Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:32 PM GMT

PDB ID	:	4FA5
Title	:	Crystal Structure of WT MauG in Complex with Pre-Methylamine Dehydrogenase Aged 20 Days
Authors	:	Yukl, E.T.; Wilmot, C.M.
Deposited on	:	2012-05-21
Resolution	:	1.94 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 ①) were used in the production of this report:

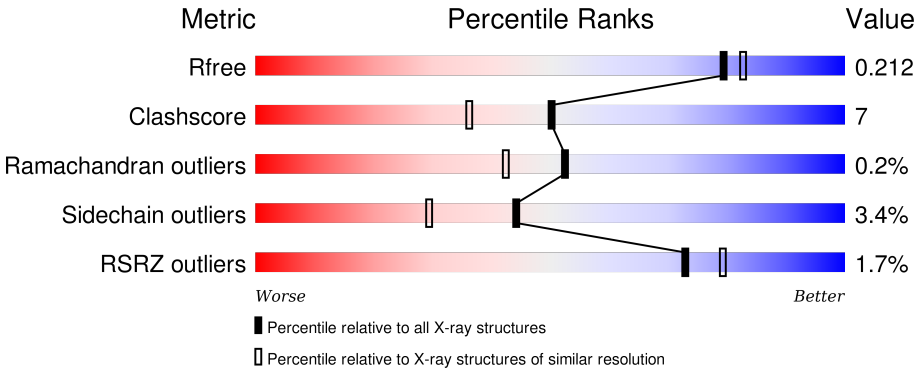
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	81% 13% • 5%
1	B	373	82% 12% •• •
2	C	137	4% 77% 15% • 6%
2	E	137	2% 69% 20% • 9%
3	D	385	3% 83% 15% ••

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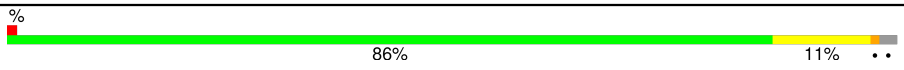
Mol	Chain	Length	Quality of chain
3	F	385	

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
2	0AF	E	57[B]	-	-	X	-
4	CA	B	401	-	-	-	X
8	MES	D	401	-	-	-	X
8	MES	F	401	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15078 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	5	0
			2779	1732	501	535	11			
1	B	357	Total	C	N	O	S	0	8	0
			2838	1765	517	544	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	129	Total	C	N	O	S	0	3	0
			1026	638	177	197	14			
2	E	125	Total	C	N	O	S	0	5	0
			1002	624	167	197	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

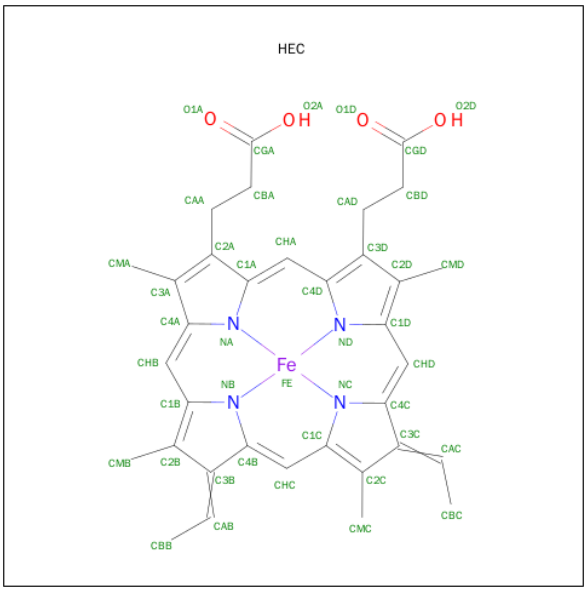
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	3	0
			2945	1865	507	564	9			
3	F	376	Total	C	N	O	S	0	5	0
			2965	1876	512	568	9			

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

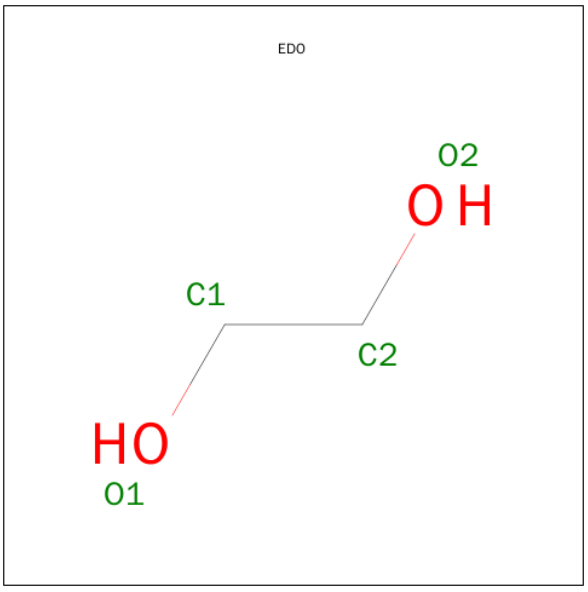
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

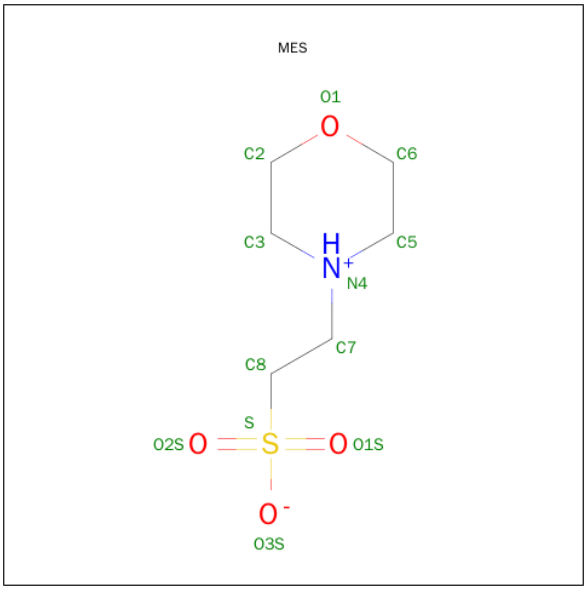


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Na 2 2	0	0
7	A	1	Total Na 1 1	0	0

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 9 is water.

