



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:17 PM GMT

PDB ID : 4L3G
Title : Crystal Structure of the E113Q-MauG/pre-Methylamine Dehydrogenase Complex Aged 120 Days
Authors : Yukl, E.T.; Wilmot, C.M.
Deposited on : 2013-06-05
Resolution : 2.05 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

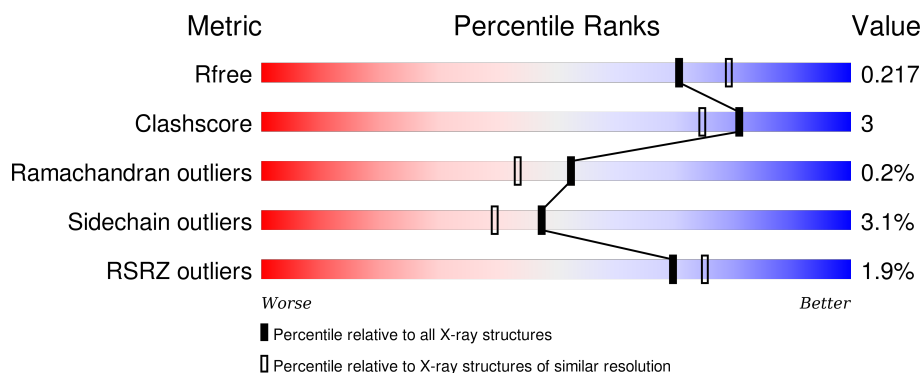
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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>3%</div> <div>87% 8% • 5%</div> </div>
1	B	373	<div> <div>%</div> <div>87% 8% 5%</div> </div>
2	C	137	<div> <div>%</div> <div>79% 11% • 9%</div> </div>
2	E	137	<div> <div>77% 12% • 9%</div> </div>
3	D	385	<div> <div>4%</div> <div>87% 11% •</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	385	<div> <div></div> <div>%</div> <div>88%</div> <div>9% ..</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
6	NA	A	405	-	-	-	X
6	NA	B	405	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14591 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	1	0
			2741	1711	492	527	11			
1	B	355	Total	C	N	O	S	0	6	0
			2787	1742	505	529	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	GLN	GLU	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	113	GLN	GLU	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
			958	592	161	191	14			
2	E	125	Total	C	N	O	S	0	2	0
			962	596	161	191	14			

There are 12 discrepancies between the modelled and reference sequences:

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

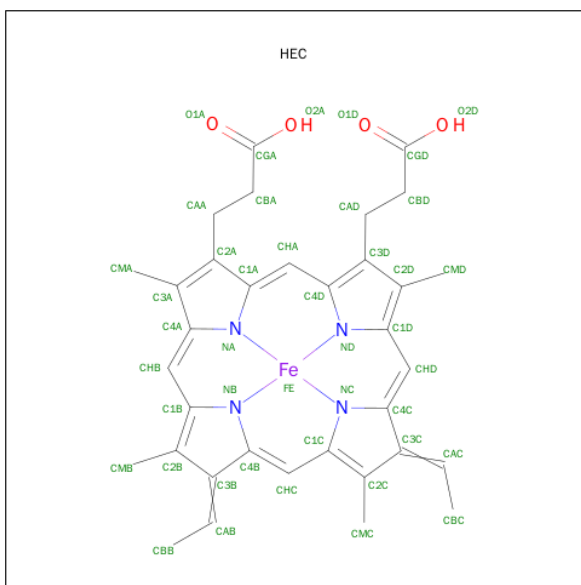
- Molecule 3 is a protein called methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	2	0
			2933	1859	505	560	9			
3	F	376	Total	C	N	O	S	0	4	0
			2948	1872	507	561	8			

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

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

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



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

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

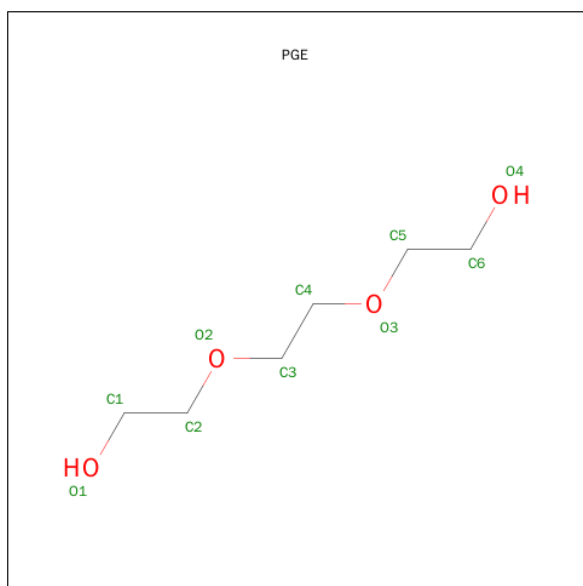
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Na		
			2	2	0	0
6	A	2	Total	Na		
			2	2	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

