Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:41 PM GMT

PDB ID	:	3RN0
Title	:	Crystal Structure of the W199K-MauG/pre-Methylamine Dehydrogenase Complex
Authors	:	Jensen, L.M.R.; Wilmot, C.M.
Deposited on	:	2011-04-21
Resolution	:	1.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

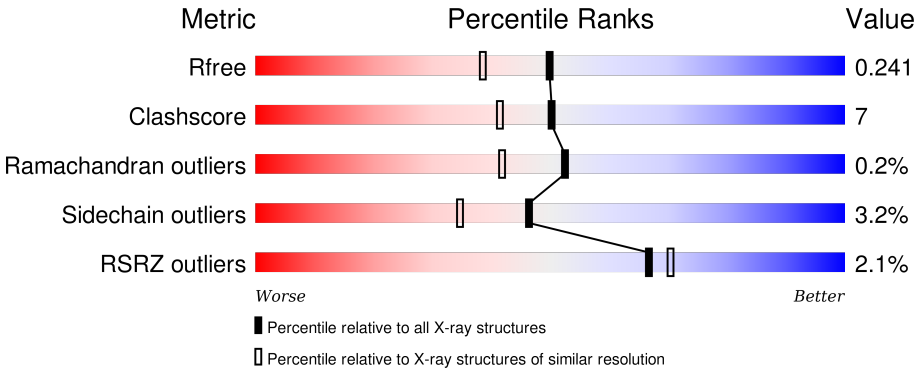
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.91 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	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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	2% 77% 16% • 5%
1	B	373	% 79% 15% • 5%
2	C	137	4% 69% 21% • 9%
2	E	137	% 74% 15% • 9%
3	D	386	4% 80% 17% • •

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Mol	Chain	Length	Quality of chain
3	F	386	2% 81% 16%

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	C	57	X	-	-	-
7	P6G	F	387	-	-	-	X
9	MES	F	389	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14657 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	2	0
			2741	1710	491	529	11			
1	B	355	Total	C	N	O	S	0	1	0
			2746	1712	494	529	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	LYS	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	LYS	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	125	Total	C	N	O	S	0	1	0
			957	592	161	190	14			
2	E	125	Total	C	N	O	S	0	1	0
			957	592	161	190	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	1	0
			2931	1858	505	560	8			
3	F	376	Total	C	N	O	S	0	0	0
			2923	1853	502	560	8			

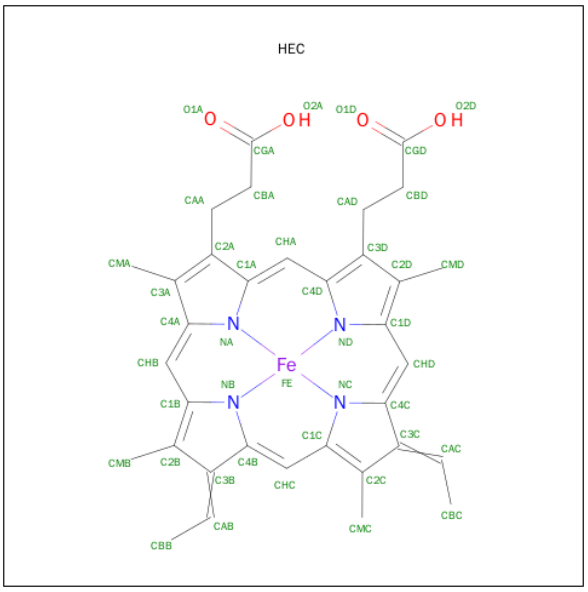
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

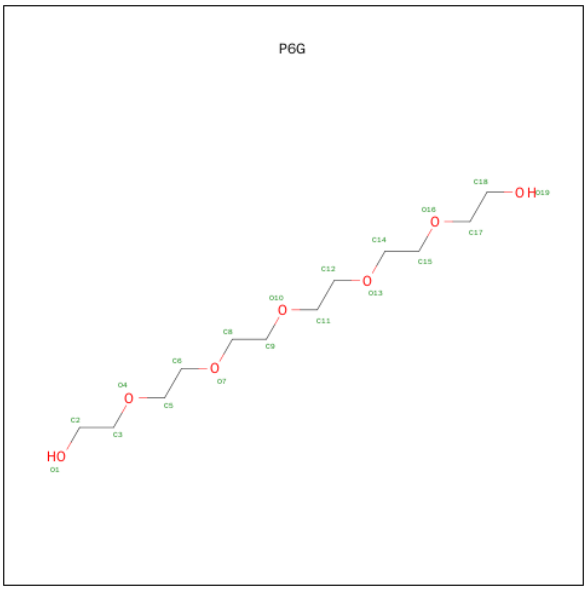
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



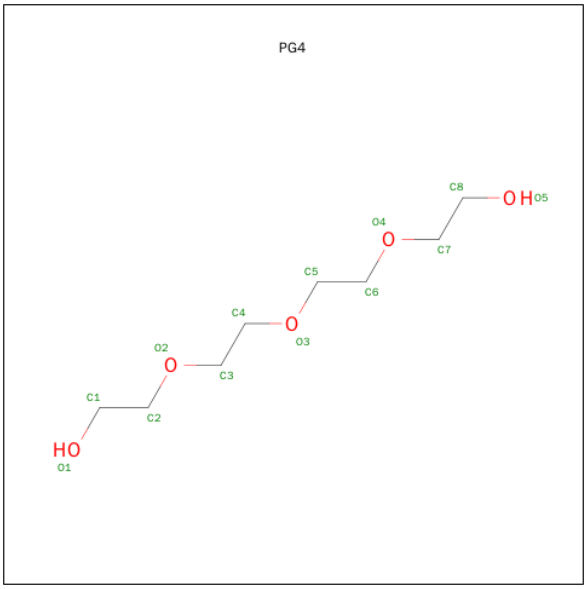
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 7 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



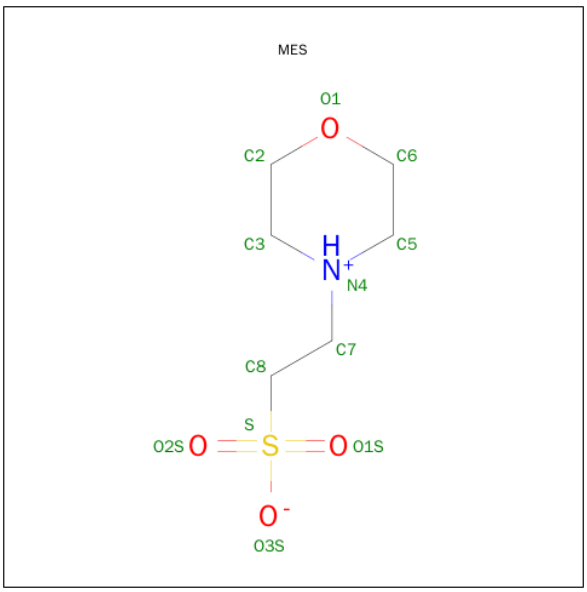
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O 19 12 7	0	0

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

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



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

- Molecule 10 is water.

