



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:25 AM GMT

PDB ID : 3ORV
Title : Crystal Structure of the Y294H-MauG/pre-Methylamine Dehydrogenase Complex
Authors : Jensen, L.M.R.; Wilmot, C.M.
Deposited on : 2010-09-07
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 ⓘ 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

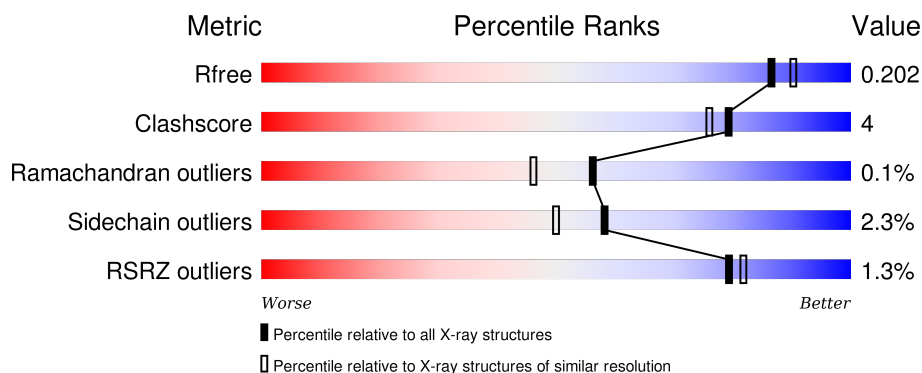
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	<div> <div>2%</div> <div>84% 9% 5%</div> </div>
1	B	373	<div> <div>2%</div> <div>85% 10% 5%</div> </div>
2	C	137	<div> <div>%</div> <div>80% 9% 9%</div> </div>
2	E	137	<div> <div></div> <div>85% 6% 9%</div> </div>
3	D	386	<div> <div>%</div> <div>88% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	386	 % 87% 11%

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	EDO	D	388	-	-	-	X
6	EDO	F	391	-	-	-	X
8	PEG	D	389	-	-	-	X
8	PEG	E	138	-	-	-	X
8	PEG	F	390	-	-	X	X
9	PG4	F	388	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 14851 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	4	0
			2760	1722	500	527	11			
1	B	355	Total	C	N	O	S	0	1	0
			2745	1712	493	529	11			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	HIS	TYR	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	294	HIS	TYR	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	124	Total	C	N	O	S	0	4	0
			965	598	163	188	16			
2	E	124	Total	C	N	O	S	0	2	0
			954	591	160	188	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	EXPRESSION TAG	UNP P22619
C	133	HIS	-	EXPRESSION TAG	UNP P22619
C	134	HIS	-	EXPRESSION TAG	UNP P22619
C	135	HIS	-	EXPRESSION TAG	UNP P22619
C	136	HIS	-	EXPRESSION TAG	UNP P22619
C	137	HIS	-	EXPRESSION TAG	UNP P22619
E	132	HIS	-	EXPRESSION TAG	UNP P22619
E	133	HIS	-	EXPRESSION TAG	UNP P22619
E	134	HIS	-	EXPRESSION TAG	UNP P22619
E	135	HIS	-	EXPRESSION TAG	UNP P22619
E	136	HIS	-	EXPRESSION TAG	UNP P22619
E	137	HIS	-	EXPRESSION TAG	UNP P22619

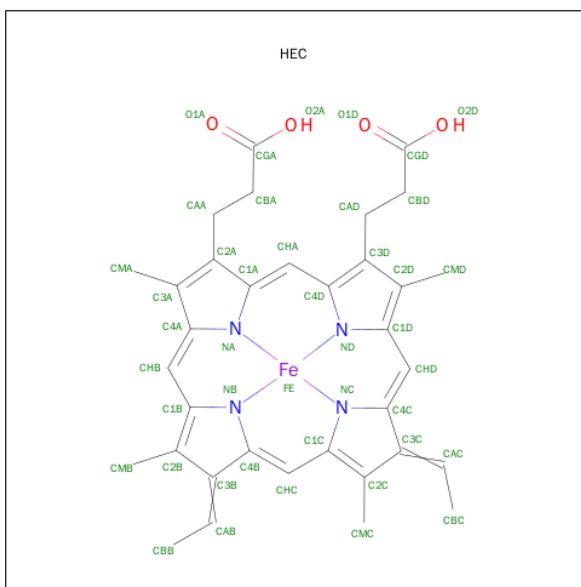
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	376	Total	C	N	O	S	0	1	0
			2931	1858	505	560	8			
3	F	376	Total	C	N	O	S	0	3	0
			2933	1860	502	561	10			

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

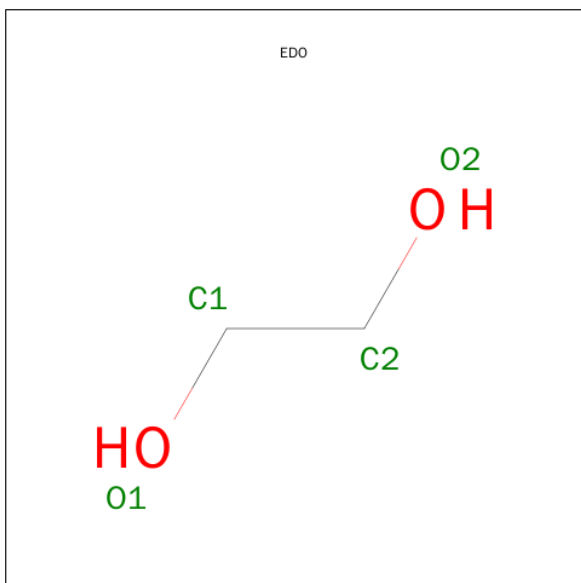
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