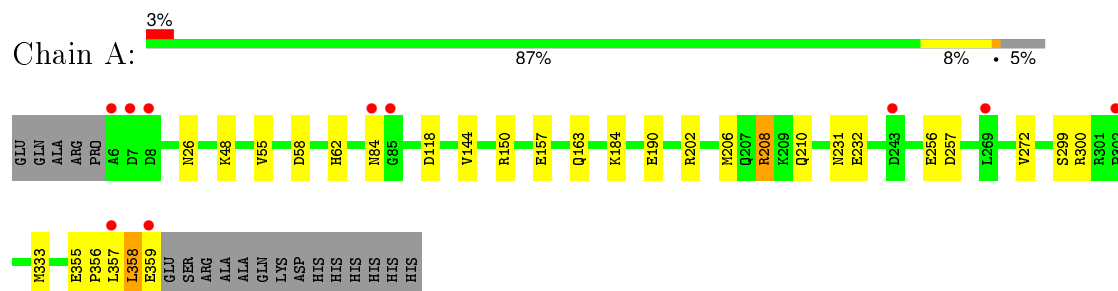
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	157	Total 157	O 157	0	0
9	B	239	Total 239	O 239	0	0
9	C	66	Total 66	O 66	0	0
9	D	203	Total 204	O 204	0	1
9	E	90	Total 90	O 90	0	0
9	F	308	Total 310	O 310	0	2

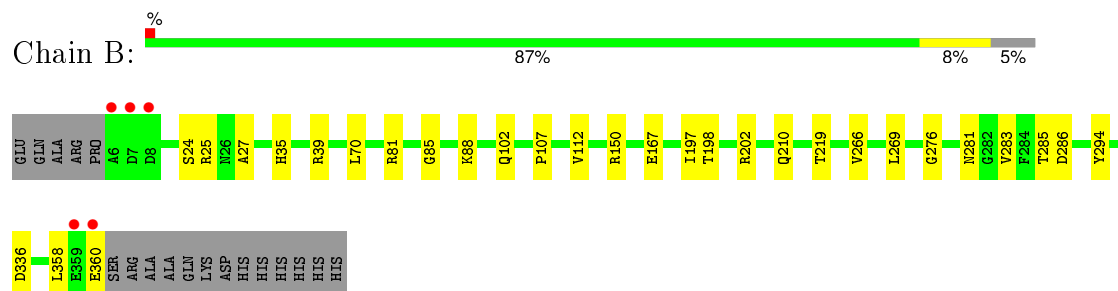
3 Residue-property plots [i](#)

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

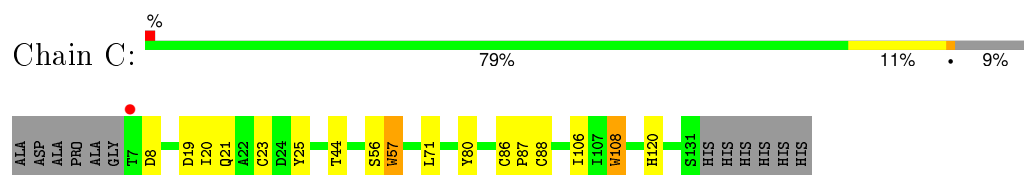
- Molecule 1: Methylamine utilization protein MauG