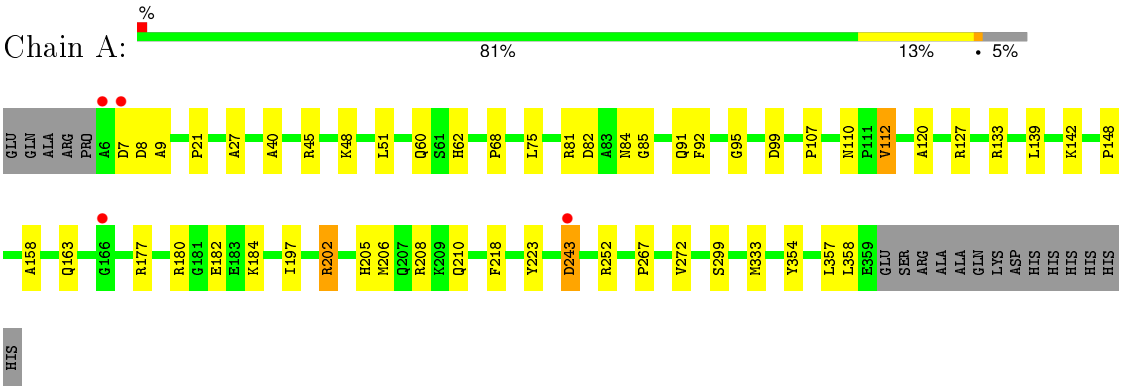
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	226	Total O 228 228	0	2
9	B	308	Total O 310 310	0	2
9	C	80	Total O 80 80	0	0
9	D	235	Total O 235 235	0	0
9	E	98	Total O 98 98	0	0
9	F	358	Total O 359 359	0	1

3 Residue-property plots (i)

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

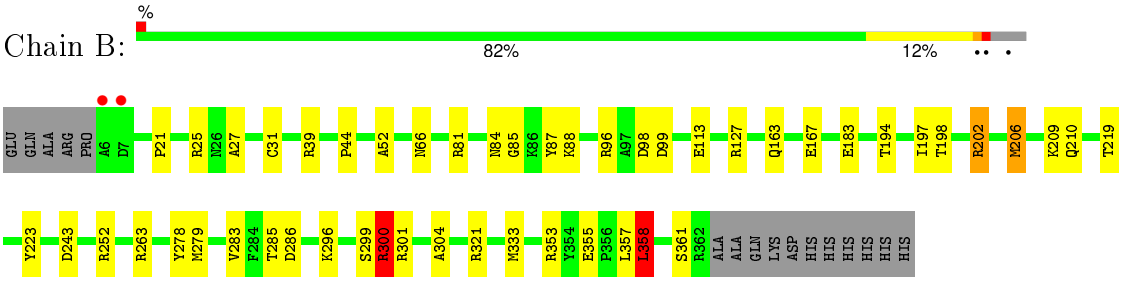
- Molecule 1: Methylamine utilization protein MauG

Chain A:



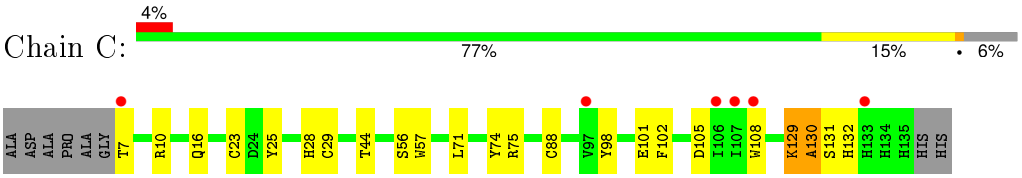
- Molecule 1: Methylamine utilization protein MauG

Chain B:



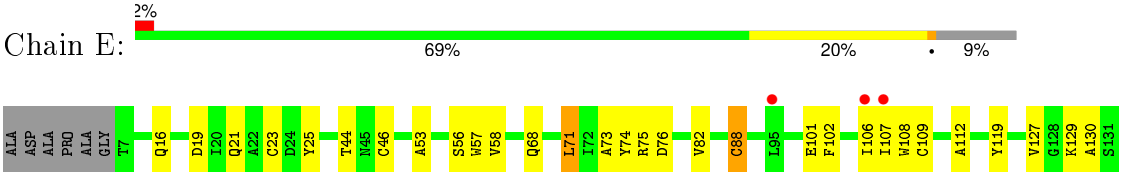
- Molecule 2: Methylamine dehydrogenase light chain

Chain C:

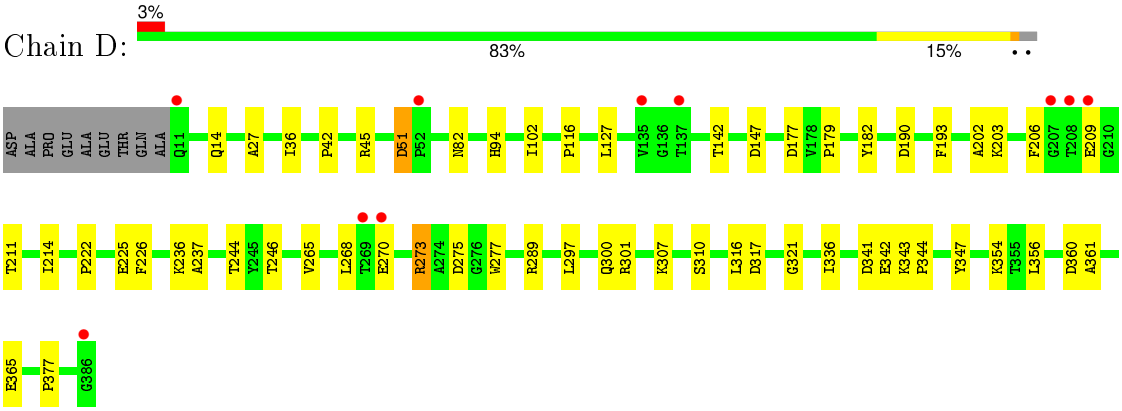


- Molecule 2: Methylamine dehydrogenase light chain

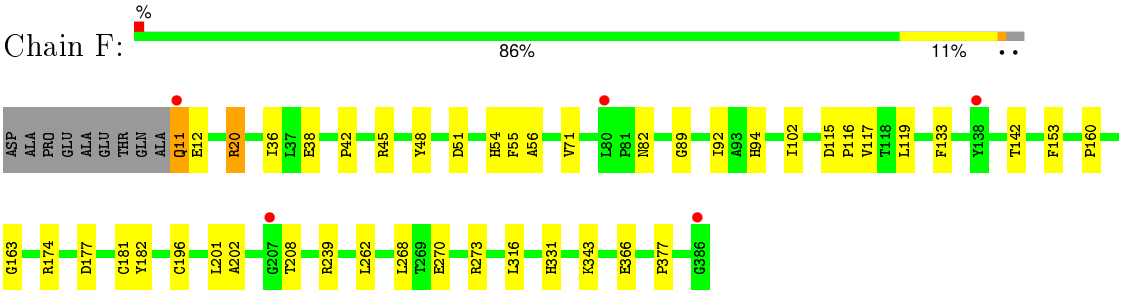
Chain E:



