



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:07 PM GMT

PDB ID : 3SXT  
Title : Crystal Structure of the Quinol Form of Methylamine Dehydrogenase in Complex with the Diferrous Form of MauG  
Authors : Jensen, L.M.R.; Wilmot, C.M.  
Deposited on : 2011-07-15  
Resolution : 1.81 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](mailto: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.

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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

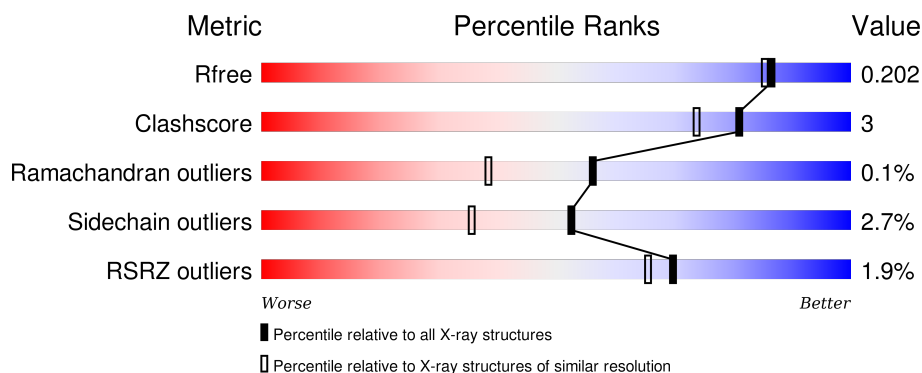
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.81 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	5422 (1.84-1.80)
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (1.84-1.80)

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  $\geq 3$ , 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	<div> <div>2%</div> <div>88% 7% 5%</div> </div>
1	B	373	<div> <div>2%</div> <div>86% 9% . .</div> </div>
2	C	137	<div> <div>%</div> <div>81% 8% . 9%</div> </div>
2	E	137	<div> <div>%</div> <div>81% 9% . 9%</div> </div>
3	D	386	<div> <div>%</div> <div>87% 10% .</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	386	

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
7	EDO	B	406	-	-	-	X
7	EDO	D	401	-	-	X	X
7	EDO	F	401	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15339 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	354	Total	C	N	O	S	0	0	0
			2734	1707	490	526	11			
1	B	357	Total	C	N	O	S	0	4	0
			2789	1740	505	532	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	125	Total	C	N	O	S	0	1	0
			961	594	161	193	13			
2	E	125	Total	C	N	O	S	0	1	0
			958	592	161	191	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	375	Total	C	N	O	S	0	4	0
			2943	1868	509	558	8			
3	F	376	Total	C	N	O	S	0	2	0
			2932	1861	502	561	8			

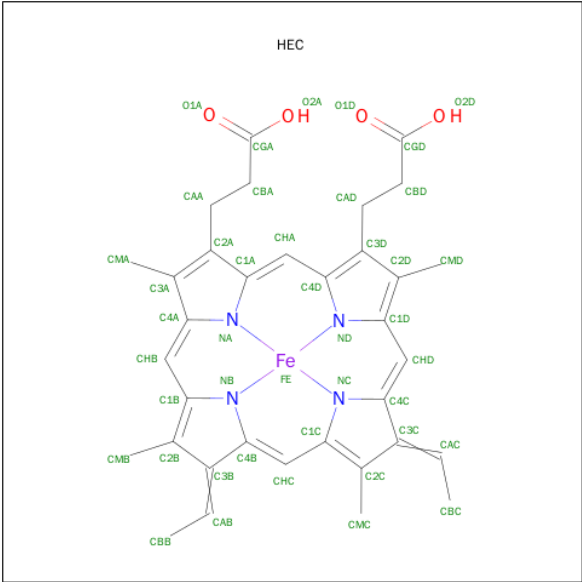
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

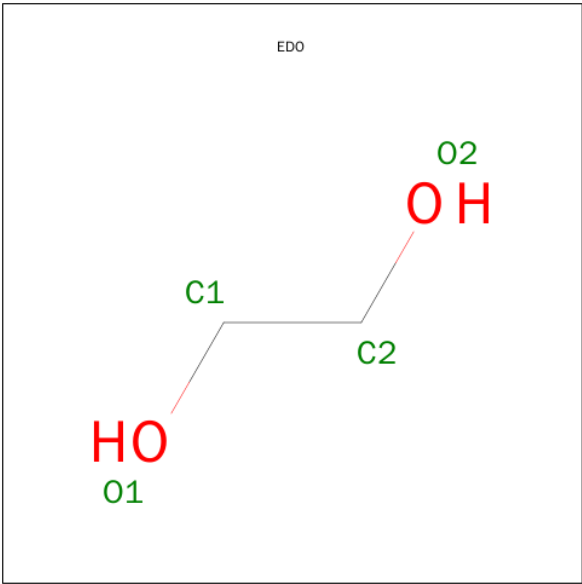
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