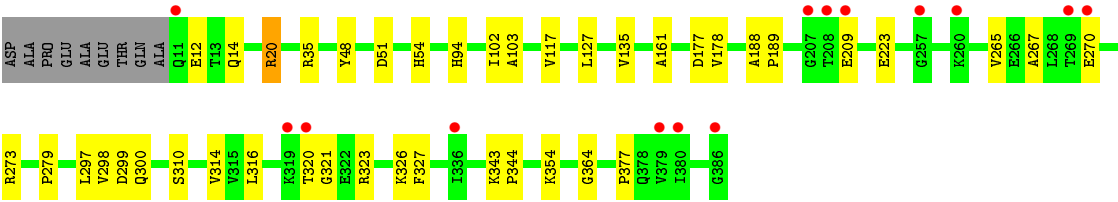


- Molecule 1: Methylamine utilization protein MauG

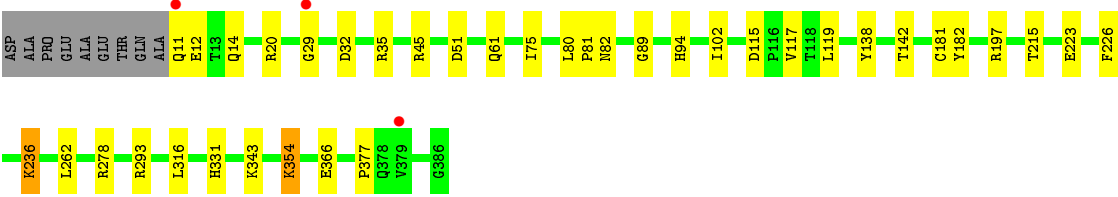
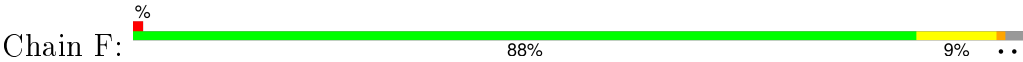


- Molecule 2: methylamine dehydrogenase light chain





• Molecule 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)	29.62 – 2.05 29.62 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.62-2.05) 85.3 (29.62-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.158 , 0.210 0.165 , 0.217	Depositor DCC
R_{free} test set	5450 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 106501 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14591	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PGE, NA, CA, HEC, HYP, ACT, TRQ