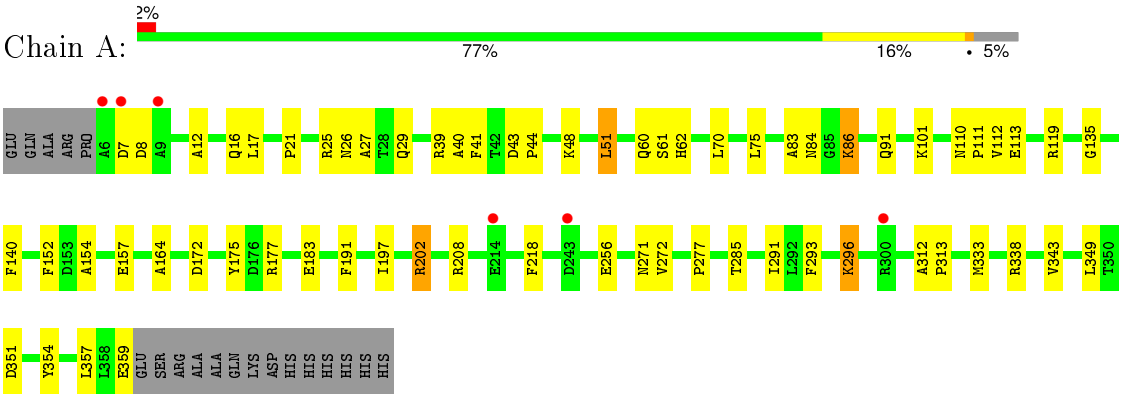
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	206	Total	O	0	0
			206	206		
10	B	265	Total	O	0	0
			265	265		
10	C	83	Total	O	0	0
			83	83		
10	D	223	Total	O	0	0
			223	223		
10	E	89	Total	O	0	0
			89	89		
10	F	314	Total	O	0	0
			314	314		

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.

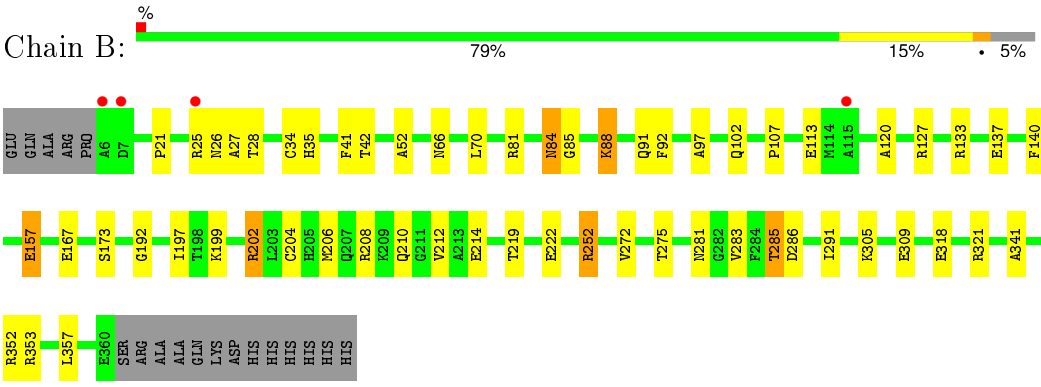
- Molecule 1: Methylamine utilization protein MauG

Chain A:



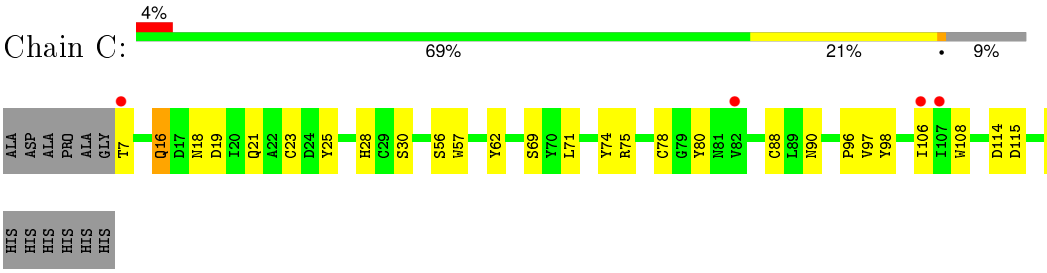
- Molecule 1: Methylamine utilization protein MauG

Chain B:



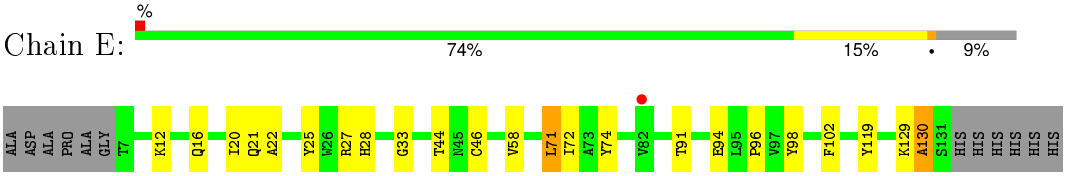
- Molecule 2: Methylamine dehydrogenase light chain

Chain C:



