



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:01 am GMT

PDB ID : 3RLM
Title : Structure of the W199F MauG/pre-Methylamine Dehydrogenase complex after treatment with hydrogen peroxide
Authors : Yukl, E.T.; Wilmot, C.M.
Deposited on : 2011-04-19
Resolution : 2.13 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

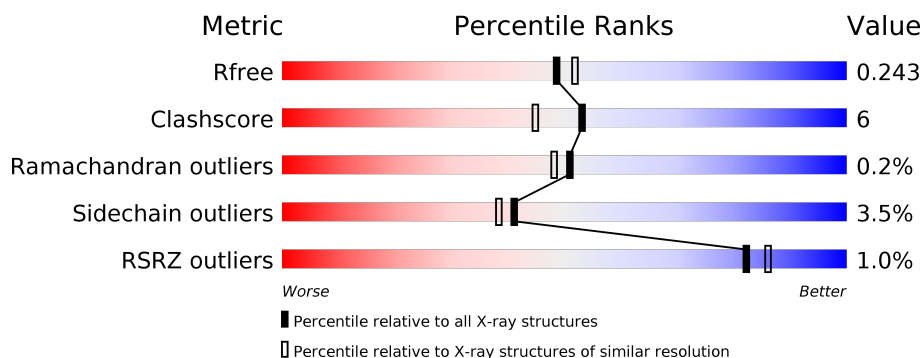
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (2.16-2.12)

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

Mol	Chain	Length	Quality of chain
1	A	373	<div> <div>81% 13% 5%</div> </div>
1	B	373	<div> <div>79% 16% 5%</div> </div>
2	C	137	<div> <div>77% 17% ..</div> </div>
2	E	137	<div> <div>68% 23% 9%</div> </div>
3	D	386	<div> <div>82% 16%</div> </div>
3	F	386	<div> <div>86% 11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CA	B	400	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14548 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	3	0
			2757	1720	495	531	11			
1	B	355	Total	C	N	O	S	0	3	0
			2773	1728	502	532	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	PHE	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	PHE	TRP	ENGINEERED MUTATION	UNP Q51658
B	368	HIS	-	EXPRESSION TAG	UNP Q51658
B	369	HIS	-	EXPRESSION TAG	UNP Q51658
B	370	HIS	-	EXPRESSION TAG	UNP Q51658
B	371	HIS	-	EXPRESSION TAG	UNP Q51658
B	372	HIS	-	EXPRESSION TAG	UNP Q51658
B	373	HIS	-	EXPRESSION TAG	UNP Q51658

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	131	Total	C	N	O	S	0	2	0
			1023	632	179	198	14			
2	E	125	Total	C	N	O	S	0	2	0
			960	594	161	190	15			

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

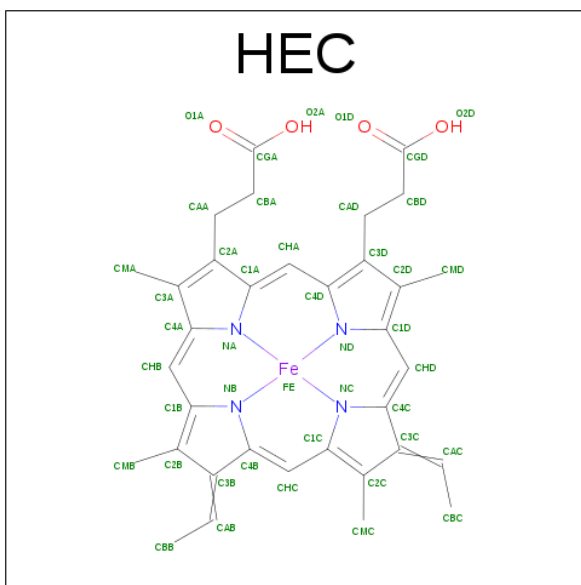
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	1	0
			2934	1859	506	561	8			
3	F	376	Total	C	N	O	S	0	3	0
			2941	1865	504	563	9			

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

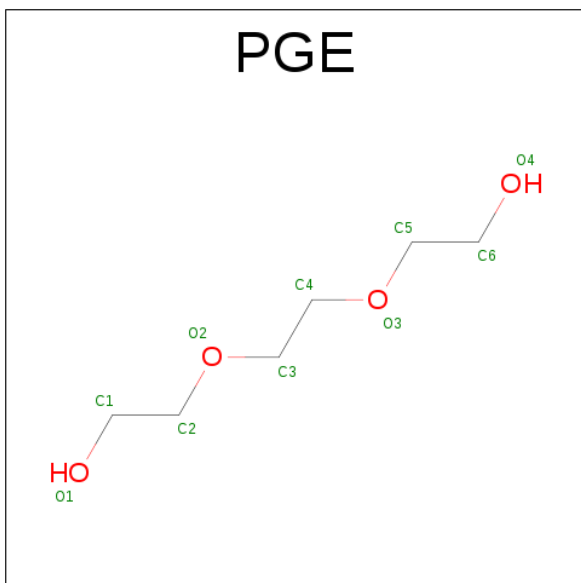
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



