



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:20 AM GMT

PDB ID : 2YEV  
Title : Structure of caa3-type cytochrome oxidase  
Authors : Lyons, J.A.; Aragao, D.; Soulimane, T.; Caffrey, M.  
Deposited on : 2011-03-31  
Resolution : 2.36 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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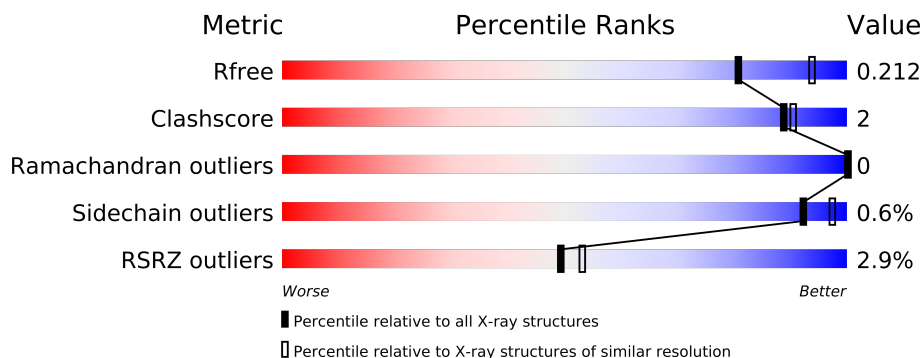
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.36 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))
$R_{free}$	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	791	
1	D	791	
2	B	337	
2	E	337	
3	C	66	
3	F	66	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	CUA	B	585	-	X
12	7E9	B	701	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
13	CL	C	101	-	X
13	CL	F	101	-	X
6	CU	A	1017	-	X
6	CU	D	1017	-	X
7	4AG	A	1200	-	X
8	7E8	A	1300	-	X
8	7E8	A	1301	-	X
9	MG	A	1801	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 19587 atoms, of which 0 are hydrogen and 0 are deuterium.

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 CYTOCHROME C OXIDASE POLYPEPTIDE I+III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	0	1	0
			6281	4244	992	1022	23			
1	D	780	Total	C	N	O	S	0	0	0
			6276	4241	992	1020	23			

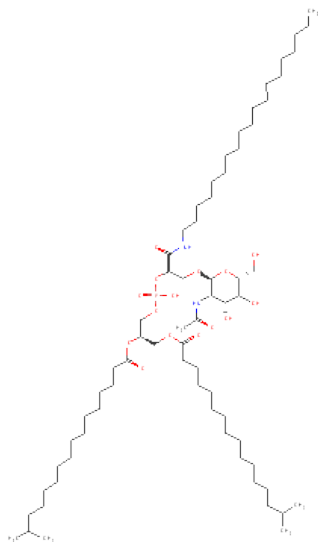
- Molecule 2 is a protein called CYTOCHROME C OXIDASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	319	Total	C	N	O	S	0	0	0
			2507	1637	422	439	9			
2	E	319	Total	C	N	O	S	0	0	0
			2507	1637	422	439	9			

- Molecule 3 is a protein called CAA3-TYPE CYTOCHROME OXIDASE SUBUNIT IV.

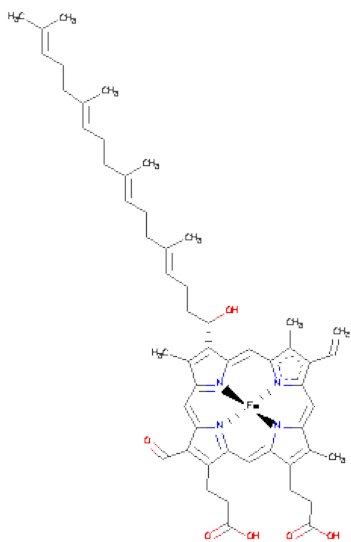
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	64	Total	C	N	O	S	0	0	0
			502	344	76	79	3			
3	F	63	Total	C	N	O	S	0	0	0
			492	338	73	78	3			

- Molecule 4 is (1R,4S,6R)-6-({[2-(ACETYLAMINO)-2-DEOXY-ALPHA-D-GLUCOPYRANOSYL]OXY}METHYL)-4-HYDROXY-1-{{[(15-METHYLHEXADECANOYL)OXY]METHYL}-4-OXIDO-7-OXO-3,5-DIOXA-8-AZA-4-PHOSPHAHEPTACOS-1-YL15-METHYLHEXADECANOATE (three-letter code: 5PL) (formula: C<sub>67</sub>H<sub>129</sub>N<sub>2</sub>O<sub>15</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			85	67	2	15	1		
4	D	1	Total	C	N	O	P	0	0
			85	67	2	15	1		

- Molecule 5 is HEME-AS (three-letter code: HAS) (formula: C<sub>54</sub>H<sub>64</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		
5	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

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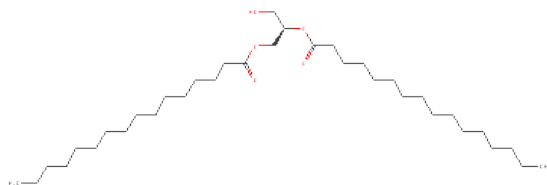
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	Fe	N	O	
			65	54	1	4	6	
5	D	1	Total	C	Fe	N	O	
			65	54	1	4	6	

- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

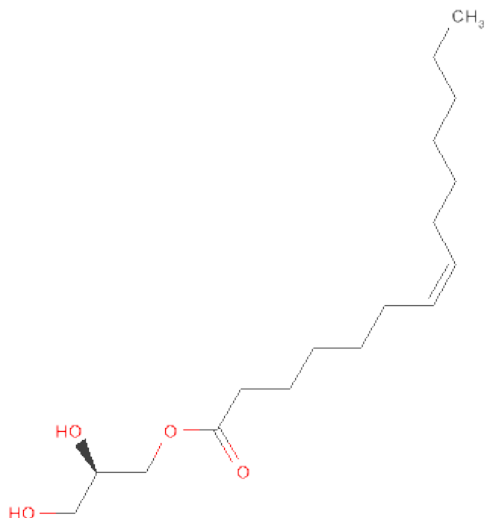
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cu		
			1	1	0	0
6	D	1	Total	Cu		
			1	1	0	0