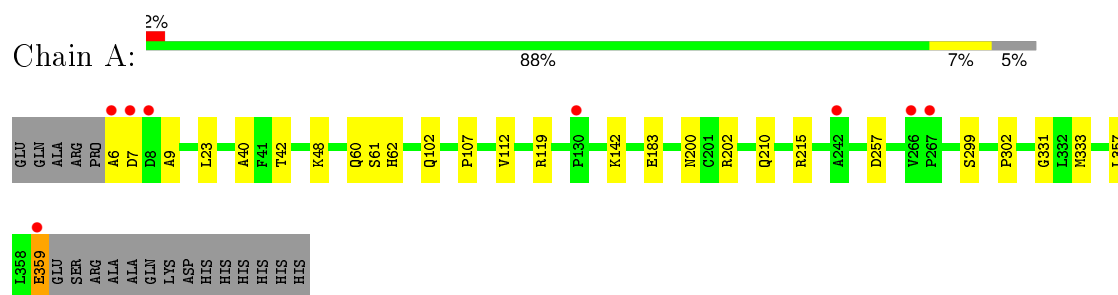
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	340	Total O 340 340	0	0
8	B	358	Total O 358 358	0	0
8	C	123	Total O 123 123	0	0
8	D	452	Total O 452 452	0	0
8	E	138	Total O 138 138	0	0
8	F	413	Total O 413 413	0	0

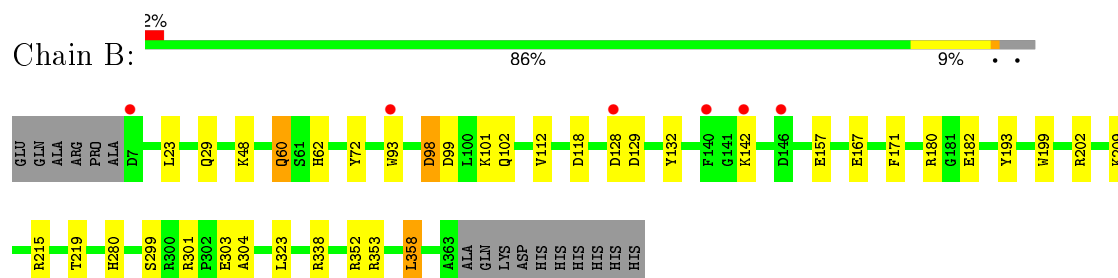
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

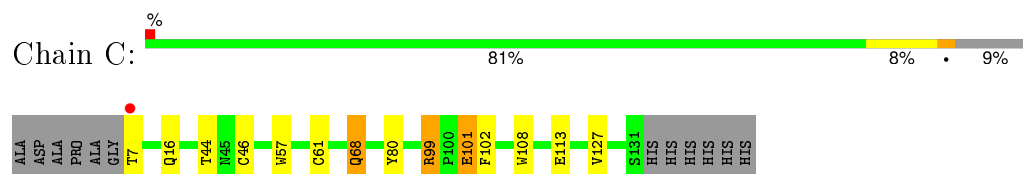
- Molecule 1: Methylamine utilization protein MauG



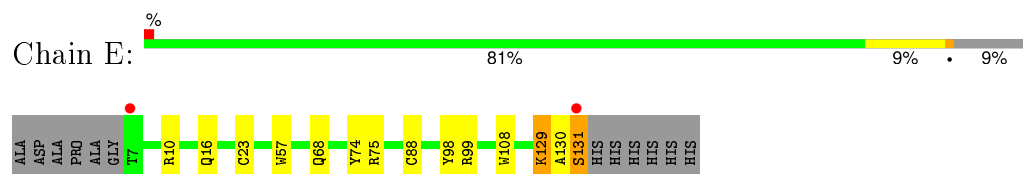
- Molecule 1: Methylamine utilization protein MauG



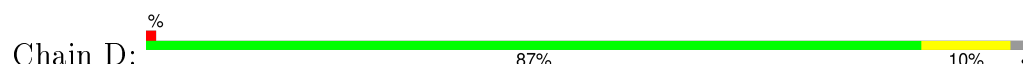
- Molecule 2: Methylamine dehydrogenase light chain



