



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:46 pm BST

PDB ID : 1XVB  
Title : soluble methane monooxygenase hydroxylase: 6-bromohexanol soaked structure  
Authors : Sazinsky, M.H.; Lippard, S.J.  
Deposited on : 2004-10-27  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

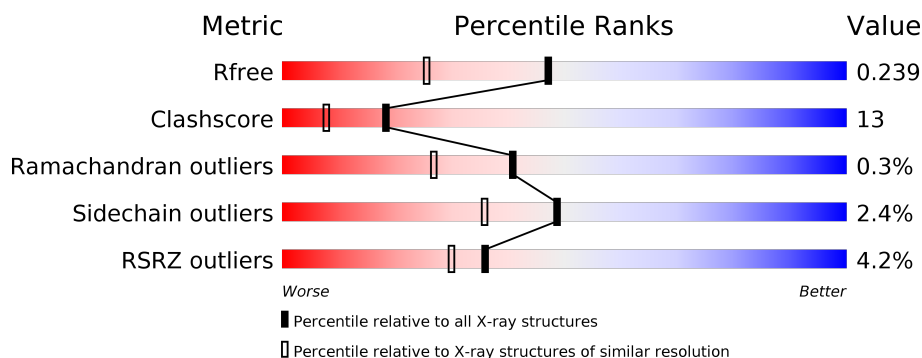
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 respectively. 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	527	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 75%; height: 10px; background-color: green;"></div> <div style="width: 20%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>75%</span> <span>20%</span> <span>• •</span> </div> </div>
1	B	527	<div> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 72%; height: 10px; background-color: green;"></div> <div style="width: 23%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>72%</span> <span>23%</span> <span>• •</span> </div> </div>
2	C	389	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 76%; height: 10px; background-color: green;"></div> <div style="width: 23%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>76%</span> <span>23%</span> <span>•</span> </div> </div>
2	D	389	<div> <div style="width: 10%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 68%; height: 10px; background-color: green;"></div> <div style="width: 31%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>68%</span> <span>31%</span> <span>•</span> </div> </div>
3	E	170	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 77%; height: 10px; background-color: green;"></div> <div style="width: 19%; height: 10px; background-color: yellow;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>77%</span> <span>19%</span> <span>• •</span> </div> </div>
3	F	170	<div> <div style="width: 19%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <div style="width: 58%; height: 10px; background-color: green;"></div> <div style="width: 38%; height: 10px; background-color: yellow;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>58%</span> <span>38%</span> <span>• •</span> </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
5	BHL	A	1210	-	-	X	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 18520 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 Methane monooxygenase component A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4138	2649	709	762	18			
1	B	510	Total	C	N	O	S	0	0	0
			4137	2646	711	762	18			

- Molecule 2 is a protein called Methane monooxygenase component A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	0	0	0
			3163	2036	545	574	8			
2	D	388	Total	C	N	O	S	0	0	0
			3151	2028	543	572	8			

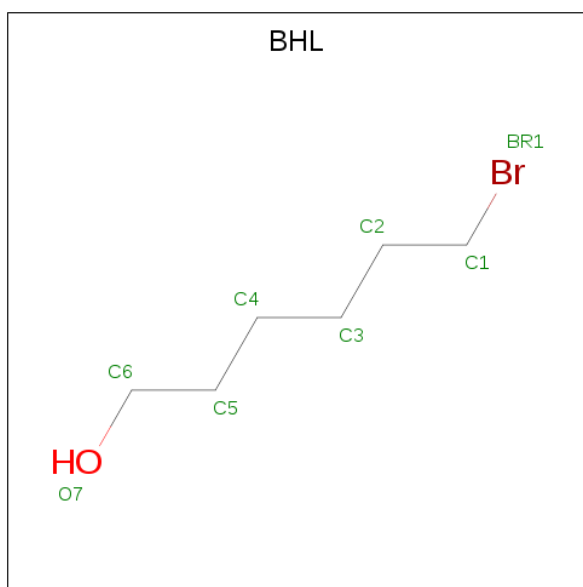
- Molecule 3 is a protein called Methane monooxygenase component A gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1364	864	245	250	5			
3	F	166	Total	C	N	O	S	0	0	0
			1358	860	243	250	5			

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

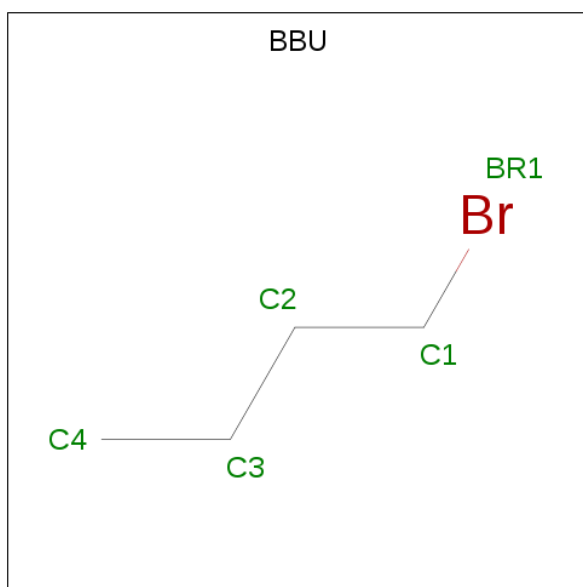
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Fe	0	0
			2	2		
4	A	2	Total	Fe	0	0
			2	2		

- Molecule 5 is 6-BROMOHEXAN-1-OL (three-letter code: BHL) (formula: C<sub>6</sub>H<sub>13</sub>BrO).



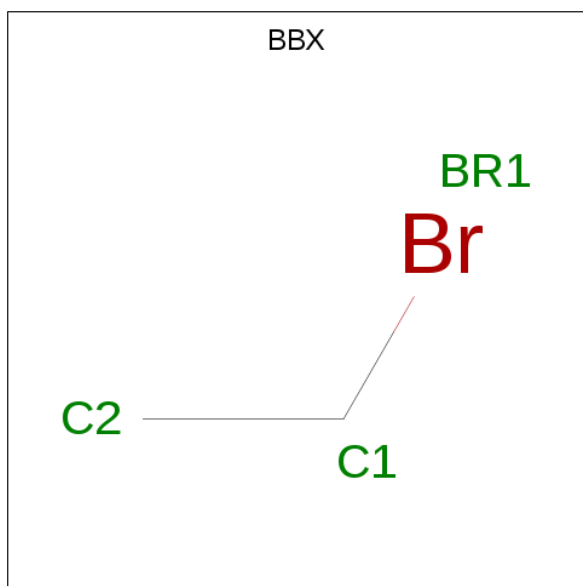
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Br	C	O	0	0
			8	1	6	1		
5	A	1	Total	Br	C	O	0	0
			8	1	6	1		
5	A	1	Total	Br	C	O	0	0
			8	1	6	1		
5	A	1	Total	Br			0	0
			1	1				
5	A	1	Total	C	O		0	0
			7	6	1			
5	B	1	Total	Br	C	O	0	0
			8	1	6	1		
5	B	1	Total	Br	C	O	0	0
			8	1	6	1		
5	B	1	Total	Br	C	O	0	0
			8	1	6	1		
5	B	1	Total	Br	C	O	0	0
			8	1	6	1		

- Molecule 6 is 1-BROMOBUTANE (three-letter code: BBU) (formula: C<sub>4</sub>H<sub>9</sub>Br).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Br	C	0	0
			5	1	4		

- Molecule 7 is 1-BROMOETHANE (three-letter code: BBX) (formula:  $C_2H_5Br$ ).