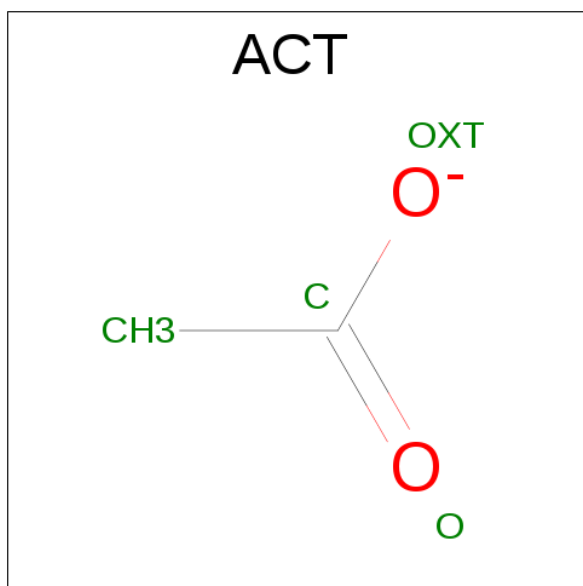
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $\text{C}_6\text{H}_{14}\text{O}_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

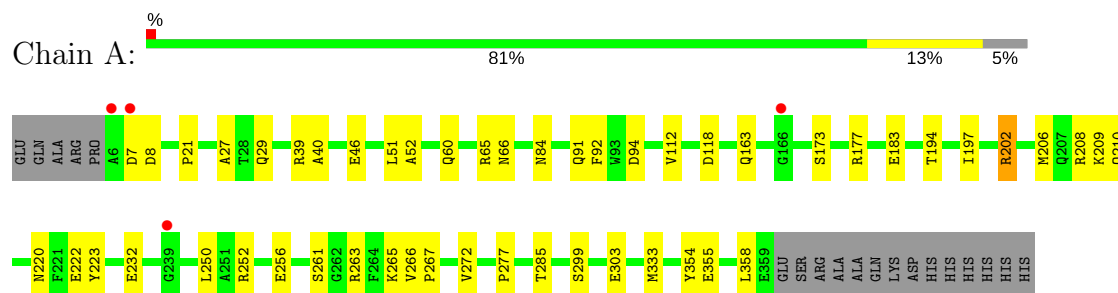
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	146	Total	O	0	1
			147	147		
8	B	219	Total	O	0	1
			220	220		
8	C	59	Total	O	0	0
			59	59		
8	D	168	Total	O	0	0
			168	168		
8	E	80	Total	O	0	0
			80	80		
8	F	294	Total	O	0	0
			294	294		

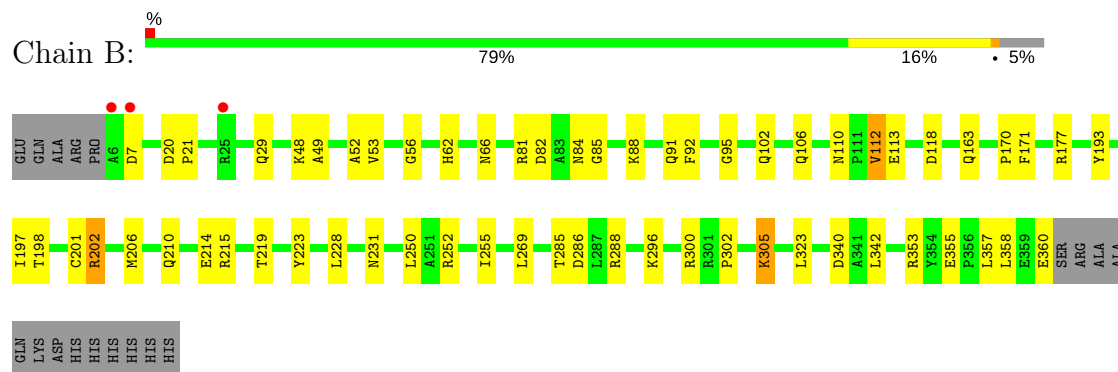
3 Residue-property plots [i](#)

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

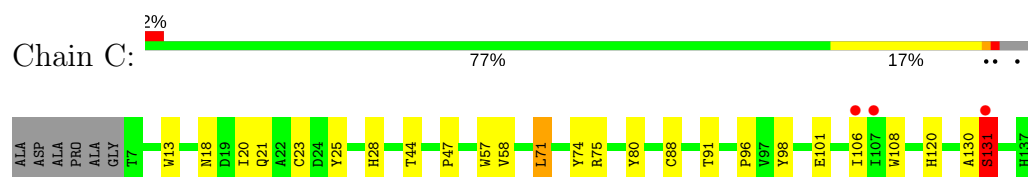
• Molecule 1: Methylamine utilization protein MauG