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	0.85	0/2798	0.87	4/3794 (0.1%)
1	B	0.91	1/2859 (0.0%)	0.91	2/3873 (0.1%)
2	C	0.91	0/969	0.92	2/1323 (0.2%)
2	E	1.04	0/976	0.97	1/1333 (0.1%)
3	D	0.85	1/3017 (0.0%)	0.88	1/4110 (0.0%)
3	F	1.01	0/3037	1.01	7/4136 (0.2%)
All	All	0.92	2/13656 (0.0%)	0.92	17/18569 (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
1	B	0	1
2	C	0	4
2	E	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	294	TYR	CE1-CZ	-5.44	1.31	1.38
3	D	48	TYR	CG-CD1	5.21	1.46	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	A	257	ASP	CB-CG-OD1	6.91	124.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	236[A]	LYS	CA-C-O	6.28	133.29	120.10
3	F	236[B]	LYS	CA-C-O	6.28	133.29	120.10
3	F	138	TYR	CB-CG-CD1	5.98	124.59	121.00
2	C	19	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	58	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	B	150	ARG	NE-CZ-NH1	5.60	123.10	120.30
3	F	197	ARG	NE-CZ-NH2	5.55	123.07	120.30
2	E	99	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	336	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	58	ASP	CB-CG-OD1	5.32	123.09	118.30
3	F	236[A]	LYS	N-CA-C	5.07	124.68	111.00
3	F	236[B]	LYS	N-CA-C	5.07	124.68	111.00
2	C	8	ASP	CB-CG-OD1	5.04	122.84	118.30
3	D	35	ARG	NE-CZ-NH1	5.01	122.81	120.30
3	F	35	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	107	HYP	Mainchain
2	C	108	TRP	Mainchain
2	C	56	SER	Mainchain,Peptide
2	C	57	TRQ	Mainchain
2	E	56	SER	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2741	0	2617	13	0
1	B	2787	0	2692	16	0
2	C	958	0	862	9	0
2	E	962	0	871	15	0
3	D	2933	0	2821	18	0
3	F	2948	0	2852	20	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	86	0	60	3	0
5	B	86	0	60	3	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	C	4	0	3	1	0
7	F	4	0	3	0	0
8	F	10	0	14	0	0
9	A	157	0	0	1	0
9	B	239	0	0	2	0
9	C	66	0	0	1	0
9	D	204	0	0	2	0
9	E	90	0	0	3	0
9	F	310	0	0	6	0
All	All	14591	0	12855	85	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (85) 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:210:GLN:HE22	2:E:44:THR:HG21	1.52	0.74
1:A:208:ARG:NH2	3:F:29:GLY:O	2.23	0.71
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.39	0.69
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.59	0.66
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.77	0.65
1:B:285:THR:HG22	1:B:286:ASP:OD1	1.97	0.65
1:B:198:THR:HG22	2:E:58[A]:VAL:HG13	1.78	0.64
7:C:201:ACT:H3	9:C:318:HOH:O	1.97	0.64
3:D:314:VAL:HG12	3:D:326:LYS:HG3	1.80	0.62
5:B:402:HEC:HBB3	5:B:402:HEC:HMB1	1.83	0.60
3:F:12:GLU:OE2	3:F:20:ARG:NH1	2.34	0.60
3:F:278:ARG:NH1	9:F:621:HOH:O	2.25	0.60
5:A:402:HEC:HBC3	5:A:402:HEC:HMC1	1.83	0.60
3:F:236[A]:LYS:NZ	9:F:785:HOH:O	2.36	0.59
1:B:39[A]:ARG:NH2	1:B:276:GLY:O	2.34	0.59
1:A:231:ASN:C	1:A:231:ASN:OD1	2.40	0.57
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.38	0.56
1:B:197:ILE:O	1:B:202:ARG:CD	2.54	0.55
3:D:12:GLU:OE1	3:D:20[A]:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:57:TRQ:HB2	2:C:108:TRP:NE1	2.22	0.54
3:D:265:VAL:HG21	3:D:321:GLY:HA2	1.90	0.54
1:A:357:LEU:O	1:A:359:GLU:N	2.41	0.54
3:D:54:HIS:HD2	9:D:585:HOH:O	1.91	0.53
1:A:144:VAL:HA	1:A:150:ARG:NH1	2.23	0.53
3:F:181:CYS:C	3:F:182:TYR:CD1	2.82	0.53
2:E:95:LEU:HD22	3:F:226:PHE:CE1	2.44	0.52
1:B:281:ASN:OD1	1:B:283:VAL:HB	2.08	0.52