- Molecule 7 is (2R)-3-HYDROXYPROPANE-1,2-DIYLDIHEXADECANOATE (three-letter code: 4AG) (formula: C<sub>35</sub>H<sub>68</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O		
			40	35	5	0	0

- Molecule 8 is (2R)-2,3-DIHYDROXYPROPYL(7Z)-TETRADEC-7-ENOATE (three-letter code: 7E8) (formula: C<sub>17</sub>H<sub>32</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			21	17	4		
8	A	1	Total	C	O	0	0
			21	17	4		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

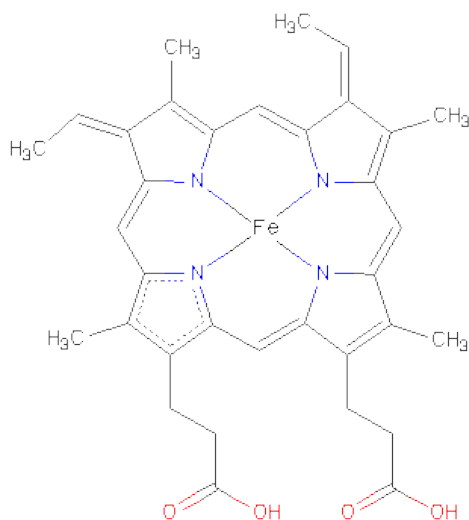
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

- Molecule 10 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	Cu			0	0
			2	2				
10	E	1	Total	Cu			0	0
			2	2				

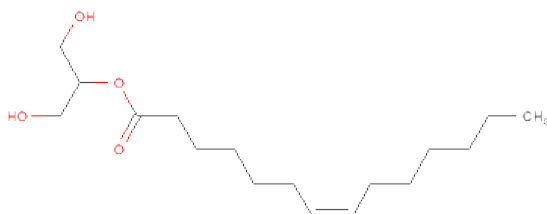
- Molecule 11 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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



- Molecule 12 is 1,3-DIHYDROXYPROPAN-2-YL(Z)-TETRADEC-7-ENOATE (three-letter code: 7E9) (formula: C<sub>17</sub>H<sub>32</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			21	17	4		

- Molecule 13 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	D	1	Total	Cl	0	0
			1	1		
13	C	1	Total	Cl	0	0
			1	1		
13	F	1	Total	Cl	0	0
			1	1		

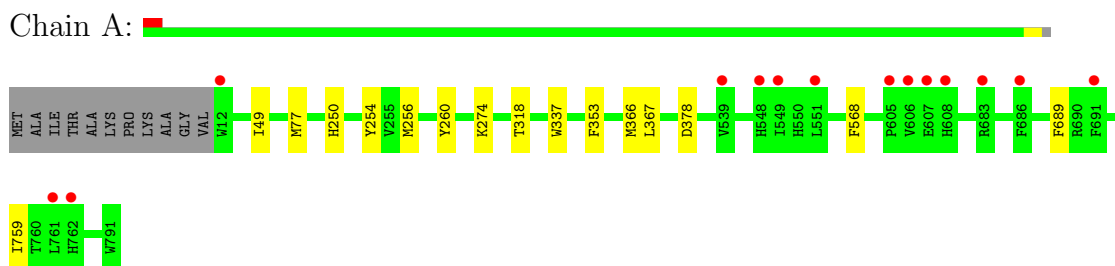
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	157	Total	O	0	0
			157	157		
14	B	90	Total	O	0	0
			90	90		
14	D	111	Total	O	0	0
			111	111		
14	E	34	Total	O	0	0
			34	34		

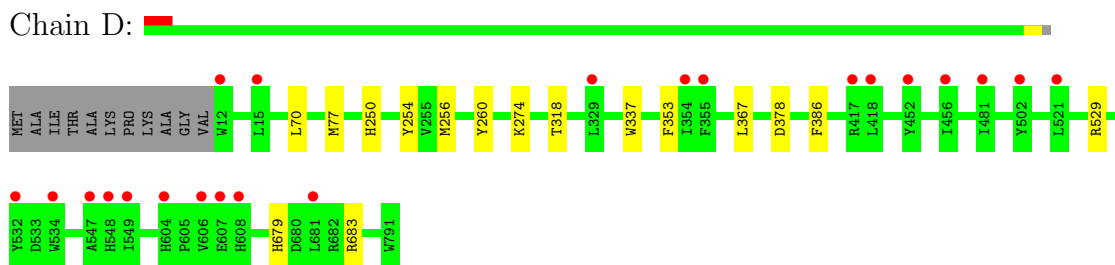
### 3 Residue-property plots

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.

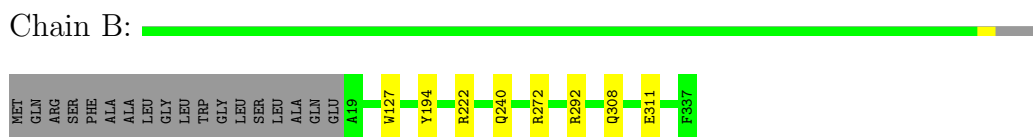
- Molecule 1: CYTOCHROME C OXIDASE POLYPEPTIDE I+III



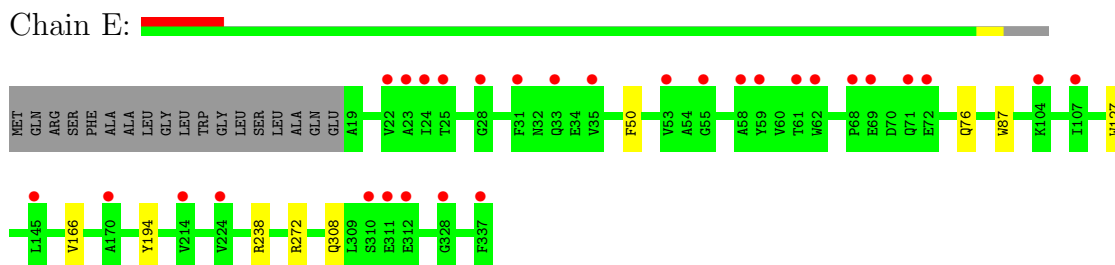
- Molecule 1: CYTOCHROME C OXIDASE POLYPEPTIDE I+III



- Molecule 2: CYTOCHROME C OXIDASE SUBUNIT 2

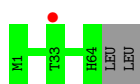


- Molecule 2: CYTOCHROME C OXIDASE SUBUNIT 2



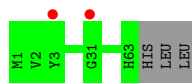
- Molecule 3: CAA3-TYPE CYTOCHROME OXIDASE SUBUNIT IV