• Molecule 3: Methylamine dehydrogenase heavy chain



• Molecule 3: Methylamine dehydrogenase heavy chain



4 Data and refinement statistics (i)

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)	44.49 – 1.94 44.49 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.49-1.94) 86.1 (44.49-1.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.152 , 0.204 0.168 , 0.212	Depositor DCC
R_{free} test set	6440 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 125460 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15078	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0AF, NA, CA, EDO, MES, 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	0.97	1/2846 (0.0%)	0.93	5/3860 (0.1%)
1	B	1.11	2/2902 (0.1%)	0.99	9/3932 (0.2%)
2	C	0.99	1/1029 (0.1%)	0.89	0/1406
2	E	1.16	3/1001 (0.3%)	1.03	0/1368
3	D	0.95	1/3026 (0.0%)	0.91	3/4122 (0.1%)
3	F	1.12	1/3045 (0.0%)	1.01	3/4147 (0.1%)
All	All	1.05	9/13849 (0.1%)	0.96	20/18835 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	88[A]	CYS	CB-SG	-5.78	1.72	1.81
2	E	88[B]	CYS	CB-SG	-5.78	1.72	1.81
3	D	27	ALA	CA-CB	5.50	1.64	1.52
2	E	112	ALA	CA-CB	5.45	1.63	1.52
3	F	71	VAL	CB-CG1	5.41	1.64	1.52
1	A	158	ALA	CA-CB	5.30	1.63	1.52
2	C	101	GLU	CG-CD	5.17	1.59	1.51
1	B	283	VAL	CB-CG2	5.15	1.63	1.52
1	B	31	CYS	CB-SG	-5.10	1.73	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	127	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	300[A]	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	300[B]	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	208	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	252	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	99	ASP	CB-CG-OD2	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	ASP	CB-CG-OD1	5.38	123.14	118.30
3	D	360	ASP	CB-CG-OD2	5.34	123.10	118.30
3	F	239	ARG	NE-CZ-NH2	-5.32	117.64	120.30
3	F	239	ARG	NE-CZ-NH1	5.32	122.96	120.30
3	F	201	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	B	358	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	45	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	99	ASP	CB-CG-OD2	5.15	122.94	118.30
3	D	147	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	353	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	75	LEU	CA-CB-CG	-5.09	103.60	115.30
1	B	206[A]	MET	CG-SD-CE	-5.06	92.11	100.20
1	B	206[B]	MET	CG-SD-CE	-5.06	92.11	100.20
3	D	51	ASP	CB-CG-OD1	-5.02	113.78	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2779	0	2648	40	0
1	B	2838	0	2708	31	0
2	C	1026	0	907	23	0
2	E	1002	0	893	32	0
3	D	2945	0	2826	47	0
3	F	2965	0	2844	28	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	60	4	0
5	B	86	0	60	3	0
6	A	8	0	12	0	0
6	B	4	0	6	0	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
8	D	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	12	0	12	0	0
9	A	228	0	0	4	0
9	B	310	0	0	4	0
9	C	80	0	0	5	0
9	D	235	0	0	2	0
9	E	98	0	0	4	0
9	F	359	0	0	4	0
All	All	15078	0	12988	187	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 7.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57[B]:0AF:CB	2:E:57[B]:0AF:CA	1.76	1.61
3:D:273[B]:ARG:CG	3:D:273[B]:ARG:HH11	1.66	1.08
3:D:270:GLU:HA	3:D:273[A]:ARG:HH12	1.11	1.08
3:D:273[B]:ARG:HG2	3:D:273[B]:ARG:NH1	1.55	1.05
1:A:206:MET:HE2	1:A:206:MET:HA	1.35	1.02
3:D:273[A]:ARG:HH11	3:D:273[A]:ARG:HB2	1.29	0.97
3:D:265:VAL:HG21	3:D:321:GLY:HA3	1.53	0.89
3:F:11:GLN:HB3	9:F:853:HOH:O	1.74	0.87
3:D:273[A]:ARG:CB	3:D:273[A]:ARG:HH11	1.85	0.87
3:D:273[B]:ARG:HG2	3:D:273[B]:ARG:HH11	0.74	0.87
9:B:797:HOH:O	2:E:127:VAL:HG12	1.74	0.86
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.58	0.85
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.25	0.84
1:B:197:ILE:O	1:B:202[B]:ARG:HD2	1.75	0.84
1:A:127[A]:ARG:HD2	9:A:708:HOH:O	1.77	0.83
2:C:57[B]:0AF:HBC1	2:C:108[B]:TRP:NE1	1.95	0.82
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.43	0.82
3:D:265:VAL:HG21	3:D:321:GLY:CA	2.10	0.81
3:D:342:GLU:HA	9:D:733:HOH:O	1.81	0.80
3:D:273[A]:ARG:CG	3:D:273[A]:ARG:HH11	1.92	0.80
9:C:273:HOH:O	3:F:36:ILE:HD11	1.87	0.74
