



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2018 – 02:18 PM EST

PDB ID : 1D2V  
Title : CRYSTAL STRUCTURE OF BROMIDE-BOUND HUMAN MYELOPER-  
OXIDASE ISOFORM C AT PH 5.5  
Authors : Fiedler, T.J.; Davey, C.A.; Fenna, R.E.  
Deposited on : 1999-09-28  
Resolution : 1.75 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

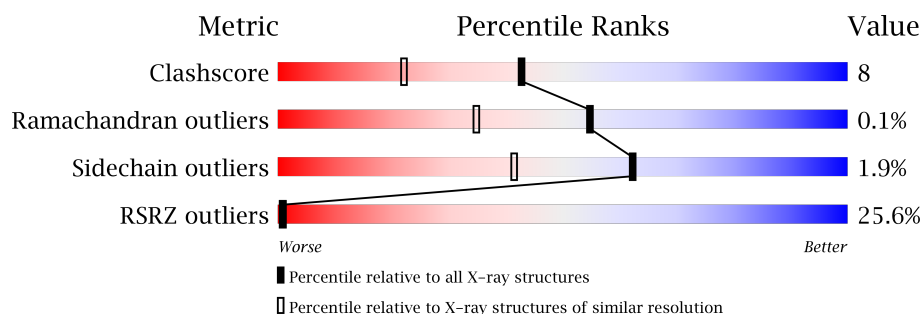
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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. 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	104	<div> <div>18%</div> <div> <div></div> <div>80%</div> <div>20%</div> </div> </div>
1	B	104	<div> <div>26%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
2	C	466	<div> <div>23%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>.</div> </div> </div>
2	D	466	<div> <div>30%</div> <div> <div></div> <div>82%</div> <div>18%</div> <div>.</div> </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
11	ACT	C	1606	-	-	X	X
11	ACT	D	2604	-	-	X	-
4	BR	A	843	-	-	X	-
8	BMA	C	1642	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 10306 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 MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			
1	B	104	Total	C	N	O	S	0	0	0
			838	529	148	156	5			

- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			
2	D	466	Total	C	N	O	S	0	0	0
			3733	2351	687	668	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	150	CSO	CYS	MODIFIED RESIDUE	UNP P05164
D	150	CSO	CYS	MODIFIED RESIDUE	UNP P05164

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Br	0	0
			4	4		

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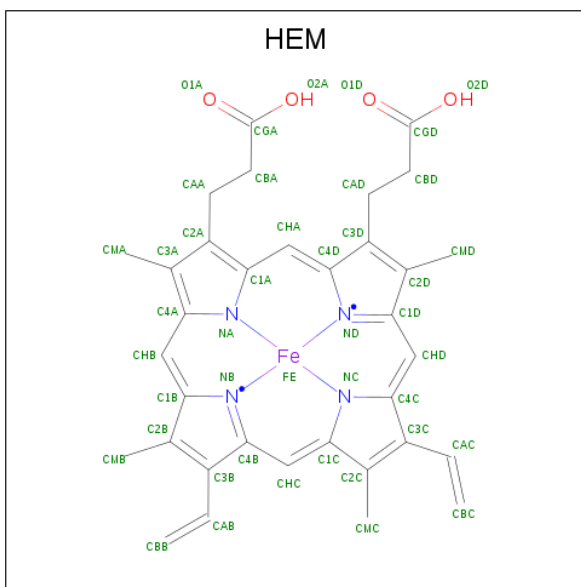
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Br	0	0
			4	4		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