- Molecule 3: CAA3-TYPE CYTOCHROME OXIDASE SUBUNIT IV

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.25Å 76.03Å 300.27Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	77.18 – 2.36 115.49 – 2.36	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.18-2.36) 100.0 (115.49-2.36)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.37Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.4_486)	Depositor
R, $R_{free}$	0.171 , 0.218 0.163 , 0.212	Depositor DCC
$R_{free}$ test set	5971 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.2	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.5	EDS
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 118259 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5PL, 7E8, CL, MG, HAS, 4AG, CUA, HEC, 7E9, FME, CU

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	0.32	0/6523	0.44	0/8921
1	D	0.31	0/6515	0.44	0/8910
2	B	0.32	0/2586	0.46	0/3523
2	E	0.31	0/2586	0.46	0/3523
3	C	0.26	0/502	0.38	0/683
3	F	0.25	0/491	0.39	0/668
All	All	0.31	0/19203	0.44	0/26228

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6281	0	0	13	0
1	D	6276	0	0	15	0
2	B	2507	0	0	5	0
2	E	2507	0	0	4	0
3	C	502	0	0	0	0
3	F	492	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	85	0	128	2	0
4	D	85	0	128	2	0
5	A	130	0	124	9	0
5	D	130	0	124	9	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	A	40	0	68	1	0
8	A	42	0	64	1	0
9	A	1	0	0	0	0
9	D	1	0	0	0	0
10	B	2	0	0	0	0
10	E	2	0	0	0	0
11	B	43	0	30	2	0
11	E	43	0	30	1	0
12	B	21	0	32	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	F	1	0	0	0	0
14	A	157	0	0	1	0
14	B	90	0	0	2	0
14	D	111	0	0	0	0
14	E	34	0	0	1	0
All	All	19587	0	728	46	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (46) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:367:LEU:CB	5:D:1016:HAS:HMD	2.15	0.77
1:A:367:LEU:CB	5:A:1016:HAS:HMD	2.25	0.67
5:D:1016:HAS:HMC1	5:D:1016:HAS:HBC1	1.82	0.60
2:B:127:TRP:CD1	11:B:587:HEC:HAD1	2.38	0.59
2:E:127:TRP:CD1	11:E:587:HEC:HAD1	2.38	0.58
1:D:529:ARG:NH2	2:E:76:GLN:OE1	2.36	0.58
1:A:568:PHE:CZ	4:A:900:5PL:H202	2.39	0.58
1:A:77:MET:CB	5:A:1015:HAS:CAC	2.87	0.52
1:A:49:ILE:CG2	5:A:1015:HAS:HMD	2.40	0.52
1:A:366:MET:SD	7:A:1200:4AG:H352	2.50	0.51
1:D:679:HIS:CE1	1:D:683:ARG:CZ	2.94	0.50
11:B:587:HEC:HBB3	11:B:587:HEC:HMB1	1.94	0.50
1:D:77:MET:CB	5:D:1015:HAS:CAC	2.91	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:222:ARG:NH1	14:B:2044:HOH:O	2.46	0.48
1:D:367:LEU:C	5:D:1016:HAS:HMD	2.34	0.48
2:E:308:GLN:N	2:E:308:GLN:OE1	2.48	0.47
5:A:1016:HAS:HMC1	5:A:1016:HAS:HBC1	1.97	0.47
2:B:308:GLN:N	2:B:308:GLN:OE1	2.47	0.47
1:A:318:THR:CG2	5:A:1016:HAS:HMB2	2.44	0.47
1:D:256:MET:O	1:D:260:TYR:CD2	2.68	0.46
1:A:353:PHE:CD1	1:A:353:PHE:C	2.89	0.46
1:A:77:MET:CB	5:A:1015:HAS:HAC	2.46	0.46
1:D:679:HIS:CE1	1:D:683:ARG:NH1	2.84	0.45
1:D:318:THR:CG2	5:D:1016:HAS:HMB2	2.47	0.45
1:D:70:LEU:CD1	5:D:1015:HAS:HBD1	2.46	0.45
1:A:256:MET:O	1:A:260:TYR:CD2	2.70	0.45
1:A:250:HIS:CE1	1:A:254:TYR:OH	2.68	0.45
1:D:353:PHE:CD1	1:D:353:PHE:C	2.90	0.45
5:A:1015:HAS:H281	5:A:1015:HAS:H251	1.65	0.45
4:D:900:5PL:HAY1	4:D:900:5PL:OCO	2.16	0.44
2:B:292:ARG:NH2	2:B:311:GLU:OE1	2.51	0.44
2:E:166:VAL:N	14:E:2012:HOH:O	2.50	0.44
2:B:240:GLN:NE2	14:B:2049:HOH:O	2.49	0.43
1:D:250:HIS:CE1	1:D:254:TYR:OH	2.71	0.43
1:D:250:HIS:CD2	1:D:250:HIS:C	2.91	0.43
4:A:900:5PL:OCO	4:A:900:5PL:HAY1	2.19	0.43
1:D:386:PHE:CG	5:D:1016:HAS:HMA2	2.54	0.43
8:A:1301:7E8:H191	14:A:2010:HOH:O	2.18	0.43
5:A:1015:HAS:HAD2	5:A:1015:HAS:HHA	1.88	0.42
1:D:274:LYS:NZ	1:D:337:TRP:O	2.51	0.42
1:A:274:LYS:NZ	1:A:337:TRP:O	2.53	0.42
4:D:900:5PL:HBH	4:D:900:5PL:OCO	2.19	0.41
1:D:386:PHE:CD2	5:D:1016:HAS:HAA1	2.56	0.41
1:A:250:HIS:CD2	1:A:250:HIS:C	2.94	0.41
1:A:367:LEU:CB	5:A:1016:HAS:CMD	2.98	0.41
5:D:1015:HAS:H281	5:D:1015:HAS:H251	1.35	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	779/791 (98%)	762 (98%)	17 (2%)	0	100	100
1	D	778/791 (98%)	759 (98%)	19 (2%)	0	100	100
2	B	317/337 (94%)	308 (97%)	9 (3%)	0	100	100
2	E	317/337 (94%)	307 (97%)	10 (3%)	0	100	100
3	C	62/66 (94%)	62 (100%)	0	0	100	100
3	F	61/66 (92%)	61 (100%)	0	0	100	100
All	All	2314/2388 (97%)	2259 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	640/646 (99%)	637 (100%)	3 (0%)	94	98
1	D	639/646 (99%)	638 (100%)	1 (0%)	96	99
2	B	261/274 (95%)	259 (99%)	2 (1%)	89	95
2	E	261/274 (95%)	256 (98%)	5 (2%)	69	84
3	C	51/53 (96%)	51 (100%)	0	100	100
3	F	50/53 (94%)	50 (100%)	0	100	100
All	All	1902/1946 (98%)	1891 (99%)	11 (1%)	92	97