1:A:107:PRO:HG3	9:A:661[B]:HOH:O	1.88	0.73
3:F:11:GLN:NE2	3:F:11:GLN:HA	2.06	0.71
3:D:265:VAL:CG2	3:D:321:GLY:HA3	2.20	0.70
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.56	0.70
1:A:206:MET:HE1	1:A:218:PHE:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:273[B]:ARG:CG	3:D:273[B]:ARG:NH1	2.36	0.68
2:E:58[A]:VAL:HG12	2:E:73:ALA:HA	1.74	0.68
1:B:285:THR:HG22	1:B:286:ASP:OD1	1.93	0.68
1:A:206:MET:CE	1:A:218:PHE:CD2	2.77	0.68
3:F:11:GLN:HE21	3:F:11:GLN:HA	1.59	0.67
2:E:57[A]:0AF:CE3	2:E:108[A]:TRP:CD1	2.79	0.66
2:E:57[B]:0AF:HBC1	2:E:108[B]:TRP:NE1	2.11	0.66
3:D:270:GLU:HA	3:D:273[A]:ARG:NH1	1.97	0.66
3:D:273[A]:ARG:NH1	3:D:273[A]:ARG:CG	2.54	0.66
1:B:301:ARG:NH2	3:F:177[B]:ASP:OD1	2.30	0.65
2:C:129:LYS:O	2:C:130:ALA:CB	2.45	0.65
3:D:273[A]:ARG:HG3	3:D:273[A]:ARG:NH1	2.12	0.64
3:D:270:GLU:CA	3:D:273[A]:ARG:HH12	1.99	0.64
1:A:133:ARG:NH1	1:A:133:ARG:HB2	2.14	0.62
1:A:68:PRO:HG2	5:A:402:HEC:HBA1	1.82	0.62
1:A:110:ASN:OD1	1:A:112:VAL:HG13	2.00	0.62
1:A:133:ARG:HB2	1:A:133:ARG:CZ	2.29	0.61
2:E:23:CYS:SG	2:E:88[B]:CYS:HB2	2.40	0.61
2:E:57[B]:0AF:CB	2:E:57[B]:0AF:HA	2.16	0.61
1:B:300[A]:ARG:HG2	1:B:300[A]:ARG:O	1.98	0.61
3:F:12:GLU:OE1	3:F:20:ARG:HD3	2.02	0.60
3:F:270[B]:GLU:HB2	3:F:273[B]:ARG:NH2	2.17	0.59
2:E:57[B]:0AF:CA	2:E:57[B]:0AF:CG	2.73	0.58
3:D:51:ASP:HA	3:D:377:PRO:HA	1.85	0.58
3:D:343:LYS:HE3	3:D:343:LYS:HA	1.85	0.58
2:E:57[B]:0AF:CB	2:E:57[B]:0AF:N	2.62	0.57
3:D:273[A]:ARG:NH1	3:D:273[A]:ARG:HB2	2.10	0.57
1:A:206:MET:HE3	1:A:218:PHE:HD2	1.69	0.57
2:C:57[A]:0AF:CE3	2:C:108[A]:TRP:CD1	2.88	0.57
1:A:48:LYS:H	1:A:62:HIS:HE1	1.52	0.56
1:A:180[B]:ARG:HD3	1:A:182:GLU:CD	2.26	0.56
1:A:243[A]:ASP:N	1:A:243[A]:ASP:OD2	2.37	0.56
1:A:206:MET:HE2	1:A:206:MET:CA	2.24	0.56
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.19	0.56
3:F:82:ASN:HB3	3:F:142:THR:HB	1.88	0.56
2:C:129:LYS:NZ	9:C:247:HOH:O	2.39	0.55
3:F:51:ASP:HA	3:F:377:PRO:HA	1.89	0.55
1:B:198:THR:HG22	2:E:58[A]:VAL:HG13	1.87	0.55
1:B:299:SER:HB2	1:B:333:MET:HG3	1.88	0.54
1:B:300[A]:ARG:NH1	9:F:855:HOH:O	2.40	0.54
3:D:246:THR:O	3:D:273[A]:ARG:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:236:LYS:HD3	3:D:289:ARG:NH1	2.24	0.53
1:B:197:ILE:HA	1:B:202[A]:ARG:HG3	1.91	0.53
1:B:296:LYS:NZ	9:B:570:HOH:O	2.37	0.53
2:C:57[B]:0AF:HZ3	9:C:225:HOH:O	2.08	0.53
3:D:265:VAL:HG21	3:D:321:GLY:HA2	1.89	0.53
2:E:19:ASP:O	2:E:25:TYR:HB2	2.09	0.53
1:A:272:VAL:HG21	5:A:403:HEC:HMA3	1.90	0.52
1:B:197:ILE:O	1:B:202[B]:ARG:CD	2.55	0.51
1:A:205:HIS:O	1:A:206:MET:CE	2.59	0.51
1:A:21:PRO:O	1:A:27:ALA:HA	2.11	0.51
2:C:57[B]:0AF:HBC1	2:C:108[B]:TRP:HE1	1.71	0.51
1:A:9:ALA:HB3	1:A:139:LEU:HD21	1.93	0.50
3:D:179:PRO:HD3	3:D:214:ILE:HD13	1.94	0.50
1:A:163:GLN:HE22	5:A:402:HEC:HMA1	1.77	0.50
3:D:347:TYR:HB3	3:D:356:LEU:HD11	1.94	0.50
3:F:331:HIS:HE1	3:F:366:GLU:OE1	1.95	0.49
1:A:243[B]:ASP:HB3	9:A:629:HOH:O	2.12	0.49
3:F:54:HIS:HE1	9:F:706:HOH:O	1.94	0.49
2:E:57[A]:0AF:HE3	2:E:108[A]:TRP:CD1	2.47	0.49
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.94	0.49
2:E:56:SER:CB	2:E:74:TYR:O	2.60	0.49
9:E:242:HOH:O	3:F:54:HIS:HD2	1.95	0.49
2:E:56:SER:HB2	2:E:74:TYR:O	2.12	0.49
2:C:129:LYS:O	2:C:130:ALA:HB3	2.12	0.49
5:B:403:HEC:HBC3	5:B:403:HEC:HMC1	1.95	0.49
3:D:336:ILE:HA	3:D:347:TYR:O	2.12	0.49
1:A:120:ALA:HA	1:A:148:PRO:HB3	1.94	0.49
1:B:52:ALA:O	1:B:66:ASN:HA	2.13	0.49
1:B:194:THR:HG21	2:E:101[B]:GLU:HG3	1.95	0.48
3:F:268:LEU:O	3:F:273[B]:ARG:NH1	2.46	0.48
3:D:36:ILE:HD13	2:E:46:CYS:HB2	1.95	0.48
2:E:75:ARG:HA	9:E:289:HOH:O	2.12	0.48
2:C:75:ARG:HD2	9:C:279:HOH:O	2.12	0.48
2:E:71:LEU:HD22	2:E:129:LYS:O	2.14	0.48
2:E:76:ASP:HB2	2:E:108[B]:TRP:O	2.14	0.47
1:A:177:ARG:HG2	1:A:180[B]:ARG:HH11	1.78	0.47
3:D:222:PRO:HG2	3:D:225:GLU:HB2	1.96	0.47
2:E:58[B]:VAL:O	2:E:102:PHE:HD1	1.98	0.47
1:B:163:GLN:HE22	5:B:402:HEC:HMA1	1.79	0.47
3:F:45:ARG:NH2	3:F:343:LYS:O	2.47	0.47
1:B:243[B]:ASP:OD2	9:B:635[B]:HOH:O	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:275:ASP:HB2	9:D:715:HOH:O	2.13	0.46
3:D:344:PRO:HG2	3:D:361:ALA:HB3	1.97	0.46
1:B:197:ILE:HG22	1:B:206[A]:MET:CE	2.46	0.46