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



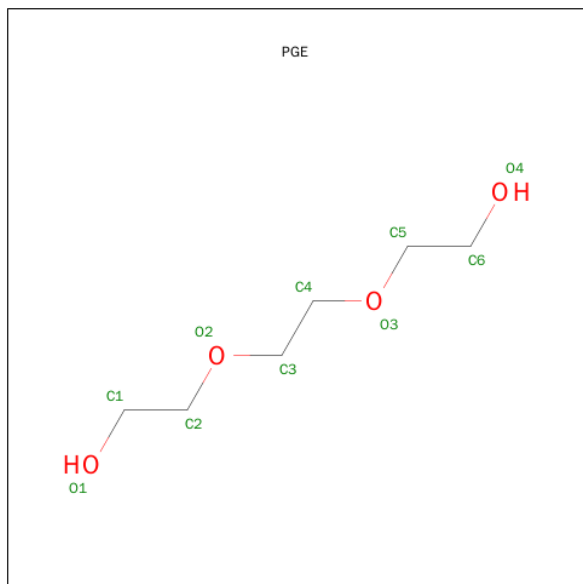
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



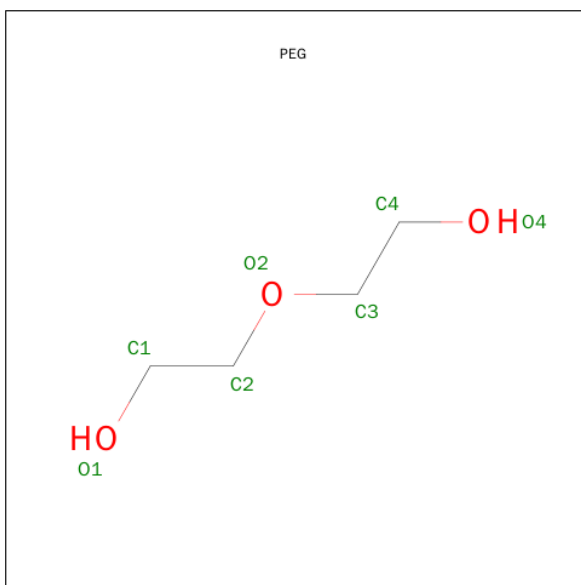
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



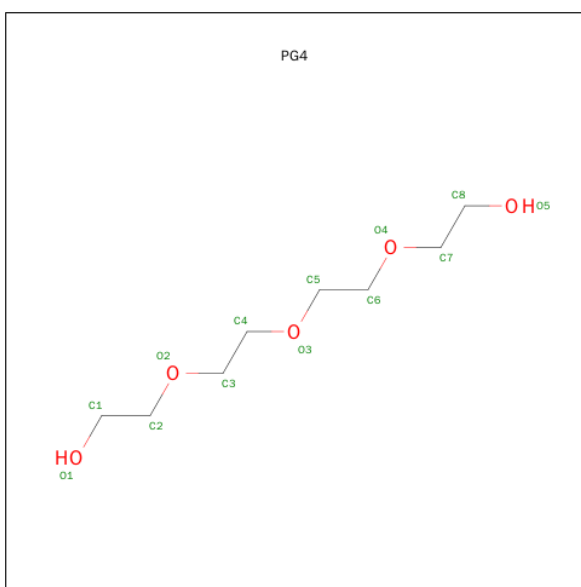
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			7	4	3		
8	E	1	Total	C	O	0	0
			7	4	3		
8	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



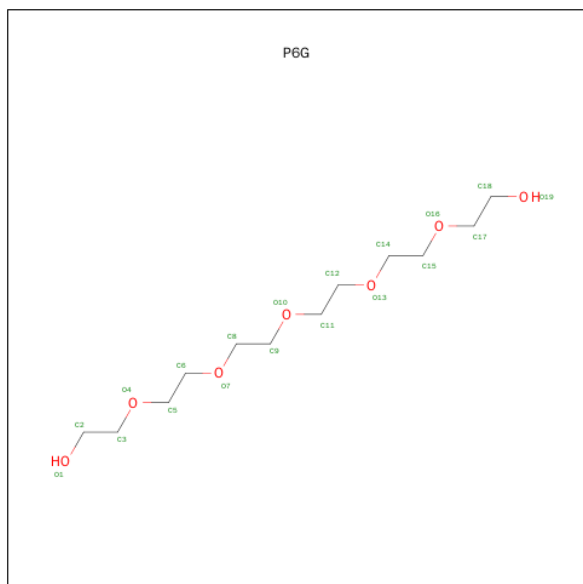
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	F	1	Total	C	O	0	0
			13	8	5		