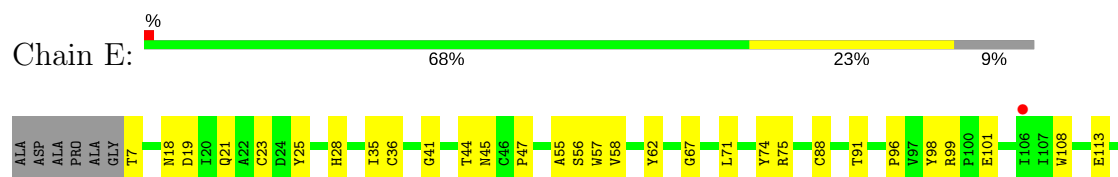
• Molecule 1: Methylamine utilization protein MauG

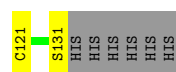


• Molecule 2: Methylamine dehydrogenase light chain

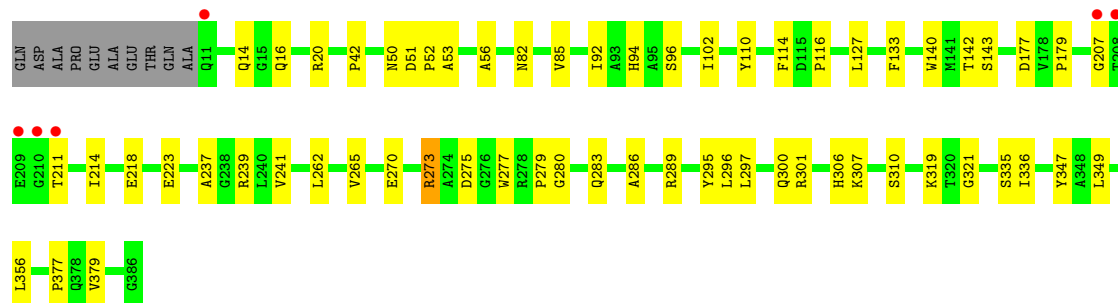
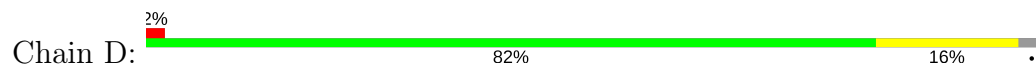


• Molecule 2: Methylamine dehydrogenase light chain

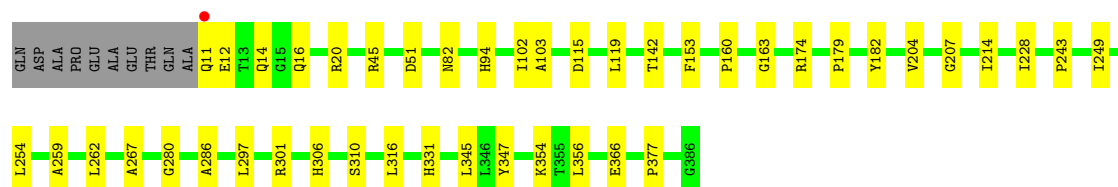
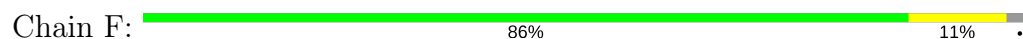




• Molecule 3: Methylamine dehydrogenase heavy chain



• Molecule 3: Methylamine dehydrogenase heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	44.49 – 2.13 44.49 – 2.13	Depositor EDS
% Data completeness (in resolution range)	95.4 (44.49-2.13) 84.1 (44.49-2.13)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.181 , 0.237 0.190 , 0.243	Depositor DCC
R_{free} test set	4676 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14548	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, CA, PGE, 0AF, HEC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.50	0/2823	0.64	2/3828 (0.1%)
1	B	0.56	0/2836	0.66	1/3844 (0.0%)
2	C	0.54	0/1044	0.70	0/1425
2	E	0.70	0/975	0.74	0/1331
3	D	0.51	0/3011	0.62	0/4102
3	F	0.62	0/3024	0.71	0/4119
All	All	0.56	0/13713	0.67	3/18649 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	39	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	252	ARG	NE-CZ-NH2	-5.11	117.75	120.30

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	2757	0	2632	27	1
1	B	2773	0	2649	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1023	0	912	23	0
2	E	960	0	869	28	0
3	D	2934	0	2820	37	0
3	F	2941	0	2830	22	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	6	0
6	B	10	0	14	0	0
7	D	4	0	3	0	0
7	F	4	0	3	0	0
8	A	147	0	0	3	0
8	B	220	0	0	10	1
8	C	59	0	0	1	0
8	D	168	0	0	1	0
8	E	80	0	0	4	0
8	F	294	0	0	1	0
All	All	14548	0	12852	163	1

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 6.