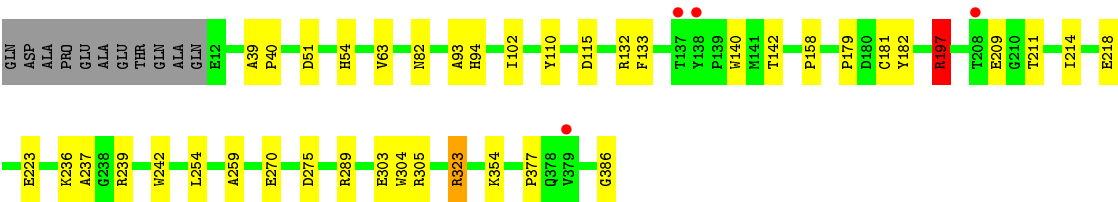
- Molecule 2: Methylamine dehydrogenase light chain



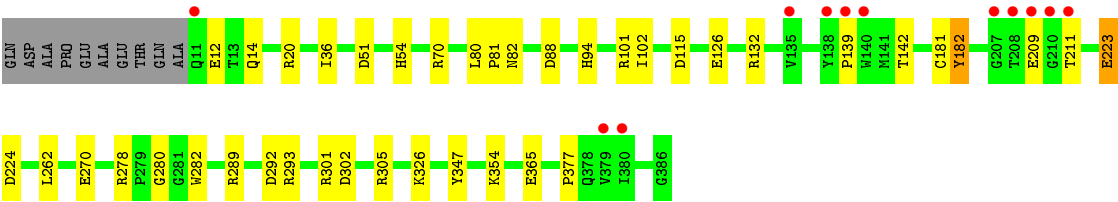
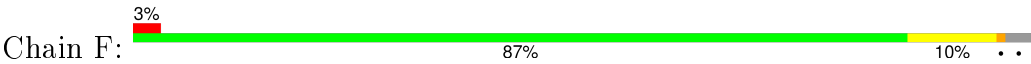
- Molecule 3: Methylamine dehydrogenase heavy chain







● Molecule 3: Methylamine dehydrogenase heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.64Å 135.66Å 111.56Å 90.00° 97.37° 90.00°	Depositor
Resolution (Å)	35.01 – 1.81 35.01 – 1.81	Depositor EDS
% Data completeness (in resolution range)	97.9 (35.01-1.81) 97.9 (35.01-1.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.145 , 0.187 0.162 , 0.202	Depositor DCC
$R_{free}$ test set	8245 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.0	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 163981 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15339	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, CA, TOQ, EDO, 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	1.13	1/2798 (0.0%)	0.94	2/3797 (0.1%)
1	B	1.22	6/2865 (0.2%)	1.03	13/3883 (0.3%)
2	C	1.28	5/972 (0.5%)	0.98	1/1327 (0.1%)
2	E	1.35	2/969 (0.2%)	1.04	2/1323 (0.2%)
3	D	1.23	6/3032 (0.2%)	1.05	5/4129 (0.1%)
3	F	1.19	4/3015 (0.1%)	1.01	12/4109 (0.3%)
All	All	1.21	24/13651 (0.2%)	1.01	35/18568 (0.2%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	303	GLU	CD-OE1	8.33	1.34	1.25
2	C	80	TYR	CD1-CE1	6.52	1.49	1.39
3	F	347	TYR	CD2-CE2	6.14	1.48	1.39
1	B	199	TRP	CB-CG	5.91	1.60	1.50
3	F	282	TRP	CB-CG	5.80	1.60	1.50
1	B	182	GLU	CB-CG	-5.80	1.41	1.52
2	C	113	GLU	CB-CG	-5.67	1.41	1.52
2	C	61	CYS	CB-SG	5.61	1.91	1.82
3	D	242	TRP	CE3-CZ3	5.59	1.48	1.38
3	D	63	VAL	CB-CG2	5.48	1.64	1.52
1	A	40	ALA	CA-CB	5.40	1.63	1.52
2	E	98	TYR	CD2-CE2	5.39	1.47	1.39
3	D	140	TRP	CE3-CZ3	5.27	1.47	1.38
1	B	157	GLU	CG-CD	-5.27	1.44	1.51
3	D	93	ALA	CA-CB	5.27	1.63	1.52
3	D	110	TYR	CD2-CE2	5.24	1.47	1.39
1	B	72	TYR	CD1-CE1	5.19	1.47	1.39
1	B	193	TYR	CD2-CE2	5.13	1.47	1.39
3	F	182	TYR	CG-CD2	5.13	1.45	1.39
2	E	74	TYR	CD1-CE1	5.13	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	101[A]	GLU	CD-OE1	-5.05	1.20	1.25
2	C	101[B]	GLU	CD-OE1	-5.05	1.20	1.25
3	D	133	PHE	CD1-CE1	5.03	1.49	1.39
3	F	270	GLU	CD-OE2	-5.02	1.20	1.25