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

- Molecule 10 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



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

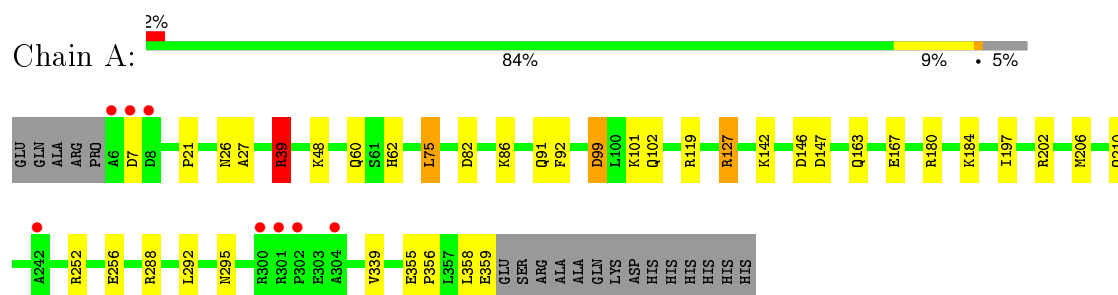
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	234	Total	O	0	0
			234	234		
11	B	289	Total	O	0	0
			289	289		
11	C	84	Total	O	0	0
			84	84		
11	D	236	Total	O	0	0
			236	236		
11	E	105	Total	O	0	0
			105	105		
11	F	353	Total	O	0	0
			353	353		

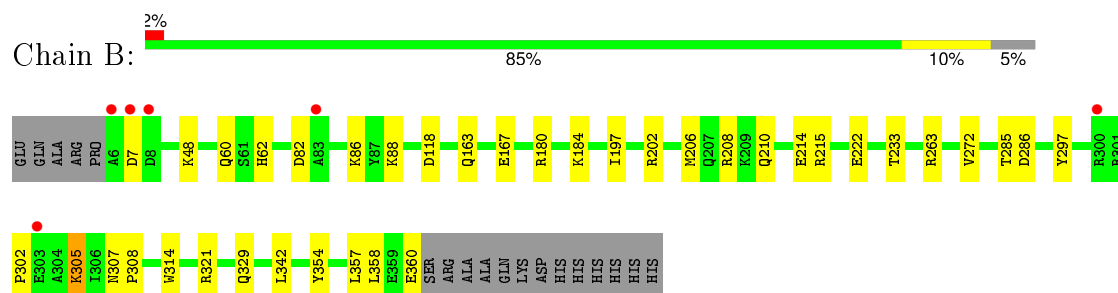
3 Residue-property plots [i](#)

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

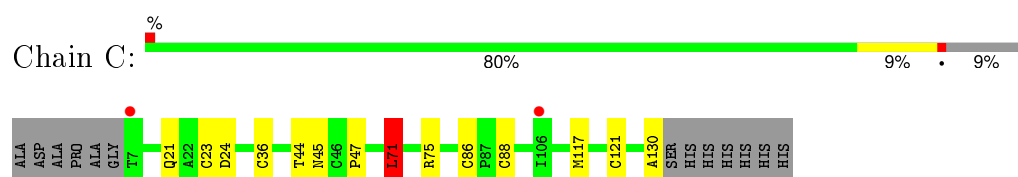
- Molecule 1: Methylamine utilization protein mauG



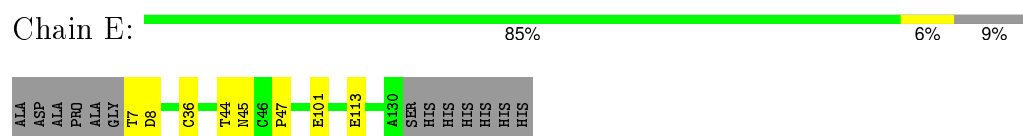
- Molecule 1: Methylamine utilization protein mauG



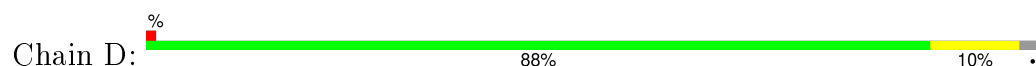
- Molecule 2: Methylamine dehydrogenase light chain

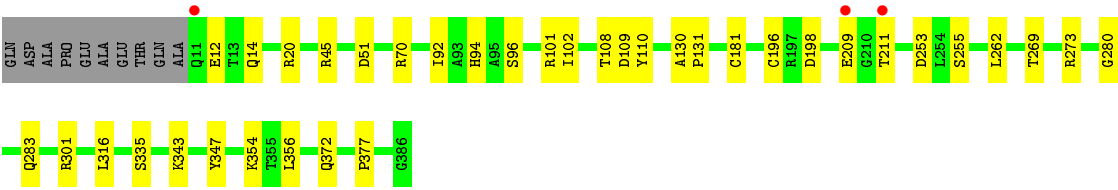


- Molecule 2: Methylamine dehydrogenase light chain

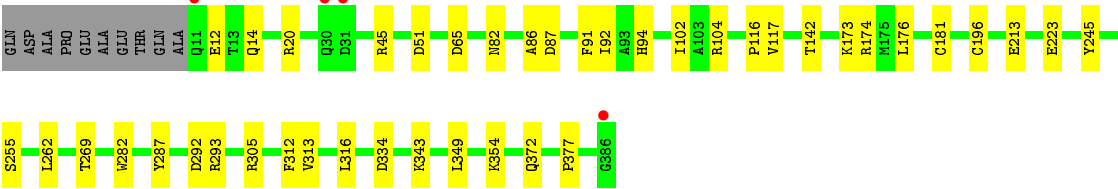
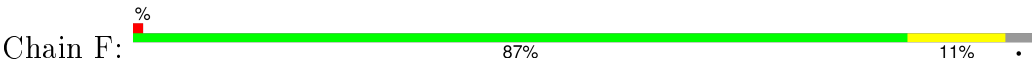