All (163) 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:C:130:ALA:HA	2:C:131:SER:HB3	1.27	1.09
3:D:273[A]:ARG:HG3	3:D:273[A]:ARG:HH11	1.08	1.07
3:D:273[A]:ARG:CG	3:D:273[A]:ARG:HH11	1.69	1.03
2:E:36[B]:CYS:SG	2:E:41:GLY:HA3	2.08	0.94
2:C:130:ALA:CA	2:C:131:SER:HB3	2.02	0.89
2:E:56:SER:HB2	2:E:74:TYR:O	1.81	0.81
3:D:273[A]:ARG:NH1	3:D:273[A]:ARG:HB2	1.99	0.78
3:F:249:ILE:HD11	3:F:267:ALA:HB2	1.69	0.74
3:D:273[A]:ARG:HG3	3:D:273[A]:ARG:NH1	1.91	0.74
2:E:36[B]:CYS:SG	2:E:45:ASN:O	2.47	0.72
1:B:81:ARG:HD3	8:B:505:HOH:O	1.89	0.71
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.54	0.71
2:C:57:0AF:CE3	2:C:108:TRP:CD1	2.75	0.69
3:D:273[A]:ARG:NH1	3:D:273[A]:ARG:CG	2.40	0.68
1:B:88:LYS:HE2	8:B:439:HOH:O	1.93	0.68
3:D:273[A]:ARG:NH1	3:D:273[A]:ARG:CB	2.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:113:GLU:OE2	8:E:465:HOH:O	2.14	0.66
8:B:546:HOH:O	2:E:101:GLU:HG3	1.95	0.65
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.42	0.65
5:B:600:HEC:HBC3	5:B:600:HEC:HMC1	1.79	0.65
3:F:51:ASP:HA	3:F:377:PRO:HA	1.79	0.64
3:D:273[A]:ARG:CB	3:D:273[A]:ARG:HH11	2.11	0.63
1:B:250:LEU:O	8:B:470:HOH:O	2.16	0.63
1:A:8:ASP:HB2	8:A:494:HOH:O	1.97	0.63
1:B:300:ARG:NH1	8:B:453:HOH:O	2.27	0.62
1:A:197:ILE:O	1:A:202:ARG:HD2	2.00	0.62
1:A:197:ILE:HA	1:A:202:ARG:HB3	1.82	0.61
1:A:299:SER:HB2	1:A:333:MET:HG3	1.84	0.59
3:F:331:HIS:HE1	3:F:366:GLU:OE1	1.86	0.59
2:C:23:CYS:HB3	2:C:88[B]:CYS:SG	2.42	0.59
3:D:42:PRO:HG3	3:D:116:PRO:HB2	1.85	0.58
2:C:74:TYR:O	2:C:75:ARG:HG3	2.04	0.58
1:B:255:ILE:O	8:B:470:HOH:O	2.17	0.57
1:B:91:GLN:O	1:B:92:PHE:HB2	2.04	0.57
1:B:95:GLY:HA3	1:B:223:TYR:OH	2.05	0.57
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.53	0.57
1:A:65:ARG:HH12	1:A:94:ASP:CG	2.08	0.57
1:A:163:GLN:HE22	5:A:500:HEC:HMA1	1.70	0.57
1:B:91:GLN:HE21	5:B:500:HEC:HAA1	1.70	0.56
1:B:202:ARG:HB2	1:B:206:MET:HG3	1.87	0.56
1:B:177[B]:ARG:NH2	1:B:355:GLU:OE2	2.37	0.56
3:F:179:PRO:HD3	3:F:214:ILE:HD13	1.87	0.56
1:A:177[A]:ARG:NE	1:A:183:GLU:OE1	2.30	0.56
3:F:297:LEU:HD22	3:F:310:SER:HB2	1.88	0.55
2:E:74:TYR:O	2:E:75:ARG:HG3	2.06	0.55
3:D:280:GLY:HA3	3:D:301:ARG:CZ	2.36	0.55
1:A:250:LEU:HD22	1:A:261:SER:HB2	1.88	0.55
2:C:91:THR:HB	3:D:306:HIS:CE1	2.42	0.55
1:A:91:GLN:O	1:A:92:PHE:HB2	2.08	0.54
2:E:56:SER:CB	2:E:74:TYR:O	2.54	0.54
3:D:349:LEU:HD21	3:D:377:PRO:HB2	1.89	0.53
3:D:277:TRP:CE2	3:D:300:GLN:HG3	2.43	0.53
3:D:82:ASN:HB3	3:D:142:THR:HB	1.90	0.53
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.89	0.53
1:A:21:PRO:O	1:A:27:ALA:HA	2.09	0.52
1:A:250:LEU:O	8:A:492:HOH:O	2.19	0.52
2:C:13:TRP:HZ3	8:C:306:HOH:O	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:0AF:CE3	2:E:108:TRP:CD1	2.93	0.52
3:F:45:ARG:HD3	3:F:345:LEU:HD11	1.91	0.52
2:E:36[B]:CYS:SG	2:E:47:PRO:HD3	2.49	0.52
1:B:231:ASN:OD1	8:B:410:HOH:O	2.19	0.51
3:D:179:PRO:HD3	3:D:214:ILE:HD13	1.90	0.51
1:A:194:THR:HG21	2:C:101[B]:GLU:HG3	1.92	0.51
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.93	0.50
1:B:285:THR:HG22	1:B:286:ASP:OD1	2.12	0.49
3:D:283:GLN:HB2	3:D:335:SER:HB3	1.93	0.49
1:A:177[B]:ARG:NH2	1:A:355:GLU:OE2	2.40	0.49
1:B:305:LYS:HE3	8:B:582:HOH:O	2.12	0.49
3:D:51:ASP:HA	3:D:377:PRO:HA	1.94	0.49
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.77	0.49
1:B:113:GLU:HG2	5:B:500:HEC:HBC2	1.94	0.49
1:A:202:ARG:NE	8:A:510:HOH:O	2.46	0.49
2:C:23:CYS:CB	2:C:88[B]:CYS:SG	3.01	0.49
1:A:52:ALA:O	1:A:66:ASN:HA	2.13	0.49
2:C:57:0AF:HE3	2:C:108:TRP:CD1	2.47	0.49
1:B:52:ALA:O	1:B:66:ASN:HA	2.12	0.48
3:D:96:SER:HB3	3:D:110:TYR:CZ	2.48	0.48
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.48	0.48
3:D:92:ILE:HG13	3:D:114:PHE:HB2	1.95	0.48