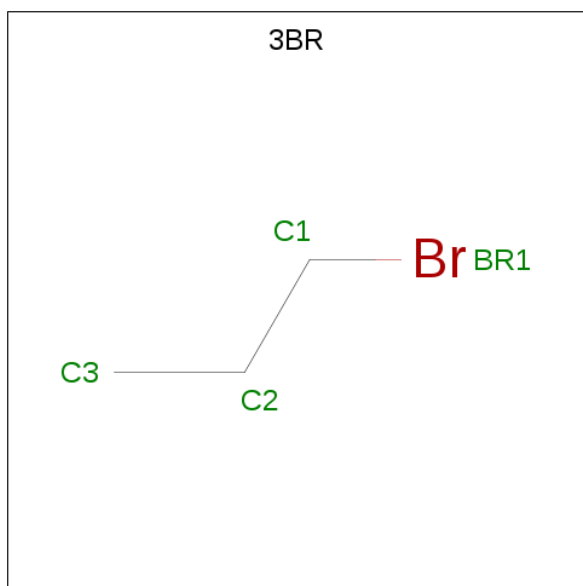


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Br	C	0	0
			3	1	2		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Ca 1 1	0	0

- Molecule 9 is 1-BROMOPROPANE (three-letter code: 3BR) (formula: C<sub>3</sub>H<sub>7</sub>Br).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Br C 4 1 3	0	0
9	C	1	Total Br C 4 1 3	0	0

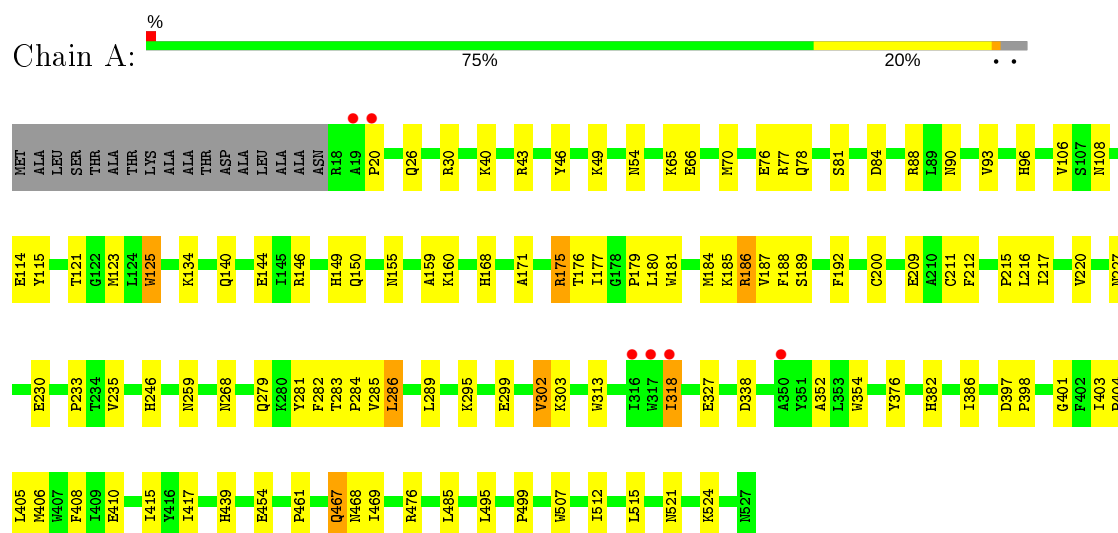
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	282	Total O 282 282	0	0
10	B	250	Total O 250 250	0	0
10	C	270	Total O 270 270	0	0
10	D	127	Total O 127 127	0	0
10	E	147	Total O 147 147	0	0
10	F	40	Total O 40 40	0	0

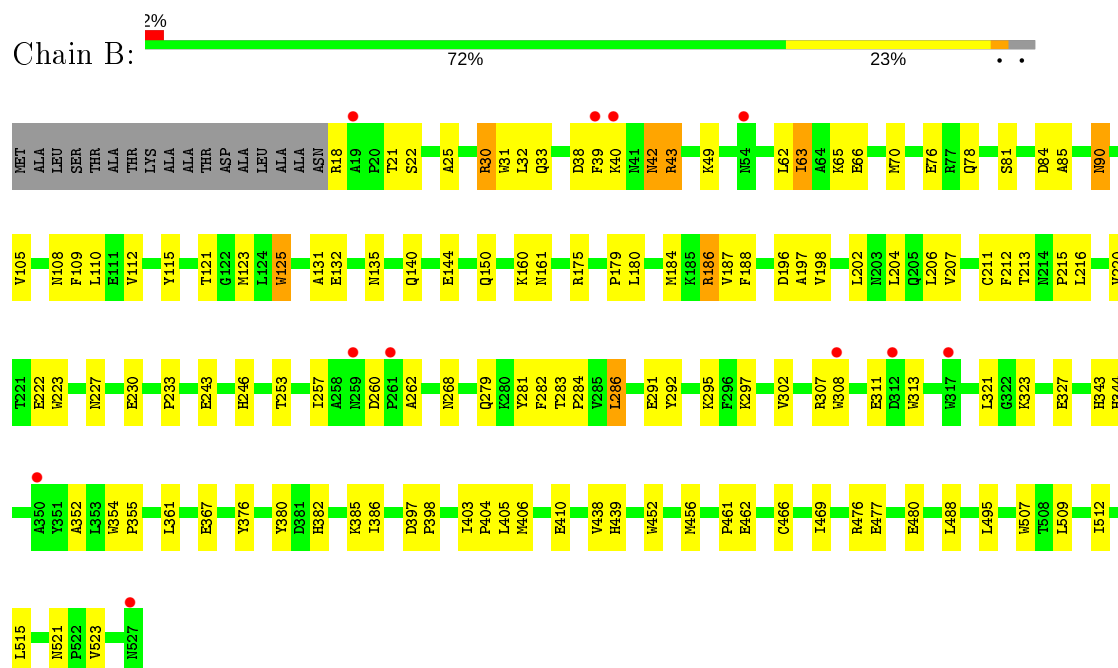
### 3 Residue-property plots [i](#)