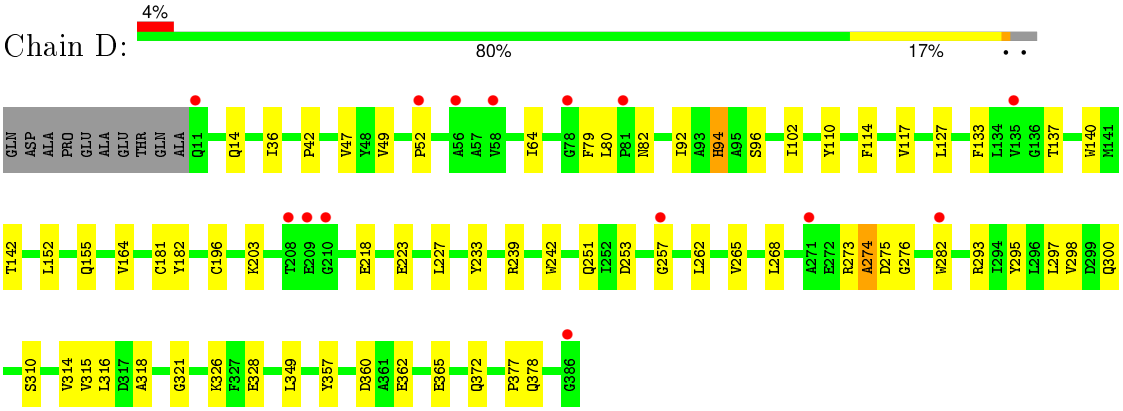
- Molecule 2: Methylamine dehydrogenase light chain

Chain E:



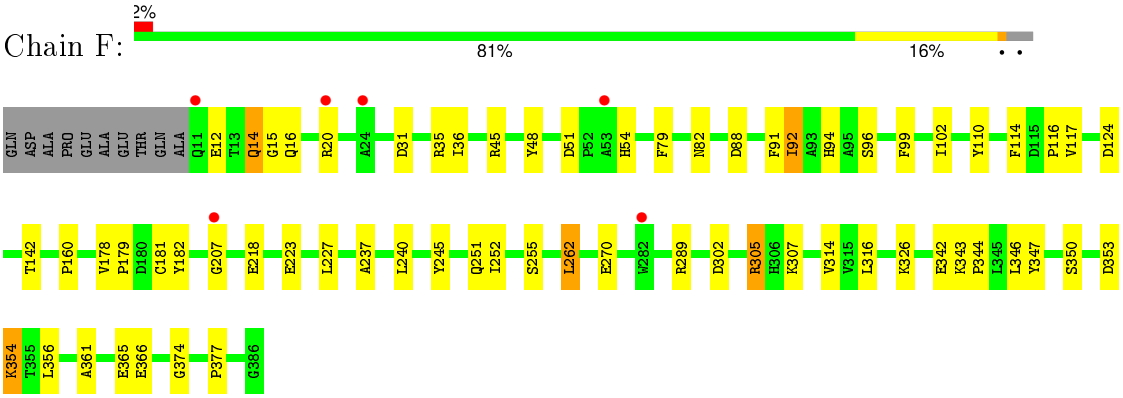
• Molecule 3: Methylamine dehydrogenase heavy chain

Chain D:



• Molecule 3: Methylamine dehydrogenase heavy chain

Chain F:



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)	39.58 – 1.91 39.57 – 1.91	Depositor EDS
% Data completeness (in resolution range)	86.4 (39.58-1.91) 76.5 (39.57-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.173 , 0.230 0.190 , 0.241	Depositor DCC
R_{free} test set	5868 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 116920 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14657	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 5.80% 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, PG4, MES, P6G, 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	1.01	1/2809 (0.0%)	0.97	4/3809 (0.1%)
1	B	1.20	5/2811 (0.2%)	1.10	9/3811 (0.2%)
2	C	0.98	0/969	0.98	1/1323 (0.1%)
2	E	1.22	2/969 (0.2%)	1.04	2/1323 (0.2%)
3	D	1.01	4/3011 (0.1%)	0.96	1/4102 (0.0%)
3	F	1.22	6/3000 (0.2%)	1.06	7/4088 (0.2%)
All	All	1.11	18/13569 (0.1%)	1.02	24/18456 (0.1%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	74	TYR	CD2-CE2	6.59	1.49	1.39
3	F	79	PHE	CE1-CZ	6.37	1.49	1.37
3	F	245	TYR	CD1-CE1	6.19	1.48	1.39
3	F	270	GLU	CG-CD	5.98	1.60	1.51
3	D	357	TYR	CD2-CE2	5.98	1.48	1.39
2	E	22	ALA	CA-CB	5.72	1.64	1.52
3	F	99	PHE	CE2-CZ	5.66	1.48	1.37
1	B	97	ALA	CA-CB	5.59	1.64	1.52
1	B	318	GLU	CD-OE1	5.58	1.31	1.25
1	B	212	VAL	CB-CG2	5.46	1.64	1.52
1	B	222	GLU	CD-OE1	5.33	1.31	1.25
3	D	218	GLU	CB-CG	5.25	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	34	CYS	CB-SG	-5.14	1.73	1.81
3	F	223	GLU	CG-CD	5.05	1.59	1.51
3	D	282	TRP	CB-CG	-5.04	1.41	1.50
1	A	164	ALA	CA-CB	5.02	1.62	1.52
3	D	49	VAL	CB-CG1	5.02	1.63	1.52
3	F	366	GLU	CG-CD	5.00	1.59	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	252	ARG	NE-CZ-NH2	-18.61	111.00	120.30
1	B	252	ARG	NE-CZ-NH1	13.52	127.06	120.30
1	B	206	MET	CG-SD-CE	-10.75	83.00	100.20
3	F	35	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	75	LEU	CA-CB-CG	-7.97	96.98	115.30
3	F	305	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	B	321	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	B	321	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	B	127	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	B	208	ARG	NE-CZ-NH1	-6.65	116.97	120.30
3	F	88	ASP	CB-CG-OD1	6.12	123.81	118.30
3	F	124	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	39	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	A	17	LEU	CB-CG-CD2	-5.60	101.48	111.00
3	F	346	LEU	CB-CG-CD1	5.38	120.15	111.00
2	E	71	LEU	CB-CG-CD1	5.33	120.07	111.00
3	F	305	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	351	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	B	150	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	E	27	ARG	NE-CZ-NH1	-5.24	117.68	120.30
3	F	302	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	B	150	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	D	274	ALA	N-CA-C	-5.20	96.97	111.00
2	C	78	CYS	CA-CB-SG	-5.19	104.65	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	57	0AF	CA