2:E:57[B]:0AF:HBC1	2:E:108[B]:TRP:HE1	1.80	0.46
1:A:60:GLN:O	1:A:62:HIS:HD2	1.98	0.46
3:F:153:PHE:CZ	3:F:163:GLY:HA3	2.50	0.46
3:D:45:ARG:NH2	3:D:343:LYS:O	2.49	0.46
1:A:205:HIS:O	1:A:206:MET:HE3	2.15	0.46
1:B:202[A]:ARG:HH22	1:B:209:LYS:HA	1.81	0.46
3:D:82:ASN:HB3	3:D:142:THR:HB	1.97	0.45
2:C:25:TYR:HB3	2:C:28:HIS:CD2	2.51	0.45
3:D:226:PHE:O	3:D:244:THR:HA	2.16	0.45
2:C:23:CYS:SG	2:C:88[B]:CYS:HB2	2.56	0.45
3:D:341:ASP:N	3:D:341:ASP:OD1	2.40	0.45
3:D:277:TRP:CE2	3:D:300:GLN:HG3	2.51	0.45
2:E:53:ALA:HB2	2:E:109:CYS:HA	1.98	0.45
1:B:355:GLU:O	1:B:358:LEU:HB2	2.16	0.45
1:A:180[B]:ARG:HD3	1:A:182:GLU:OE1	2.17	0.45
3:D:36:ILE:CD1	2:E:46:CYS:HB2	2.46	0.45
1:A:299:SER:HB2	1:A:333:MET:HG3	1.99	0.45
3:D:190:ASP:HB2	3:D:206:PHE:O	2.17	0.44
2:E:75:ARG:HD2	9:E:269:HOH:O	2.17	0.44
2:C:75:ARG:HA	9:C:272:HOH:O	2.17	0.44
1:B:81:ARG:HB2	1:B:87:TYR:CE2	2.53	0.44
1:B:197:ILE:HG22	1:B:206[A]:MET:HE3	2.00	0.44
2:C:23:CYS:SG	2:C:88[B]:CYS:SG	3.15	0.44
3:F:115:ASP:O	3:F:119:LEU:HA	2.17	0.44
2:C:105:ASP:OD1	3:D:307:LYS:NZ	2.47	0.44
3:F:89:GLY:HA2	9:F:571:HOH:O	2.17	0.43
2:E:101[B]:GLU:HG2	2:E:102:PHE:CD2	2.53	0.43
1:B:81:ARG:NH1	1:B:85:GLY:HA2	2.32	0.43
1:B:202[A]:ARG:NH2	9:B:699:HOH:O	2.51	0.43
1:A:82:ASP:C	1:A:82:ASP:OD2	2.55	0.43
1:A:206:MET:HE3	1:A:218:PHE:CD2	2.44	0.43
1:A:210:GLN:NE2	2:C:44:THR:HG21	2.28	0.43
2:C:23:CYS:HB3	2:C:88[B]:CYS:SG	2.59	0.43
1:B:21:PRO:O	1:B:27:ALA:HA	2.19	0.43
1:A:81:ARG:CZ	1:A:85:GLY:HA2	2.48	0.43
3:D:42:PRO:HG3	3:D:116:PRO:HB2	2.01	0.42
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.54	0.42
2:E:130:ALA:HB3	9:E:287:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:HD2	1:B:44:PRO:HB3	2.00	0.42
1:A:91:GLN:O	1:A:92:PHE:HB2	2.18	0.42
2:C:10:ARG:HB3	3:D:301:ARG:HB3	2.02	0.42
2:E:107:ILE:HD12	2:E:119:TYR:HB2	2.01	0.42
1:A:133:ARG:NH1	1:A:133:ARG:CB	2.81	0.42
1:A:48:LYS:HD2	1:A:62:HIS:NE2	2.34	0.42
1:A:95:GLY:HA3	1:A:223:TYR:OH	2.19	0.42
3:F:48:TYR:CZ	3:F:92:ILE:HG21	2.55	0.42
1:A:267:PRO:HD3	5:A:403:HEC:CAD	2.50	0.42
1:A:197:ILE:HA	1:A:202:ARG:HB3	2.02	0.41
2:E:82:VAL:HG12	3:F:56:ALA:HA	2.02	0.41
3:D:268:LEU:HD22	3:D:277:TRP:HB3	2.01	0.41
3:F:38:GLU:HB3	3:F:117:VAL:CG1	2.49	0.41
1:B:278:TYR:O	1:B:279:MET:HB2	2.21	0.41
2:C:57[A]:0AF:HE3	2:C:108[A]:TRP:CD1	2.55	0.41
3:D:203:LYS:O	3:D:214:ILE:HA	2.21	0.41
1:A:206:MET:HE1	1:A:218:PHE:CE2	2.55	0.41
2:C:23:CYS:CB	2:C:88[B]:CYS:SG	3.08	0.41
1:A:202:ARG:NE	9:A:697:HOH:O	2.47	0.41
3:F:38:GLU:HB3	3:F:117:VAL:HG13	2.02	0.41
3:F:42:PRO:HG3	3:F:116:PRO:HB2	2.02	0.41
2:C:98:TYR:HA	3:D:182:TYR:CE1	2.56	0.41
3:D:236:LYS:HD3	3:D:289:ARG:HH12	1.86	0.41
1:B:113:GLU:HG2	5:B:402:HEC:HBC2	2.03	0.41
3:F:174[B]:ARG:CZ	3:F:208:THR:HA	2.51	0.41
1:B:88[A]:LYS:HB3	1:B:88[A]:LYS:HE2	1.97	0.41
2:C:56:SER:CB	2:C:74:TYR:O	2.69	0.41
1:B:96:ARG:HA	1:B:252[B]:ARG:HG3	2.02	0.40
3:F:54:HIS:O	3:F:55:PHE:HB2	2.21	0.40
1:B:223:TYR:HB3	1:B:263:ARG:HB3	2.03	0.40
1:B:299:SER:HB3	1:B:304:ALA:CB	2.51	0.40
3:F:181[B]:CYS:HA	3:F:196:CYS:HA	2.03	0.40
3:F:196:CYS:SG	3:F:202:ALA:HB2	2.61	0.40
2:E:106:ILE:HG12	3:F:133:PHE:CZ	2.57	0.40
2:C:57[B]:0AF:HBC1	2:C:108[B]:TRP:CE2	2.56	0.40
2:C:102:PHE:HE1	2:C:132:HIS:CE1	2.39	0.40
3:D:193:PHE:HA	3:D:202:ALA: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	357/373 (96%)	348 (98%)	9 (2%)	0	100	100
1	B	363/373 (97%)	351 (97%)	12 (3%)	0	100	100
2	C	128/137 (93%)	123 (96%)	4 (3%)	1 (1%)	24	10
2	E	126/137 (92%)	124 (98%)	2 (2%)	0	100	100
3	D	377/385 (98%)	359 (95%)	17 (4%)	1 (0%)	46	35
3	F	379/385 (98%)	366 (97%)	12 (3%)	1 (0%)	46	35
All	All	1730/1790 (97%)	1671 (97%)	56 (3%)	3 (0%)	52	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	130	ALA
3	F	102	ILE
3	D	102	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/292 (96%)	269 (96%)	12 (4%)	35	19
1	B	287/292 (98%)	273 (95%)	14 (5%)	31	14
2	C	110/112 (98%)	104 (94%)	6 (6%)	27	11
2	E	108/112 (96%)	105 (97%)	3 (3%)	51	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	307/310 (99%)	296 (96%)	11 (4%)	42 27
3	F	309/310 (100%)	303 (98%)	6 (2%)	65 56
All	All	1402/1428 (98%)	1350 (96%)	52 (4%)	44 26