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

- Molecule 1: Methane monooxygenase component A alpha chain

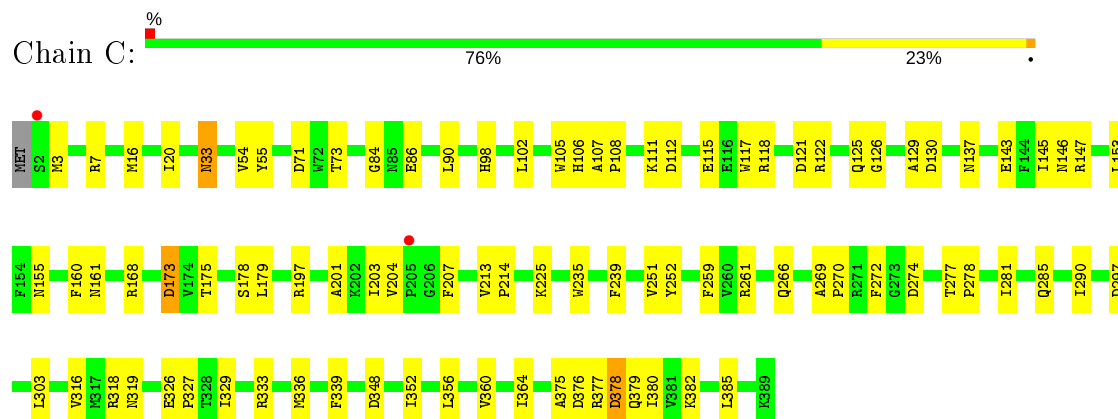


- Molecule 1: Methane monooxygenase component A alpha chain

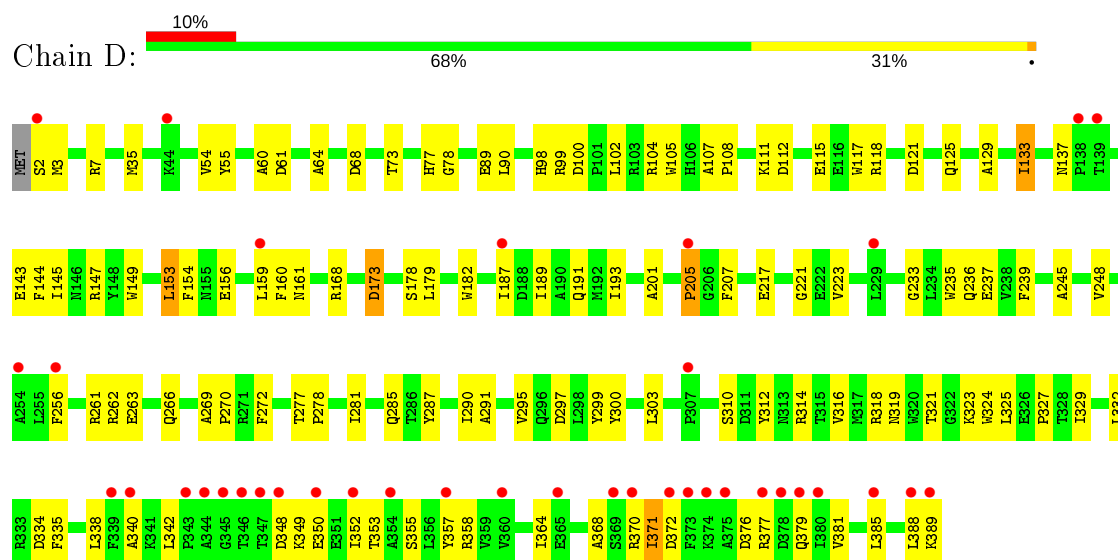




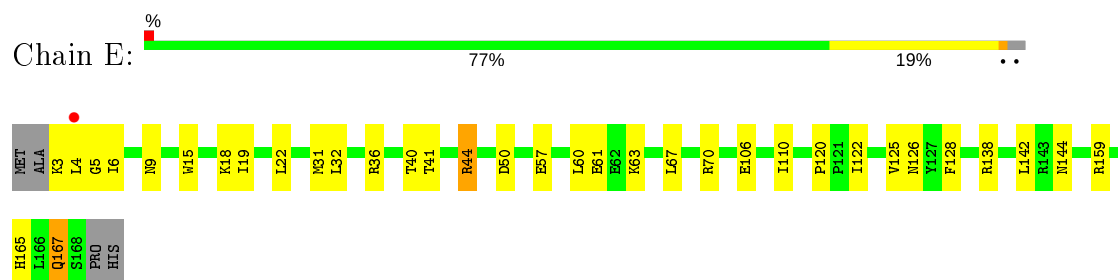
- Molecule 2: Methane monooxygenase component A beta chain



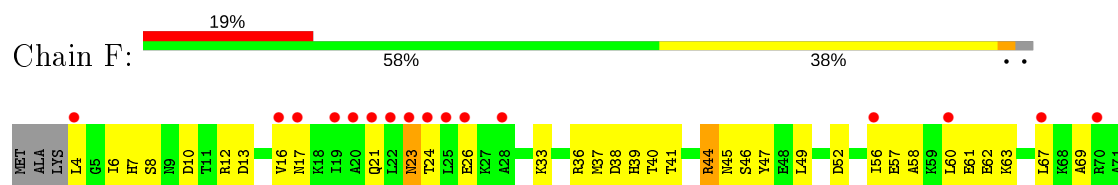
- Molecule 2: Methane monooxygenase component A beta chain

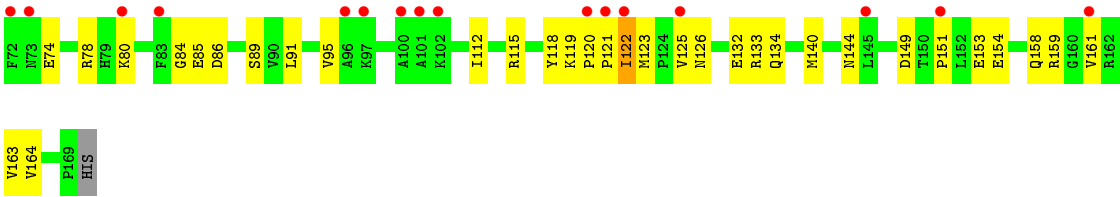


- Molecule 3: Methane monooxygenase component A gamma chain



- Molecule 3: Methane monooxygenase component A gamma chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.63Å 171.87Å 220.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.85 – 1.80 29.85 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.1 (29.85-1.80) 91.2 (29.85-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 1.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.219 , 0.251 0.207 , 0.239	Depositor DCC
$R_{free}$ test set	22694 reflections (9.29%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3BR, BHL, CA, FE, BBX, BBU

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	0.34	0/4263	0.58	0/5797
1	B	0.33	0/4262	0.55	0/5796
2	C	0.38	0/3259	0.58	0/4430
2	D	0.32	0/3247	0.52	0/4417
3	E	0.34	0/1392	0.59	0/1876
3	F	0.27	0/1387	0.49	0/1873
All	All	0.34	0/17810	0.56	0/24189

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	TYR	Sidechain

### 5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4138	0	3897	121	0
1	B	4137	0	3888	120	0
2	C	3163	0	2986	80	0
2	D	3151	0	2960	103	0
3	E	1364	0	1352	30	0
3	F	1358	0	1335	61	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	32	0	43	18	0
5	B	40	0	54	10	0
6	A	5	0	7	0	0
7	B	3	0	0	0	0
8	C	1	0	0	0	0
9	C	8	0	10	0	0
10	A	282	0	0	11	0
10	B	250	0	0	4	0
10	C	270	0	0	9	0
10	D	127	0	0	1	0
10	E	147	0	0	0	0
10	F	40	0	0	1	0
All	All	18520	0	16532	452	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 13.