- Molecule 3: Methylamine dehydrogenase heavy chain





• Molecule 3: Methylamine dehydrogenase heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	44.49 – 1.91 44.48 – 1.91	Depositor EDS
% Data completeness (in resolution range)	93.9 (44.49-1.91) 83.6 (44.48-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.139 , 0.187 0.157 , 0.202	Depositor DCC
R_{free} test set	6318 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 126229 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14851	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, P6G, CA, EDO, PG4, 0AF, HEC, PEG

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	1.10	0/2836	1.07	11/3846 (0.3%)
1	B	1.19	2/2812 (0.1%)	0.97	7/3816 (0.2%)
2	C	1.14	1/986 (0.1%)	0.95	3/1345 (0.2%)
2	E	1.27	1/969 (0.1%)	1.01	1/1323 (0.1%)
3	D	1.06	0/3011	0.94	5/4102 (0.1%)
3	F	1.29	8/3019 (0.3%)	1.01	8/4114 (0.2%)
All	All	1.17	12/13633 (0.1%)	0.99	35/18546 (0.2%)

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	A	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	117	VAL	CB-CG2	-6.21	1.39	1.52
2	C	121	CYS	CB-SG	6.02	1.92	1.82
3	F	245	TYR	CD1-CE1	5.95	1.48	1.39
3	F	213	GLU	CD-OE2	5.89	1.32	1.25
2	E	101	GLU	CB-CG	5.74	1.63	1.52
3	F	223	GLU	CG-CD	5.58	1.60	1.51
1	B	314	TRP	CE3-CZ3	5.44	1.47	1.38
3	F	287	TYR	CE1-CZ	5.39	1.45	1.38
3	F	312	PHE	CE2-CZ	5.39	1.47	1.37
3	F	313	VAL	CB-CG2	5.31	1.64	1.52
1	B	222	GLU	CG-CD	5.29	1.59	1.51
3	F	282	TRP	CE3-CZ3	5.12	1.47	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	ARG	NE-CZ-NH2	-22.78	108.91	120.30
1	A	39	ARG	NE-CZ-NH1	21.62	131.11	120.30
1	A	39	ARG	CD-NE-CZ	9.34	136.67	123.60
1	B	208	ARG	NE-CZ-NH1	-7.23	116.69	120.30
3	D	101	ARG	NE-CZ-NH2	-6.87	116.87	120.30
3	F	104	ARG	CG-CD-NE	-6.72	97.69	111.80
3	F	349	LEU	CB-CG-CD2	-6.36	100.18	111.00
1	A	39	ARG	CG-CD-NE	-6.29	98.59	111.80
1	A	252	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	B	180	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	99	ASP	CB-CG-OD2	6.04	123.73	118.30
3	F	305	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	B	321	ARG	NE-CZ-NH2	-5.77	117.42	120.30
3	F	334	ASP	CB-CG-OD1	-5.76	113.12	118.30
2	C	71	LEU	CB-CG-CD1	5.59	120.50	111.00
1	A	147	ASP	CB-CG-OD1	5.54	123.28	118.30
2	E	8	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	263	ARG	NE-CZ-NH2	-5.47	117.56	120.30
2	C	117	MET	CG-SD-CE	5.46	108.94	100.20
3	D	109	ASP	CB-CG-OD1	5.45	123.20	118.30
3	F	65	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	127	ARG	NE-CZ-NH1	5.41	123.01	120.30
3	F	292	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	342	LEU	CB-CG-CD1	-5.38	101.85	111.00
3	D	198	ASP	CB-CG-OD1	5.38	123.14	118.30
3	D	354	LYS	CD-CE-NZ	-5.33	99.43	111.70
1	A	180	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	75	LEU	CA-CB-CG	-5.15	103.45	115.30
1	A	82	ASP	CB-CG-OD2	5.15	122.93	118.30
3	D	253	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	118	ASP	CB-CG-OD1	5.12	122.91	118.30
3	F	104	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	82	ASP	CB-CG-OD1	5.03	122.82	118.30
3	F	293	ARG	CG-CD-NE	-5.02	101.26	111.80
2	C	24	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	ARG	Sidechain

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	2760	0	2649	19	0
1	B	2745	0	2620	23	0
2	C	965	0	881	11	0
2	E	954	0	863	3	0
3	D	2931	0	2823	18	0
3	F	2933	0	2827	20	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	60	1	0
5	B	86	0	60	2	0
6	B	4	0	6	0	0
6	D	4	0	6	0	0
6	F	4	0	6	0	0
7	D	10	0	14	3	0
8	D	7	0	10	0	0
8	E	7	0	10	0	0
8	F	7	0	10	5	0
9	F	26	0	36	3	0
10	F	19	0	26	3	0
11	A	234	0	0	3	0
11	B	289	0	0	6	0
11	C	84	0	0	0	0
11	D	236	0	0	4	0
11	E	105	0	0	0	0
11	F	353	0	0	6	0
All	All	14851	0	12907	91	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 4.