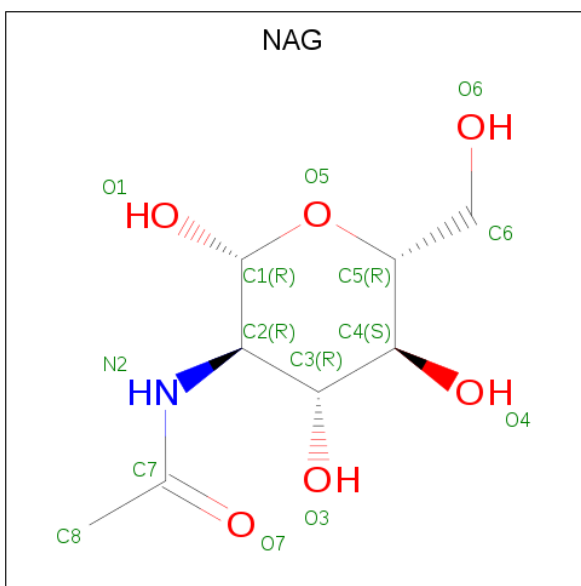
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



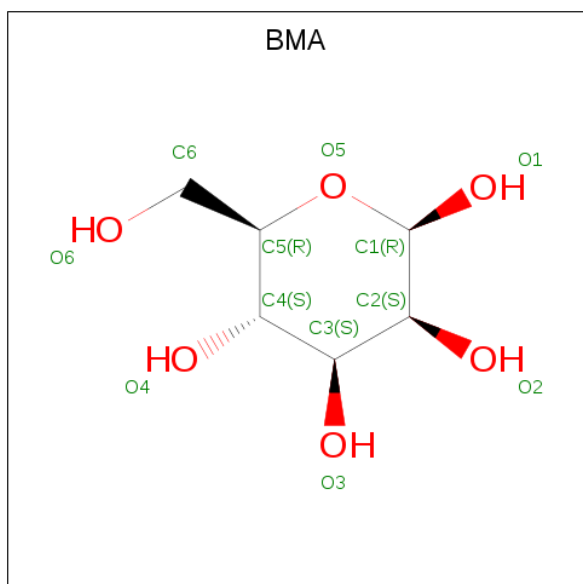
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total 14	C 8	N 1	O 5	0	0
7	C	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



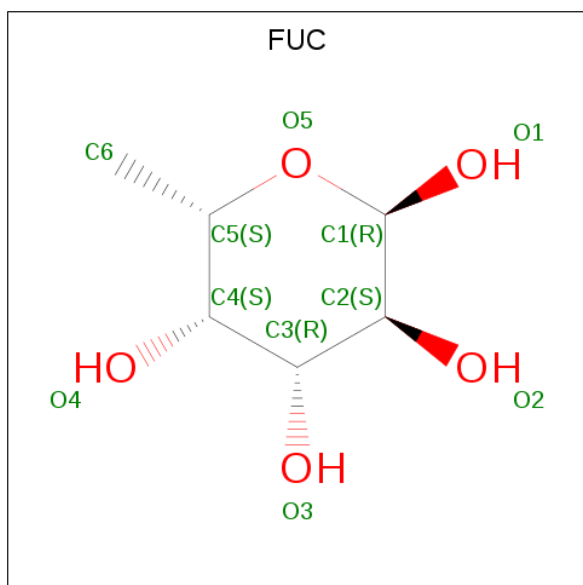
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			11	6	5		
9	C	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		

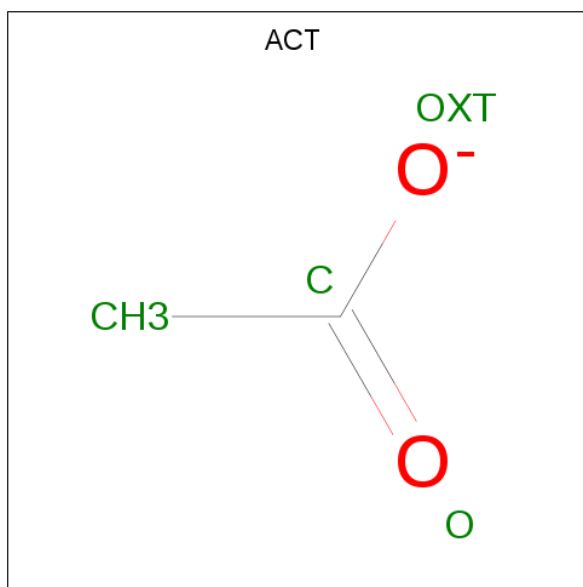
- Molecule 10 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).