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	132	ARG	NE-CZ-NH1	8.71	124.65	120.30
3	D	305	ARG	NE-CZ-NH2	-7.81	116.39	120.30
3	D	197	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	180	ARG	NE-CZ-NH2	7.05	123.83	120.30
2	C	99	ARG	NE-CZ-NH1	-6.97	116.81	120.30
3	F	88	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	257	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	B	353	ARG	NE-CZ-NH1	6.50	123.55	120.30
3	F	101	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	180	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	B	358	LEU	CB-CG-CD2	6.31	121.73	111.00
3	F	132	ARG	NE-CZ-NH2	-6.29	117.15	120.30
2	E	10	ARG	NE-CZ-NH1	6.13	123.37	120.30
3	D	239	ARG	NE-CZ-NH1	6.08	123.34	120.30
3	F	224	ASP	CB-CG-OD1	6.08	123.77	118.30
3	F	278	ARG	CG-CD-NE	-6.03	99.13	111.80
1	B	202	ARG	NE-CZ-NH2	6.02	123.31	120.30
3	D	115	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	257	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	118	ASP	CB-CG-OD1	5.87	123.58	118.30
3	F	278	ARG	NE-CZ-NH2	-5.83	117.39	120.30
3	F	305	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	99	ASP	CB-CG-OD2	5.60	123.34	118.30
2	E	75	ARG	NE-CZ-NH1	-5.55	117.53	120.30
3	F	224	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	98	ASP	CB-CG-OD1	5.42	123.18	118.30
3	F	302	ASP	CB-CG-OD1	-5.37	113.46	118.30
3	F	115	ASP	CB-CG-OD1	5.37	123.13	118.30
3	F	292	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	98	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	301	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	338	ARG	NE-CZ-NH2	-5.13	117.73	120.30
3	F	132	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	352[A]	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352[B]	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	2734	0	2607	20	0
1	B	2789	0	2679	12	0
2	C	961	0	864	10	0
2	E	958	0	864	10	0
3	D	2943	0	2850	18	0
3	F	2932	0	2826	20	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	1	0
6	B	86	0	60	2	0
7	A	8	0	12	2	0
7	B	4	0	6	0	0
7	D	4	0	6	4	0
7	F	4	0	6	3	0
8	A	340	0	0	5	0
8	B	358	0	0	2	0
8	C	123	0	0	1	0
8	D	452	0	0	9	0
8	E	138	0	0	0	0
8	F	413	0	0	6	0
All	All	15339	0	12840	88	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 3.