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	ASP
1	A	689	PHE
1	A	759	ILE
2	B	194	TYR
2	B	272	ARG
1	D	378	ASP

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Mol	Chain	Res	Type
2	E	50	PHE
2	E	87	TRP
2	E	194	TYR
2	E	238	ARG
2	E	272	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z  > 2$
3	FME	C	1	3	9,9,10	5.94	2 (22%)	6,9,11	1.21	1 (16%)
3	FME	F	1	3	9,9,10	6.12	2 (22%)	6,9,11	0.40	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
3	FME	C	1	3	-	0/7/9/11	0/0/0/0
3	FME	F	1	3	-	0/7/9/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	FME	O-C	18.13	1.23	1.11
3	C	1	FME	O-C	17.64	1.23	1.11
3	F	1	FME	CA-C	2.78	1.53	1.48
3	C	1	FME	CA-C	2.56	1.53	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	-2.80	118.33	122.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 7 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	HAS	A	1015	1	72,72,72	2.03	14 (19%)	86,109,109	2.50	33 (38%)
5	HAS	A	1016	1,14	72,72,72	2.19	15 (20%)	86,109,109	2.48	32 (37%)
7	4AG	A	1200	-	39,39,39	1.01	2 (5%)	41,41,41	1.18	3 (7%)
8	7E8	A	1300	-	20,20,20	0.98	1 (5%)	21,21,21	1.00	1 (4%)
8	7E8	A	1301	-	20,20,20	0.95	1 (5%)	21,21,21	1.04	2 (9%)
4	5PL	A	900	-	85,85,85	0.77	2 (2%)	101,101,101	1.04	5 (4%)
10	CUA	B	585	2	0,1,1	0.00	-	0,0,0	0.00	-
11	HEC	B	587	2	50,50,50	2.60	14 (28%)	56,82,82	2.12	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	7E9	B	701	-	20,20,20	1.03	1 (5%)	21,21,21	1.19	1 (4%)
5	HAS	D	1015	1	72,72,72	2.15	13 (18%)	86,109,109	2.52	33 (38%)
5	HAS	D	1016	1,14	72,72,72	2.00	15 (20%)	86,109,109	2.67	37 (43%)
4	5PL	D	900	-	85,85,85	0.77	2 (2%)	101,101,101	1.05	7 (6%)
10	CUA	E	585	2	0,1,1	0.00	-	0,0,0	0.00	-
11	HEC	E	587	2	50,50,50	2.71	14 (28%)	56,82,82	2.24	15 (26%)

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	HAS	A	1015	1	-	0/36/82/82	0/0/8/8
5	HAS	A	1016	1,14	-	0/36/82/82	0/0/8/8
7	4AG	A	1200	-	-	0/41/41/41	0/0/0/0
8	7E8	A	1300	-	1/1/2/4	0/20/20/20	0/0/0/0
8	7E8	A	1301	-	-	0/20/20/20	0/0/0/0
4	5PL	A	900	-	-	0/87/107/107	0/1/1/1
10	CUA	B	585	2	-	0/0/0/0	0/0/0/0
11	HEC	B	587	2	-	0/10/54/54	0/0/8/8
12	7E9	B	701	-	-	0/21/21/21	0/0/0/0
5	HAS	D	1015	1	-	0/36/82/82	0/0/8/8
5	HAS	D	1016	1,14	-	2/36/82/82	0/0/8/8
4	5PL	D	900	-	-	0/87/107/107	0/1/1/1
10	CUA	E	585	2	-	0/0/0/0	0/0/0/0
11	HEC	E	587	2	-	0/10/54/54	0/0/8/8