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	2741	0	2624	34	0
1	B	2746	0	2629	42	0
2	C	957	0	863	24	0
2	E	957	0	864	16	0
3	D	2931	0	2821	46	0
3	F	2923	0	2808	35	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	86	0	60	3	0
6	B	86	0	61	9	0
7	F	19	0	26	4	0
8	F	13	0	18	1	0
9	F	12	0	12	0	0
10	A	206	0	0	4	0
10	B	265	0	0	8	0
10	C	83	0	0	2	0
10	D	223	0	0	6	0
10	E	89	0	0	0	0
10	F	314	0	0	4	0
All	All	14657	0	12786	185	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 (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:CYS:SG	6:B:600:HEC:CAC	2.02	1.47
3:D:52:PRO:HG2	3:D:378:GLN:HE21	1.16	1.05
3:F:207:GLY:HA3	10:F:1052:HOH:O	1.61	1.00
1:B:204:CYS:SG	6:B:600:HEC:HAC	2.01	0.95
1:A:48:LYS:H	1:A:62:HIS:HE1	1.17	0.91
1:B:107:PRO:HG3	10:B:1182:HOH:O	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1121:HOH:O	3:F:36:ILE:HD11	1.69	0.91
3:D:314:VAL:HG12	3:D:326:LYS:HG3	1.55	0.88
3:D:52:PRO:HG2	3:D:378:GLN:NE2	1.89	0.88
1:B:197:ILE:O	1:B:202:ARG:HD3	1.74	0.86
1:B:204:CYS:SG	6:B:600:HEC:C3C	2.64	0.86
1:A:48:LYS:H	1:A:62:HIS:CE1	1.97	0.82
3:F:218:GLU:HG2	7:F:387:P6G:H31	1.66	0.76
1:B:204:CYS:SG	6:B:600:HEC:CBC	2.73	0.76
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.51	0.75
1:A:113:GLU:HG2	6:A:500:HEC:HBC2	1.71	0.72
3:F:218:GLU:HG2	7:F:387:P6G:C3	2.20	0.71
3:F:255:SER:HA	8:F:388:PG4:H32	1.72	0.71
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.37	0.70
3:D:360:ASP:OD1	3:D:362:GLU:HB3	1.92	0.70
1:A:272:VAL:HG21	6:A:600:HEC:HMA3	1.76	0.67
1:B:352:ARG:HD2	10:B:1181:HOH:O	1.94	0.67
3:D:265:VAL:HG21	3:D:321:GLY:HA3	1.76	0.67
3:D:268:LEU:HD21	3:D:298:VAL:HG11	1.78	0.66
3:F:218:GLU:CG	7:F:387:P6G:H31	2.25	0.65
3:F:342:GLU:HA	10:F:870:HOH:O	1.99	0.63
2:C:16:GLN:HE22	2:C:19:ASP:H	1.47	0.63
2:C:16:GLN:NE2	2:C:18:ASN:H	1.97	0.62
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.32	0.62
2:C:56:SER:HB2	2:C:74:TYR:O	2.01	0.61
3:D:36:ILE:CD1	2:E:46:CYS:HB2	2.31	0.60
1:B:285:THR:HG22	1:B:286:ASP:OD1	2.01	0.60
3:F:347:TYR:HB3	3:F:356:LEU:HD11	1.83	0.60
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.50	0.59
2:C:21:GLN:HE22	3:F:14:GLN:NE2	2.00	0.59
3:D:181:CYS:C	3:D:182:TYR:CD1	2.76	0.59
3:D:295:TYR:CD2	3:D:315:VAL:HG22	2.38	0.58
3:F:237:ALA:HB2	3:F:289:ARG:HG3	1.84	0.58
2:C:18:ASN:O	3:F:16:GLN:HA	2.04	0.58
2:E:91:THR:HG21	3:F:307:LYS:HD2	1.87	0.57
1:A:110:ASN:OD1	1:A:111:PRO:HD2	2.04	0.57
1:B:202:ARG:HH11	1:B:202:ARG:HG2	1.70	0.57
3:D:265:VAL:CG2	3:D:321:GLY:HA3	2.34	0.56
6:B:600:HEC:HBC3	6:B:600:HEC:HMC1	1.87	0.56
3:D:36:ILE:HD12	2:E:46:CYS:HB2	1.88	0.56
3:F:365:GLU:OE1	3:F:365:GLU:HA	2.05	0.56
2:C:19:ASP:OD1	3:F:15:GLY:HA3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:NZ	1:A:157:GLU:OE2	2.32	0.55
3:F:51:ASP:HA	3:F:377:PRO:HA	1.88	0.55
2:C:16:GLN:C	2:C:16:GLN:HE21	2.08	0.55
1:B:81:ARG:HD2	10:B:1180:HOH:O	2.05	0.55
3:D:274:ALA:HB3	10:D:838:HOH:O	2.07	0.55
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.89	0.54
3:D:181:CYS:HA	3:D:196:CYS:HA	1.89	0.54
3:F:240:LEU:HD23	3:F:252:ILE:HD13	1.90	0.54
2:C:16:GLN:HE21	2:C:18:ASN:H	1.57	0.53
1:B:202:ARG:HH11	1:B:202:ARG:CG	2.21	0.53
1:B:42:THR:HG21	1:B:275:THR:HB	1.91	0.53
