2.76	1.47	1.39
6	A	600	HEC	C4D-C3D	2.72	1.48	1.43
6	B	600	HEC	FE-NC	2.68	2.03	1.92
6	A	600	HEC	C4C-CHD	2.65	1.46	1.38
6	A	600	HEC	C4A-CHB	2.64	1.46	1.38
6	B	500	HEC	C4A-CHB	2.61	1.46	1.38
6	A	600	HEC	O2A-CGA	-2.50	1.21	1.30
6	B	500	HEC	C1D-CHD	2.42	1.46	1.39
6	A	600	HEC	C1A-CHA	2.36	1.45	1.38
6	A	600	HEC	C1C-NC	-2.33	1.32	1.36
6	A	500	HEC	C4A-C3A	2.30	1.51	1.43
6	A	600	HEC	C1B-CHB	2.27	1.46	1.39
6	B	600	HEC	FE-NB	2.26	2.02	1.92
6	A	600	HEC	C4D-CHA	2.25	1.46	1.39
6	A	500	HEC	C4A-NA	-2.23	1.33	1.37
6	B	600	HEC	C1C-CHC	2.22	1.46	1.39
6	B	600	HEC	C4A-CHB	2.17	1.45	1.38
6	B	500	HEC	C4D-CHA	2.04	1.45	1.39
6	B	600	HEC	FE-ND	2.03	2.01	1.92
6	A	500	HEC	C4C-NC	-2.03	1.34	1.37

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	HEC	C2D-C1D-ND	9.11	116.29	109.41
6	B	600	HEC	CBB-CAB-C3B	-8.88	103.43	128.44
6	A	500	HEC	C4B-C3B-C2B	-8.44	101.29	106.68
6	A	600	HEC	CBB-CAB-C3B	-8.17	105.43	128.44
6	B	500	HEC	C2D-C1D-ND	8.05	115.49	109.41
6	A	600	HEC	CMC-C2C-C3C	7.60	134.11	125.72
6	A	600	HEC	CBD-CAD-C3D	-7.53	99.43	112.69
6	B	600	HEC	C3B-C2B-C1B	-7.47	102.10	107.07
6	A	500	HEC	C2B-C1B-NB	7.46	115.04	109.41
6	A	500	HEC	CBB-CAB-C3B	-7.43	107.53	128.44
6	B	600	HEC	C2B-C1B-NB	7.32	114.94	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	500	HEC	CBB-CAB-C3B	-7.30	107.89	128.44
6	B	600	HEC	C4A-C3A-C2A	-7.21	102.31	106.89
6	B	600	HEC	C3A-C4A-NA	7.07	114.75	109.41
6	B	600	HEC	CBD-CAD-C3D	-7.01	100.35	112.69
6	A	600	HEC	C2B-C1B-NB	6.92	114.63	109.41
6	A	600	HEC	C3A-C4A-NA	6.76	114.52	109.41
6	B	600	HEC	C2D-C1D-ND	6.66	114.44	109.41
6	B	500	HEC	C2B-C1B-NB	6.59	114.39	109.41
6	A	600	HEC	CBC-CAC-C3C	-6.55	110.01	128.44
6	B	500	HEC	C2C-C1C-NC	6.39	114.24	109.41
6	A	500	HEC	C4A-C3A-C2A	-6.35	102.85	106.89
6	A	600	HEC	C3B-C2B-C1B	-6.27	102.90	107.07
6	A	500	HEC	C3A-C4A-NA	6.22	114.11	109.41
6	A	600	HEC	C1D-C2D-C3D	-6.16	102.71	107.00
6	A	500	HEC	C2D-C1D-ND	6.14	114.05	109.41
6	B	600	HEC	C1D-C2D-C3D	-6.03	102.80	107.00
6	A	600	HEC	C2C-C1C-NC	5.95	113.91	109.41
6	B	600	HEC	CMB-C2B-C3B	5.53	131.83	125.72
6	A	600	HEC	C3C-C2C-C1C	-5.40	103.48	107.07
6	B	600	HEC	C2A-C1A-NA	5.36	113.66	109.64
6	B	500	HEC	CBD-CAD-C3D	-5.32	103.31	112.69
6	B	600	HEC	C4C-C3C-C2C	-5.15	103.39	106.68
6	A	500	HEC	C2A-C1A-NA	4.99	113.38	109.64
6	B	500	HEC	C4C-C3C-C2C	-4.95	103.52	106.68
6	B	500	HEC	C2A-C1A-NA	4.91	113.32	109.64
6	A	500	HEC	CMB-C2B-C3B	4.78	131.00	125.72
6	B	600	HEC	CBC-CAC-C3C	-4.76	115.04	128.44
6	B	500	HEC	C3D-C4D-ND	4.74	116.32	109.73