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	587	HEC	C3C-CAC	9.50	1.55	1.35
11	B	587	HEC	C3B-CAB	9.27	1.54	1.35
11	B	587	HEC	C3C-CAC	9.14	1.54	1.35
11	E	587	HEC	C3B-CAB	9.01	1.54	1.35
5	A	1016	HAS	C4A-C3A	7.68	1.49	1.40
5	A	1016	HAS	C1C-C2C	7.62	1.49	1.40
5	D	1015	HAS	C4A-C3A	7.62	1.49	1.40
5	D	1016	HAS	C4A-C3A	7.36	1.49	1.40
5	A	1015	HAS	C1C-C2C	7.25	1.49	1.40
5	A	1015	HAS	C4A-C3A	7.25	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1015	HAS	C1C-C2C	6.97	1.48	1.40
5	D	1016	HAS	C1C-C2C	6.66	1.48	1.40
5	D	1015	HAS	FE-NB	6.10	2.18	1.92
5	A	1015	HAS	FE-NB	5.98	2.18	1.92
5	A	1016	HAS	FE-NB	5.57	2.16	1.92
5	D	1015	HAS	C4C-C3C	5.41	1.48	1.41
5	A	1016	HAS	C4C-C3C	5.37	1.48	1.41
11	E	587	HEC	C3D-C2D	5.21	1.53	1.37
5	D	1016	HAS	FE-NB	5.17	2.14	1.92
5	A	1016	HAS	FE-NC	5.16	2.14	1.92
5	A	1016	HAS	C2D-C1D	5.13	1.48	1.40
5	D	1016	HAS	C4C-C3C	5.06	1.47	1.41
5	D	1015	HAS	C2D-C1D	5.00	1.48	1.40
11	B	587	HEC	C3D-C2D	4.92	1.52	1.37
5	A	1015	HAS	C4C-C3C	4.83	1.47	1.41
5	D	1015	HAS	FE-ND	4.79	2.13	1.92
5	A	1015	HAS	C2D-C1D	4.72	1.47	1.40
11	E	587	HEC	C1B-C2B	4.69	1.46	1.40
5	D	1015	HAS	FE-NA	4.59	2.12	1.92
5	A	1015	HAS	FE-NA	4.49	2.11	1.92
5	A	1016	HAS	FE-ND	4.42	2.11	1.92
5	D	1016	HAS	FE-NA	4.35	2.11	1.92
4	D	900	5PL	OCK-CBU	4.33	1.47	1.34
5	A	1016	HAS	FE-NA	4.33	2.11	1.92
7	A	1200	4AG	O17-C16	4.22	1.46	1.33
11	B	587	HEC	C1D-C2D	4.21	1.45	1.40
11	E	587	HEC	C1C-C2C	4.18	1.45	1.40
8	A	1300	7E8	O16-C8	4.15	1.46	1.33
4	A	900	5PL	OCL-CBL	4.13	1.46	1.33
4	A	900	5PL	OCK-CBU	4.09	1.46	1.34
11	E	587	HEC	C1D-C2D	4.00	1.45	1.40
8	A	1301	7E8	O16-C8	3.99	1.45	1.33
5	D	1016	HAS	C3B-C11	-3.98	1.48	1.52
12	B	701	7E9	O1-C80	3.96	1.46	1.34
7	A	1200	4AG	O21-C22	3.94	1.46	1.34
5	D	1015	HAS	FE-NC	3.93	2.09	1.92
5	A	1016	HAS	C3B-C11	-3.91	1.48	1.52
5	D	1016	HAS	C2D-C1D	3.91	1.46	1.40
11	E	587	HEC	C3B-C2B	-3.88	1.33	1.41
5	D	1015	HAS	C3B-C11	-3.88	1.48	1.52
11	B	587	HEC	C1C-C2C	3.80	1.44	1.40
11	B	587	HEC	C3B-C2B	-3.75	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1016	HAS	FE-ND	3.74	2.08	1.92
4	D	900	5PL	OCL-CBL	3.68	1.44	1.33
11	B	587	HEC	C1B-C2B	3.66	1.44	1.40
5	D	1016	HAS	C1A-C2A	3.66	1.49	1.43
11	E	587	HEC	FE-NB	3.64	2.08	1.92
11	B	587	HEC	C3C-C2C	-3.63	1.33	1.41
11	E	587	HEC	C3C-C2C	-3.56	1.33	1.41
5	A	1015	HAS	C3B-C11	-3.49	1.49	1.52
11	E	587	HEC	FE-NA	3.49	2.07	1.92
5	D	1016	HAS	FE-NC	3.30	2.06	1.92
11	E	587	HEC	FE-ND	3.27	2.06	1.92
5	A	1015	HAS	FE-NC	3.26	2.06	1.92
5	A	1016	HAS	C1A-C2A	3.22	1.49	1.43
5	D	1015	HAS	C2D-C3D	3.21	1.47	1.41
5	A	1016	HAS	C2D-C3D	3.15	1.46	1.41
5	D	1015	HAS	C1A-C2A	3.10	1.48	1.43
5	A	1015	HAS	C2A-C3A	3.08	1.46	1.37
5	D	1016	HAS	C2A-C3A	3.07	1.46	1.37
5	A	1016	HAS	C2A-C3A	3.06	1.46	1.37
11	E	587	HEC	C3C-C4C	3.05	1.45	1.41
5	A	1015	HAS	FE-ND	2.95	2.05	1.92
11	B	587	HEC	C3C-C4C	2.91	1.45	1.41
5	A	1015	HAS	C1A-C2A	2.90	1.48	1.43
5	D	1015	HAS	C2A-C3A	2.81	1.46	1.37
11	B	587	HEC	FE-NB	2.76	2.04	1.92
5	D	1016	HAS	C2D-C3D	2.58	1.45	1.41
11	B	587	HEC	FE-ND	2.58	2.03	1.92
5	A	1015	HAS	C2D-C3D	2.55	1.45	1.41
5	D	1015	HAS	C3C-C2C	2.54	1.45	1.41
5	A	1016	HAS	C3C-C2C	2.44	1.45	1.41
11	B	587	HEC	FE-NC	2.42	2.02	1.92
11	B	587	HEC	C3B-C4B	2.40	1.44	1.41
5	A	1015	HAS	C3C-C2C	2.38	1.45	1.41
5	A	1016	HAS	C1B-C2B	2.34	1.51	1.43
5	D	1016	HAS	C3C-C2C	2.33	1.45	1.41
11	B	587	HEC	FE-NA	2.31	2.02	1.92
11	E	587	HEC	FE-NC	2.30	2.02	1.92
11	E	587	HEC	C3B-C4B	2.22	1.44	1.41
5	A	1016	HAS	C4B-C3B	2.17	1.50	1.43
5	D	1016	HAS	C4B-C3B	2.12	1.50	1.43
5	A	1015	HAS	C4B-C3B	2.07	1.50	1.43
5	D	1016	HAS	C4D-C3D	2.02	1.50	1.43