All (91) 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)
3:F:196[B]:CYS:SG	11:F:609:HOH:O	2.08	1.08
3:D:14:GLN:HE22	3:D:70:ARG:HB2	1.26	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LYS:H	1:B:62:HIS:HE1	1.07	0.97
3:D:209:GLU:HB2	11:D:1178:HOH:O	1.72	0.88
1:B:48:LYS:H	1:B:62:HIS:CE1	1.93	0.85
3:D:181:CYS:HG	3:D:196:CYS:HG	1.19	0.83
3:F:269[B]:THR:HG22	11:F:935:HOH:O	1.79	0.82
1:A:48:LYS:H	1:A:62:HIS:HE1	1.27	0.79
3:D:255:SER:HA	7:D:387:PGE:H22	1.68	0.74
10:F:389:P6G:H21	11:F:840:HOH:O	1.86	0.74
1:B:233[A]:THR:CG2	11:B:825:HOH:O	2.35	0.72
1:A:197:ILE:O	1:A:202:ARG:HD2	1.90	0.72
1:A:288[A]:ARG:HG3	1:A:339:VAL:HG11	1.73	0.70
3:D:255:SER:HA	7:D:387:PGE:C2	2.21	0.70
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.43	0.67
3:F:181[A]:CYS:HG	3:F:196[A]:CYS:HG	0.83	0.66
1:B:285:THR:HG22	1:B:286:ASP:OD1	1.96	0.66
1:A:48:LYS:H	1:A:62:HIS:CE1	2.12	0.65
2:C:71:LEU:HD13	2:C:130:ALA:HB2	1.77	0.65
1:B:302:PRO:O	1:B:305:LYS:HG2	1.98	0.64
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.63	0.64
2:C:86:CYS:H	3:F:372:GLN:HE22	1.46	0.63
3:D:372:GLN:NE2	11:D:1095:HOH:O	2.32	0.62
1:A:119[B]:ARG:CZ	11:A:830:HOH:O	2.48	0.61
1:A:202:ARG:HA	1:A:206:MET:HG3	1.85	0.59
3:D:283:GLN:HB2	3:D:335:SER:HB3	1.84	0.58
1:B:202:ARG:HB2	1:B:206:MET:CE	2.32	0.58
1:A:292:LEU:O	1:A:295:ASN:HB2	2.04	0.57
1:A:288[A]:ARG:HG3	1:A:339:VAL:CG1	2.33	0.57
2:C:23[B]:CYS:HB2	2:C:88[B]:CYS:SG	2.45	0.57
1:B:202:ARG:HB2	1:B:206:MET:HE2	1.86	0.57
1:A:99:ASP:OD2	1:A:102[A]:GLN:HG2	2.06	0.56
1:B:233[A]:THR:HG22	11:B:825:HOH:O	2.03	0.55
3:D:209:GLU:CB	11:D:1178:HOH:O	2.40	0.55
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.70	0.55
1:B:272:VAL:HG21	5:B:600:HEC:HMA3	1.88	0.55
10:F:389:P6G:C2	11:F:840:HOH:O	2.50	0.54
2:C:86:CYS:H	3:F:372:GLN:NE2	2.05	0.53
1:B:214:GLU:HG2	1:B:215:ARG:HG3	1.90	0.53
3:F:51:ASP:HA	3:F:377:PRO:HA	1.91	0.53
1:A:163:GLN:HE22	5:A:500:HEC:HMA1	1.74	0.53
1:B:233[B]:THR:HG23	11:B:994:HOH:O	2.09	0.53
3:F:87:ASP:H	8:F:390:PEG:C3	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36[B]:CYS:SG	2:C:45:ASN:O	2.67	0.52
1:A:86:LYS:HD3	11:A:501:HOH:O	2.09	0.52
3:F:45:ARG:NH2	3:F:343:LYS:O	2.43	0.51
1:A:210:GLN:NE2	2:C:44:THR:HG21	2.24	0.51
3:D:12:GLU:OE1	3:D:20[A]:ARG:NE	2.28	0.50
1:A:60:GLN:O	1:A:62:HIS:HD2	1.97	0.48
2:E:36[B]:CYS:SG	2:E:47:PRO:HD3	2.53	0.48
3:D:273:ARG:HG2	11:D:647:HOH:O	2.14	0.48
2:C:21:GLN:HE22	3:F:14:GLN:NE2	2.12	0.47