6	B	600	HEC	C2C-C1C-NC	4.65	112.92	109.41
6	B	500	HEC	C3C-C2C-C1C	-4.63	103.99	107.07
6	B	500	HEC	C4D-C3D-C2D	-4.62	102.14	106.92
6	B	500	HEC	C4D-ND-C1D	-4.58	100.73	106.76
6	B	500	HEC	CMB-C2B-C3B	4.54	130.73	125.72
6	A	500	HEC	CBC-CAC-C3C	-4.49	115.79	128.44
6	A	500	HEC	CMC-C2C-C3C	4.45	130.63	125.72
6	B	500	HEC	C3B-C2B-C1B	-4.38	104.16	107.07
6	A	500	HEC	CBD-CAD-C3D	-4.34	105.05	112.69
6	B	500	HEC	CMC-C2C-C3C	4.13	130.28	125.72
6	B	600	HEC	CBA-CAA-C2A	-4.11	104.67	112.35
6	A	600	HEC	C4C-C3C-C2C	-4.10	104.06	106.68
6	B	500	HEC	CBC-CAC-C3C	-4.05	117.04	128.44
6	B	500	HEC	C1A-C2A-C3A	-4.05	103.49	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	HEC	CMC-C2C-C1C	-4.04	122.41	128.62
6	A	600	HEC	CMB-C2B-C3B	4.03	130.17	125.72
6	A	500	HEC	C3C-C2C-C1C	-4.01	104.40	107.07
6	B	500	HEC	C4C-CHD-C1D	-3.99	122.22	127.47
6	B	600	HEC	C3C-C2C-C1C	-3.95	104.44	107.07
6	A	500	HEC	C2C-C1C-NC	3.91	112.36	109.41
6	B	600	HEC	C4B-CHC-C1C	-3.90	122.33	127.47
6	A	500	HEC	C4B-NB-C1B	-3.80	101.76	106.76
6	B	500	HEC	C4B-C3B-C2B	-3.77	104.27	106.68
6	A	600	HEC	CBA-CAA-C2A	-3.76	105.32	112.35
6	A	600	HEC	C1A-C2A-C3A	-3.74	103.73	106.69
6	A	600	HEC	C4D-ND-C1D	-3.73	101.85	106.76
6	A	500	HEC	C4C-C3C-C2C	-3.73	104.30	106.68
6	A	600	HEC	C4A-C3A-C2A	-3.70	104.54	106.89
6	A	500	HEC	C4D-C3D-C2D	-3.60	103.19	106.92
6	B	500	HEC	CMA-C3A-C2A	3.56	131.66	124.94
6	A	500	HEC	C3D-C4D-ND	3.55	114.66	109.73
6	B	500	HEC	C4A-CHB-C1B	-3.52	122.84	127.47
6	A	500	HEC	C3B-C4B-NB	3.49	116.56	111.52
6	A	600	HEC	CHD-C1D-ND	-3.35	118.99	124.58
6	A	500	HEC	C4C-CHD-C1D	-3.34	123.08	127.47
6	A	600	HEC	CMD-C2D-C3D	3.33	131.22	124.94
6	A	500	HEC	C3B-C2B-C1B	-3.31	104.87	107.07
6	B	600	HEC	C1A-CHA-C4D	-3.21	123.25	127.47
6	B	600	HEC	CMA-C3A-C2A	3.21	130.99	124.94
6	B	500	HEC	C1D-C2D-C3D	-3.14	104.81	107.00
6	A	600	HEC	C4B-CHC-C1C	-3.06	123.45	127.47
6	A	500	HEC	C1A-C2A-C3A	-3.05	104.28	106.69
6	B	500	HEC	C4B-NB-C1B	-3.01	102.80	106.76
6	B	500	HEC	C3D-C4D-CHA	-3.01	120.30	126.00
6	A	600	HEC	C3D-C4D-ND	2.96	113.85	109.73
6	A	500	HEC	CMB-C2B-C1B	-2.93	124.11	128.62
6	A	500	HEC	C1D-C2D-C3D	-2.93	104.96	107.00
6	B	500	HEC	CMD-C2D-C3D	2.89	130.40	124.94
6	A	500	HEC	C4D-ND-C1D	-2.85	103.01	106.76
6	A	500	HEC	C2C-C1C-CHC	-2.79	120.72	126.00
6	B	500	HEC	C3A-C4A-NA	2.71	111.46	109.41
6	A	600	HEC	C4B-C3B-C2B	-2.59	105.02	106.68
6	B	600	HEC	CMC-C2C-C3C	2.57	128.56	125.72
6	A	600	HEC	C2A-C1A-NA	2.51	111.52	109.64
6	B	500	HEC	CMD-C2D-C1D	-2.51	124.76	128.62