All (452) 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:282:PHE:HB2	5:B:1205:BHL:O7	1.29	1.28
3:E:19:ILE:HD12	3:E:60:LEU:HD13	1.47	0.95
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.14	0.94
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.18	0.92
1:A:77:ARG:HG2	1:B:84:ASP:HB2	1.52	0.91
1:B:282:PHE:CB	5:B:1205:BHL:O7	2.20	0.89
3:F:41:THR:O	3:F:44:ARG:HD2	1.72	0.88
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.55	0.88
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.74	0.88
1:B:268:ASN:HD21	1:B:327:GLU:H	1.18	0.87
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.57	0.86
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:HD21	1:A:295:LYS:H	1.24	0.85
2:C:84:GLY:HA3	10:C:1335:HOH:O	1.74	0.85
1:B:160:LYS:HE3	1:B:161:ASN:OD1	1.79	0.83
1:A:268:ASN:HD21	1:A:327:GLU:H	1.27	0.82
1:B:282:PHE:HB2	5:B:1205:BHL:HO7	1.40	0.81
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.25	0.80
3:E:15:TRP:O	3:E:19:ILE:HG12	1.82	0.79
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.64	0.78
3:E:36:ARG:HH12	3:E:122:ILE:HD13	1.49	0.77
2:C:86:GLU:HG2	10:C:1335:HOH:O	1.85	0.77
2:D:325:LEU:O	2:D:329:ILE:HG12	1.85	0.76
1:A:216:LEU:HD21	5:A:1207:BHL:BR1	2.41	0.76
3:E:41:THR:O	3:E:44:ARG:HD2	1.85	0.76
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.68	0.75
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.22	0.75
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.68	0.75
1:A:467:GLN:HE22	2:C:71:ASP:H	1.35	0.74
2:D:371:ILE:H	2:D:371:ILE:HD13	1.51	0.74
1:A:408:PHE:HB3	5:A:1210:BHL:O7	1.87	0.73
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.70	0.73
1:B:43:ARG:HD2	1:B:43:ARG:O	1.88	0.72
1:A:401:GLY:HA2	1:A:515:LEU:HD21	1.70	0.72
1:A:467:GLN:HE21	1:A:467:GLN:H	1.34	0.72
1:B:268:ASN:ND2	1:B:327:GLU:H	1.88	0.72
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.72	0.71
1:A:405:LEU:CD1	5:A:1210:BHL:H41	2.21	0.71
2:D:349:LYS:HG3	2:D:352:ILE:HD11	1.72	0.71
1:A:217:ILE:HG12	5:A:1203:BHL:BR1	2.46	0.70
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.22	0.69
2:D:133:ILE:HD13	2:D:133:ILE:O	1.92	0.69
1:A:77:ARG:CG	1:B:84:ASP:HB2	2.23	0.69
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.91	0.68
3:F:13:ASP:O	3:F:16:VAL:HG22	1.94	0.68
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.29	0.68
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.76	0.68
2:C:318:ARG:NH2	10:C:1387:HOH:O	2.27	0.68
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.40	0.68
2:D:340:ALA:HA	2:D:389:LYS:HE2	1.76	0.67
3:E:19:ILE:CD1	3:E:60:LEU:HD13	2.24	0.67
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.76	0.67
1:A:282:PHE:CE2	1:A:286:LEU:HD12	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ARG:HD3	1:B:30:ARG:C	2.14	0.67
1:B:125:TRP:HE1	2:D:161:ASN:ND2	1.91	0.67
2:D:262:ARG:HA	2:D:266:GLN:HB3	1.77	0.67
1:B:33:GLN:HE22	1:B:132:GLU:H	1.40	0.66
2:D:277:THR:HG22	2:D:281:ILE:HD13	1.76	0.66
1:B:307:ARG:HH21	1:B:308:TRP:HE1	1.44	0.66
1:A:467:GLN:NE2	1:A:467:GLN:H	1.94	0.66
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.95	0.66
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.78	0.66
1:A:20:PRO:HG3	2:C:129:ALA:HB2	1.77	0.65
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.27	0.65
1:A:405:LEU:HD21	5:A:1210:BHL:C1	2.27	0.65
3:F:57:GLU:O	3:F:61:GLU:HG3	1.98	0.64
1:A:268:ASN:ND2	1:A:327:GLU:H	1.95	0.64
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.79	0.64
3:E:67:LEU:HD23	3:E:70:ARG:HH21	1.62	0.64
2:C:360:VAL:O	2:C:364:ILE:HG12	1.98	0.63
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.28	0.63
3:E:165:HIS:HE1	3:E:167:GLN:NE2	1.96	0.63
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.80	0.63
1:B:282:PHE:CE2	1:B:286:LEU:HD12	2.33	0.63
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.81	0.63
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.82	0.62
1:B:367:GLU:HG3	10:B:1347:HOH:O	1.98	0.62
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.14	0.62
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.47	0.62
1:A:160:LYS:HE3	10:A:1404:HOH:O	2.00	0.62
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.34	0.62
1:A:405:LEU:HD12	5:A:1210:BHL:H41	1.80	0.62
1:B:283:THR:HB	1:B:284:PRO:HD3	1.81	0.62
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.97	0.62
1:A:114:GLU:OE1	5:A:1203:BHL:H62	2.00	0.62
1:A:405:LEU:CD1	5:A:1210:BHL:C4	2.78	0.62
1:A:467:GLN:NE2	2:C:71:ASP:H	1.97	0.62
1:B:462:GLU:HG3	3:F:112:ILE:HD11	1.82	0.62
1:A:40:LYS:HD2	10:A:1314:HOH:O	1.99	0.61
1:B:33:GLN:NE2	1:B:132:GLU:H	1.97	0.61
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.81	0.61
1:B:227:ASN:HD21	1:B:295:LYS:H	1.46	0.61
1:A:382:HIS:O	1:A:386:ILE:HG12	2.01	0.61
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:41:THR:O	3:E:44:ARG:CD	2.49	0.61
1:B:123:MET:HB2	2:D:168:ARG:HD3	1.83	0.60
2:C:336:MET:CE	2:C:385:LEU:HD23	2.32	0.60
1:A:66:GLU:O	1:A:70:MET:HG2	2.02	0.60
1:B:281:TYR:O	1:B:284:PRO:HD2	2.02	0.60
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.83	0.60
2:D:223:VAL:HG13	2:D:335:PHE:HA	1.83	0.60
1:A:417:ILE:HD11	1:A:469:ILE:HG12	1.84	0.59
3:E:36:ARG:NH1	3:E:122:ILE:HD13	2.18	0.59
1:B:18:ARG:O	2:D:129:ALA:HA	2.02	0.59
2:C:143:GLU:HG3	10:C:1363:HOH:O	2.01	0.59
1:A:227:ASN:ND2	1:A:295:LYS:H	1.97	0.59
1:B:382:HIS:O	1:B:386:ILE:HG12	2.02	0.59
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.67	0.58
2:C:145:ILE:HD11	2:C:274:ASP:OD2	2.03	0.58
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.50	0.58
2:C:329:ILE:HD11	2:C:380:ILE:HD12	1.85	0.58
1:B:216:LEU:HD21	5:B:1205:BHL:BR1	2.58	0.58
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.85	0.58
2:C:364:ILE:HD12	2:C:375:ALA:HB3	1.86	0.58
1:B:216:LEU:O	1:B:220:VAL:HG23	2.04	0.58
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.50	0.58
1:A:77:ARG:HG3	1:A:77:ARG:HH21	1.67	0.57
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.38	0.57
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.04	0.57
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.38	0.57
1:A:76:GLU:OE1	1:B:76:GLU:HG2	2.04	0.57
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.86	0.57
2:D:376:ASP:OD2	2:D:379:GLN:HG2	2.04	0.57
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.86	0.57
1:B:361:LEU:HD21	5:B:1202:BHL:H32	1.87	0.57
1:A:417:ILE:CD1	1:A:468:ASN:HB2	2.34	0.57
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.38	0.57
1:B:186:ARG:HA	2:D:73:THR:OG1	2.05	0.57
1:A:405:LEU:HD11	5:A:1210:BHL:C4	2.35	0.57
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.85	0.57
1:B:268:ASN:HD21	1:B:327:GLU:N	1.97	0.57
2:C:98:HIS:HE1	2:C:178:SER:OG	1.87	0.57
2:D:319:ASN:OD1	3:F:78:ARG:HD3	2.04	0.57
1:A:406:MET:O	1:A:410:GLU:HG3	2.04	0.56
3:F:58:ALA:O	3:F:62:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:SER:OG	1:B:84:ASP:HB3	2.04	0.56
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.96	0.56
2:C:333:ARG:HD2	10:C:1380:HOH:O	2.04	0.56
1:A:318:ILE:HD13	1:A:318:ILE:O	2.06	0.56
1:B:43:ARG:HD2	1:B:43:ARG:C	2.26	0.56
1:A:186:ARG:HA	2:C:73:THR:OG1	2.06	0.55
1:B:42:ASN:HD22	2:D:236:GLN:HE21	1.54	0.55
1:A:26:GLN:HG2	10:A:1310:HOH:O	2.07	0.55
1:B:180:LEU:HD13	5:B:1202:BHL:BR1	2.62	0.55
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.40	0.55
3:E:57:GLU:O	3:E:61:GLU:HG3	2.05	0.55
1:B:302:VAL:HG12	10:B:1342:HOH:O	2.07	0.55
2:D:153:LEU:HD12	2:D:153:LEU:C	2.27	0.55
1:A:209:GLU:HG2	5:A:1203:BHL:H32	1.88	0.54
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.42	0.54
2:D:352:ILE:HG13	2:D:353:THR:N	2.23	0.54
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.54	0.54
3:F:23:ASN:HD22	3:F:23:ASN:N	2.05	0.54
3:F:52:ASP:O	3:F:56:ILE:HG13	2.08	0.54
1:A:405:LEU:HD11	5:A:1210:BHL:H41	1.89	0.54
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.26	0.54
1:A:108:ASN:HD21	1:A:175:ARG:HH21	1.54	0.54
3:F:44:ARG:HG3	3:F:46:SER:O	2.08	0.54
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.90	0.54
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.37	0.54
3:F:36:ARG:HA	3:F:40:THR:HG23	1.90	0.54
1:B:108:ASN:HD21	1:B:175:ARG:HH21	1.54	0.54
1:B:123:MET:HE3	1:B:197:ALA:HA	1.89	0.54
1:A:108:ASN:ND2	1:A:175:ARG:HH21	2.05	0.53
1:A:302:VAL:HG13	10:A:1360:HOH:O	2.09	0.53
2:C:146:ASN:O	2:C:214:PRO:HG3	2.08	0.53
2:D:312:TYR:O	2:D:316:VAL:HG23	2.08	0.53
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.07	0.53
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.91	0.53
2:D:159:LEU:HD22	2:D:248:VAL:HG13	1.91	0.53
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.91	0.53
1:A:417:ILE:HD12	1:A:468:ASN:HB2	1.90	0.53
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.55	0.53
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.90	0.53
1:A:121:THR:HG21	1:A:140:GLN:CG	2.39	0.53
1:B:144:GLU:HA	1:B:144:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:MET:O	2:C:20:ILE:HG12	2.09	0.53
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.89	0.53
1:A:140:GLN:O	1:A:144:GLU:HG2	2.09	0.53
1:B:476:ARG:HH12	3:F:6:ILE:HD12	1.72	0.53
2:D:310:SER:O	2:D:314:ARG:HG3	2.09	0.53
1:A:302:VAL:HG22	1:A:376:TYR:OH	2.09	0.53
3:F:6:ILE:N	3:F:6:ILE:HD12	2.24	0.53
2:C:348:ASP:O	2:C:352:ILE:HG12	2.08	0.52
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.06	0.52
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.91	0.52
2:C:336:MET:HE3	2:C:385:LEU:HD23	1.92	0.52
3:E:32:LEU:HD23	3:E:122:ILE:HD11	1.90	0.52
1:A:121:THR:HG21	1:A:140:GLN:HG2	1.92	0.52
1:A:302:VAL:HG22	1:A:376:TYR:CZ	2.45	0.52
3:E:3:LYS:HG2	3:E:9:ASN:HA	1.92	0.52
3:F:61:GLU:O	3:F:121:PRO:HG2	2.10	0.52
2:C:111:LYS:O	2:C:115:GLU:HG3	2.09	0.51
1:A:417:ILE:HD13	10:A:1227:HOH:O	2.09	0.51
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.10	0.51
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.45	0.51
2:D:352:ILE:CD1	2:D:388:LEU:HD11	2.40	0.51
1:A:216:LEU:O	1:A:220:VAL:HG23	2.09	0.51
1:B:488:LEU:HD21	1:B:509:LEU:HD13	1.93	0.51
2:C:339:PHE:CE2	2:C:352:ILE:HD12	2.45	0.51
1:A:106:VAL:HG13	5:A:1207:BHL:BR1	2.67	0.51
1:A:84:ASP:HB3	1:B:81:SER:OG	2.11	0.51
1:B:361:LEU:CD2	5:B:1202:BHL:H32	2.42	0.50
3:F:153:GLU:CD	3:F:153:GLU:H	2.14	0.50
1:B:198:VAL:O	1:B:202:LEU:HG	2.11	0.50
2:D:300:TYR:CE1	2:D:370:ARG:HG3	2.46	0.50
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.93	0.50
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.76	0.50
1:A:405:LEU:HD21	5:A:1200:BHL:BR1	2.66	0.50
3:F:86:ASP:HB3	3:F:89:SER:OG	2.11	0.50
2:D:2:SER:HB2	10:D:494:HOH:O	2.10	0.50
3:F:91:LEU:O	3:F:95:VAL:HG23	2.12	0.50
1:B:25:ALA:CB	1:B:63:ILE:HD12	2.42	0.50
2:C:352:ILE:O	2:C:356:LEU:HD23	2.11	0.50
2:D:105:TRP:O	2:D:108:PRO:HD2	2.11	0.50
2:D:149:TRP:CE2	2:D:193:ILE:HD12	2.47	0.50
2:D:263:GLU:HA	2:D:263:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:MET:HE3	1:B:187:VAL:CG2	2.42	0.49
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.76	0.49
2:D:143:GLU:O	2:D:147:ARG:HB3	2.12	0.49
3:F:17:ASN:O	3:F:21:GLN:HG2	2.13	0.49
3:F:118:TYR:HB3	3:F:123:MET:HB2	1.93	0.49
1:B:140:GLN:O	1:B:144:GLU:HG2	2.12	0.49
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.47	0.49