3:F:86:ALA:HA	8:F:390:PEG:H31	1.97	0.47
3:F:269[B]:THR:CG2	11:F:935:HOH:O	2.47	0.47
3:D:108:THR:OG1	9:F:388:PG4:H82	2.15	0.46
1:B:297:TYR:O	1:B:329:GLN:HG2	2.13	0.46
1:A:355:GLU:N	1:A:356:PRO:CD	2.78	0.46
3:D:96:SER:HB3	3:D:110:TYR:CZ	2.51	0.46
1:B:233[A]:THR:HG22	11:B:994:HOH:O	2.15	0.46
1:A:21:PRO:O	1:A:27:ALA:HA	2.16	0.45
1:B:88:LYS:HD2	11:B:818:HOH:O	2.16	0.45
3:F:12:GLU:OE2	3:F:20:ARG:NH1	2.49	0.45
3:D:255:SER:HA	7:D:387:PGE:H2	1.96	0.45
2:E:36[B]:CYS:SG	2:E:45:ASN:O	2.74	0.45
9:F:388:PG4:H22	11:F:528:HOH:O	2.16	0.45
3:D:347:TYR:HB3	3:D:356:LEU:HD11	1.98	0.45
1:B:202:ARG:CB	1:B:206:MET:HE2	2.47	0.44
1:A:91:GLN:O	1:A:92:PHE:HB2	2.17	0.44
3:F:255:SER:HA	9:F:387:PG4:H32	1.99	0.43
1:B:305:LYS:HE2	1:B:305:LYS:HB3	1.55	0.43
3:D:280:GLY:HA3	3:D:301:ARG:CZ	2.48	0.43
1:B:197:ILE:O	1:B:202:ARG:CD	2.67	0.43
1:B:163:GLN:HE22	5:B:500:HEC:HMA1	1.83	0.42
2:C:23[B]:CYS:CB	2:C:88[B]:CYS:SG	3.07	0.42
2:C:36[B]:CYS:SG	2:C:47:PRO:HD3	2.60	0.42
3:F:91:PHE:HA	3:F:116:PRO:HD3	2.01	0.42
3:F:87:ASP:H	8:F:390:PEG:H32	1.84	0.41
3:D:51:ASP:HA	3:D:377:PRO:HA	2.02	0.41
1:B:354:TYR:O	1:B:357:LEU:HB2	2.20	0.41
1:B:60:GLN:O	1:B:62:HIS:HD2	2.03	0.41
3:D:130:ALA:N	3:D:131:PRO:HD3	2.35	0.41
3:F:87:ASP:HB2	8:F:390:PEG:H32	2.03	0.41
1:A:127:ARG:HD2	1:A:146:ASP:OD2	2.21	0.41
3:F:174:ARG:CZ	3:F:176:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:87:ASP:H	8:F:390:PEG:H31	1.85	0.41
10:F:389:P6G:H52	10:F:389:P6G:H81	1.88	0.41
1:B:307:ASN:HA	1:B:308:PRO:HD2	1.90	0.40
3:D:45:ARG:NH2	3:D:343:LYS:O	2.55	0.40
1:A:26:ASN:ND2	11:A:836:HOH:O	2.54	0.40
1:B:86:LYS:HD3	11:B:671:HOH:O	2.21	0.40
3:F:82:ASN:HB3	3:F:142:THR:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	356/373 (95%)	348 (98%)	8 (2%)	0	100	100
1	B	354/373 (95%)	346 (98%)	8 (2%)	0	100	100
2	C	125/137 (91%)	123 (98%)	2 (2%)	0	100	100
2	E	123/137 (90%)	120 (98%)	3 (2%)	0	100	100
3	D	375/386 (97%)	365 (97%)	9 (2%)	1 (0%)	46	34
3	F	377/386 (98%)	365 (97%)	11 (3%)	1 (0%)	46	34
All	All	1710/1792 (95%)	1667 (98%)	41 (2%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	102	ILE
3	F	102	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/292 (96%)	270 (96%)	10 (4%)	42	29
1	B	278/292 (95%)	272 (98%)	6 (2%)	60	52
2	C	107/112 (96%)	104 (97%)	3 (3%)	51	41
2	E	105/112 (94%)	103 (98%)	2 (2%)	65	58
3	D	305/311 (98%)	299 (98%)	6 (2%)	63	56
3	F	307/311 (99%)	301 (98%)	6 (2%)	63	56
All	All	1382/1430 (97%)	1349 (98%)	33 (2%)	58	48