6	B	600	HEC	C4C-CHD-C1D	-2.48	124.21	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	500	HEC	O2A-CGA-CBA	2.41	122.73	114.22
6	B	600	HEC	C2B-C1B-CHB	-2.38	121.48	126.00
6	A	500	HEC	CMC-C2C-C1C	-2.38	124.97	128.62
6	B	600	HEC	C2D-C1D-CHD	-2.35	121.55	126.00
6	B	600	HEC	C3C-C4C-NC	2.33	114.89	111.52
6	A	600	HEC	CAD-CBD-CGD	-2.29	106.10	113.47
6	B	500	HEC	CMB-C2B-C1B	-2.28	125.11	128.62
6	A	600	HEC	CMA-C3A-C2A	2.25	129.18	124.94
6	B	500	HEC	CAA-C2A-C1A	2.24	128.71	124.67
6	A	600	HEC	CHA-C4D-ND	-2.21	120.89	124.58
6	B	600	HEC	C2C-C1C-CHC	-2.17	121.88	126.00
6	A	600	HEC	C2B-C1B-CHB	-2.15	121.92	126.00
6	B	500	HEC	C4C-NC-C1C	-2.13	103.96	106.76
6	B	600	HEC	C4B-NB-C1B	-2.10	103.99	106.76
6	B	600	HEC	CMD-C2D-C3D	2.09	128.89	124.94
6	B	500	HEC	CBA-CAA-C2A	-2.08	108.46	112.35
6	A	500	HEC	O2D-CGD-CBD	2.05	121.45	114.22
6	B	500	HEC	C4A-C3A-C2A	-2.04	105.60	106.89
6	B	500	HEC	CHB-C1B-NB	-2.01	121.22	124.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	354/373 (94%)	-0.55	2 (0%) 86 91	8, 17, 31, 49	0
1	B	355/373 (95%)	-0.46	3 (0%) 83 88	9, 19, 34, 59	0
2	C	131/137 (95%)	-0.23	2 (1%) 70 77	9, 13, 38, 54	0
2	E	124/137 (90%)	-0.40	0 100 100	8, 13, 23, 37	0
3	D	376/386 (97%)	-0.45	5 (1%) 74 81	9, 16, 31, 55	0
3	F	376/386 (97%)	-0.52	2 (0%) 88 93	7, 13, 25, 47	0
All	All	1716/1792 (95%)	-0.47	14 (0%) 83 88	7, 16, 32, 59	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	ASP	4.6
1	B	7	ASP	4.4
1	A	6	ALA	4.4
3	D	209	GLU	4.1
3	D	207	GLY	3.9
3	D	208	THR	3.5
3	D	11	GLN	3.1
1	B	6	ALA	3.0
3	F	386	GLY	3.0
2	C	137	HIS	2.8
3	F	11	GLN	2.7
3	D	211	THR	2.6
1	B	300	ARG	2.3
2	C	133	HIS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	0AF	E	57	15/16	0.12	1.49	10,12,14,17	0
2	0AF	C	57	15/16	0.10	0.19	12,14,17,17	0

6.3 Carbohydrates ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
10	ACT	F	389	4/4	0.12	5.74	23,25,28,28	0
9	PG4	F	388	13/13	0.12	2.13	41,47,56,57	0
8	1PE	F	387	16/16	0.12	1.92	22,34,45,47	0
4	CA	A	400	1/1	0.07	1.66	11,11,11,11	0
7	EDO	B	374	4/4	0.13	1.35	33,37,39,41	0
5	NA	B	401	1/1	0.13	1.18	36,36,36,36	0
6	HEC	A	500	43/43	0.07	0.66	7,12,16,19	0
6	HEC	B	600	43/43	0.08	-0.02	4,8,11,14	0
4	CA	B	400	1/1	0.06	-0.27	10,10,10,10	0
5	NA	B	402	1/1	0.07	-0.29	24,24,24,24	0
6	HEC	B	500	43/43	0.06	-0.34	7,12,16,18	0
6	HEC	A	600	43/43	0.07	-0.37	8,10,12,15	0
5	NA	A	401	1/1	0.06	-0.62	23,23,23,23	0
5	NA	A	402	1/1	0.03	-3.98	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.