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.95	0.49
1:B:227:ASN:ND2	1:B:295:LYS:H	2.09	0.49
3:F:38:ASP:HA	3:F:45:ASN:HB2	1.95	0.49
2:D:277:THR:HB	2:D:278:PRO:HD3	1.95	0.49
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.48	0.49
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.94	0.48
1:A:415:ILE:HD12	5:A:1210:BHL:H62	1.96	0.48
2:C:143:GLU:O	2:C:147:ARG:HB3	2.14	0.48
3:E:106:GLU:O	3:E:110:ILE:HG12	2.12	0.48
1:B:213:THR:OG1	1:B:243:GLU:HG2	2.13	0.48
2:D:223:VAL:HG11	2:D:338:LEU:HB2	1.95	0.48
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.48	0.48
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.49	0.48
1:B:63:ILE:H	1:B:63:ILE:HD13	1.78	0.48
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.31	0.48
1:A:175:ARG:HG2	1:A:176:THR:N	2.27	0.48
2:D:187:ILE:O	2:D:191:GLN:HG3	2.13	0.48
1:A:88:ARG:NH2	10:A:1456:HOH:O	2.35	0.48
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.49	0.48
1:A:81:SER:HB3	1:B:85:ALA:HB2	1.96	0.47
3:F:125:VAL:HG23	3:F:126:ASN:N	2.28	0.47
3:E:4:LEU:HG	3:E:4:LEU:O	2.14	0.47
1:A:408:PHE:CB	5:A:1210:BHL:O7	2.59	0.47
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.12	0.47
2:C:153:LEU:HD12	2:C:153:LEU:C	2.34	0.47
2:D:277:THR:HG22	2:D:281:ILE:CD1	2.42	0.47
2:D:381:VAL:O	2:D:385:LEU:HB2	2.14	0.47
3:F:63:LYS:NZ	3:F:67:LEU:HD21	2.28	0.47
1:B:257:ILE:HD12	1:B:257:ILE:C	2.34	0.47
1:B:30:ARG:HD3	1:B:30:ARG:O	2.15	0.47
2:D:291:ALA:O	2:D:295:VAL:HG23	2.15	0.47
1:B:323:LYS:HG2	10:B:1458:HOH:O	2.14	0.47
3:F:4:LEU:HD11	3:F:10:ASP:OD2	2.15	0.47
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:1350:HOH:O	3:E:125:VAL:HG22	2.13	0.47
1:A:171:ALA:O	1:A:175:ARG:HB3	2.15	0.47
1:A:88:ARG:NE	10:A:1456:HOH:O	2.35	0.47
2:C:266:GLN:HB2	2:C:281:ILE:HG21	1.97	0.47
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.97	0.46
10:A:1388:HOH:O	3:E:6:ILE:HD13	2.15	0.46
3:F:33:LYS:O	3:F:37:MET:HG2	2.15	0.46
1:B:30:ARG:HD2	1:B:31:TRP:CE2	2.50	0.46
2:D:153:LEU:HD12	2:D:154:PHE:N	2.30	0.46
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.51	0.46
2:D:324:TRP:HA	2:D:327:PRO:HD2	1.96	0.46
3:F:154:GLU:O	3:F:158:GLN:HG3	2.15	0.46
3:F:44:ARG:HD3	3:F:47:TYR:CE1	2.50	0.46
1:A:289:LEU:HD23	5:A:1206:BHL:H42	1.98	0.46
3:E:22:LEU:HD21	3:E:31:MET:CE	2.46	0.46
1:A:246:HIS:N	1:A:246:HIS:CD2	2.83	0.46
1:B:121:THR:HG21	1:B:140:GLN:CG	2.46	0.46
1:B:186:ARG:HD3	1:B:186:ARG:O	2.15	0.46
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.46	0.46
1:A:282:PHE:HB2	5:A:1207:BHL:O7	2.16	0.46
2:C:122:ARG:HD3	10:C:1361:HOH:O	2.14	0.46
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.51	0.46
10:B:1320:HOH:O	2:D:187:ILE:HD12	2.15	0.46
3:E:138:ARG:NH2	3:E:142:LEU:HD21	2.31	0.46
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.51	0.46
1:B:21:THR:HG22	1:B:22:SER:N	2.32	0.45
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.50	0.45
2:D:266:GLN:HB2	2:D:281:ILE:HG21	1.99	0.45
2:C:239:PHE:HB2	3:E:126:ASN:HA	1.98	0.45
1:A:115:TYR:OH	2:C:173:ASP:HA	2.16	0.45
1:A:180:LEU:HD13	5:A:1206:BHL:BR1	2.71	0.45
2:C:102:LEU:HD11	2:C:290:ILE:HG12	1.97	0.45
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.99	0.45
3:E:122:ILE:HD12	3:E:122:ILE:N	2.30	0.45
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.99	0.45
2:D:223:VAL:CG1	2:D:335:PHE:HA	2.47	0.45
1:B:38:ASP:O	1:B:39:PHE:HB3	2.17	0.45
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.98	0.45
2:C:378:ASP:O	2:C:382:LYS:HG3	2.15	0.45
2:D:179:LEU:HD23	2:D:182:TRP:CZ3	2.52	0.45
3:F:4:LEU:HA	3:F:8:SER:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HD21	1:A:175:ARG:NH2	2.15	0.45
2:D:189:ILE:O	2:D:193:ILE:HG12	2.17	0.45
1:A:93:VAL:HG11	2:D:3:MET:HG2	1.98	0.45
2:D:98:HIS:CD2	2:D:99:ARG:N	2.84	0.45
1:B:204:LEU:HD11	5:B:1201:BHL:H51	1.98	0.45
1:B:62:LEU:HD21	1:B:70:MET:HE1	1.99	0.45
1:A:54:ASN:HB2	10:A:1467:HOH:O	2.15	0.45
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.16	0.45
1:B:466:CYS:HB2	2:D:73:THR:HA	1.99	0.45
2:C:54:VAL:O	2:C:55:TYR:HB2	2.16	0.45
1:A:318:ILE:HD13	10:A:1464:HOH:O	2.16	0.45
1:A:77:ARG:CG	1:A:77:ARG:HH21	2.29	0.45
2:D:60:ALA:HA	2:D:68:ASP:HB3	1.99	0.45
3:F:24:THR:HG22	3:F:26:GLU:HB3	1.98	0.45
1:A:78:GLN:HE21	1:A:235:VAL:HA	1.82	0.45
3:F:80:LYS:CE	3:F:84:GLY:HA2	2.39	0.45
1:A:212:PHE:HA	1:A:215:PRO:HG2	1.99	0.44
1:A:318:ILE:HD13	1:A:318:ILE:C	2.36	0.44
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.00	0.44
2:C:98:HIS:HD2	2:C:297:ASP:OD1	2.00	0.44
2:D:145:ILE:O	2:D:149:TRP:HB3	2.17	0.44
2:C:33:ASN:HD22	2:C:33:ASN:N	2.13	0.44
1:B:196:ASP:HB2	3:F:140:MET:SD	2.57	0.44
1:A:268:ASN:HD21	1:A:327:GLU:N	2.05	0.44
1:B:476:ARG:HH12	3:F:6:ILE:CD1	2.30	0.44
2:D:98:HIS:HE1	2:D:178:SER:OG	1.99	0.44
2:D:377:ARG:O	2:D:381:VAL:HG23	2.17	0.44
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.81	0.44
3:F:56:ILE:O	3:F:60:LEU:HD13	2.18	0.44
2:C:376:ASP:HB3	2:C:379:GLN:HB2	2.00	0.44
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.53	0.44
2:D:54:VAL:O	2:D:55:TYR:HB2	2.18	0.44
1:B:204:LEU:CD1	5:B:1201:BHL:H51	2.48	0.44
1:B:32:LEU:HD21	1:B:135:ASN:HB2	1.99	0.44
3:F:115:ARG:O	3:F:119:LYS:HB2	2.18	0.44
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.66	0.43
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.53	0.43
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.48	0.43
2:D:121:ASP:O	2:D:125:GLN:HG3	2.18	0.43
2:D:348:ASP:HB2	2:D:350:GLU:OE1	2.18	0.43
1:B:405:LEU:HD22	5:B:1212:BHL:H22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:175:THR:O	2:C:179:LEU:HB2	2.18	0.43
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.17	0.43
2:D:353:THR:O	2:D:357:TYR:HD1	2.01	0.43
1:B:186:ARG:HD3	1:B:186:ARG:C	2.38	0.43
2:D:235:TRP:CD1	2:D:235:TRP:C	2.91	0.43
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.53	0.43
1:A:417:ILE:CD1	1:A:469:ILE:HG12	2.46	0.43
2:C:352:ILE:O	2:C:356:LEU:CD2	2.67	0.43
1:A:230:GLU:C	1:A:233:PRO:HD2	2.39	0.43
2:C:339:PHE:CZ	2:C:352:ILE:HD12	2.54	0.43
1:A:283:THR:HB	1:A:284:PRO:CD	2.48	0.43
1:B:105:VAL:O	1:B:109:PHE:HB2	2.19	0.43
2:C:235:TRP:CD1	2:C:235:TRP:C	2.92	0.43
2:C:33:ASN:HD22	2:C:33:ASN:H	1.66	0.43
2:D:111:LYS:O	2:D:115:GLU:HG3	2.18	0.43
2:D:144:PHE:CZ	2:D:342:LEU:HD23	2.53	0.43
1:B:212:PHE:HA	1:B:215:PRO:HG2	2.00	0.43
1:B:223:TRP:CZ3	1:B:297:LYS:HA	2.53	0.43
1:A:159:ALA:O	2:C:33:ASN:HB2	2.18	0.43
3:E:44:ARG:NH2	3:E:50:ASP:OD1	2.52	0.43
1:B:406:MET:O	1:B:410:GLU:HG3	2.18	0.43
2:D:239:PHE:HB2	3:F:126:ASN:HA	2.01	0.43
1:A:192:PHE:O	1:A:200:CYS:HB3	2.19	0.43
1:B:108:ASN:ND2	1:B:175:ARG:HH21	2.17	0.43
2:C:137:ASN:HB3	2:C:272:PHE:HB3	2.01	0.43
2:D:321:THR:O	2:D:325:LEU:HB2	2.18	0.43
2:D:368:ALA:O	2:D:371:ILE:HD13	2.19	0.43
3:F:6:ILE:H	3:F:6:ILE:HD12	1.83	0.43
1:A:299:GLU:CG	1:A:303:LYS:HD3	2.49	0.43
1:A:403:ILE:CD1	1:A:515:LEU:HD12	2.49	0.43
1:B:207:VAL:O	1:B:211:CYS:HB3	2.19	0.43
2:C:7:ARG:HB2	2:C:7:ARG:NH1	2.34	0.43
1:A:134:LYS:HD3	2:C:161:ASN:HD21	1.83	0.42
1:A:186:ARG:C	1:A:186:ARG:HD3	2.39	0.42
1:B:216:LEU:HG	1:B:286:LEU:HD11	2.01	0.42
2:C:364:ILE:CD1	2:C:375:ALA:HB3	2.48	0.42
3:F:12:ARG:O	3:F:16:VAL:HG13	2.19	0.42
1:A:417:ILE:HD13	1:A:468:ASN:HB2	2.01	0.42
2:D:352:ILE:HD12	2:D:388:LEU:HD11	2.00	0.42
1:A:283:THR:HB	1:A:284:PRO:HD3	2.01	0.42
1:A:403:ILE:HG22	1:A:405:LEU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:126:GLY:O	2:C:130:ASP:HB2	2.19	0.42
3:E:40:THR:C	3:E:41:THR:HG23	2.39	0.42
1:B:90:ASN:OD1	2:C:3:MET:O	2.38	0.42
1:B:230:GLU:C	1:B:233:PRO:HD2	2.39	0.42
2:C:102:LEU:HD13	10:C:1407:HOH:O	2.19	0.42
2:D:137:ASN:HB3	2:D:272:PHE:HB3	2.02	0.42
2:D:314:ARG:O	2:D:318:ARG:HG3	2.20	0.42
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.55	0.42
2:D:77:HIS:CG	3:F:140:MET:HG2	2.54	0.42
1:A:299:GLU:OE1	1:A:303:LYS:HE2	2.20	0.42
2:C:121:ASP:O	2:C:125:GLN:HG3	2.20	0.42
2:D:78:GLY:O	3:F:112:ILE:HD13	2.20	0.42
3:F:38:ASP:HB2	3:F:39:HIS:CE1	2.54	0.42
1:B:216:LEU:C	1:B:216:LEU:HD23	2.40	0.42
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.38	0.42
1:B:452:TRP:O	1:B:456:MET:HG3	2.19	0.42
2:C:376:ASP:O	2:C:380:ILE:HG12	2.19	0.42
1:A:184:MET:HE3	1:A:187:VAL:CG2	2.50	0.42
1:A:246:HIS:CE1	10:A:1309:HOH:O	2.72	0.42
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.14	0.42
2:D:89:GLU:OE2	3:F:125:VAL:HG22	2.20	0.42
1:B:49:LYS:HD3	3:F:140:MET:HB3	2.02	0.42
1:B:405:LEU:HD12	1:B:406:MET:N	2.35	0.41
2:D:349:LYS:O	2:D:352:ILE:HG12	2.19	0.41
2:D:355:SER:HA	2:D:358:ARG:CZ	2.49	0.41
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.51	0.41
2:C:336:MET:HE2	2:C:385:LEU:HA	2.01	0.41
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.56	0.41
1:B:343:HIS:H	1:B:343:HIS:CD2	2.39	0.41
1:B:63:ILE:HD13	1:B:66:GLU:HB3	2.00	0.41
2:C:259:PHE:CE1	2:C:356:LEU:HD22	2.56	0.41
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.20	0.41
3:F:133:ARG:NH1	3:F:134:GLN:HG3	2.35	0.41
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.86	0.41
1:B:253:THR:O	1:B:257:ILE:HG13	2.21	0.41
2:C:277:THR:N	2:C:278:PRO:CD	2.84	0.41
1:B:246:HIS:N	1:B:246:HIS:CD2	2.87	0.41
2:C:155:ASN:ND2	2:C:252:TYR:OH	2.53	0.41
3:F:23:ASN:ND2	3:F:23:ASN:N	2.65	0.41
2:C:225:LYS:HB3	10:C:1375:HOH:O	2.19	0.41
2:D:262:ARG:HA	2:D:266:GLN:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:132:GLU:HG3	10:F:878:HOH:O	2.20	0.41
1:A:96:HIS:HB2	2:C:20:ILE:HD12	2.03	0.41
1:B:380:TYR:HE1	1:B:385:LYS:HZ3	1.66	0.41
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.88	0.41
2:D:233:GLY:O	2:D:237:GLU:HB2	2.20	0.41
2:D:319:ASN:ND2	3:F:74:GLU:HA	2.35	0.41
1:B:477:GLU:O	1:B:480:GLU:HB2	2.19	0.41
2:C:90:LEU:HD13	2:C:303:LEU:HD13	2.03	0.41
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.56	0.41
2:D:312:TYR:CD1	3:F:69:ALA:HB2	2.56	0.41
2:D:340:ALA:HA	2:D:389:LYS:CE	2.47	0.41
1:A:185:LYS:O	1:A:189:SER:HB2	2.21	0.41
1:B:65:LYS:HB3	2:D:117:TRP:CG	2.56	0.41
2:D:217:GLU:O	2:D:221:GLY:HA3	2.21	0.41
3:F:120:PRO:HA	3:F:122:ILE:N	2.36	0.41
1:A:177:ILE:HG12	1:A:485:LEU:HB2	2.02	0.40
2:D:314:ARG:NH1	2:D:372:ASP:OD1	2.54	0.40
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.85	0.40
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.55	0.40
2:D:277:THR:O	2:D:281:ILE:HD13	2.21	0.40
3:E:22:LEU:O	3:E:63:LYS:HE2	2.21	0.40
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.21	0.40
1:A:495:LEU:HD11	1:A:512:ILE:HG13	2.04	0.40
1:B:121:THR:HG21	1:B:140:GLN:CD	2.42	0.40
1:B:403:ILE:HD11	1:B:515:LEU:HD12	2.02	0.40
3:F:85:GLU:OE1	3:F:118:TYR:HE2	2.04	0.40
1:A:521:ASN:HB3	1:A:524:LYS:HG2	2.01	0.40
1:B:115:TYR:OH	2:D:173:ASP:HA	2.21	0.40
2:C:316:VAL:O	2:C:319:ASN:HB3	2.22	0.40
3:E:15:TRP:CZ3	3:E:18:LYS:HD3	2.56	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	508/527 (96%)	488 (96%)	20 (4%)	0	100	100
1	B	508/527 (96%)	486 (96%)	21 (4%)	1 (0%)	47	33
2	C	386/389 (99%)	374 (97%)	11 (3%)	1 (0%)	41	27
2	D	386/389 (99%)	360 (93%)	24 (6%)	2 (0%)	29	15
3	E	164/170 (96%)	161 (98%)	2 (1%)	1 (1%)	25	12
3	F	164/170 (96%)	152 (93%)	11 (7%)	1 (1%)	25	12
All	All	2116/2172 (97%)	2021 (96%)	89 (4%)	6 (0%)	41	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	205	PRO
3	F	122	ILE
2	D	64	ALA
3	E	5	GLY
2	C	251	VAL