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	587	HEC	CBD-CAD-C3D	-8.09	98.45	112.69
11	E	587	HEC	CBD-CAD-C3D	-7.95	98.69	112.69
11	B	587	HEC	CBB-CAB-C3B	-7.41	107.59	128.44
11	E	587	HEC	CBB-CAB-C3B	-7.33	107.81	128.44
5	A	1016	HAS	C4D-C3D-C2D	-7.24	100.79	106.80
5	D	1016	HAS	CMC-C2C-C3C	7.22	136.34	124.97
5	D	1016	HAS	C4D-C3D-C2D	-7.21	100.82	106.80
5	A	1015	HAS	C4D-C3D-C2D	-7.18	100.84	106.80
5	A	1016	HAS	CMC-C2C-C3C	7.14	136.22	124.97
5	D	1016	HAS	CMA-C3A-C4A	-7.13	117.65	128.62
5	D	1015	HAS	CMC-C2C-C3C	6.88	135.80	124.97
5	D	1015	HAS	C4D-C3D-C2D	-6.49	101.41	106.80
5	D	1016	HAS	CMC-C2C-C1C	-6.37	118.82	128.62
5	A	1015	HAS	CMC-C2C-C3C	6.35	134.98	124.97
5	A	1016	HAS	CMC-C2C-C1C	-6.15	119.16	128.62
5	A	1016	HAS	CMA-C3A-C4A	-6.07	119.28	128.62
5	A	1015	HAS	CMA-C3A-C4A	-6.00	119.39	128.62
5	D	1015	HAS	CMC-C2C-C1C	-5.84	119.64	128.62
5	D	1016	HAS	CMA-C3A-C2A	5.62	135.54	124.94
5	D	1016	HAS	CMB-C2B-C3B	5.50	135.31	124.94
5	D	1015	HAS	CBA-CAA-C2A	-5.44	103.11	112.69
5	D	1016	HAS	C1D-C2D-CMD	-5.40	119.33	128.19
5	D	1015	HAS	CMB-C2B-C3B	5.16	134.67	124.94
5	A	1016	HAS	CAD-CBD-CGD	-5.10	97.07	113.47
11	E	587	HEC	CBC-CAC-C3C	-5.07	114.16	128.44
5	A	1015	HAS	CMA-C3A-C2A	5.05	134.46	124.94
5	A	1015	HAS	CMC-C2C-C1C	-5.00	120.92	128.62
5	D	1015	HAS	CMA-C3A-C4A	-4.99	120.95	128.62
5	A	1015	HAS	C3C-C2C-C1C	-4.96	104.10	107.00
5	A	1016	HAS	CMA-C3A-C2A	4.77	133.93	124.94
5	D	1015	HAS	C1D-C2D-CMD	-4.76	120.38	128.19
5	A	1016	HAS	C1D-C2D-CMD	-4.69	120.50	128.19
5	A	1015	HAS	C1D-C2D-CMD	-4.68	120.50	128.19
5	D	1016	HAS	C1A-C2A-C3A	-4.58	102.17	106.92
5	D	1016	HAS	C13-C12-C11	-4.52	106.78	114.06
5	A	1015	HAS	C1A-C2A-C3A	-4.38	102.38	106.92
5	D	1016	HAS	CAD-CBD-CGD	-4.37	99.43	113.47
5	D	1016	HAS	C13-C14-C15	-4.34	118.43	127.80
5	A	1015	HAS	CBA-CAA-C2A	-4.30	105.12	112.69
5	A	1015	HAS	CMB-C2B-C3B	4.29	133.03	124.94
11	B	587	HEC	CMC-C2C-C1C	-4.24	122.09	128.62
5	A	1015	HAS	OMD-CMD-C2D	-4.22	116.20	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	900	5PL	OCK-CBU-CBV	4.21	120.78	111.56
5	A	1016	HAS	C1A-C2A-C3A	-4.21	102.56	106.92
5	D	1015	HAS	C3C-C2C-C1C	-4.18	104.55	107.00
5	A	1015	HAS	C3D-C4D-ND	4.18	112.77	109.64
4	A	900	5PL	OCK-CBU-CBV	4.12	120.58	111.56
5	D	1015	HAS	CMA-C3A-C2A	4.08	132.63	124.94
5	A	1016	HAS	C3C-C2C-C1C	-4.07	104.62	107.00
7	A	1200	4AG	O21-C22-C23	4.02	120.37	111.56
5	D	1015	HAS	C4C-NC-C1C	3.95	111.97	106.76
12	B	701	7E9	O1-C80-C2	3.95	120.20	111.56
11	E	587	HEC	CBA-CAA-C2A	-3.82	105.20	112.35
5	D	1015	HAS	C21-C22-C23	-3.80	119.59	127.80
5	D	1016	HAS	CAD-C3D-C4D	3.79	131.51	124.67
5	D	1015	HAS	C13-C14-C15	-3.78	119.65	127.80
5	A	1016	HAS	C13-C14-C15	-3.75	119.72	127.80
5	D	1015	HAS	CAD-CBD-CGD	-3.71	101.53	113.47
11	E	587	HEC	C4D-ND-C1D	3.70	111.64	106.76
5	D	1016	HAS	C3C-C2C-C1C	-3.70	104.83	107.00
5	A	1016	HAS	CMB-C2B-C3B	3.67	131.87	124.94
5	A	1016	HAS	C13-C12-C11	-3.62	108.23	114.06
5	A	1015	HAS	C3C-CAC-CBC	-3.62	118.46	125.95
5	D	1016	HAS	C1B-C2B-C3B	-3.60	104.90	107.00
5	D	1015	HAS	C4B-NB-C1B	3.57	110.94	105.58
5	D	1015	HAS	C13-C12-C11	-3.56	108.33	114.06
5	A	1016	HAS	CAA-CBA-CGA	-3.55	102.04	113.47
5	A	1015	HAS	C4C-NC-C1C	3.54	111.43	106.76
5	A	1016	HAS	C3D-C4D-ND	3.52	112.28	109.64
5	D	1015	HAS	C1A-C2A-C3A	-3.47	103.32	106.92
5	A	1015	HAS	C26-C15-C16	3.46	120.66	115.39
5	A	1015	HAS	CAD-CBD-CGD	-3.38	102.60	113.47
4	D	900	5PL	CBH-OCK-CBU	-3.37	109.61	117.92
5	A	1016	HAS	OMD-CMD-C2D	-3.34	118.12	125.32
5	A	1015	HAS	C4B-NB-C1B	3.30	110.53	105.58
5	D	1016	HAS	C3D-C4D-ND	3.28	112.09	109.64
4	A	900	5PL	O1-C1-C2	3.26	112.06	107.27
5	D	1016	HAS	CMB-C2B-C1B	-3.23	119.79	126.16
8	A	1301	7E8	O16-C8-C7	3.21	122.02	111.94
5	D	1015	HAS	CMB-C2B-C1B	-3.21	119.83	126.16
5	A	1016	HAS	C21-C22-C23	-3.17	120.95	127.80
5	D	1016	HAS	C4C-NC-C1C	3.16	110.93	106.76
5	A	1016	HAS	C4C-NC-C1C	3.16	110.92	106.76
5	D	1015	HAS	C17-C18-C19	-3.15	121.00	127.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	5PL	CBH-OCK-CBU	-3.15	110.15	117.92
5	A	1015	HAS	C1B-C2B-C3B	-3.13	105.17	107.00
5	A	1015	HAS	C25-C23-C24	3.12	120.13	115.39
11	B	587	HEC	CBC-CAC-C3C	-3.11	119.67	128.44
5	D	1016	HAS	C27-C19-C20	3.09	120.09	115.39
5	D	1016	HAS	C26-C15-C16	3.07	120.05	115.39