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.57	0.52
3:F:115:ASP:O	3:F:119:LEU:HA	2.10	0.52
3:D:20[A]:ARG:HG2	9:D:545:HOH:O	2.09	0.52
3:D:188:ALA:HB1	3:D:189:PRO:HD2	1.92	0.52
1:B:81[B]:ARG:CZ	1:B:85:GLY:HA2	2.41	0.51
1:A:163:GLN:HE22	5:A:402:HEC:HMA1	1.75	0.51
3:F:51:ASP:HA	3:F:377:PRO:HA	1.93	0.51
3:F:45:ARG:NH2	3:F:343:LYS:O	2.44	0.50
1:B:197:ILE:O	1:B:202:ARG:HD2	2.12	0.50
1:A:26:ASN:ND2	9:A:583:HOH:O	2.44	0.50
3:D:270:GLU:HA	3:D:273:ARG:NH1	2.26	0.50
1:A:55:VAL:HG22	1:A:62:HIS:CE1	2.47	0.50
1:B:210:GLN:NE2	2:E:44:THR:HG21	2.25	0.49
2:E:56:SER:CB	2:E:74:TYR:O	2.61	0.49
2:C:23:CYS:HB3	2:C:88[B]:CYS:SG	2.53	0.48
2:E:75:ARG:HD2	9:E:276:HOH:O	2.13	0.48
2:E:131:SER:HB2	9:E:268:HOH:O	2.13	0.47
2:E:56:SER:HB3	2:E:74:TYR:O	2.15	0.47
1:A:272:VAL:HG21	5:A:403:HEC:HMA3	1.96	0.47
3:D:103:ALA:HB3	9:F:704:HOH:O	2.15	0.45
1:A:357:LEU:C	1:A:359:GLU:H	2.19	0.45
2:E:57:TRQ:HB2	2:E:108:TRP:NE1	2.31	0.44
3:F:80:LEU:N	3:F:81:PRO:HD3	2.32	0.44
2:E:101:GLU:HA	9:E:272:HOH:O	2.18	0.44
3:D:327:PHE:CD1	3:D:364:GLY:HA3	2.53	0.44
2:C:86:CYS:N	2:C:87:PRO:CD	2.81	0.44
3:D:343:LYS:N	3:D:344:PRO:CD	2.81	0.43
2:C:20:ILE:HG22	2:C:25:TYR:CZ	2.53	0.43
3:F:354:LYS:NZ	9:F:676:HOH:O	2.51	0.43
2:E:58[B]:VAL:HG22	2:E:59:ALA:N	2.33	0.43
3:F:182:TYR:CD1	3:F:182:TYR:N	2.87	0.43
1:A:299:SER:HB2	1:A:333:MET:HG3	2.00	0.43
1:B:198:THR:CG2	2:E:58[A]:VAL:HG13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ILE:O	1:B:202:ARG:HD3	2.18	0.43
3:F:12:GLU:CD	3:F:20:ARG:NH1	2.72	0.43
1:A:355:GLU:N	1:A:356:PRO:CD	2.82	0.42
1:A:48:LYS:H	1:A:62:HIS:CE1	2.38	0.42
3:D:279:PRO:HA	3:D:298:VAL:HA	2.01	0.42
3:D:299:ASP:OD1	3:D:300:GLN:N	2.50	0.42
1:B:360:GLU:C	9:B:726:HOH:O	2.58	0.42
3:F:331:HIS:HE1	3:F:366:GLU:OE1	2.03	0.42
3:F:215:THR:HG21	9:F:679:HOH:O	2.19	0.42
1:B:24:SER:OG	1:B:27:ALA:HA	2.19	0.41
2:E:71:LEU:HD22	2:E:129:LYS:O	2.19	0.41
3:F:82:ASN:HB3	3:F:142:THR:HB	2.01	0.41
2:E:77:CYS:O	2:E:120:HIS:HB3	2.20	0.41
3:D:51:ASP:HA	3:D:377:PRO:HA	2.03	0.41
2:C:23:CYS:CB	2:C:88[B]:CYS:SG	3.09	0.41
2:C:106:ILE:HA	3:D:135:VAL:HG23	2.01	0.41
1:B:35:HIS:CE1	1:B:70:LEU:HD21	2.56	0.41
3:F:89:GLY:HA2	9:F:505:HOH:O	2.21	0.41
3:D:267:ALA:O	3:D:323:ARG:NH2	2.51	0.40
1:B:266:VAL:HG22	5:B:403:HEC:HMD3	2.02	0.40
1:B:25:ARG:NH1	9:B:718:HOH:O	2.48	0.40
3:D:161:ALA:HA	3:D:178:VAL:HG22	2.03	0.40
2:C:80:TYR:HB2	2:C:120:HIS:HB2	2.04	0.40
3:F:61:GLN:HB3	3:F:75[A]:ILE:HB	2.03	0.40
5:B:402:HEC:HBB3	5:B:402:HEC:CMB	2.50	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	352/373 (94%)	339 (96%)	12 (3%)	1 (0%)	46 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	358/373 (96%)	346 (97%)	12 (3%)	0	100	100
2	C	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
2	E	124/137 (90%)	120 (97%)	4 (3%)	0	100	100
3	D	376/385 (98%)	362 (96%)	13 (4%)	1 (0%)	46	36
3	F	377/385 (98%)	363 (96%)	12 (3%)	2 (0%)	34	22
All	All	1710/1790 (96%)	1650 (96%)	56 (3%)	4 (0%)	52	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LEU
3	D	102	ILE
3	F	32	ASP
3	F	102	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/291 (95%)	264 (96%)	12 (4%)	35	27
1	B	282/291 (97%)	274 (97%)	8 (3%)	51	44
2	C	105/112 (94%)	104 (99%)	1 (1%)	82	81
2	E	106/112 (95%)	102 (96%)	4 (4%)	40	31
3	D	306/310 (99%)	295 (96%)	11 (4%)	42	34
3	F	308/310 (99%)	299 (97%)	9 (3%)	50	42
All	All	1383/1426 (97%)	1338 (97%)	45 (3%)	47	37