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	39	ARG
1	A	75	LEU
1	A	101	LYS
1	A	142	LYS
1	A	167	GLU
1	A	184	LYS
1	A	256	GLU
1	A	358	LEU
1	A	359	GLU
1	B	7	ASP
1	B	167	GLU
1	B	184	LYS
1	B	305	LYS
1	B	358	LEU
1	B	360	GLU
2	C	71	LEU
2	C	75[A]	ARG
2	C	75[B]	ARG
3	D	92	ILE
3	D	94	HIS
3	D	211	THR

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Mol	Chain	Res	Type
3	D	262	LEU
3	D	269	THR
3	D	316	LEU
2	E	7	THR
2	E	113	GLU
3	F	92	ILE
3	F	94	HIS
3	F	173	LYS
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	GLN
1	A	62	HIS
1	A	163	GLN
1	A	210	GLN
1	B	62	HIS
1	B	163	GLN
1	B	210	GLN
3	D	14	GLN
2	E	68	GLN
3	F	14	GLN
3	F	300	GLN
3	F	372	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	1.35	1 (7%)	10,22,24	2.54	4 (40%)
2	0AF	E	57	2	13,16,17	1.45	3 (23%)	10,22,24	1.83	3 (30%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CB-CA	-2.17	1.49	1.53
2	E	57	0AF	CZ3-CE3	2.31	1.42	1.36
2	E	57	0AF	CB-CG	2.50	1.58	1.51
2	C	57	0AF	CZ3-CE3	2.54	1.42	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	0AF	CB-CG-CD1	-5.63	121.01	127.97
2	E	57	0AF	O-C-CA	-4.15	114.68	125.49
2	C	57	0AF	O-C-CA	-3.53	116.30	125.49
2	E	57	0AF	CB-CG-CD1	-2.04	125.44	127.97
2	E	57	0AF	CE3-CD2-CE2	2.10	121.37	117.03
2	C	57	0AF	CH2-CZ2-CE2	2.20	122.90	120.15
2	C	57	0AF	CZ3-CE3-CD2	2.27	124.10	120.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	24,50,50	1.58	6 (25%)	19,82,82	3.22	9 (47%)
5	HEC	A	600	1	24,50,50	2.08	10 (41%)	19,82,82	3.68	8 (42%)
6	EDO	B	374	-	3,3,3	0.57	0	2,2,2	0.19	0
5	HEC	B	500	1	24,50,50	1.54	7 (29%)	19,82,82	3.62	10 (52%)
5	HEC	B	600	1	24,50,50	1.67	7 (29%)	19,82,82	3.83	10 (52%)
7	PGE	D	387	-	9,9,9	0.64	0	8,8,8	0.53	0
6	EDO	D	388	-	3,3,3	0.79	0	2,2,2	0.79	0
8	PEG	D	389	-	6,6,6	0.61	0	5,5,5	0.65	0
8	PEG	E	138	-	6,6,6	0.94	0	5,5,5	0.62	0
9	PG4	F	387	-	12,12,12	0.71	0	11,11,11	0.64	0
9	PG4	F	388	-	12,12,12	0.83	0	11,11,11	0.71	0
10	P6G	F	389	-	18,18,18	0.53	0	17,17,17	0.58	0
8	PEG	F	390	-	6,6,6	0.72	0	5,5,5	0.84	0
6	EDO	F	391	-	3,3,3	0.54	0	2,2,2	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	A	500	1	-	0/6/54/54	0/0/8/8
5	HEC	A	600	1	-	0/6/54/54	0/0/8/8
6	EDO	B	374	-	-	0/1/1/1	0/0/0/0
5	HEC	B	500	1	-	0/6/54/54	0/0/8/8
5	HEC	B	600	1	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGE	D	387	-	-	0/7/7/7	0/0/0/0
6	EDO	D	388	-	-	0/1/1/1	0/0/0/0
8	PEG	D	389	-	-	0/4/4/4	0/0/0/0
8	PEG	E	138	-	-	0/4/4/4	0/0/0/0
9	PG4	F	387	-	-	0/10/10/10	0/0/0/0
9	PG4	F	388	-	-	0/10/10/10	0/0/0/0
10	P6G	F	389	-	-	0/16/16/16	0/0/0/0
8	PEG	F	390	-	-	0/4/4/4	0/0/0/0
6	EDO	F	391	-	-	0/1/1/1	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	HEC	C3B-C2B	-4.68	1.35	1.40
5	A	600	HEC	C4B-NB	-4.16	1.31	1.36
5	A	600	HEC	C4C-NC	-3.72	1.31	1.36
5	B	500	HEC	C1A-NA	-2.94	1.32	1.36
5	B	600	HEC	C1A-NA	-2.92	1.32	1.36
5	A	600	HEC	C4A-NA	-2.81	1.32	1.36
5	B	500	HEC	C4C-NC	-2.63	1.33	1.36
5	A	600	HEC	C1A-NA	-2.27	1.33	1.36
5	B	500	HEC	C3B-C2B	-2.14	1.38	1.40
5	B	500	HEC	C3C-C2C	-2.13	1.38	1.40
5	B	600	HEC	C4C-NC	-2.04	1.33	1.36
5	A	600	HEC	C1B-CHB	2.00	1.45	1.39
5	A	600	HEC	C4D-CHA	2.08	1.45	1.39
5	B	500	HEC	C1C-CHC	2.12	1.45	1.39
5	A	600	HEC	C3C-C4C	2.13	1.47	1.42
5	B	600	HEC	C4D-CHA	2.18	1.45	1.39
5	A	500	HEC	C3C-C4C	2.22	1.47	1.42
5	A	600	HEC	C3B-C4B	2.26	1.47	1.42
5	B	600	HEC	C1D-CHD	2.32	1.46	1.39
5	B	600	HEC	C3C-C2C	2.33	1.43	1.40
5	B	500	HEC	C3C-C4C	2.37	1.48	1.42
5	A	500	HEC	C4D-CHA	2.47	1.46	1.39
5	A	500	HEC	C1B-CHB	2.96	1.48	1.39
5	A	500	HEC	C3B-C4B	3.06	1.49	1.42
5	B	500	HEC	C1B-CHB	3.14	1.48	1.39
5	A	600	HEC	C1C-CHC	3.15	1.48	1.39
5	B	600	HEC	C1B-CHB	3.17	1.48	1.39
5	A	500	HEC	C1C-CHC	3.32	1.49	1.39
5	A	500	HEC	C1D-CHD	3.40	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	600	HEC	C1C-CHC	3.40	1.49	1.39