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	ASP
1	A	51	LEU
1	A	84	ASN
1	A	112	VAL
1	A	142	LYS
1	A	184	LYS
1	A	202	ARG
1	A	243[A]	ASP
1	A	243[B]	ASP
1	A	357	LEU
1	A	358	LEU
1	B	25	ARG
1	B	84	ASN
1	B	167	GLU
1	B	183	GLU
1	B	202[A]	ARG
1	B	202[B]	ARG
1	B	219	THR
1	B	300[A]	ARG
1	B	300[B]	ARG
1	B	321[A]	ARG
1	B	321[B]	ARG
1	B	357	LEU
1	B	358	LEU
1	B	361	SER
2	C	7	THR
2	C	16	GLN
2	C	29	CYS
2	C	71	LEU
2	C	129	LYS
2	C	131	SER
3	D	94	HIS
3	D	127	LEU

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Mol	Chain	Res	Type
3	D	177	ASP
3	D	209	GLU
3	D	211	THR
3	D	273[A]	ARG
3	D	273[B]	ARG
3	D	316	LEU
3	D	317	ASP
3	D	354	LYS
3	D	365	GLU
2	E	16	GLN
2	E	68	GLN
2	E	71	LEU
3	F	11	GLN
3	F	20	ARG
3	F	94	HIS
3	F	160	PRO
3	F	262	LEU
3	F	316	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	62	HIS
1	A	91	GLN
1	A	163	GLN
1	A	210	GLN
1	B	84	ASN
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
3	D	14	GLN
3	D	30	GLN
2	E	68	GLN
3	F	11	GLN
3	F	30	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

4 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[A]	2	13,16,17	1.33	1 (7%)	10,22,24	1.38	1 (10%)
2	0AF	C	57[B]	2	13,16,17	2.14	4 (30%)	10,22,24	2.64	3 (30%)
2	0AF	E	57[A]	2	13,16,17	1.69	3 (23%)	10,22,24	2.00	3 (30%)
2	0AF	E	57[B]	2	13,16,17	3.80	4 (30%)	10,22,24	3.23	4 (40%)