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	118	ASP

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Mol	Chain	Res	Type
1	A	157	GLU
1	A	184	LYS
1	A	190	GLU
1	A	202	ARG
1	A	206	MET
1	A	208	ARG
1	A	232	GLU
1	A	256	GLU
1	A	300	ARG
1	A	358	LEU
1	B	88	LYS
1	B	102	GLN
1	B	112	VAL
1	B	167	GLU
1	B	219	THR
1	B	269[A]	LEU
1	B	269[B]	LEU
1	B	358	LEU
2	C	71	LEU
3	D	20[A]	ARG
3	D	20[B]	ARG
3	D	94	HIS
3	D	117	VAL
3	D	127	LEU
3	D	177	ASP
3	D	209	GLU
3	D	223	GLU
3	D	316	LEU
3	D	320	THR
3	D	354	LYS
2	E	7	THR
2	E	16	GLN
2	E	71	LEU
2	E	131	SER
3	F	11[A]	GLN
3	F	11[B]	GLN
3	F	94	HIS
3	F	117	VAL
3	F	223	GLU
3	F	262	LEU
3	F	293	ARG
3	F	316	LEU

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Mol	Chain	Res	Type
3	F	354	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) 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	A	163	GLN
1	A	210	GLN
1	B	16	GLN
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
2	E	21	GLN
2	E	68	GLN
3	F	14	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$
1	HYP	A	107	1	7,8,9	0.96	0	5,10,12	2.07	2 (40%)
1	HYP	B	107	1	7,8,9	0.88	0	5,10,12	2.30	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRQ	C	57	2	14,17,18	1.87	3 (21%)	8,24,26	3.99	3 (37%)
2	TRQ	E	57	2	14,17,18	2.34	6 (42%)	8,24,26	4.02	5 (62%)