5	D	1016	HAS	C21-C22-C23	-3.01	121.31	127.80
11	B	587	HEC	C4B-C3B-C2B	2.99	108.59	106.68
11	B	587	HEC	C4A-CHB-C1B	-2.98	123.55	127.47
5	D	1016	HAS	CHB-C1D-ND	2.96	129.52	124.58
11	B	587	HEC	C4D-ND-C1D	2.95	110.65	106.76
5	A	1016	HAS	C4D-ND-C1D	2.94	110.64	106.76
5	D	1015	HAS	C27-C19-C20	2.94	119.86	115.39
11	E	587	HEC	CMC-C2C-C1C	-2.93	124.11	128.62
11	E	587	HEC	C4B-C3B-C2B	2.93	108.55	106.68
5	D	1015	HAS	C25-C23-C24	2.91	119.82	115.39
5	D	1016	HAS	C3C-CAC-CBC	-2.90	119.94	125.95
5	A	1015	HAS	C17-C18-C19	-2.90	121.53	127.80
5	D	1015	HAS	C3C-CAC-CBC	-2.90	119.95	125.95
5	D	1015	HAS	C3D-C4D-ND	2.89	111.80	109.64
5	D	1015	HAS	C2B-C3B-C11	2.87	132.27	126.14
5	D	1016	HAS	C3D-C2D-CMD	2.87	131.57	124.21
5	A	1016	HAS	C27-C19-C20	2.86	119.73	115.39
5	D	1015	HAS	C4D-ND-C1D	2.83	110.49	106.76
11	B	587	HEC	C1D-C2D-C3D	-2.82	105.04	107.00
5	D	1015	HAS	C4A-NA-C1A	2.79	110.44	106.76
5	D	1015	HAS	C3D-C2D-CMD	2.79	131.37	124.21
11	E	587	HEC	C3C-C4C-NC	-2.79	107.50	111.52
5	D	1016	HAS	C4B-NB-C1B	2.76	109.72	105.58
5	A	1016	HAS	C4B-C3B-C2B	-2.75	104.95	106.87
4	D	900	5PL	OCL-CBL-CBM	2.75	120.58	111.94
5	D	1016	HAS	OMD-CMD-C2D	-2.74	119.40	125.32
4	A	900	5PL	CAY-CAX-NCB	-2.74	103.97	112.21
5	D	1015	HAS	C3C-C4C-NC	-2.73	107.57	111.52
5	A	1015	HAS	C21-C22-C23	-2.73	121.91	127.80
5	D	1016	HAS	C17-C18-C19	-2.71	121.95	127.80
5	D	1015	HAS	OMD-CMD-C2D	-2.71	119.46	125.32
5	A	1016	HAS	C17-C18-C19	-2.71	121.96	127.80
5	A	1015	HAS	C2B-C3B-C11	2.70	131.91	126.14
5	D	1016	HAS	CAA-CBA-CGA	-2.70	104.80	113.47
7	A	1200	4AG	O17-C16-C15	2.70	120.42	111.94
11	E	587	HEC	C4A-C3A-C2A	2.70	108.61	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1015	HAS	C26-C15-C16	2.67	119.45	115.39
5	A	1015	HAS	C13-C12-C11	-2.65	109.80	114.06
5	A	1015	HAS	C13-C14-C15	-2.62	122.14	127.80
8	A	1300	7E8	O16-C8-C7	2.62	120.18	111.94
5	D	1015	HAS	C4B-C3B-C2B	-2.57	105.07	106.87
5	D	1015	HAS	C1B-C2B-C3B	-2.56	105.50	107.00
11	E	587	HEC	C4C-C3C-C2C	2.56	108.31	106.68
4	A	900	5PL	OCL-CBL-CBM	2.53	119.91	111.94
5	A	1016	HAS	C4B-NB-C1B	2.53	109.38	105.58
4	D	900	5PL	C3-C2-N2	-2.52	105.21	110.56
4	D	900	5PL	O1-C1-C2	2.49	110.92	107.27
5	A	1016	HAS	C2A-C1A-CHA	-2.49	121.28	126.00
11	E	587	HEC	C2B-C1B-NB	-2.48	107.54	109.41
5	A	1016	HAS	C1B-C2B-C3B	-2.47	105.56	107.00
11	E	587	HEC	C3B-C4B-NB	-2.45	107.98	111.52
5	D	1016	HAS	C2A-C1A-CHA	-2.45	121.35	126.00
5	A	1015	HAS	C3C-C4C-NC	-2.45	107.98	111.52
11	E	587	HEC	C3A-C4A-NA	-2.44	107.57	109.41
11	B	587	HEC	C3C-C4C-NC	-2.40	108.05	111.52
7	A	1200	4AG	C6-O21-C22	-2.38	112.06	117.92
5	D	1016	HAS	C4B-C3B-C2B	-2.37	105.21	106.87
5	D	1016	HAS	C25-C23-C24	2.37	118.99	115.39
5	D	1016	HAS	C26-C15-C14	-2.36	118.85	123.52
5	A	1016	HAS	C3D-C2D-CMD	2.35	130.24	124.21
5	A	1015	HAS	C4D-ND-C1D	2.34	109.84	106.76
5	A	1016	HAS	C26-C15-C16	2.33	118.94	115.39
5	D	1016	HAS	C2D-C1D-CHB	-2.31	121.63	126.00
5	A	1015	HAS	C26-C15-C14	-2.29	118.98	123.52
11	E	587	HEC	CMC-C2C-C3C	-2.29	123.19	125.72
11	B	587	HEC	C3B-C4B-NB	-2.29	108.21	111.52
5	A	1016	HAS	C25-C23-C24	2.27	118.85	115.39
5	A	1016	HAS	C2C-C3C-CAC	2.26	131.96	127.33
5	D	1015	HAS	CBD-CAD-C3D	2.26	116.57	112.35
5	A	1016	HAS	C2B-C3B-C11	2.25	130.94	126.14
5	A	1015	HAS	C3D-C2D-CMD	2.24	129.97	124.21
4	D	900	5PL	OCG-CAN-CAM	2.24	110.61	106.23
11	E	587	HEC	C4B-CHC-C1C	-2.23	124.54	127.47
11	B	587	HEC	C4C-C3C-C2C	2.23	108.10	106.68
5	D	1016	HAS	C2B-C3B-C11	2.22	130.88	126.14
5	A	1015	HAS	CMB-C2B-C1B	-2.21	121.79	126.16
5	D	1016	HAS	CHC-C1C-NC	2.19	128.23	124.58
5	D	1015	HAS	C32-C30-C31	2.18	120.19	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	900	5PL	O5-C5-C4	2.17	113.78	109.76
5	A	1015	HAS	O1D-CGD-CBD	-2.15	115.64	123.03
5	A	1015	HAS	CBD-CAD-C3D	2.15	116.36	112.35
8	A	1301	7E8	O16-C8-O15	-2.14	117.58	123.43
5	A	1016	HAS	CAD-C3D-C4D	2.12	128.49	124.67
5	A	1015	HAS	C2A-C1A-NA	2.08	112.63	109.73
5	A	1016	HAS	O1A-CGA-CBA	-2.08	115.86	123.03
5	A	1016	HAS	C32-C30-C31	2.06	119.88	114.62
5	A	1015	HAS	O2D-CGD-CBD	2.06	121.51	114.22
5	D	1016	HAS	C3C-C4C-NC	-2.05	108.55	111.52
5	D	1016	HAS	C32-C30-C31	2.05	119.86	114.62
11	B	587	HEC	O2A-CGA-CBA	2.02	121.35	114.22
5	D	1016	HAS	C2B-C1B-NB	2.01	110.93	109.41