1:A:119:ARG:HG2	1:A:152:PHE:CG	2.44	0.53
3:F:45:ARG:NH2	3:F:343:LYS:O	2.42	0.52
3:F:82:ASN:HB3	3:F:142:THR:HB	1.91	0.52
1:A:208:ARG:NH1	3:F:31:ASP:HB2	2.25	0.52
1:B:21:PRO:O	1:B:27:ALA:HA	2.09	0.52
3:D:155:GLN:NE2	10:D:632:HOH:O	2.41	0.52
3:F:54:HIS:HE1	10:F:595:HOH:O	1.93	0.52
1:A:60:GLN:O	1:A:62:HIS:HD2	1.93	0.51
3:D:251:GLN:HE22	3:D:318:ALA:HB1	1.75	0.51
1:A:218:PHE:CE1	1:A:349:LEU:HD22	2.45	0.51
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.21	0.51
3:F:181:CYS:C	3:F:182:TYR:CD1	2.84	0.51
3:D:349:LEU:HD21	3:D:377:PRO:HB2	1.92	0.51
1:B:285:THR:HB	1:B:309:GLU:OE1	2.10	0.50
1:B:272:VAL:HG21	6:B:600:HEC:HMA3	1.94	0.50
3:D:372:GLN:NE2	10:D:1077:HOH:O	2.27	0.49
3:F:354:LYS:HG2	3:F:374:GLY:O	2.13	0.49
3:D:140:TRP:CE2	3:D:233:TYR:HB3	2.48	0.49
1:A:26:ASN:ND2	10:A:819:HOH:O	2.43	0.49
1:B:81:ARG:HH11	1:B:85:GLY:HA2	1.77	0.49
3:D:203:LYS:HE3	3:D:257:GLY:O	2.12	0.49
3:D:293:ARG:HD2	3:D:295:TYR:OH	2.13	0.48
1:A:25:ARG:HH11	1:A:26:ASN:HD21	1.61	0.48
1:B:291:ILE:HD11	1:B:346:LEU:HD12	1.95	0.48
3:D:92:ILE:HG13	3:D:114:PHE:HB2	1.96	0.48
1:A:51:LEU:HB3	1:A:277:PRO:HD3	1.95	0.48
2:C:25:TYR:HB3	2:C:28:HIS:CD2	2.49	0.47
3:F:227:LEU:N	3:F:227:LEU:HD12	2.30	0.47
1:A:86:LYS:HG3	10:A:501:HOH:O	2.15	0.47
2:E:25:TYR:HB3	2:E:28:HIS:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:96:SER:HB3	3:F:110:TYR:CZ	2.50	0.47
2:E:94:GLU:HG2	2:E:102:PHE:O	2.16	0.46
2:C:23:CYS:SG	2:C:88[B]:CYS:HB2	2.56	0.46
1:B:291:ILE:HG12	6:B:600:HEC:HMB2	1.96	0.46
3:D:96:SER:HB3	3:D:110:TYR:CZ	2.50	0.46
3:D:275:ASP:OD1	10:D:1136:HOH:O	2.21	0.46
3:D:253:ASP:HB2	3:D:262:LEU:CD1	2.46	0.46
3:F:344:PRO:HG2	3:F:361:ALA:HB3	1.97	0.46
2:C:56:SER:HB3	2:C:75:ARG:HD2	1.97	0.46
1:A:12:ALA:O	1:A:16:GLN:HG2	2.15	0.46
1:A:140:PHE:CE1	1:A:154:ALA:HB1	2.51	0.46
3:D:47:VAL:HG13	3:D:64:ILE:HB	1.98	0.45
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.50	0.45
3:D:82:ASN:HB3	3:D:142:THR:HB	1.97	0.45
2:E:20:ILE:HG22	2:E:25:TYR:CZ	2.51	0.45
2:C:62:TYR:HB2	10:C:1114:HOH:O	2.16	0.45
2:C:130:ALA:O	2:C:131:SER:CB	2.65	0.45
3:D:276:GLY:O	3:D:300:GLN:HA	2.16	0.45
1:B:192:GLY:N	1:B:341:ALA:HB1	2.31	0.45
3:F:48:TYR:CZ	3:F:92:ILE:HG21	2.52	0.45
1:B:88:LYS:NZ	10:B:758:HOH:O	2.50	0.45
3:D:239:ARG:HH11	3:D:251:GLN:NE2	2.15	0.45
2:E:96:PRO:HB2	2:E:98:TYR:CE1	2.52	0.45
3:F:350:SER:HB3	3:F:353:ASP:HB2	1.99	0.45
7:F:387:P6G:H142	7:F:387:P6G:H171	1.57	0.44
3:D:227:LEU:HB3	3:D:242:TRP:NE1	2.33	0.44
2:C:88[B]:CYS:SG	2:C:90:ASN:ND2	2.90	0.44
1:B:88:LYS:HD3	10:B:802:HOH:O	2.18	0.44
2:E:12:LYS:HE2	10:F:971:HOH:O	2.18	0.44
2:E:58:VAL:HA	2:E:72:ILE:O	2.18	0.44
3:D:265:VAL:HG21	3:D:321:GLY:CA	2.45	0.44
1:A:312:ALA:O	1:A:313:PRO:C	2.56	0.43
3:D:239:ARG:HD2	3:D:251:GLN:HE21	1.83	0.43
1:B:35:HIS:CE1	1:B:70:LEU:HD21	2.53	0.43
1:A:293:PHE:CE1	1:A:296:LYS:CD	3.02	0.43
3:F:91:PHE:HA	3:F:116:PRO:HD3	2.00	0.43
2:C:106:ILE:HG12	3:D:133:PHE:CZ	2.53	0.43
1:A:48:LYS:N	1:A:62:HIS:HE1	1.98	0.43
3:D:152:LEU:HD23	3:D:164:VAL:HA	2.00	0.43
1:A:61:SER:HB3	1:A:112:VAL:HB	2.01	0.43
3:D:273:ARG:HG2	10:D:643:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:57:0AF:CE3	2:C:108:TRP:CD1	3.02	0.43