All (88) 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:A:215:ARG:HH12	7:A:406:EDO:H12	1.09	1.15
7:D:401:EDO:H22	8:D:555:HOH:O	1.50	1.12
2:E:130:ALA:O	2:E:131:SER:HB2	1.48	1.06
3:F:126:GLU:H	7:F:401:EDO:H21	1.29	0.97
1:B:48:LYS:H	1:B:62:HIS:HE1	1.15	0.94
1:A:215:ARG:NH1	7:A:406:EDO:H12	1.81	0.94
2:E:99:ARG:NH1	3:F:223:GLU:HG3	1.93	0.83
8:C:295:HOH:O	3:F:36[A]:ILE:HD11	1.79	0.83
1:B:98:ASP:H	1:B:102:GLN:HE21	1.29	0.80
2:E:68:GLN:HB3	2:E:129:LYS:HE3	1.63	0.79
1:A:48:LYS:H	1:A:62:HIS:HE1	1.31	0.79
3:F:126:GLU:H	7:F:401:EDO:C2	2.00	0.74
3:F:326:LYS:HE3	8:F:864:HOH:O	1.88	0.73
1:B:48:LYS:H	1:B:62:HIS:CE1	2.03	0.73
3:D:54:HIS:HD2	8:D:858:HOH:O	1.73	0.70
1:A:359:GLU:N	1:A:359:GLU:OE1	2.23	0.70
3:F:126:GLU:N	7:F:401:EDO:H21	2.06	0.69
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.29	0.64
1:B:98:ASP:H	1:B:102:GLN:NE2	1.95	0.64
3:F:12:GLU:CD	3:F:20:ARG:HH12	2.02	0.63
1:B:171:PHE:CE1	1:B:215[B]:ARG:HD2	2.33	0.63
1:A:202:ARG:NE	2:C:127:VAL:HB	2.16	0.61
2:C:68:GLN:HA	2:C:68:GLN:HE21	1.64	0.60
1:B:60:GLN:O	1:B:62:HIS:HD2	1.84	0.60
1:A:202:ARG:HE	2:C:127:VAL:HB	1.65	0.60
1:A:119:ARG:NE	8:A:656:HOH:O	2.34	0.59
3:F:14:GLN:HE21	3:F:70:ARG:HH11	1.50	0.59
1:A:48:LYS:H	1:A:62:HIS:CE1	2.19	0.58
6:B:404:HEC:HBC3	6:B:404:HEC:HMC1	1.86	0.58
2:E:57:TOQ:HB	2:E:108:TRP:NE1	2.18	0.57
3:F:293:ARG:HG3	8:F:769:HOH:O	2.03	0.57
1:A:119:ARG:CZ	8:A:656:HOH:O	2.53	0.56
2:E:23:CYS:SG	2:E:88[B]:CYS:HB2	2.46	0.55
2:C:101[B]:GLU:OE2	3:D:197:ARG:NH2	2.38	0.54
2:E:130:ALA:O	2:E:131:SER:CB	2.34	0.53
1:A:6:ALA:HA	1:A:9:ALA:HB3	1.91	0.53
2:C:57:TOQ:HB	2:C:108:TRP:NE1	2.23	0.53
3:D:218:GLU:HG2	8:D:785:HOH:O	2.07	0.53
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.74	0.53
3:F:54:HIS:HE1	8:F:663:HOH:O	1.91	0.53
3:F:51:ASP:HA	3:F:377:PRO:HA	1.91	0.52
2:E:23:CYS:SG	2:E:88[B]:CYS:SG	3.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:280:GLY:HA3	3:F:301:ARG:CZ	2.40	0.52
3:F:326:LYS:CE	8:F:864:HOH:O	2.54	0.51
7:D:401:EDO:H21	8:D:722:HOH:O	2.11	0.50
3:D:323[A]:ARG:HD3	8:D:754:HOH:O	2.12	0.50
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.93	0.50
1:A:183:GLU:HB2	8:A:783:HOH:O	2.13	0.48
2:E:23:CYS:SG	2:E:88[B]:CYS:CB	3.01	0.48
1:A:61:SER:HB3	1:A:112:VAL:HB	1.95	0.48
3:D:82:ASN:HB3	3:D:142:THR:HB	1.96	0.47
1:A:107:PRO:HG3	8:A:834:HOH:O	2.14	0.47
1:A:200:ASN:O	6:A:405:HEC:HMC3	2.14	0.47