3:D:283:GLN:HB2	3:D:335:SER:CB	2.43	0.48
1:A:206:MET:O	1:A:220:ASN:HB3	2.12	0.48
1:A:272:VAL:HG21	5:A:600:HEC:HMA3	1.94	0.48
2:C:20:ILE:HG22	2:C:25:TYR:CZ	2.49	0.48
2:C:47:PRO:HG2	2:C:120:HIS:CD2	2.48	0.48
2:E:23:CYS:HB3	2:E:88[B]:CYS:SG	2.54	0.48
1:B:110:ASN:HB3	1:B:113:GLU:HB2	1.95	0.47
2:E:23:CYS:SG	2:E:88[B]:CYS:HB2	2.54	0.47
2:E:55:ALA:O	2:E:75:ARG:HG2	2.15	0.47
8:D:480:HOH:O	3:F:103:ALA:HB3	2.14	0.47
1:B:170:PRO:HG3	1:B:353:ARG:HH12	1.78	0.47
2:C:71:LEU:HD22	2:C:130:ALA:HB3	1.96	0.47
1:A:277:PRO:HB3	1:A:285:THR:HA	1.96	0.47
3:F:228:ILE:HD11	3:F:243:PRO:HD2	1.96	0.47
1:B:29:GLN:HE22	1:B:56:GLY:HA2	1.80	0.47
2:E:36[B]:CYS:HA	2:E:121:CYS:SG	2.54	0.47
2:E:99:ARG:HD3	8:E:187:HOH:O	2.13	0.47
2:C:80:TYR:HB2	2:C:120:HIS:HB2	1.96	0.47
1:A:40:ALA:HA	1:A:354:TYR:CE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:106:ILE:HG12	3:D:133:PHE:HZ	1.79	0.46
3:D:279:PRO:HB3	3:D:296:LEU:HD21	1.96	0.46
1:B:193:TYR:O	1:B:197:ILE:HG12	2.16	0.46
1:B:49:ALA:HB3	1:B:53:VAL:HG22	1.97	0.46
3:F:82:ASN:HB3	3:F:142:THR:HB	1.98	0.46
1:B:81:ARG:HH11	1:B:85:GLY:HA2	1.82	0.45
3:F:174:ARG:NH2	3:F:207:GLY:O	2.38	0.45
2:E:96:PRO:HB2	2:E:98:TYR:CE1	2.52	0.45
1:B:163:GLN:HE22	5:B:500:HEC:HMA1	1.82	0.45
3:D:265:VAL:HG21	3:D:321:GLY:CA	2.47	0.45
3:D:347:TYR:HB3	3:D:356:LEU:HD11	1.98	0.45
2:E:131:SER:HA	8:E:176:HOH:O	2.16	0.45
1:B:302:PRO:O	1:B:305:LYS:HD2	2.18	0.44
3:D:85:VAL:HG22	3:D:92:ILE:HG22	1.99	0.44
2:E:35:ILE:HD11	2:E:88[A]:CYS:SG	2.57	0.44
2:C:96:PRO:HB2	2:C:98:TYR:CE1	2.53	0.44
1:B:228:LEU:HB2	8:B:423:HOH:O	2.18	0.44
1:B:342:LEU:HD13	5:B:600:HEC:HMB1	2.00	0.44
3:D:140:TRP:HE3	3:D:143:SER:HG	1.66	0.44
3:F:115:ASP:O	3:F:119:LEU:HA	2.16	0.44
1:A:223:TYR:CE2	1:A:265:LYS:HB2	2.52	0.43
1:B:82:ASP:OD1	1:B:84:ASN:HB2	2.18	0.43
3:D:270:GLU:HA	3:D:273[A]:ARG:HH12	1.83	0.43
3:F:153:PHE:CE1	3:F:163:GLY:HA3	2.54	0.43
1:A:173:SER:O	1:A:177[B]:ARG:HG2	2.18	0.43
3:D:286:ALA:HB3	3:D:295:TYR:HB2	2.01	0.43
3:D:50:ASN:O	3:D:52:PRO:HD3	2.18	0.43
3:F:286:ALA:HA	8:F:604:HOH:O	2.18	0.43
2:C:91:THR:HG21	3:D:307:LYS:HD2	2.01	0.43
1:B:198:THR:HG22	2:E:58:VAL:HG13	2.01	0.43
3:F:254:LEU:HD23	3:F:259:ALA:HA	2.01	0.42
1:A:222:GLU:O	1:A:266:VAL:HG23	2.19	0.42
3:D:239:ARG:HG3	3:D:241:VAL:HG23	2.00	0.42
3:F:204:VAL:HG22	3:F:214:ILE:HG12	2.01	0.42
1:A:223:TYR:HB3	1:A:263:ARG:HB3	2.00	0.42
3:D:336:ILE:HA	3:D:347:TYR:O	2.19	0.42
2:E:62:TYR:OH	2:E:67:GLY:HA2	2.20	0.42
1:B:110:ASN:OD1	1:B:112:VAL:HG13	2.19	0.42
2:E:91:THR:HB	3:F:306:HIS:CE1	2.53	0.42
2:E:19:ASP:O	2:E:25:TYR:HB2	2.20	0.42
1:B:170:PRO:HG3	1:B:353:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:PHE:CZ	1:B:215:ARG:HB3	2.54	0.41
3:D:53:ALA:HB3	3:D:56:ALA:HB3	2.02	0.41
2:C:130:ALA:CA	2:C:131:SER:CB	2.85	0.41
1:A:29:GLN:HE22	5:A:500:HEC:HBC3	1.86	0.41
1:B:214:GLU:HG2	1:B:215:ARG:HG3	2.03	0.41
3:D:283:GLN:OE1	3:D:379:VAL:HA	2.20	0.41
1:A:267:PRO:HD3	5:A:600:HEC:C3D	2.50	0.41
2:C:18:ASN:O	3:F:16:GLN:HA	2.20	0.41
1:B:106:GLN:HB3	8:B:407:HOH:O	2.20	0.41
2:E:25:TYR:HB3	2:E:28:HIS:CD2	2.55	0.41
2:C:25:TYR:HB3	2:C:28:HIS:CD2	2.56	0.41
2:E:75:ARG:HA	8:E:155:HOH:O	2.20	0.41
3:F:347:TYR:HB3	3:F:356:LEU:HD11	2.03	0.41
1:B:288:ARG:NH1	1:B:340:ASP:OD1	2.49	0.41
2:C:23:CYS:SG	2:C:88[B]:CYS:HB2	2.61	0.41
2:E:36[B]:CYS:HB2	2:E:121:CYS:SG	2.61	0.40
1:B:48:LYS:HG3	1:B:62:HIS:CE1	2.56	0.40
3:D:16:GLN:HA	2:E:18:ASN:O	2.21	0.40
3:F:280:GLY:HA3	3:F:301:ARG:CZ	2.52	0.40
1:B:202:ARG:NH2	2:E:75:ARG:HD2	2.37	0.40
1:B:201:CYS:HA	5:B:600:HEC:CHC	2.52	0.40
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.48	0.40
1:B:20:ASP:HA	1:B:21:PRO:HD2	1.83	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46[A]:GLU:OE2	8:B:586:HOH:O[1_544]	2.12	0.08