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
1	HYP	A	107	1	-	0/0/11/13	0/1/1/1
1	HYP	B	107	1	-	0/0/11/13	0/1/1/1
2	TRQ	C	57	2	-	0/3/19/21	0/2/2/2
2	TRQ	E	57	2	-	0/3/19/21	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	TRQ	CD1-NE1	-3.63	1.30	1.36
2	E	57	TRQ	CD2-CE2	-2.63	1.37	1.40
2	E	57	TRQ	CZ3-CH2	-2.48	1.39	1.45
2	C	57	TRQ	CD1-NE1	-2.04	1.33	1.36
2	E	57	TRQ	CD2-CG	2.55	1.43	1.40
2	E	57	TRQ	CZ3-CE3	3.58	1.40	1.34
2	C	57	TRQ	CZ3-CE3	3.73	1.40	1.34
2	C	57	TRQ	CD2-CE3	3.84	1.53	1.44
2	E	57	TRQ	CD2-CE3	4.86	1.55	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	TRQ	CB-CG-CD1	-9.76	115.91	127.97
2	E	57	TRQ	CB-CG-CD1	-9.10	116.73	127.97
1	B	107	HYP	O-C-CA	-3.42	116.41	125.44
2	E	57	TRQ	O7-CZ2-CE2	-3.41	118.31	122.10
2	E	57	TRQ	O-C-CA	-3.39	116.66	125.49
2	C	57	TRQ	CD1-NE1-CE2	2.05	109.65	104.34
1	A	107	HYP	OD1-CG-CD	2.17	115.19	110.47
2	E	57	TRQ	CD1-NE1-CE2	2.37	110.46	104.34
1	B	107	HYP	CG-CB-CA	2.47	107.43	103.90
1	B	107	HYP	CB-CG-CD	2.60	106.35	103.14
1	A	107	HYP	CG-CB-CA	3.27	108.59	103.90
2	E	57	TRQ	CB-CG-CD2	4.05	133.93	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	TRQ	CB-CG-CD2	4.40	134.75	124.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	57	TRQ	1	0
2	E	57	TRQ	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	$\# Z > 2$
5	HEC	A	402	1	24,50,50	2.20	12 (50%)	19,82,82	3.07	8 (42%)
5	HEC	A	403	1	24,50,50	2.25	9 (37%)	19,82,82	3.29	7 (36%)
5	HEC	B	402	1	24,50,50	1.80	7 (29%)	19,82,82	3.34	8 (42%)
5	HEC	B	403	1	24,50,50	1.93	6 (25%)	19,82,82	3.75	8 (42%)
7	ACT	C	201	-	1,3,3	0.50	0	0,3,3	0.00	-
7	ACT	F	401	-	1,3,3	2.31	1 (100%)	0,3,3	0.00	-
8	PGE	F	402	-	9,9,9	0.63	0	8,8,8	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	A	402	1	-	0/6/54/54	0/0/8/8
5	HEC	A	403	1	-	0/6/54/54	0/0/8/8
5	HEC	B	402	1	-	0/6/54/54	0/0/8/8
5	HEC	B	403	1	-	0/6/54/54	0/0/8/8
7	ACT	C	201	-	-	0/0/0/0	0/0/0/0
7	ACT	F	401	-	-	0/0/0/0	0/0/0/0
8	PGE	F	402	-	-	0/7/7/7	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	403	HEC	C4B-NB	-5.27	1.29	1.36
5	B	403	HEC	C4A-NA	-5.04	1.29	1.36
5	A	402	HEC	C4C-NC	-4.49	1.30	1.36
5	A	402	HEC	C3C-C2C	-4.48	1.36	1.40
5	A	403	HEC	C3B-C2B	-4.07	1.36	1.40
5	B	402	HEC	C4C-NC	-4.04	1.31	1.36
5	A	403	HEC	C4C-NC	-3.94	1.31	1.36
5	B	403	HEC	C3C-C2C	-3.85	1.36	1.40
5	A	403	HEC	C4A-NA	-3.71	1.31	1.36
5	A	402	HEC	C1A-NA	-3.63	1.31	1.36
5	A	402	HEC	C3B-C2B	-3.59	1.37	1.40
5	A	403	HEC	C1A-NA	-2.80	1.32	1.36
5	B	402	HEC	C3C-C2C	-2.74	1.37	1.40
5	B	402	HEC	C4B-NB	-2.50	1.33	1.36
5	B	403	HEC	C4B-NB	-2.47	1.33	1.36
5	B	402	HEC	C3B-C2B	-2.45	1.38	1.40
5	A	402	HEC	C4B-NB	-2.04	1.33	1.36
5	B	403	HEC	C3B-C2B	-2.02	1.38	1.40
5	A	402	HEC	C4A-NA	-2.02	1.34	1.36
5	A	403	HEC	C1C-CHC	2.01	1.45	1.39
5	A	402	HEC	C1B-CHB	2.06	1.45	1.39
5	A	403	HEC	C1D-CHD	2.09	1.45	1.39
5	B	403	HEC	C4D-CHA	2.11	1.45	1.39
5	A	402	HEC	C1C-CHC	2.26	1.46	1.39
7	F	401	ACT	CH3-C	2.31	1.52	1.48
5	A	402	HEC	C3B-C4B	2.32	1.48	1.42
5	B	403	HEC	C3C-C4C	2.36	1.48	1.42
5	B	402	HEC	C1C-CHC	2.55	1.46	1.39
5	A	402	HEC	C4D-CHA	2.55	1.46	1.39
5	A	403	HEC	C3C-C4C	2.69	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	402	HEC	C1D-CHD	2.76	1.47	1.39
5	B	402	HEC	C1D-CHD	2.81	1.47	1.39
5	A	402	HEC	C3C-C4C	2.84	1.49	1.42
5	B	402	HEC	C1B-CHB	2.87	1.47	1.39
5	A	403	HEC	C4D-CHA	3.11	1.48	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	403	HEC	CBB-CAB-C3B	-12.36	99.89	127.35