2:C:101[B]:GLU:HG2	2:C:102:PHE:CD2	2.50	0.46
1:A:60:GLN:O	1:A:62:HIS:HD2	1.97	0.46
1:A:331:GLY:O	3:D:158:PRO:HA	2.16	0.46
1:A:299:SER:HB2	1:A:333:MET:HG3	1.97	0.46
3:D:54:HIS:CD2	8:D:858:HOH:O	2.57	0.46
2:E:57:TOQ:HB	2:E:108:TRP:HE1	1.79	0.46
1:B:29:GLN:HB3	8:B:640:HOH:O	2.16	0.46
3:F:293:ARG:CG	8:F:769:HOH:O	2.63	0.45
3:F:181:CYS:C	3:F:182:TYR:CD1	2.89	0.45
3:D:303:GLU:HG3	3:D:304:TRP:CD1	2.52	0.45
6:B:405:HEC:HBC3	6:B:405:HEC:HMC1	1.98	0.45
2:C:101[B]:GLU:H	2:C:101[B]:GLU:CD	2.20	0.45
3:D:51:ASP:HA	3:D:377:PRO:HA	1.98	0.45
3:D:197:ARG:HG2	3:D:197:ARG:O	2.17	0.44
3:D:179:PRO:HD3	3:D:214:ILE:HD13	1.99	0.44
2:C:99:ARG:NH1	3:D:223:GLU:O	2.48	0.44
1:A:359:GLU:H	1:A:359:GLU:CD	2.18	0.44
3:F:80:LEU:N	3:F:81:PRO:HD3	2.33	0.44
3:D:236:LYS:NZ	3:D:386:GLY:O	2.45	0.43
3:F:82:ASN:HB3	3:F:142:THR:HB	2.00	0.43
2:C:46:CYS:HB2	3:F:36[B]:ILE:HD13	1.99	0.43
2:E:129:LYS:HA	2:E:129:LYS:HD2	1.82	0.43
7:D:401:EDO:O2	8:D:873:HOH:O	2.21	0.43
3:D:181:CYS:C	3:D:182:TYR:CD1	2.93	0.42
1:B:299:SER:HB3	1:B:304:ALA:CB	2.49	0.42
1:B:209:LYS:HG3	8:B:820:HOH:O	2.19	0.42
3:F:289:ARG:NH2	8:F:893:HOH:O	2.53	0.42
1:A:42:THR:HB	8:A:526:HOH:O	2.20	0.42
1:B:129:ASP:HB3	1:B:132:TYR:CD1	2.55	0.41
3:D:254:LEU:HD23	3:D:259:ALA:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:39:ALA:HB1	3:D:40:PRO:HD2	2.03	0.41
1:B:101:LYS:HD2	1:B:101:LYS:C	2.41	0.41
1:B:93:TRP:CE2	1:B:280:HIS:HA	2.56	0.41
7:D:401:EDO:C2	8:D:722:HOH:O	2.69	0.40
3:D:211:THR:HB	8:D:740:HOH:O	2.22	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	352/373 (94%)	345 (98%)	7 (2%)	0	100	100
1	B	359/373 (96%)	349 (97%)	10 (3%)	0	100	100
2	C	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
2	E	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
3	D	377/386 (98%)	367 (97%)	8 (2%)	2 (0%)	34	17
3	F	376/386 (97%)	363 (96%)	12 (3%)	1 (0%)	46	29
All	All	1710/1792 (95%)	1666 (97%)	41 (2%)	3 (0%)	56	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	102[A]	ILE
3	D	102[B]	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	276/292 (94%)	269 (98%)	7 (2%)	55	39
1	B	283/292 (97%)	274 (97%)	9 (3%)	46	28
2	C	105/112 (94%)	102 (97%)	3 (3%)	50	33
2	E	105/112 (94%)	102 (97%)	3 (3%)	50	33
3	D	307/311 (99%)	299 (97%)	8 (3%)	54	37
3	F	306/311 (98%)	298 (97%)	8 (3%)	54	37
All	All	1382/1430 (97%)	1344 (97%)	38 (3%)	52	36