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	355/373 (95%)	345 (97%)	10 (3%)	0	100	100
1	B	356/373 (95%)	345 (97%)	11 (3%)	0	100	100
2	C	130/137 (95%)	119 (92%)	10 (8%)	1 (1%)	22	13
2	E	124/137 (90%)	119 (96%)	5 (4%)	0	100	100
3	D	375/386 (97%)	358 (96%)	15 (4%)	2 (0%)	32	24
3	F	377/386 (98%)	364 (97%)	12 (3%)	1 (0%)	44	39
All	All	1717/1792 (96%)	1650 (96%)	63 (4%)	4 (0%)	51	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	131	SER
3	D	102	ILE
3	F	102	ILE
3	D	207	GLY

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	279/292 (96%)	266 (95%)	13 (5%)	30	25
1	B	280/292 (96%)	267 (95%)	13 (5%)	31	26
2	C	112/112 (100%)	109 (97%)	3 (3%)	50	50
2	E	106/112 (95%)	104 (98%)	2 (2%)	62	65
3	D	305/311 (98%)	293 (96%)	12 (4%)	37	34
3	F	307/311 (99%)	301 (98%)	6 (2%)	60	63
All	All	1389/1430 (97%)	1340 (96%)	49 (4%)	41	38

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP

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Mol	Chain	Res	Type
1	A	51	LEU
1	A	60	GLN
1	A	84	ASN
1	A	112	VAL
1	A	118	ASP
1	A	202	ARG
1	A	208	ARG
1	A	209	LYS
1	A	232	GLU
1	A	256	GLU
1	A	303	GLU
1	A	358	LEU
1	B	7	ASP
1	B	102	GLN
1	B	112	VAL
1	B	118	ASP
1	B	202	ARG
1	B	219	THR
1	B	269	LEU
1	B	296	LYS
1	B	305	LYS
1	B	323	LEU
1	B	357	LEU
1	B	358	LEU
1	B	360	GLU
2	C	58	VAL
2	C	71	LEU
2	C	131	SER
3	D	20	ARG
3	D	94	HIS
3	D	127	LEU
3	D	177	ASP
3	D	211	THR
3	D	218	GLU
3	D	223	GLU
3	D	262	LEU
3	D	273[A]	ARG
3	D	273[B]	ARG
3	D	275	ASP
3	D	319	LYS
2	E	7	THR
2	E	71	LEU