1:B:173:SER:HB2	1:B:348:THR:O	2.18	0.43
3:D:137:THR:HA	10:D:389:HOH:O	2.19	0.42
2:E:129:LYS:O	2:E:130:ALA:HB2	2.18	0.42
1:A:135:GLY:HA2	10:A:1122:HOH:O	2.20	0.42
1:B:133:ARG:O	1:B:137:GLU:HG3	2.19	0.42
1:B:25:ARG:HD3	10:B:1124:HOH:O	2.19	0.42
3:F:92:ILE:HG12	3:F:114:PHE:HB2	2.00	0.42
1:A:271:ASN:O	1:A:272:VAL:C	2.58	0.42
3:D:182:TYR:CD1	3:D:182:TYR:N	2.87	0.42
3:D:82:ASN:O	3:D:94:HIS:HA	2.20	0.42
2:C:106:ILE:HG12	3:D:133:PHE:HZ	1.84	0.42
1:B:84:ASN:OD1	1:B:84:ASN:N	2.52	0.42
1:B:113:GLU:HG2	6:B:500:HEC:HBC2	2.00	0.42
2:C:96:PRO:HB2	2:C:98:TYR:CE1	2.55	0.42
1:B:202:ARG:NH1	1:B:202:ARG:CG	2.80	0.42
1:A:175:TYR:C	1:A:175:TYR:CD2	2.93	0.42
3:F:305:ARG:HD2	3:F:305:ARG:HA	1.89	0.42
3:D:79:PHE:O	3:D:80:LEU:C	2.58	0.42
1:B:252:ARG:HD3	10:B:811:HOH:O	2.20	0.41
2:C:80:TYR:HB2	2:C:120:HIS:HB2	2.02	0.41
1:A:197:ILE:O	1:A:202:ARG:HD2	2.20	0.41
3:D:326:LYS:HB3	3:D:326:LYS:HE2	1.84	0.41
1:B:81:ARG:CD	10:B:1180:HOH:O	2.65	0.41
1:B:192:GLY:CA	1:B:341:ALA:HB1	2.51	0.41
1:A:83:ALA:N	10:A:1003:HOH:O	2.51	0.41
1:A:191:PHE:CZ	1:A:338:ARG:HG2	2.55	0.41
2:C:56:SER:CB	2:C:74:TYR:O	2.67	0.41
3:D:297:LEU:HA	3:D:297:LEU:HD23	1.88	0.41
1:B:204:CYS:CB	6:B:600:HEC:C3C	2.98	0.41
2:E:129:LYS:O	2:E:130:ALA:CB	2.68	0.41
2:C:114:ASP:O	2:C:115:ASP:HB2	2.21	0.41
1:B:140:PHE:HZ	1:B:157:GLU:HG2	1.85	0.41
1:B:120:ALA:HA	1:B:148:PRO:HB3	2.02	0.41
3:F:251:GLN:O	3:F:262:LEU:HB2	2.20	0.41
1:A:21:PRO:O	1:A:27:ALA:HA	2.21	0.41
1:A:43:ASP:HA	1:A:44:PRO:HD2	1.65	0.41
3:D:253:ASP:HB2	3:D:262:LEU:HD11	2.02	0.41
1:B:281:ASN:OD1	1:B:283:VAL:HB	2.20	0.41
3:F:178:VAL:HB	3:F:179:PRO:CD	2.50	0.41
3:F:314:VAL:HG12	3:F:326:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:97:VAL:HG23	2:C:106:ILE:HD11	2.02	0.41
1:B:91:GLN:O	1:B:92:PHE:HB2	2.21	0.40
1:A:172:ASP:O	1:A:177:ARG:NH1	2.54	0.40
1:B:41:PHE:HE2	1:B:353:ARG:HH21	1.69	0.40
1:A:291:ILE:HD12	1:A:343:VAL:HG23	2.02	0.40
1:B:52:ALA:O	1:B:66:ASN:HA	2.21	0.40
3:D:36:ILE:HD13	2:E:46:CYS:HB2	2.04	0.40
1:A:277:PRO:HB3	1:A:285:THR:HA	2.02	0.40
1:A:41:PHE:HB2	1:A:70:LEU:H	1.86	0.40
3:D:42:PRO:HD3	3:D:117:VAL:HG12	2.03	0.40
2:E:33:GLY:HA3	2:E:119:TYR:OH	2.22	0.40
1:B:199:LYS:O	1:B:202:ARG:NH1	2.54	0.40
1:A:91:GLN:HB3	6:A:500:HEC:HAA1	2.03	0.40
2:C:16:GLN:NE2	2:C:19:ASP:H	2.15	0.40
1:B:26:ASN:HB2	1:B:28:THR:HG23	2.04	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	354/373 (95%)	336 (95%)	18 (5%)	0	100	100
1	B	354/373 (95%)	341 (96%)	13 (4%)	0	100	100
2	C	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
2	E	123/137 (90%)	119 (97%)	3 (2%)	1 (1%)	24	11
3	D	375/386 (97%)	356 (95%)	17 (4%)	2 (0%)	34	20
3	F	374/386 (97%)	360 (96%)	13 (4%)	1 (0%)	46	34
All	All	1703/1792 (95%)	1633 (96%)	66 (4%)	4 (0%)	52	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	130	ALA
3	D	102	ILE
3	D	223	GLU
3	F	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	278/292 (95%)	265 (95%)	13 (5%)	32	19
1	B	278/292 (95%)	267 (96%)	11 (4%)	38	25
2	C	105/112 (94%)	100 (95%)	5 (5%)	31	18
2	E	105/112 (94%)	103 (98%)	2 (2%)	65	58
3	D	305/311 (98%)	300 (98%)	5 (2%)	70	65
3	F	304/311 (98%)	296 (97%)	8 (3%)	54	44
All	All	1375/1430 (96%)	1331 (97%)	44 (3%)	46	35