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	HEC	CBB-CAB-C3B	-11.21	102.45	127.35
5	B	600	HEC	CBB-CAB-C3B	-10.77	103.41	127.35
5	A	500	HEC	CBB-CAB-C3B	-9.84	105.48	127.35
5	A	600	HEC	CBB-CAB-C3B	-8.82	107.76	127.35
5	A	600	HEC	CBC-CAC-C3C	-7.53	110.62	127.35
5	B	600	HEC	CBC-CAC-C3C	-6.72	112.43	127.35
5	A	600	HEC	CBA-CAA-C2A	-6.17	101.47	112.53
5	A	600	HEC	CBD-CAD-C3D	-6.14	101.53	112.53
5	B	600	HEC	CBA-CAA-C2A	-5.64	102.41	112.53
5	B	500	HEC	CBC-CAC-C3C	-5.58	114.95	127.35
5	B	600	HEC	CBD-CAD-C3D	-5.31	103.01	112.53
5	A	500	HEC	CBC-CAC-C3C	-5.17	115.87	127.35
5	B	500	HEC	CBD-CAD-C3D	-4.07	105.23	112.53
5	A	500	HEC	CBD-CAD-C3D	-3.79	105.73	112.53
5	A	600	HEC	C4C-C3C-C2C	-3.43	102.64	106.35
5	B	600	HEC	C4C-C3C-C2C	-3.33	102.75	106.35
5	B	500	HEC	CMC-C2C-C1C	-3.24	123.00	128.36
5	A	500	HEC	C4B-C3B-C2B	-3.23	102.86	106.35
5	B	500	HEC	C4C-C3C-C2C	-3.17	102.92	106.35
5	B	500	HEC	CMB-C2B-C1B	-2.99	123.42	128.36
5	B	600	HEC	CAA-CBA-CGA	-2.97	107.30	112.75
5	B	600	HEC	CMC-C2C-C1C	-2.95	123.49	128.36
5	A	500	HEC	C4C-C3C-C2C	-2.92	103.20	106.35
5	B	500	HEC	C4B-C3B-C2B	-2.73	103.40	106.35
5	B	600	HEC	CMD-C2D-C1D	-2.70	123.90	128.36
5	A	500	HEC	CMB-C2B-C1B	-2.60	124.06	128.36
5	A	600	HEC	CAD-CBD-CGD	-2.47	108.23	112.75
5	B	600	HEC	CAA-C2A-C1A	-2.14	124.69	127.01
5	A	600	HEC	CMC-C2C-C1C	-2.13	124.83	128.36
5	B	500	HEC	C3B-C4B-NB	2.19	115.08	110.94
5	B	600	HEC	CMD-C2D-C3D	2.33	130.12	125.24
5	A	500	HEC	C3B-C4B-NB	2.45	115.57	110.94
5	A	500	HEC	CMA-C3A-C2A	2.66	130.81	125.24
5	A	500	HEC	CAD-C3D-C4D	2.67	129.90	127.01
5	A	600	HEC	CMA-C3A-C2A	3.14	131.80	125.24
5	B	500	HEC	CAD-C3D-C4D	3.32	130.62	127.01
5	B	500	HEC	CAD-CBD-CGD	3.43	119.03	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	HEC	1	0
5	B	500	HEC	1	0
5	B	600	HEC	1	0
7	D	387	PGE	3	0
9	F	387	PG4	1	0
9	F	388	PG4	2	0
10	F	389	P6G	3	0
8	F	390	PEG	5	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	354/373 (94%)	-0.32	8 (2%) 64 67	20, 29, 48, 68	0
1	B	355/373 (95%)	-0.36	6 (1%) 73 76	17, 26, 45, 64	0
2	C	123/137 (89%)	-0.06	2 (1%) 74 78	16, 25, 38, 56	0
2	E	123/137 (89%)	-0.14	0 100 100	17, 22, 33, 45	0
3	D	376/386 (97%)	-0.10	3 (0%) 87 89	18, 32, 53, 72	0
3	F	376/386 (97%)	-0.33	4 (1%) 82 84	15, 22, 37, 61	0
All	All	1707/1792 (95%)	-0.25	23 (1%) 79 82	15, 27, 48, 72	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ASP	5.9
1	A	6	ALA	5.1
1	B	6	ALA	5.1
1	A	7	ASP	4.8
1	A	302	PRO	3.6
3	D	11	GLN	3.6
2	C	106	ILE	3.4
1	A	301	ARG	3.1
1	B	83	ALA	3.0
3	D	209	GLU	3.0
1	A	304	ALA	3.0
1	B	8	ASP	2.9
1	A	300	ARG	2.7
2	C	7	THR	2.5
1	B	303	GLU	2.5
3	F	386	GLY	2.5
3	D	211	THR	2.4
3	F	30	GLN	2.3
3	F	11	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	8	ASP	2.2
3	F	31	ASP	2.2
1	A	242	ALA	2.1
1	B	300	ARG	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	C	57	15/16	0.97	0.12	-	21,24,25,26	0
2	0AF	E	57	15/16	0.97	0.16	-	16,19,22,24	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
8	PEG	E	138	7/7	0.85	0.21	4.84	43,45,49,55	0
9	PG4	F	388	13/13	0.87	0.21	3.69	37,45,60,61	0
8	PEG	F	390	7/7	0.91	0.12	3.42	29,34,42,44	0
6	EDO	F	391	4/4	0.86	0.12	2.49	52,54,54,54	0
8	PEG	D	389	7/7	0.88	0.15	2.36	46,49,53,53	0
6	EDO	D	388	4/4	0.88	0.14	2.19	38,39,41,41	0
4	CA	B	400	1/1	1.00	0.08	1.69	19,19,19,19	0
7	PGE	D	387	10/10	0.89	0.09	1.27	56,60,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	P6G	F	389	19/19	0.93	0.11	1.24	29,42,55,58	0
4	CA	A	400	1/1	0.99	0.08	0.69	20,20,20,20	0
5	HEC	A	600	43/43	0.99	0.09	0.12	18,21,23,24	0
9	PG4	F	387	13/13	0.89	0.11	0.11	50,53,64,65	0
5	HEC	A	500	43/43	0.99	0.07	0.03	19,22,25,26	0
6	EDO	B	374	4/4	0.86	0.08	-0.27	43,44,46,47	0
5	HEC	B	600	43/43	0.99	0.08	-0.30	12,16,19,21	0
5	HEC	B	500	43/43	0.99	0.06	-0.58	14,19,22,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.