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Mol	Chain	Res	Type
3	F	11	GLN
3	F	94	HIS
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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	163	GLN
1	A	210	GLN
1	B	16	GLN
1	B	29	GLN
1	B	60	GLN
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
2	C	134	HIS
3	D	14	GLN
3	D	30	GLN
2	E	68	GLN
3	F	11	GLN
3	F	14	GLN
3	F	331	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	14,16,17	1.00	0	12,22,24	1.28	2 (16%)
2	0AF	E	57	2	14,16,17	1.11	2 (14%)	12,22,24	1.64	3 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0AF	C	57	2	-	0/3/6/8	0/2/2/2
2	0AF	E	57	2	-	0/3/6/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CZ2-CE2	-2.07	1.39	1.42
2	E	57	0AF	CZ3-CE3	2.06	1.41	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	57	0AF	CB-CG-CD1	-3.74	123.34	127.97
2	C	57	0AF	CE3-CD2-CG	-2.13	130.51	134.42
2	E	57	0AF	CB-CG-CD2	2.28	129.80	126.25
2	C	57	0AF	CB-CA-C	2.31	115.86	111.41
2	E	57	0AF	CB-CA-C	2.48	116.19	111.41

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	0AF	2	0
2	E	57	0AF	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 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
5	HEC	A	500	1,8	28,50,50	1.71	8 (28%)	16,82,82	2.29	5 (31%)
5	HEC	A	600	1	28,50,50	1.87	10 (35%)	16,82,82	2.85	7 (43%)
6	PGE	B	374	-	9,9,9	0.55	0	8,8,8	0.46	0
5	HEC	B	500	1,8	28,50,50	1.72	7 (25%)	16,82,82	2.04	7 (43%)
5	HEC	B	600	1	28,50,50	1.71	9 (32%)	16,82,82	2.66	8 (50%)
7	ACT	D	387	-	1,3,3	1.45	0	0,3,3	0.00	-
7	ACT	F	387	-	1,3,3	0.98	0	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	A	500	1,8	-	0/6/54/54	0/0/8/8
5	HEC	A	600	1	-	0/6/54/54	0/0/8/8
6	PGE	B	374	-	-	0/7/7/7	0/0/0/0
5	HEC	B	500	1,8	-	0/6/54/54	0/0/8/8
5	HEC	B	600	1	-	0/6/54/54	0/0/8/8
7	ACT	D	387	-	-	0/0/0/0	0/0/0/0
7	ACT	F	387	-	-	0/0/0/0	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	HEC	C4B-NB	-3.83	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	HEC	C4C-NC	-3.48	1.32	1.36
5	A	600	HEC	C4B-NB	-3.23	1.33	1.36
5	A	600	HEC	C4A-NA	-3.11	1.33	1.36
5	B	600	HEC	C4B-NB	-2.76	1.33	1.36
5	A	500	HEC	C4C-NC	-2.73	1.33	1.36
5	B	600	HEC	C1A-NA	-2.63	1.33	1.36
5	B	600	HEC	C4A-NA	-2.60	1.33	1.36
5	A	600	HEC	C4C-NC	-2.59	1.33	1.36
5	A	500	HEC	C4A-NA	-2.48	1.33	1.36
5	A	600	HEC	C3B-C2B	-2.38	1.38	1.40
5	B	600	HEC	C4D-CHA	2.11	1.45	1.40
5	B	600	HEC	C1D-CHD	2.12	1.45	1.40
5	B	600	HEC	C1B-CHB	2.35	1.46	1.40
5	A	600	HEC	C1B-CHB	2.41	1.46	1.40
5	B	500	HEC	C1C-CHC	2.57	1.47	1.40
5	B	600	HEC	C1C-CHC	2.63	1.47	1.40
5	B	500	HEC	C3B-C4B	2.68	1.48	1.43
5	B	500	HEC	C1B-CHB	2.74	1.47	1.40
5	B	500	HEC	C4D-CHA	2.76	1.47	1.40
5	A	500	HEC	C4D-CHA	2.83	1.47	1.40
5	B	600	HEC	C3C-C4C	2.83	1.48	1.43
5	A	600	HEC	C1D-CHD	2.84	1.47	1.40
5	A	600	HEC	C3B-C4B	2.87	1.48	1.43
5	A	500	HEC	C3B-C4B	2.89	1.48	1.43
5	A	500	HEC	C1B-CHB	2.95	1.48	1.40
5	A	500	HEC	C3C-C4C	3.00	1.48	1.43
5	A	600	HEC	C1C-CHC	3.02	1.48	1.40
5	A	500	HEC	C1D-CHD	3.04	1.48	1.40
5	A	600	HEC	C3C-C4C	3.30	1.49	1.43