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	23	LEU
1	A	102	GLN
1	A	142	LYS
1	A	302	PRO
1	A	357	LEU
1	A	359	GLU
1	B	23	LEU
1	B	60	GLN
1	B	112	VAL
1	B	128	ASP
1	B	142	LYS
1	B	167	GLU
1	B	219	THR
1	B	323	LEU
1	B	358	LEU
2	C	7	THR
2	C	16	GLN
2	C	68	GLN
3	D	94	HIS
3	D	197	ARG
3	D	209	GLU

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Mol	Chain	Res	Type
3	D	270	GLU
3	D	275	ASP
3	D	323[A]	ARG
3	D	323[B]	ARG
3	D	354	LYS
2	E	16	GLN
2	E	129	LYS
2	E	131	SER
3	F	94	HIS
3	F	139	PRO
3	F	209	GLU
3	F	211	THR
3	F	223	GLU
3	F	262	LEU
3	F	354	LYS
3	F	365	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	62	HIS
1	A	210	GLN
1	B	60	GLN
1	B	62	HIS
1	B	102	GLN
3	D	30	GLN
3	D	235	GLN
3	D	378	GLN
2	E	21	GLN
3	F	14	GLN
3	F	30	GLN
3	F	54	HIS
3	F	378	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	TOQ	C	57	2	14,17,18	1.13	1 (7%)	11,24,26	1.82	2 (18%)
2	TOQ	E	57	2	14,17,18	1.46	3 (21%)	11,24,26	2.50	4 (36%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	TOQ	CZ2-CE2	-2.92	1.37	1.42
2	E	57	TOQ	CD1-NE1	-2.73	1.31	1.36
2	E	57	TOQ	CE3-CZ3	2.04	1.40	1.36
2	E	57	TOQ	CD1-CG	2.33	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	TOQ	CB-CG-CD1	-6.57	119.85	127.97
2	C	57	TOQ	CB-CG-CD1	-4.63	122.24	127.97
2	E	57	TOQ	CE3-CZ3-CH2	-2.65	117.65	120.31
2	E	57	TOQ	CG-CD2-CE2	-2.42	105.64	109.82
2	C	57	TOQ	CZ3-CE3-CD2	-2.14	118.32	121.13
2	E	57	TOQ	CZ3-CH2-CZ2	2.34	122.16	120.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	404	1,8	24,50,50	1.41	2 (8%)	19,82,82	3.55	8 (42%)
6	HEC	A	405	1	24,50,50	1.50	6 (25%)	19,82,82	3.90	10 (52%)
7	EDO	A	406	-	3,3,3	0.32	0	2,2,2	0.68	0
7	EDO	A	407	-	3,3,3	0.42	0	2,2,2	1.00	0
6	HEC	B	404	1	24,50,50	1.68	6 (25%)	19,82,82	3.04	8 (42%)
6	HEC	B	405	1	24,50,50	1.58	5 (20%)	19,82,82	3.64	7 (36%)
7	EDO	B	406	-	3,3,3	0.58	0	2,2,2	0.46	0
7	EDO	D	401	-	3,3,3	0.72	0	2,2,2	0.42	0
7	EDO	F	401	-	3,3,3	0.58	0	2,2,2	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEC	A	404	1,8	-	0/6/54/54	0/0/8/8
6	HEC	A	405	1	-	0/6/54/54	0/0/8/8
7	EDO	A	406	-	-	0/1/1/1	0/0/0/0
7	EDO	A	407	-	-	0/1/1/1	0/0/0/0
6	HEC	B	404	1	-	0/6/54/54	0/0/8/8
6	HEC	B	405	1	-	0/6/54/54	0/0/8/8
7	EDO	B	406	-	-	0/1/1/1	0/0/0/0
7	EDO	D	401	-	-	0/1/1/1	0/0/0/0
7	EDO	F	401	-	-	0/1/1/1	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	405	HEC	C4A-NA	-3.55	1.31	1.36
6	B	405	HEC	C1A-NA	-2.94	1.32	1.36
6	A	405	HEC	C4C-NC	-2.88	1.32	1.36
6	B	404	HEC	C4C-NC	-2.69	1.33	1.36
6	A	405	HEC	C1A-NA	-2.59	1.33	1.36
6	B	404	HEC	C1A-NA	-2.23	1.33	1.36
6	A	405	HEC	C4D-CHA	2.06	1.45	1.39
6	B	405	HEC	C1B-CHB	2.23	1.46	1.39
6	A	405	HEC	C3C-C4C	2.28	1.48	1.42
6	A	405	HEC	C3B-C4B	2.28	1.48	1.42
6	B	404	HEC	C4D-CHA	2.49	1.46	1.39
6	B	405	HEC	C3C-C4C	2.51	1.48	1.42
6	B	405	HEC	C4D-CHA	2.57	1.46	1.39
6	B	404	HEC	C1C-CHC	2.79	1.47	1.39
6	A	405	HEC	C1B-CHB	2.83	1.47	1.39
6	A	404	HEC	C1D-CHD	3.05	1.48	1.39
6	B	404	HEC	C1D-CHD	3.35	1.49	1.39
6	A	404	HEC	C1B-CHB	3.58	1.49	1.39
6	B	404	HEC	C1B-CHB	3.85	1.50	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	404	HEC	CBB-CAB-C3B	-10.35	104.36	127.35
6	A	405	HEC	CBD-CAD-C3D	-9.78	94.99	112.53
6	A	405	HEC	CBB-CAB-C3B	-9.52	106.20	127.35
6	B	405	HEC	CBB-CAB-C3B	-8.91	107.55	127.35
6	B	405	HEC	CBD-CAD-C3D	-8.90	96.57	112.53
6	B	404	HEC	CBB-CAB-C3B	-7.58	110.51	127.35