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

- Molecule 11 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	98	Total	O	0	0
			98	98		
12	C	319	Total	O	0	0
			319	319		

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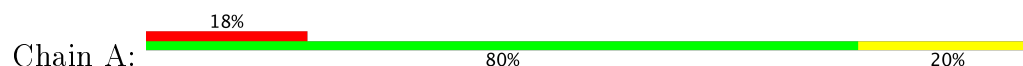
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	100	Total 100	O 100	0	0
12	D	314	Total 314	O 314	0	0

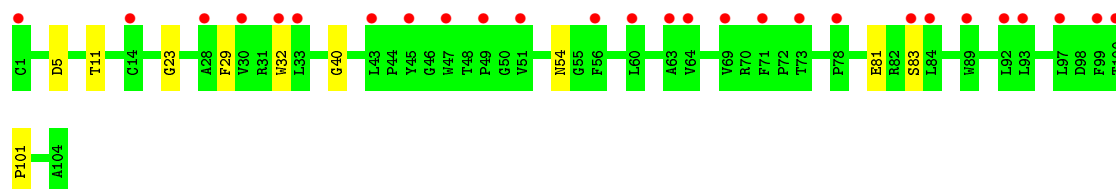
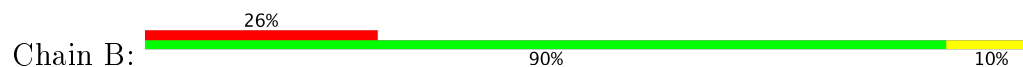
### 3 Residue-property plots [i](#)

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.

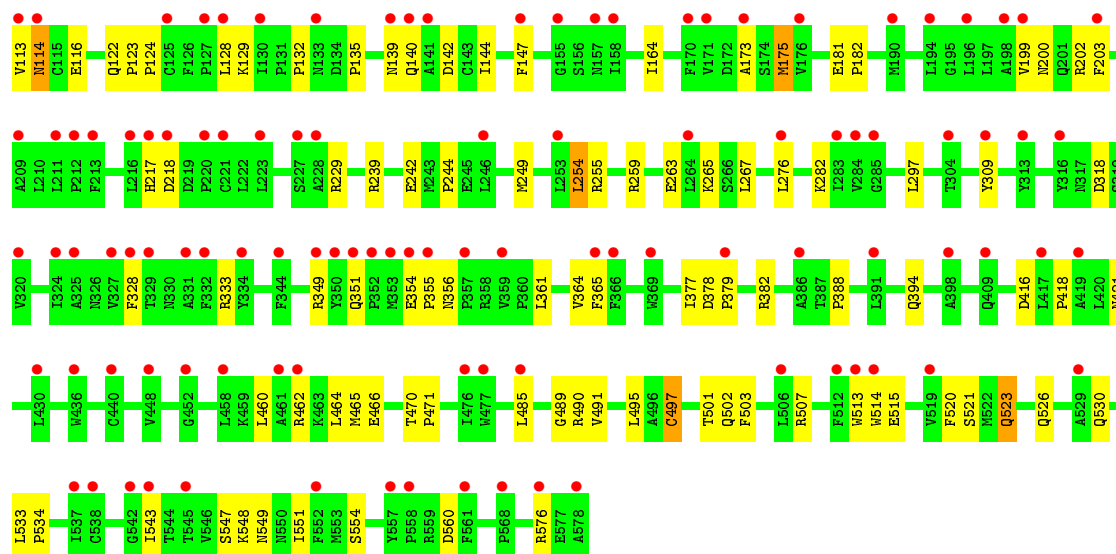
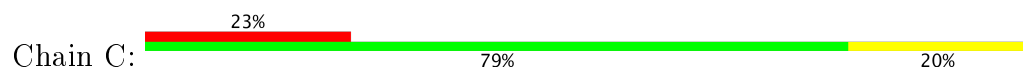
#### • Molecule 1: MYELOPEROXIDASE