### 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	423/442 (96%)	410 (97%)	13 (3%)	40	25
1	B	422/442 (96%)	410 (97%)	12 (3%)	43	30
2	C	315/323 (98%)	310 (98%)	5 (2%)	62	54
2	D	312/323 (97%)	304 (97%)	8 (3%)	46	32
3	E	143/147 (97%)	141 (99%)	2 (1%)	67	59
3	F	142/147 (97%)	139 (98%)	3 (2%)	53	42
All	All	1757/1824 (96%)	1714 (98%)	43 (2%)	49	36

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	43	ARG
1	A	90	ASN
1	A	125	TRP
1	A	175	ARG
1	A	186	ARG
1	A	259	ASN
1	A	279	GLN
1	A	286	LEU
1	A	302	VAL
1	A	318	ILE
1	A	338	ASP
1	A	467	GLN
1	B	30	ARG
1	B	42	ASN
1	B	43	ARG
1	B	63	ILE
1	B	90	ASN
1	B	110	LEU
1	B	112	VAL
1	B	125	TRP
1	B	186	ARG
1	B	279	GLN
1	B	286	LEU
1	B	311	GLU
2	C	33	ASN
2	C	160	PHE
2	C	173	ASP
2	C	377	ARG
2	C	378	ASP
2	D	35	MET
2	D	133	ILE
2	D	153	LEU
2	D	160	PHE
2	D	173	ASP
2	D	205	PRO
2	D	334	ASP
2	D	371	ILE
3	E	44	ARG
3	E	167	GLN
3	F	23	ASN
3	F	44	ARG