6	A	404	HEC	CBD-CAD-C3D	-6.89	100.18	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	405	HEC	CBC-CAC-C3C	-6.46	113.00	127.35
6	B	404	HEC	CBC-CAC-C3C	-6.32	113.31	127.35
6	B	404	HEC	CBD-CAD-C3D	-5.67	102.37	112.53
6	A	404	HEC	CBC-CAC-C3C	-5.14	115.92	127.35
6	A	405	HEC	CBC-CAC-C3C	-5.14	115.92	127.35
6	A	404	HEC	C4B-C3B-C2B	-4.27	101.75	106.35
6	A	405	HEC	CBA-CAA-C2A	-4.23	104.94	112.53
6	A	405	HEC	C4B-C3B-C2B	-3.27	102.82	106.35
6	B	404	HEC	CBA-CAA-C2A	-3.25	106.70	112.53
6	A	405	HEC	CMB-C2B-C1B	-3.03	123.34	128.36
6	B	405	HEC	CBA-CAA-C2A	-2.68	107.73	112.53
6	B	405	HEC	C4B-C3B-C2B	-2.59	103.55	106.35
6	A	404	HEC	CMB-C2B-C1B	-2.52	124.20	128.36
6	A	405	HEC	CMD-C2D-C1D	-2.51	124.22	128.36
6	A	405	HEC	CAA-C2A-C1A	-2.49	124.30	127.01
6	A	404	HEC	CBA-CAA-C2A	-2.46	108.12	112.53
6	B	404	HEC	C4B-C3B-C2B	-2.39	103.77	106.35
6	B	404	HEC	C4C-C3C-C2C	-2.38	103.78	106.35
6	A	405	HEC	CMA-C3A-C2A	2.04	129.51	125.24
6	B	405	HEC	C3B-C4B-NB	2.08	114.87	110.94
6	B	404	HEC	C3B-C4B-NB	2.14	114.98	110.94
6	A	404	HEC	C3B-C4B-NB	2.19	115.08	110.94
6	B	404	HEC	CAD-CBD-CGD	2.80	117.88	112.75
6	A	405	HEC	CMD-C2D-C3D	3.00	131.50	125.24
6	A	404	HEC	CMA-C3A-C2A	3.64	132.84	125.24
6	B	405	HEC	CMA-C3A-C2A	3.91	133.42	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	405	HEC	1	0
7	A	406	EDO	2	0
6	B	404	HEC	1	0
6	B	405	HEC	1	0
7	D	401	EDO	4	0
7	F	401	EDO	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	354/373 (94%)	-0.16	8 (2%) 64 59	22, 33, 46, 68	0
1	B	357/373 (95%)	-0.13	6 (1%) 73 69	20, 30, 50, 63	0
2	C	124/137 (90%)	-0.19	1 (0%) 87 85	19, 26, 36, 52	0
2	E	124/137 (90%)	-0.27	2 (1%) 74 71	16, 21, 31, 52	0
3	D	375/386 (97%)	-0.31	4 (1%) 82 80	17, 25, 40, 60	0
3	F	376/386 (97%)	-0.12	12 (3%) 51 45	18, 29, 46, 66	0
All	All	1710/1792 (95%)	-0.19	33 (1%) 70 65	16, 28, 45, 68	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ASP	5.5
1	A	7	ASP	5.4
1	A	6	ALA	5.0
3	F	208	THR	4.6
3	F	209	GLU	3.6
2	E	131	SER	3.5
3	F	11	GLN	3.5
2	C	7	THR	3.4
3	F	210	GLY	3.3
1	B	128	ASP	3.1
3	F	207	GLY	3.0
3	D	208	THR	2.9
2	E	7	THR	2.9
1	A	242	ALA	2.7
1	A	266	VAL	2.5
3	F	380	ILE	2.5
3	F	140	TRP	2.4
3	F	379	VAL	2.3
1	A	359	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	F	211	THR	2.2
1	B	93	TRP	2.2
1	A	8	ASP	2.2
3	F	138	TYR	2.1
3	F	139	PRO	2.1
3	D	138	TYR	2.1
1	A	130	PRO	2.1
1	A	267	PRO	2.1
3	D	379	VAL	2.1
1	B	146	ASP	2.1
1	B	140	PHE	2.0
3	D	137	THR	2.0
3	F	135	VAL	2.0
1	B	142	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	TOQ	E	57	16/17	0.97	0.12	-	20,22,28,28	0
2	TOQ	C	57	16/17	0.97	0.11	-	22,26,29,29	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
7	EDO	D	401	4/4	0.90	0.32	17.35	41,46,46,48	0
7	EDO	B	406	4/4	0.91	0.30	6.49	40,44,44,45	0
7	EDO	F	401	4/4	0.86	0.23	5.38	42,44,48,49	0
6	HEC	A	405	43/43	0.99	0.14	0.24	20,22,25,26	0
6	HEC	B	404	43/43	0.98	0.11	0.20	22,27,30,31	0
7	EDO	A	406	4/4	0.85	0.10	0.14	52,53,53,53	0
6	HEC	A	404	43/43	0.98	0.10	0.08	24,29,31,34	0
6	HEC	B	405	43/43	0.99	0.12	0.01	16,20,24,24	0
5	NA	A	403	1/1	0.98	0.10	-0.20	40,40,40,40	0
5	NA	B	403	1/1	0.97	0.09	-0.40	39,39,39,39	0
4	CA	B	401	1/1	0.99	0.10	-0.91	25,25,25,25	0
4	CA	A	401	1/1	0.99	0.08	-1.15	25,25,25,25	0
5	NA	A	402	1/1	0.97	0.05	-	34,34,34,34	0
5	NA	B	402	1/1	0.95	0.14	-	40,40,40,40	0
7	EDO	A	407	4/4	0.88	0.16	-	55,55,55,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.