5	B	500	HEC	C1D-CHD	3.30	1.48	1.40
5	A	500	HEC	C1C-CHC	3.34	1.49	1.40
5	A	600	HEC	C4D-CHA	3.35	1.49	1.40
5	B	500	HEC	C3C-C4C	3.37	1.49	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	HEC	C1D-C2D-C3D	-6.28	102.63	107.00
5	A	600	HEC	CBD-CAD-C3D	-6.09	100.85	112.48
5	A	500	HEC	C1D-C2D-C3D	-5.71	103.03	107.00
5	B	600	HEC	C1D-C2D-C3D	-5.50	103.17	107.00
5	B	600	HEC	CBD-CAD-C3D	-4.40	104.07	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	HEC	CBA-CAA-C2A	-4.27	104.33	112.47
5	B	600	HEC	CBA-CAA-C2A	-3.98	104.88	112.47
5	A	500	HEC	CBD-CAD-C3D	-3.68	105.45	112.48
5	B	500	HEC	C1D-C2D-C3D	-3.54	104.53	107.00
5	B	600	HEC	CAD-CBD-CGD	-3.21	107.17	112.66
5	B	600	HEC	C4C-C3C-C2C	-3.00	103.11	106.35
5	B	500	HEC	C4C-C3C-C2C	-2.74	103.39	106.35
5	B	500	HEC	CBA-CAA-C2A	-2.73	107.27	112.47
5	B	500	HEC	CMB-C2B-C1B	-2.64	124.41	128.46
5	B	500	HEC	C4B-C3B-C2B	-2.58	103.57	106.35
5	A	600	HEC	C4C-C3C-C2C	-2.54	103.61	106.35
5	A	500	HEC	CAA-CBA-CGA	-2.35	108.64	112.66
5	A	600	HEC	CMC-C2C-C1C	-2.28	124.96	128.46
5	A	500	HEC	C4C-C3C-C2C	-2.23	103.95	106.35
5	A	500	HEC	C4B-C3B-C2B	-2.16	104.03	106.35
5	A	600	HEC	CMD-C2D-C3D	2.11	128.93	124.94
5	A	600	HEC	CMA-C3A-C2A	2.13	128.97	124.94
5	B	500	HEC	CMD-C2D-C3D	2.17	129.04	124.94
5	B	500	HEC	C3B-C4B-NB	2.18	115.06	110.94
5	B	600	HEC	CMD-C2D-C3D	2.19	129.07	124.94
5	B	600	HEC	C3C-C4C-NC	2.48	115.62	110.94
5	B	600	HEC	CMA-C3A-C2A	2.99	130.58	124.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	HEC	2	0
5	A	600	HEC	2	0
5	B	500	HEC	3	0
5	B	600	HEC	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	354/373 (94%)	-0.13	4 (1%)	80 84	30, 42, 57, 66	0
1	B	355/373 (95%)	-0.22	3 (0%)	86 89	23, 35, 50, 65	0
2	C	130/137 (94%)	0.20	3 (2%)	61 67	23, 36, 62, 73	0
2	E	124/137 (90%)	0.02	1 (0%)	86 89	21, 28, 38, 59	0
3	D	376/386 (97%)	0.04	6 (1%)	72 77	26, 42, 66, 75	0
3	F	376/386 (97%)	-0.18	1 (0%)	93 95	21, 29, 43, 57	0
All	All	1715/1792 (95%)	-0.09	18 (1%)	82 86	21, 36, 58, 75	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	6.7
3	D	208	THR	6.3
1	B	7	ASP	5.4
3	D	209	GLU	4.1
1	B	6	ALA	3.9
3	D	207	GLY	3.5
3	D	210	GLY	3.0
3	D	11	GLN	2.9
1	A	7	ASP	2.8
3	D	211	THR	2.6
1	A	166	GLY	2.5
2	E	106	ILE	2.4
2	C	107	ILE	2.3
1	A	239	GLY	2.2
2	C	106	ILE	2.1
2	C	131	SER	2.1
1	B	25	ARG	2.0
3	F	11	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	0AF	E	57	15/16	0.94	0.17	-	32,33,34,36	0
2	0AF	C	57	15/16	0.95	0.19	-	40,42,43,45	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CA	B	400	1/1	0.99	0.11	2.33	24,24,24,24	0
5	HEC	B	600	43/43	0.98	0.12	0.33	18,24,26,29	0
5	HEC	A	500	43/43	0.97	0.10	0.32	31,37,39,40	0
5	HEC	A	600	43/43	0.98	0.11	0.15	30,33,37,41	0
5	HEC	B	500	43/43	0.98	0.10	0.07	22,26,28,31	0
4	CA	A	400	1/1	0.99	0.08	-1.25	40,40,40,40	0
7	ACT	D	387	4/4	0.97	0.08	-	40,41,41,41	0
7	ACT	F	387	4/4	0.94	0.12	-	49,49,50,50	0
6	PGE	B	374	10/10	0.71	0.18	-	71,74,76,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.