5	B	402	HEC	CBB-CAB-C3B	-10.35	104.36	127.35
5	A	403	HEC	CBB-CAB-C3B	-10.18	104.72	127.35
5	A	402	HEC	CBB-CAB-C3B	-8.48	108.51	127.35
5	B	403	HEC	CBC-CAC-C3C	-6.76	112.32	127.35
5	A	402	HEC	CBC-CAC-C3C	-6.43	113.06	127.35
5	A	403	HEC	CBD-CAD-C3D	-6.30	101.23	112.53
5	B	402	HEC	CBC-CAC-C3C	-4.58	117.17	127.35
5	A	402	HEC	CBD-CAD-C3D	-4.16	105.08	112.53
5	B	402	HEC	CBD-CAD-C3D	-4.12	105.15	112.53
5	A	403	HEC	C4C-C3C-C2C	-4.06	101.97	106.35
5	B	402	HEC	C4B-C3B-C2B	-3.73	102.32	106.35
5	B	403	HEC	C4C-C3C-C2C	-3.72	102.33	106.35
5	B	403	HEC	CBD-CAD-C3D	-3.72	105.87	112.53
5	A	403	HEC	CBC-CAC-C3C	-3.58	119.41	127.35
5	B	402	HEC	C4C-C3C-C2C	-3.24	102.85	106.35
5	B	403	HEC	CBA-CAA-C2A	-3.05	107.06	112.53
5	A	402	HEC	C4C-C3C-C2C	-3.05	103.06	106.35
5	A	403	HEC	CBA-CAA-C2A	-3.04	107.07	112.53
5	A	403	HEC	C4B-C3B-C2B	-2.83	103.30	106.35
5	A	402	HEC	C4B-C3B-C2B	-2.65	103.49	106.35
5	B	402	HEC	CMB-C2B-C1B	-2.60	124.06	128.36
5	A	403	HEC	CMC-C2C-C1C	-2.39	124.41	128.36
5	B	403	HEC	C4B-C3B-C2B	-2.13	104.05	106.35
5	A	402	HEC	CBA-CAA-C2A	-2.00	108.94	112.53
5	A	402	HEC	C3C-C4C-NC	2.26	115.20	110.94
5	B	403	HEC	CAD-C3D-C4D	2.56	129.79	127.01
5	B	402	HEC	C3B-C4B-NB	2.58	115.81	110.94
5	B	403	HEC	C3C-C4C-NC	2.63	115.90	110.94
5	B	402	HEC	CAD-CBD-CGD	2.99	118.23	112.75
5	A	402	HEC	CAA-C2A-C1A	3.24	130.52	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	HEC	2	0
5	A	403	HEC	1	0
5	B	402	HEC	2	0
5	B	403	HEC	1	0
7	C	201	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	353/373 (94%)	-0.04	10 (2%) 56 63	29, 40, 57, 90	0
1	B	354/373 (94%)	-0.23	5 (1%) 78 82	23, 35, 53, 87	0
2	C	124/137 (90%)	-0.31	1 (0%) 87 90	25, 35, 51, 84	0
2	E	124/137 (90%)	-0.37	0 100 100	23, 28, 40, 87	0
3	D	376/385 (97%)	-0.03	14 (3%) 45 51	23, 39, 63, 84	0
3	F	376/385 (97%)	-0.29	3 (0%) 87 90	21, 29, 46, 63	0
All	All	1707/1790 (95%)	-0.18	33 (1%) 70 75	21, 35, 57, 90	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	5.5
1	B	6	ALA	5.0
1	B	7	ASP	4.9
3	D	208	THR	4.2
1	B	359	GLU	4.0
1	A	7	ASP	3.4
3	D	320	THR	3.3
2	C	7	THR	3.3
3	D	11	GLN	3.0
1	B	360	GLU	3.0
1	A	8	ASP	3.0
3	F	11[A]	GLN	2.9
3	D	260	LYS	2.8
3	D	386	GLY	2.8
3	D	207	GLY	2.8
3	D	379	VAL	2.7
1	A	359	GLU	2.7
1	B	8	ASP	2.6
1	A	302	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	269	LEU	2.4
3	F	379	VAL	2.4
3	F	29	GLY	2.4
1	A	243	ASP	2.4
3	D	257	GLY	2.3
3	D	209	GLU	2.3
3	D	269	THR	2.3
3	D	270	GLU	2.3
3	D	380	ILE	2.2
1	A	357	LEU	2.2
1	A	85	GLY	2.2
1	A	84	ASN	2.1
3	D	336	ILE	2.0
3	D	319	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
1	HYP	B	107	8/9	0.97	0.13	-	30,36,39,48	0
2	TRQ	C	57	16/17	0.94	0.17	-	52,57,71,80	0
2	TRQ	E	57	16/17	0.94	0.16	-	37,42,59,77	0
1	HYP	A	107	8/9	0.95	0.12	-	37,42,43,44	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(\AA^2)	Q<0.9
6	NA	B	405	1/1	0.98	0.18	4.04	30,30,30,30	0
6	NA	A	405	1/1	0.96	0.23	3.44	30,30,30,30	0
5	HEC	A	403	43/43	0.98	0.17	0.88	29,32,34,40	0
5	HEC	B	402	43/43	0.98	0.14	0.58	29,31,33,36	0
5	HEC	A	402	43/43	0.98	0.13	0.37	30,34,38,42	0
5	HEC	B	403	43/43	0.98	0.14	0.34	22,25,27,28	0
4	CA	B	401	1/1	1.00	0.11	0.09	26,26,26,26	0
8	PGE	F	402	10/10	0.90	0.11	0.07	51,56,63,64	0
4	CA	A	401	1/1	1.00	0.07	-1.52	32,32,32,32	0
6	NA	B	404	1/1	0.85	0.12	-	42,42,42,42	0
7	ACT	F	401	4/4	0.97	0.08	-	40,43,48,48	0
6	NA	A	404	1/1	0.91	0.07	-	47,47,47,47	0
7	ACT	C	201	4/4	0.92	0.10	-	53,53,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.