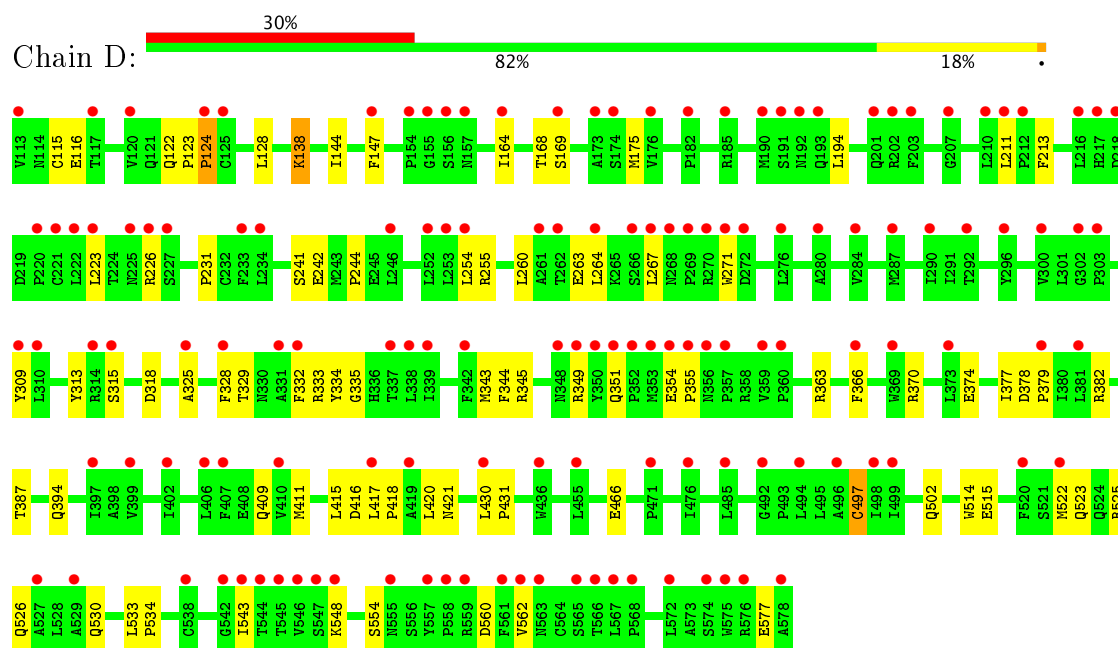
#### • Molecule 1: MYELOPEROXIDASE



#### • Molecule 2: MYELOPEROXIDASE



#### • Molecule 2: MYELOPEROXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.16 Å 63.49 Å 92.48 Å 90.00° 97.36° 90.00°	Depositor
Resolution (Å)	30.00 – 1.75 44.41 – 1.76	Depositor EDS
% Data completeness (in resolution range)	87.3 (30.00-1.75) 90.4 (44.41-1.76)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.37 (at 1.76 Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.243 , 0.296 0.238 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	12.2	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	10306	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: CSO, BMA, NAG, CA, FUC, BR, ACT, HEM, MAN, SO4

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	0.75	0/863	0.73	0/1174
1	B	0.76	0/863	0.72	0/1174
2	C	0.73	1/3811 (0.0%)	0.65	0/5168
2	D	0.70	0/3811	0.63	0/5168
All	All	0.72	1/9348 (0.0%)	0.66	0/12684