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Mol	Chain	Res	Type
3	F	149	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	168	HIS
1	A	227	ASN
1	A	249	ASN
1	A	268	ASN
1	A	273	ASN
1	A	278	GLN
1	A	279	GLN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	467	GLN
1	A	516	ASN
1	B	33	GLN
1	B	42	ASN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	116	ASN
1	B	155	ASN
1	B	168	HIS
1	B	227	ASN
1	B	249	ASN
1	B	268	ASN
1	B	273	ASN
1	B	278	GLN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	411	ASN
1	B	413	HIS
1	B	439	HIS

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Mol	Chain	Res	Type
1	B	451	GLN
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	125	GLN
2	C	146	ASN
2	C	161	ASN
2	C	285	GLN
2	C	301	ASN
2	C	379	GLN
2	D	98	HIS
2	D	125	GLN
2	D	161	ASN
2	D	285	GLN
2	D	301	ASN
3	E	45	ASN
3	E	144	ASN
3	E	165	HIS
3	E	167	GLN
3	F	7	HIS
3	F	17	ASN
3	F	23	ASN
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 19 ligands modelled in this entry, 1 is modelled with single atom and 5 are monoatomic - leaving 13 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	BHL	B	1211	-	7,7,7	0.43	0	6,6,6	0.73	0
5	BHL	B	1205	-	7,7,7	0.31	0	6,6,6	0.50	0
5	BHL	A	1203	4	7,7,7	0.31	0	6,6,6	0.81	0
5	BHL	B	1201	4	7,7,7	0.37	0	6,6,6	0.81	0
5	BHL	A	1210	5	6,6,7	0.45	0	5,5,6	0.71	0
5	BHL	A	1206	-	7,7,7	0.48	0	6,6,6	1.95	1 (16%)
5	BHL	B	1202	-	7,7,7	0.63	0	6,6,6	2.39	2 (33%)
9	3BR	C	1208	-	2,3,3	0.35	0	0,2,2	0.00	-
6	BBU	A	1209	-	4,4,4	0.35	0	2,3,3	0.54	0
7	BBX	B	1204	-	2,2,2	0.70	0	1,1,1	1.03	0
5	BHL	B	1212	-	7,7,7	0.38	0	6,6,6	0.78	0
9	3BR	C	1213	-	2,3,3	0.34	0	0,2,2	0.00	-
5	BHL	A	1207	-	7,7,7	0.56	0	6,6,6	2.21	1 (16%)