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	ASP
1	A	29	GLN
1	A	51	LEU
1	A	84	ASN
1	A	86	LYS
1	A	183	GLU
1	A	202	ARG
1	A	256	GLU
1	A	296	LYS
1	A	333	MET
1	A	357	LEU
1	A	359	GLU
1	B	84	ASN
1	B	88	LYS

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Mol	Chain	Res	Type
1	B	102	GLN
1	B	157	GLU
1	B	167	GLU
1	B	202	ARG
1	B	214	GLU
1	B	219	THR
1	B	285	THR
1	B	305	LYS
1	B	357	LEU
2	C	7	THR
2	C	16	GLN
2	C	30	SER
2	C	69	SER
2	C	71	LEU
3	D	94	HIS
3	D	127	LEU
3	D	316	LEU
3	D	328	GLU
3	D	365	GLU
2	E	16	GLN
2	E	71	LEU
3	F	14	GLN
3	F	92	ILE
3	F	94	HIS
3	F	117	VAL
3	F	160	PRO
3	F	262	LEU
3	F	316	LEU
3	F	354	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	GLN
1	A	62	HIS
1	A	91	GLN
1	B	16	GLN
1	B	29	GLN
1	B	60	GLN
1	B	91	GLN
1	B	210	GLN

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Mol	Chain	Res	Type
2	C	16	GLN
2	C	90	ASN
3	D	14	GLN
3	D	30	GLN
3	D	60	GLN
3	D	155	GLN
3	D	251	GLN
3	D	378	GLN
3	F	14	GLN
3	F	54	HIS
3	F	300	GLN
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	0AF	C	57	2	13,16,17	1.21	2 (15%)	10,22,24	1.71	2 (20%)
2	0AF	E	57	2	13,16,17	1.93	5 (38%)	10,22,24	2.17	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	2	1/1/1/2	0/3/6/8	0/2/2/2
2	0AF	E	57	2	-	0/3/6/8	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CZ2-CE2	-3.43	1.38	1.42
2	E	57	0AF	CB-CA	-2.40	1.48	1.53
2	E	57	0AF	CD1-NE1	-2.28	1.32	1.36
2	C	57	0AF	CB-CA	-2.20	1.49	1.53
2	C	57	0AF	CA-N	-2.03	1.41	1.47
2	E	57	0AF	CH2-CZ2	2.37	1.42	1.37
2	E	57	0AF	CZ3-CE3	2.68	1.42	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	57	0AF	CB-CG-CD1	-4.24	122.73	127.97
2	E	57	0AF	O-C-CA	-3.68	115.91	125.49
2	C	57	0AF	O-C-CA	-3.33	116.82	125.49
2	C	57	0AF	CB-CG-CD1	-3.05	124.20	127.97
2	E	57	0AF	O1-CZ2-CE2	-2.37	114.79	119.05
2	E	57	0AF	CE3-CZ3-CH2	-2.12	117.43	120.96

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.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	24,50,50	1.59	6 (25%)	19,82,82	3.55	9 (47%)
6	HEC	A	600	1	24,50,50	2.05	10 (41%)	19,82,82	3.82	12 (63%)
6	HEC	B	500	1,10	24,50,50	1.98	7 (29%)	19,82,82	2.92	8 (42%)
6	HEC	B	600	1	24,50,50	2.43	7 (29%)	19,82,82	4.21	11 (57%)
7	P6G	F	387	-	18,18,18	0.83	0	17,17,17	0.78	0
8	PG4	F	388	-	12,12,12	0.54	0	11,11,11	0.36	0
9	MES	F	389	-	11,12,12	0.49	0	14,16,16	3.64	9 (64%)

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	-	0/6/54/54	0/0/8/8
6	HEC	A	600	1	-	0/6/54/54	0/0/8/8
6	HEC	B	500	1,10	-	0/6/54/54	0/0/8/8
6	HEC	B	600	1	-	0/6/54/54	0/0/8/8
7	P6G	F	387	-	-	0/16/16/16	0/0/0/0
8	PG4	F	388	-	-	0/10/10/10	0/0/0/0
9	MES	F	389	-	-	0/6/14/14	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	600	HEC	C4C-NC	-6.44	1.28	1.36
6	B	600	HEC	C4B-NB	-5.64	1.29	1.36
6	B	500	HEC	C4C-NC	-5.33	1.29	1.36
6	A	600	HEC	C1A-NA	-4.55	1.30	1.36
6	B	600	HEC	C4A-NA	-3.88	1.31	1.36
6	B	600	HEC	C3C-C2C	-3.66	1.36	1.40
6	A	600	HEC	C4A-NA	-3.37	1.32	1.36
6	A	600	HEC	C4B-NB	-3.14	1.32	1.36
6	B	600	HEC	C1A-NA	-3.08	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	500	HEC	C4B-NB	-2.70	1.33	1.36
6	A	600	HEC	C4C-NC	-2.29	1.33	1.36
6	B	500	HEC	C1B-CHB	2.08	1.45	1.39
6	A	500	HEC	C1C-CHC	2.09	1.45	1.39
6	A	600	HEC	C3C-C4C	2.30	1.48	1.42
6	B	500	HEC	C4D-CHA	2.30	1.46	1.39
6	A	600	HEC	C1B-CHB	2.43	1.46	1.39
6	A	500	HEC	C1B-CHB	2.51	1.46	1.39
6	B	600	HEC	C3B-C2B	2.53	1.43	1.40
6	A	600	HEC	C1C-CHC	2.57	1.46	1.39
6	B	600	HEC	C4D-CHA	2.58	1.47	1.39
6	A	600	HEC	C4D-CHA	2.63	1.47	1.39
6	A	600	HEC	C3B-C4B	2.72	1.48	1.42
6	A	600	HEC	C1D-CHD	2.83	1.47	1.39
6	B	500	HEC	C1C-CHC	2.88	1.47	1.39
6	A	500	HEC	C4D-CHA	2.88	1.47	1.39
6	A	500	HEC	C3B-C4B	2.91	1.49	1.42
6	B	500	HEC	C3B-C4B	3.08	1.49	1.42
6	A	500	HEC	C1D-CHD	3.35	1.49	1.39
6	A	500	HEC	C3C-C4C	3.44	1.50	1.42
6	B	500	HEC	C3C-C4C	3.62	1.50	1.42