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[A]	2	-	0/3/6/8	0/2/2/2
2	0AF	C	57[B]	2	-	0/3/6/8	0/2/2/2
2	0AF	E	57[A]	2	-	0/3/6/8	0/2/2/2
2	0AF	E	57[B]	2	-	0/3/6/8	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57[B]	0AF	CZ2-CE2	-6.39	1.34	1.42
2	C	57[B]	0AF	CZ2-CE2	-5.55	1.35	1.42
2	E	57[A]	0AF	CZ2-CE2	-4.17	1.37	1.42
2	E	57[B]	0AF	CD1-NE1	-3.49	1.29	1.36
2	C	57[B]	0AF	CE2-NE1	-3.07	1.29	1.39
2	C	57[B]	0AF	CD1-NE1	-3.03	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57[B]	0AF	CE2-NE1	-3.02	1.29	1.39
2	C	57[A]	0AF	CZ2-CE2	-2.85	1.38	1.42
2	C	57[B]	0AF	CD1-CG	-2.12	1.34	1.38
2	E	57[A]	0AF	CH2-CZ2	2.18	1.42	1.37
2	E	57[A]	0AF	CZ3-CE3	2.21	1.41	1.36
2	E	57[B]	0AF	CB-CA	10.89	1.76	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	57[B]	0AF	CB-CG-CD1	-7.24	119.03	127.97
2	C	57[B]	0AF	CB-CG-CD1	-5.30	121.41	127.97
2	E	57[B]	0AF	CG-CD2-CE2	-5.06	101.06	109.82
2	C	57[B]	0AF	CG-CD2-CE2	-4.43	102.16	109.82
2	E	57[B]	0AF	CZ3-CE3-CD2	-3.82	115.48	120.88
2	C	57[B]	0AF	CZ3-CE3-CD2	-3.69	115.66	120.88
2	E	57[A]	0AF	O1-CZ2-CE2	-3.55	112.66	119.05
2	E	57[A]	0AF	CB-CG-CD1	-3.12	124.11	127.97
2	C	57[A]	0AF	CB-CG-CD1	-2.88	124.41	127.97
2	E	57[A]	0AF	CG-CD2-CE2	-2.61	105.31	109.82
2	E	57[B]	0AF	O-C-CA	-2.11	119.98	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	57[A]	0AF	2	0
2	C	57[B]	0AF	4	0
2	E	57[A]	0AF	2	0
2	E	57[B]	0AF	6	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 5 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	$\#\|Z\| > 2$
5	HEC	A	402	1,9	24,50,50	1.56	8 (33%)	19,82,82	3.09	12 (63%)
5	HEC	A	403	1	24,50,50	1.95	10 (41%)	19,82,82	4.00	6 (31%)
6	EDO	A	404	-	3,3,3	0.52	0	2,2,2	0.52	0
6	EDO	A	406	-	3,3,3	0.55	0	2,2,2	0.45	0
5	HEC	B	402	1,9	24,50,50	1.82	8 (33%)	19,82,82	3.62	12 (63%)
5	HEC	B	403	1	24,50,50	1.83	8 (33%)	19,82,82	3.87	8 (42%)
6	EDO	B	404	-	3,3,3	0.46	0	2,2,2	0.42	0
8	MES	D	401	-	11,12,12	0.68	0	14,16,16	2.78	5 (35%)
8	MES	F	401	-	11,12,12	0.66	0	14,16,16	4.29	8 (57%)

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
5	HEC	A	402	1,9	-	0/6/54/54	0/0/8/8
5	HEC	A	403	1	-	0/6/54/54	0/0/8/8
6	EDO	A	404	-	-	0/1/1/1	0/0/0/0
6	EDO	A	406	-	-	0/1/1/1	0/0/0/0
5	HEC	B	402	1,9	-	0/6/54/54	0/0/8/8
5	HEC	B	403	1	-	0/6/54/54	0/0/8/8
6	EDO	B	404	-	-	0/1/1/1	0/0/0/0
8	MES	D	401	-	-	0/6/14/14	0/1/1/1
8	MES	F	401	-	-	0/6/14/14	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	HEC	C4A-NA	-4.61	1.30	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	HEC	C4B-NB	-4.00	1.31	1.36
5	A	403	HEC	C4A-NA	-3.74	1.31	1.36
5	A	403	HEC	C4C-NC	-3.59	1.31	1.36
5	B	402	HEC	C4A-NA	-3.35	1.32	1.36
5	B	403	HEC	C4B-NB	-3.12	1.32	1.36
5	A	403	HEC	C3B-C2B	-3.03	1.37	1.40
5	B	403	HEC	C4C-NC	-2.86	1.32	1.36
5	B	402	HEC	C4C-NC	-2.71	1.33	1.36
5	A	402	HEC	C4A-NA	-2.40	1.33	1.36
5	A	403	HEC	C1A-NA	-2.36	1.33	1.36
5	A	403	HEC	C4B-NB	-2.28	1.33	1.36
5	B	402	HEC	C3C-C2C	-2.22	1.38	1.40
5	B	403	HEC	C3C-C2C	-2.04	1.38	1.40
5	A	402	HEC	C4C-NC	-2.03	1.33	1.36
5	A	402	HEC	C1A-NA	-2.00	1.34	1.36
5	A	403	HEC	C3B-C4B	2.02	1.47	1.42
5	B	403	HEC	C4D-CHA	2.21	1.45	1.39
5	B	402	HEC	C1B-CHB	2.34	1.46	1.39
5	A	403	HEC	C4D-CHA	2.36	1.46	1.39
5	B	402	HEC	C1D-CHD	2.41	1.46	1.39
5	A	402	HEC	C1C-CHC	2.46	1.46	1.39
5	A	403	HEC	C1B-CHB	2.52	1.46	1.39
5	A	403	HEC	C3C-C4C	2.53	1.48	1.42
5	A	402	HEC	C1B-CHB	2.54	1.46	1.39
5	B	403	HEC	C1C-CHC	2.62	1.47	1.39
5	B	402	HEC	C3C-C4C	2.63	1.48	1.42
5	B	402	HEC	C3B-C4B	2.64	1.48	1.42
5	A	402	HEC	C4D-CHA	2.74	1.47	1.39
5	B	403	HEC	C3C-C4C	2.76	1.49	1.42
5	A	403	HEC	C1D-CHD	2.77	1.47	1.39
5	A	402	HEC	C1D-CHD	2.85	1.47	1.39
5	B	403	HEC	C1D-CHD	2.87	1.47	1.39
5	A	402	HEC	C3C-C4C	3.13	1.49	1.42