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1300	7E8	C18

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1016	HAS	OMD-CMD-C2D-C1D
5	D	1016	HAS	OMD-CMD-C2D-C3D

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	780/791 (98%)	0.11	14 (1%) 65 68	32, 48, 91, 174	0
1	D	780/791 (98%)	0.15	22 (2%) 50 54	33, 53, 89, 153	0
2	B	319/337 (94%)	0.13	0 100 100	33, 50, 85, 163	0
2	E	319/337 (94%)	0.55	29 (9%) 9 11	38, 67, 105, 189	0
3	C	64/66 (96%)	-0.04	1 (1%) 68 72	44, 63, 112, 152	0
3	F	63/66 (95%)	0.14	2 (3%) 45 49	45, 65, 104, 153	0
All	All	2325/2388 (97%)	0.18	68 (2%) 49 53	32, 53, 95, 189	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	607	GLU	7.9
2	E	69	GLU	6.1
1	D	608	HIS	5.8
1	D	548	HIS	5.3
1	D	607	GLU	5.1
1	A	606	VAL	4.9
1	A	539	VAL	4.9
2	E	72	GLU	4.5
1	A	605	PRO	4.4
1	A	761	LEU	4.3
2	E	68	PRO	4.2
1	A	762	HIS	4.1
1	D	606	VAL	3.8
1	D	355	PHE	3.6
2	E	35	VAL	3.6
1	A	686	PHE	3.5
1	D	456	ILE	3.5
2	E	25	THR	3.4
1	D	12	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	224	VAL	3.2
2	E	22	VAL	3.1
1	A	691	PHE	3.1
1	D	354	ILE	3.1
1	D	502	TYR	2.9
2	E	62	TRP	2.9
1	D	549	ILE	2.9
2	E	28	GLY	2.9
1	D	452	TYR	2.8
2	E	312	GLU	2.8
2	E	55	GLY	2.8
2	E	311	GLU	2.8
1	D	532	TYR	2.7
2	E	33	GLN	2.7
2	E	337	PHE	2.7
2	E	310	SER	2.6
1	A	12	TRP	2.6
1	D	15	LEU	2.6
3	F	3	TYR	2.6
1	D	547	ALA	2.6
1	A	683	ARG	2.6
1	D	418	LEU	2.5
1	D	681	LEU	2.5
1	D	604	HIS	2.5
2	E	328	GLY	2.5
2	E	58	ALA	2.5
1	A	608	HIS	2.4
2	E	214	VAL	2.4
2	E	24	ILE	2.4
2	E	59	TYR	2.4
3	F	31	GLY	2.4
1	D	521	LEU	2.3
2	E	53	VAL	2.3
1	D	329	LEU	2.3
2	E	31	PHE	2.3
2	E	107	ILE	2.3
2	E	104	LYS	2.3
1	D	417	ARG	2.3
1	D	534	TRP	2.2
1	A	548	HIS	2.2
2	E	71	GLN	2.2
3	C	33	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	549	ILE	2.2
1	D	481	ILE	2.1
2	E	170	ALA	2.1
2	E	145	LEU	2.1
2	E	61	THR	2.1
2	E	23	ALA	2.0
1	A	551	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FME	C	1	10/11	0.14	1.38	69,92,107,171	0
3	FME	F	1	10/11	0.17	0.38	72,91,112,160	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	CU	A	1017	1/1	0.18	14.90	37,37,37,37	0
8	7E8	A	1300	21/21	0.38	11.46	48,79,102,115	0
13	CL	F	101	1/1	0.26	10.50	70,70,70,70	0
13	CL	C	101	1/1	0.26	7.79	60,60,60,60	0
6	CU	D	1017	1/1	0.15	7.65	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	7E8	A	1301	21/21	0.30	7.43	44,80,96,118	0
9	MG	A	1801	1/1	0.19	6.71	39,39,39,39	0
7	4AG	A	1200	40/40	0.28	6.66	33,68,115,123	0
12	7E9	B	701	21/21	0.27	6.44	58,90,108,109	0
10	CUA	B	585	2/2	0.17	2.52	35,35,35,36	0
4	5PL	A	900	85/85	0.19	1.62	35,65,105,134	0
5	HAS	A	1015	65/65	0.16	1.33	24,35,102,151	0
4	5PL	D	900	85/85	0.21	1.12	37,62,107,128	0
5	HAS	D	1015	65/65	0.15	1.01	30,55,128,138	0
10	CUA	E	585	2/2	0.16	0.83	43,43,43,44	0
5	HAS	D	1016	65/65	0.17	0.76	24,47,86,103	0
11	HEC	E	587	43/43	0.16	0.54	21,54,80,91	0
13	CL	D	1701	1/1	0.17	0.25	86,86,86,86	0
11	HEC	B	587	43/43	0.14	0.07	22,34,48,52	0
5	HAS	A	1016	65/65	0.14	-0.36	22,38,59,62	0
9	MG	D	1801	1/1	0.12	-1.43	50,50,50,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.