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	600	HEC	CBB-CAB-C3B	-11.11	102.67	127.35
6	A	500	HEC	CBB-CAB-C3B	-11.10	102.68	127.35
6	A	600	HEC	CBD-CAD-C3D	-8.38	97.51	112.53
6	B	600	HEC	CBC-CAC-C3C	-7.87	109.86	127.35
6	A	600	HEC	CBB-CAB-C3B	-7.69	110.26	127.35
6	B	600	HEC	CBD-CAD-C3D	-7.64	98.84	112.53
9	F	389	MES	C2-C3-N4	-7.37	98.95	110.12
6	A	500	HEC	CBC-CAC-C3C	-7.07	111.64	127.35
6	B	500	HEC	CBB-CAB-C3B	-7.05	111.69	127.35
6	A	600	HEC	CBC-CAC-C3C	-6.64	112.59	127.35
6	B	500	HEC	CBD-CAD-C3D	-6.42	101.02	112.53
9	F	389	MES	C6-C5-N4	-4.21	103.74	110.12
6	B	600	HEC	CAA-C2A-C1A	-4.20	122.44	127.01
6	A	600	HEC	CMC-C2C-C1C	-4.04	121.68	128.36
6	B	500	HEC	CBA-CAA-C2A	-4.02	105.33	112.53
6	A	600	HEC	CAA-C2A-C1A	-4.02	122.65	127.01
6	B	500	HEC	CMC-C2C-C1C	-4.00	121.75	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	600	HEC	CBA-CAA-C2A	-3.79	105.74	112.53
6	B	600	HEC	CMC-C2C-C1C	-3.66	122.31	128.36
6	B	500	HEC	CBC-CAC-C3C	-3.38	119.84	127.35
6	A	600	HEC	C4B-C3B-C2B	-3.32	102.77	106.35
6	A	600	HEC	CBA-CAA-C2A	-3.26	106.69	112.53
6	A	500	HEC	CBD-CAD-C3D	-3.02	107.12	112.53
6	A	500	HEC	C4C-C3C-C2C	-3.01	103.10	106.35
6	A	500	HEC	CMC-C2C-C1C	-2.87	123.62	128.36
6	B	600	HEC	CAD-CBD-CGD	-2.80	107.61	112.75
9	F	389	MES	O1-C6-C5	-2.76	105.51	111.84
6	A	600	HEC	C4C-C3C-C2C	-2.66	103.47	106.35
6	B	600	HEC	C4C-C3C-C2C	-2.62	103.52	106.35
6	A	600	HEC	CMD-C2D-C1D	-2.54	124.16	128.36
6	A	600	HEC	CAA-CBA-CGA	-2.37	108.40	112.75
6	B	600	HEC	CAA-CBA-CGA	-2.37	108.40	112.75
6	B	500	HEC	C4B-C3B-C2B	-2.26	103.91	106.35
9	F	389	MES	O3S-S-O2S	-2.21	106.47	111.61
6	A	500	HEC	CMB-C2B-C1B	-2.11	124.88	128.36
6	A	500	HEC	CBA-CAA-C2A	-2.08	108.80	112.53
6	B	500	HEC	CAD-C3D-C4D	2.19	129.38	127.01
6	B	600	HEC	C3C-C4C-NC	2.42	115.52	110.94
6	A	600	HEC	CMA-C3A-C2A	2.51	130.49	125.24
6	B	500	HEC	C3B-C4B-NB	2.62	115.90	110.94
6	A	500	HEC	CMA-C3A-C2A	2.86	131.22	125.24
6	B	600	HEC	CAD-C3D-C4D	3.06	130.33	127.01
9	F	389	MES	C5-N4-C3	3.13	115.67	108.90
6	A	500	HEC	CMD-C2D-C3D	3.17	131.86	125.24
6	A	600	HEC	CMD-C2D-C3D	3.50	132.55	125.24
9	F	389	MES	C7-N4-C3	4.06	121.68	111.27
9	F	389	MES	C7-N4-C5	4.42	122.59	111.27
9	F	389	MES	O1S-S-C8	4.76	110.97	106.91
9	F	389	MES	O2S-S-C8	5.41	111.52	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	500	HEC	2	0
6	A	600	HEC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	500	HEC	1	0
6	B	600	HEC	8	0
7	F	387	P6G	4	0
8	F	388	PG4	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%)	-0.06	6 (1%) 73 76	26, 37, 51, 70	0
1	B	355/373 (95%)	-0.17	4 (1%) 82 84	19, 30, 47, 66	0
2	C	124/137 (90%)	0.35	5 (4%) 42 46	24, 35, 52, 69	0
2	E	124/137 (90%)	0.19	1 (0%) 87 89	19, 26, 35, 60	0
3	D	376/386 (97%)	0.19	14 (3%) 45 49	24, 40, 66, 77	0
3	F	376/386 (97%)	0.01	6 (1%) 74 78	19, 28, 45, 61	0
All	All	1709/1792 (95%)	0.04	36 (2%) 67 70	19, 33, 55, 77	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ALA	6.1
1	A	6	ALA	5.5
1	B	7	ASP	5.3
1	A	7	ASP	4.6
2	C	106	ILE	3.7
2	C	82	VAL	3.7
3	D	208	THR	3.3
3	D	135	VAL	3.2
3	D	58	VAL	3.0
3	D	257	GLY	2.8
3	D	56	ALA	2.8
1	A	214	GLU	2.7
3	D	209	GLU	2.7
1	B	115	ALA	2.6
3	F	11	GLN	2.6
3	F	53	ALA	2.6
2	C	130	ALA	2.5
3	F	20	ARG	2.5
2	C	7	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	82	VAL	2.5
3	D	11	GLN	2.5
3	F	207	GLY	2.4
3	D	210	GLY	2.4
3	D	52	PRO	2.4
1	A	243	ASP	2.3
1	A	300	ARG	2.2
3	D	386	GLY	2.2
1	B	25	ARG	2.2
2	C	107	ILE	2.1
3	D	81	PRO	2.1
3	D	78	GLY	2.1
3	D	271	ALA	2.1
3	F	24	ALA	2.1
3	F	282	TRP	2.0
3	D	282	TRP	2.0
1	A	9	ALA	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	C	57	15/16	0.93	0.13	-	32,35,36,38	0
2	0AF	E	57	15/16	0.96	0.17	-	21,25,27,27	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^{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
9	MES	F	389	12/12	0.90	0.17	4.79	20,33,37,37	12
7	P6G	F	387	19/19	0.86	0.16	2.79	43,49,62,62	0
8	PG4	F	388	13/13	0.85	0.16	1.80	58,61,78,78	0
6	HEC	B	600	43/43	0.98	0.14	1.17	12,17,21,24	0
4	CA	A	400	1/1	0.99	0.11	0.74	29,29,29,29	0
6	HEC	A	500	43/43	0.97	0.09	0.13	26,30,33,35	0
4	CA	B	400	1/1	1.00	0.08	0.00	20,20,20,20	0
6	HEC	B	500	43/43	0.97	0.09	-0.06	18,23,27,28	0
6	HEC	A	600	43/43	0.98	0.10	-0.58	18,28,30,32	0
5	NA	B	402	1/1	0.94	0.07	-1.55	35,35,35,35	0
5	NA	A	402	1/1	0.98	0.06	-4.05	37,37,37,37	0
5	NA	B	401	1/1	0.97	0.22	-	41,41,41,41	0
5	NA	A	401	1/1	0.82	0.10	-	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.