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	BHL	B	1211	-	-	4/5/5/5	-
5	BHL	B	1205	-	-	1/5/5/5	-
5	BHL	A	1203	4	-	1/5/5/5	-
5	BHL	B	1201	4	-	1/5/5/5	-
5	BHL	A	1210	5	-	4/4/4/5	-
5	BHL	A	1206	-	-	4/5/5/5	-
5	BHL	B	1202	-	-	4/5/5/5	-
6	BBU	A	1209	-	-	1/2/2/2	-
9	3BR	C	1208	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BHL	B	1212	-	-	4/5/5/5	-
9	3BR	C	1213	-	-	0/1/1/1	-
5	BHL	A	1207	-	-	2/5/5/5	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1207	BHL	BR1-C1-C2	5.00	133.45	112.26
5	B	1202	BHL	BR1-C1-C2	4.76	132.45	112.26
5	A	1206	BHL	C4-C3-C2	4.43	136.90	114.42
5	B	1202	BHL	C4-C3-C2	2.80	128.62	114.42

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1211	BHL	C1-C2-C3-C4
5	A	1203	BHL	BR1-C1-C2-C3
5	B	1212	BHL	C1-C2-C3-C4
5	A	1207	BHL	C1-C2-C3-C4
5	B	1201	BHL	BR1-C1-C2-C3
5	A	1206	BHL	BR1-C1-C2-C3
5	B	1202	BHL	BR1-C1-C2-C3
5	A	1207	BHL	BR1-C1-C2-C3
5	A	1210	BHL	C2-C3-C4-C5
5	B	1211	BHL	C2-C3-C4-C5
5	B	1212	BHL	C2-C3-C4-C5
5	B	1202	BHL	C3-C4-C5-C6
5	B	1211	BHL	C3-C4-C5-C6
5	A	1210	BHL	C3-C4-C5-C6
5	A	1206	BHL	C3-C4-C5-C6
5	B	1212	BHL	C3-C4-C5-C6
6	A	1209	BBU	C1-C2-C3-C4
5	A	1206	BHL	C1-C2-C3-C4
5	B	1202	BHL	C1-C2-C3-C4
5	A	1210	BHL	C1-C2-C3-C4
5	B	1211	BHL	C4-C5-C6-O7
5	A	1210	BHL	C4-C5-C6-O7
5	B	1212	BHL	C4-C5-C6-O7
5	A	1206	BHL	C4-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
5	B	1202	BHL	C4-C5-C6-O7
5	B	1205	BHL	C3-C4-C5-C6

There are no ring outliers.

8 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1205	BHL	4	0
5	A	1203	BHL	3	0
5	B	1201	BHL	2	0
5	A	1210	BHL	9	0
5	A	1206	BHL	2	0
5	B	1202	BHL	3	0
5	B	1212	BHL	1	0
5	A	1207	BHL	3	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, 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	510/527 (96%)	-0.05	6 (1%) 79 76	20, 31, 51, 76	0
1	B	510/527 (96%)	0.00	11 (2%) 62 57	22, 33, 53, 77	0
2	C	388/389 (99%)	-0.25	2 (0%) 91 89	18, 26, 47, 87	0
2	D	388/389 (99%)	0.65	38 (9%) 7 5	24, 42, 71, 99	0
3	E	166/170 (97%)	-0.18	1 (0%) 89 87	20, 30, 48, 64	0
3	F	166/170 (97%)	1.19	32 (19%) 1 0	36, 55, 75, 87	0
All	All	2128/2172 (97%)	0.14	90 (4%) 36 30	18, 34, 62, 99	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	2	SER	13.2
2	D	389	LYS	8.3
2	D	375	ALA	5.4
2	D	352	ILE	4.9
3	E	4	LEU	4.6
3	F	70	ARG	4.5
3	F	100	ALA	4.4
2	D	344	ALA	4.1
3	F	21	GLN	4.0
2	D	205	PRO	3.9
3	F	72	PHE	3.9
3	F	23	ASN	3.8
3	F	83	PHE	3.8
3	F	22	LEU	3.8
2	D	350	GLU	3.7
2	D	388	LEU	3.7
2	D	374	LYS	3.6
2	D	343	PRO	3.6
3	F	80	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	187	ILE	3.5
3	F	102	LYS	3.5
3	F	101	ALA	3.4
3	F	25	LEU	3.4
2	D	365	GLU	3.4
2	D	370	ARG	3.4
2	D	2	SER	3.4
3	F	67	LEU	3.4
3	F	151	PRO	3.1
2	D	385	LEU	3.1
3	F	4	LEU	3.1
2	D	347	THR	3.1
2	D	357	TYR	3.1
2	D	380	ILE	3.1
2	D	379	GLN	3.0
1	B	312	ASP	2.9
1	B	259	ASN	2.8
3	F	26	GLU	2.8
3	F	96	ALA	2.7
3	F	16	VAL	2.7
1	B	40	LYS	2.7
3	F	121	PRO	2.7
1	A	318	ILE	2.7
1	B	39	PHE	2.7
2	D	373	PHE	2.6
1	B	350	ALA	2.6
2	D	345	GLY	2.6
3	F	161	VAL	2.6
1	B	317	TRP	2.6
1	A	20	PRO	2.6
2	D	44	LYS	2.6
1	A	19	ALA	2.5
2	D	369	SER	2.5
2	D	340	ALA	2.5
2	D	254	ALA	2.5
1	B	308	TRP	2.5
1	B	527	ASN	2.5
3	F	17	ASN	2.5
3	F	125	VAL	2.5
1	A	316	ILE	2.5
3	F	24	THR	2.4
1	B	261	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	20	ALA	2.3
2	D	377	ARG	2.3
1	A	350	ALA	2.3
2	D	139	THR	2.3
2	D	354	ALA	2.3
2	D	307	PRO	2.3
2	D	346	THR	2.3
2	D	256	PHE	2.2
2	D	229	LEU	2.2
2	D	138	PRO	2.2
1	A	317	TRP	2.2
3	F	120	PRO	2.2
2	D	348	ASP	2.2
3	F	97	LYS	2.2
3	F	122	ILE	2.2
2	D	159	LEU	2.2
3	F	73	ASN	2.2
2	D	339	PHE	2.2
2	D	378	ASP	2.2
3	F	19	ILE	2.1
2	D	372	ASP	2.1
1	B	54	ASN	2.0
2	D	360	VAL	2.0
1	B	19	ALA	2.0
3	F	28	ALA	2.0
2	C	205	PRO	2.0
3	F	56	ILE	2.0
3	F	60	LEU	2.0
3	F	145	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	BHL	A	1210	7/8	0.56	0.53	82,82,82,82	0
5	BHL	A	1207	8/8	0.81	0.29	60,60,60,60	0
5	BHL	B	1212	8/8	0.82	0.27	63,63,63,63	0
5	BHL	A	1203	8/8	0.83	0.24	61,61,61,61	0
9	3BR	C	1213	4/4	0.87	0.23	85,85,85,85	0
5	BHL	B	1205	8/8	0.88	0.25	57,57,57,57	0
5	BHL	B	1211	8/8	0.88	0.25	75,75,75,75	0
5	BHL	B	1201	8/8	0.91	0.21	68,68,68,68	0
9	3BR	C	1208	4/4	0.94	0.21	61,61,61,61	0
7	BBX	B	1204	3/3	0.94	0.16	83,83,83,83	0
6	BBU	A	1209	5/5	0.94	0.15	71,71,71,71	0
5	BHL	A	1200	1/8	0.95	0.09	82,82,82,82	0
5	BHL	A	1206	8/8	0.97	0.20	47,47,47,47	0
5	BHL	B	1202	8/8	0.97	0.19	44,44,44,44	0
8	CA	C	1174	1/1	0.99	0.08	32,32,32,32	0
4	FE	B	1173	1/1	0.99	0.05	28,28,28,28	0
4	FE	B	1172	1/1	0.99	0.04	32,32,32,32	0
4	FE	A	1171	1/1	1.00	0.03	25,25,25,25	0
4	FE	A	1170	1/1	1.00	0.02	28,28,28,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.