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	403	HEC	CBB-CAB-C3B	-11.29	102.26	127.35
5	B	402	HEC	CBB-CAB-C3B	-10.90	103.12	127.35
5	B	403	HEC	CBB-CAB-C3B	-10.56	103.89	127.35
5	A	402	HEC	CBB-CAB-C3B	-8.30	108.90	127.35
8	F	401	MES	C2-C3-N4	-7.85	98.23	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	403	HEC	CBC-CAC-C3C	-7.74	110.16	127.35
5	A	403	HEC	CBD-CAD-C3D	-7.68	98.77	112.53
8	F	401	MES	C6-C5-N4	-7.46	98.82	110.12
5	B	403	HEC	CBD-CAD-C3D	-7.33	99.39	112.53
5	B	403	HEC	CBC-CAC-C3C	-6.77	112.31	127.35
5	B	402	HEC	CBC-CAC-C3C	-5.59	114.94	127.35
8	D	401	MES	C2-C3-N4	-5.38	101.97	110.12
5	B	403	HEC	CBA-CAA-C2A	-5.11	103.37	112.53
5	A	402	HEC	CBC-CAC-C3C	-5.05	116.14	127.35
5	A	403	HEC	CBA-CAA-C2A	-4.94	103.67	112.53
5	A	402	HEC	CBA-CAA-C2A	-4.52	104.44	112.53
5	B	402	HEC	CMB-C2B-C1B	-4.38	121.11	128.36
8	D	401	MES	C6-C5-N4	-4.30	103.61	110.12
8	F	401	MES	O1S-S-C8	-3.86	103.61	106.91
5	B	403	HEC	CAD-CBD-CGD	-3.83	105.73	112.75
5	B	402	HEC	CBD-CAD-C3D	-3.70	105.90	112.53
5	B	402	HEC	CBA-CAA-C2A	-3.64	106.01	112.53
5	B	402	HEC	C4B-C3B-C2B	-3.27	102.83	106.35
5	A	402	HEC	CMB-C2B-C1B	-3.18	123.10	128.36
5	A	402	HEC	CBD-CAD-C3D	-3.09	106.99	112.53
5	A	402	HEC	C4C-C3C-C2C	-2.93	103.19	106.35
5	A	403	HEC	C4C-C3C-C2C	-2.86	103.27	106.35
5	B	403	HEC	CAA-CBA-CGA	-2.54	108.10	112.75
5	A	402	HEC	CMC-C2C-C1C	-2.46	124.30	128.36
5	A	403	HEC	CMB-C2B-C1B	-2.45	124.31	128.36
5	A	402	HEC	CAA-CBA-CGA	-2.39	108.37	112.75
8	F	401	MES	O1-C6-C5	-2.36	106.43	111.84
5	B	403	HEC	CMB-C2B-C1B	-2.35	124.47	128.36
5	B	403	HEC	C4C-C3C-C2C	-2.18	104.00	106.35
5	B	402	HEC	CMC-C2C-C1C	-2.17	124.78	128.36
5	A	402	HEC	C4B-C3B-C2B	-2.06	104.13	106.35
5	A	402	HEC	CMD-C2D-C1D	-2.02	125.02	128.36
5	B	402	HEC	CMD-C2D-C1D	-2.01	125.03	128.36
5	B	402	HEC	CAD-C3D-C4D	2.03	129.21	127.01
5	A	402	HEC	C3C-C4C-NC	2.14	114.98	110.94
5	B	402	HEC	CMD-C2D-C3D	2.19	129.81	125.24
5	B	402	HEC	C3B-C4B-NB	2.47	115.61	110.94
5	A	402	HEC	CMD-C2D-C3D	2.54	130.55	125.24
8	F	401	MES	C7-N4-C5	2.62	117.97	111.27
5	B	402	HEC	CAA-C2A-C1A	2.90	130.16	127.01
8	D	401	MES	C7-N4-C3	3.17	119.39	111.27
8	D	401	MES	C7-N4-C5	4.31	122.32	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	401	MES	C5-N4-C3	4.32	118.26	108.90
8	F	401	MES	C5-N4-C3	4.53	118.71	108.90
8	F	401	MES	C7-N4-C3	4.67	123.23	111.27
8	F	401	MES	O2S-S-C8	8.02	113.75	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	HEC	2	0
5	A	403	HEC	2	0
5	B	402	HEC	2	0
5	B	403	HEC	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	354/373 (94%)	-0.28	4 (1%) 82 87	26, 36, 53, 68	0
1	B	357/373 (95%)	-0.33	2 (0%) 90 93	19, 29, 47, 69	0
2	C	128/137 (93%)	0.28	6 (4%) 35 44	22, 33, 56, 75	0
2	E	124/137 (90%)	0.13	3 (2%) 62 70	19, 24, 37, 63	0
3	D	376/385 (97%)	0.08	10 (2%) 58 67	22, 39, 64, 76	0
3	F	376/385 (97%)	-0.17	5 (1%) 79 84	19, 26, 42, 63	0
All	All	1715/1790 (95%)	-0.12	30 (1%) 73 79	19, 32, 55, 76	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ALA	6.0
1	A	6	ALA	5.9
3	D	208	THR	5.3
1	B	7	ASP	4.7
3	D	207	GLY	4.3
1	A	7	ASP	3.7
3	D	11	GLN	3.4
3	F	11	GLN	3.4
2	C	106	ILE	3.2
3	F	386	GLY	3.0
3	D	269	THR	2.8
2	C	108[A]	TRP	2.8
3	D	135	VAL	2.7
2	C	97	VAL	2.6
1	A	243[A]	ASP	2.6
2	C	7	THR	2.6
3	D	270	GLU	2.5
3	D	209	GLU	2.5
3	D	386	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	166	GLY	2.4
2	E	95	LEU	2.2
3	D	137	THR	2.2
2	E	106	ILE	2.2
3	F	207	GLY	2.2
2	C	107	ILE	2.1
3	F	138	TYR	2.1
3	D	52	PRO	2.1
2	C	133	HIS	2.1
2	E	107	ILE	2.0
3	F	80	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	0AF	E	57[A]	15/16	0.97	0.19	-	25,27,29,30	15
2	0AF	C	57[B]	15/16	0.94	0.22	-	36,42,44,44	15
2	0AF	C	57[A]	15/16	0.94	0.22	-	34,35,36,39	15
2	0AF	E	57[B]	15/16	0.97	0.19	-	23,33,36,37	15

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CA	B	401	1/1	1.00	0.11	5.32	22,22,22,22	0
8	MES	D	401	12/12	0.94	0.13	4.67	31,50,56,57	12
8	MES	F	401	12/12	0.93	0.16	3.98	33,53,59,60	12
6	EDO	A	404	4/4	0.94	0.17	1.20	58,59,59,60	0
5	HEC	A	402	43/43	0.98	0.08	0.15	22,31,33,34	0
5	HEC	A	403	43/43	0.99	0.09	0.12	25,29,31,33	0
6	EDO	A	406	4/4	0.75	0.13	0.04	62,63,64,66	0
4	CA	A	401	1/1	0.98	0.08	-0.11	31,31,31,31	0
5	HEC	B	402	43/43	0.98	0.08	-0.22	20,24,27,28	0
5	HEC	B	403	43/43	0.99	0.09	-0.44	13,19,22,24	0
6	EDO	B	404	4/4	0.96	0.07	-0.70	49,50,51,53	0
7	NA	A	405	1/1	0.96	0.07	-2.11	49,49,49,49	0
7	NA	B	406	1/1	0.98	0.05	-3.14	34,34,34,34	0
7	NA	B	405	1/1	0.98	0.04	-	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.