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	114	ASN	C-N	-6.21	1.19	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	838	0	798	17	0
1	B	838	0	798	8	0
2	C	3733	0	3723	65	0
2	D	3733	0	3725	65	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	0	3	0
4	B	4	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	A	43	0	30	3	0
6	B	43	0	30	2	0
7	C	56	0	49	1	0
7	D	56	0	49	0	0
8	C	11	0	8	0	0
8	D	11	0	8	0	0
9	C	22	0	20	0	0
9	D	22	0	20	0	0
10	C	10	0	10	0	0
10	D	10	0	10	0	0
11	C	12	0	9	4	0
11	D	12	0	9	3	0
12	A	98	0	0	4	0
12	B	100	0	0	1	0
12	C	319	0	0	10	0
12	D	314	0	0	4	0
All	All	10306	0	9296	147	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 8.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:355:PRO:HG2	2:C:356:ASN:HD22	1.44	0.82
2:D:333:ARG:HH11	2:D:421:ASN:HD22	1.31	0.78
2:C:132:PRO:HG3	2:C:140:GLN:NE2	2.04	0.72
2:C:355:PRO:HG2	2:C:356:ASN:ND2	2.05	0.71
2:C:200:ASN:HD22	2:C:203:PHE:H	1.36	0.70
2:C:123:PRO:HB3	11:C:1606:ACT:H3	1.74	0.69
2:D:122:GLN:HA	2:D:122:GLN:HE21	1.55	0.69
2:D:349:ARG:HG3	2:D:351:GLN:HG2	1.73	0.69
2:C:349:ARG:HG3	2:C:351:GLN:HG2	1.76	0.69
7:C:1620:NAG:H5	12:C:1250(A):HOH:O	1.92	0.68
2:D:211:LEU:HD23	2:D:254:LEU:HD22	1.76	0.66
2:D:333:ARG:HH11	2:D:421:ASN:ND2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:1243(A):HOH:O	2:C:129:LYS:HD3	1.98	0.64
2:D:128:LEU:HB2	2:D:144:ILE:HB	1.80	0.64
2:D:411:MET:HE2	2:D:415:LEU:HD21	1.80	0.63
2:C:514:TRP:CE2	2:C:515:GLU:HG3	2.33	0.63
1:B:5:ASP:HB3	12:B:1272(B):HOH:O	1.99	0.62
2:D:548:LYS:HE2	2:D:562:VAL:HG13	1.83	0.61
6:A:605:HEM:HBB2	2:C:242:GLU:OE1	2.00	0.61
2:C:200:ASN:ND2	2:C:203:PHE:H	1.98	0.60
2:D:122:GLN:HA	2:D:122:GLN:NE2	2.17	0.59
4:A:843:BR:BR	2:C:242:GLU:HG3	2.57	0.59
2:D:263:GLU:HG3	12:D:921(B):HOH:O	2.02	0.58
1:A:2:PRO:HD2	12:A:791(A):HOH:O	2.04	0.58
2:D:522:MET:HG3	11:D:2604:ACT:H1	1.84	0.58
2:D:122:GLN:HE21	2:D:123:PRO:CD	2.15	0.58
2:C:333:ARG:HH11	2:C:421:ASN:HD22	1.52	0.57
2:C:135:PRO:HG2	12:C:1204(A):HOH:O	2.05	0.56
2:D:122:GLN:HE21	2:D:123:PRO:HD3	1.71	0.56
4:A:843:BR:BR	12:C:957(A):HOH:O	2.73	0.56
2:C:354:GLU:HB3	2:C:355:PRO:HA	1.88	0.56
1:A:101:PRO:HB2	12:A:1247(A):HOH:O	2.05	0.55
2:C:382:ARG:NH1	12:C:777(A):HOH:O	2.37	0.54
1:A:83:SER:HB3	2:C:554:SER:O	2.08	0.54
2:C:485:LEU:HD13	2:C:490:ARG:HA	1.88	0.53
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.91	0.53
2:D:378:ASP:HB2	2:D:379:PRO:HD3	1.91	0.53
2:D:548:LYS:HE2	2:D:562:VAL:CG1	2.38	0.53
2:D:271:TRP:HE1	2:D:577:GLU:CD	2.12	0.52
2:D:382:ARG:HG3	2:D:543:ILE:CD1	2.39	0.52
2:D:411:MET:CE	2:D:415:LEU:HD21	2.40	0.51
2:D:138:LYS:HZ3	2:D:138:LYS:HA	1.76	0.51
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.92	0.51
1:B:83:SER:HB3	2:D:554:SER:O	2.10	0.51
2:C:113:VAL:HG12	2:C:114:ASN:N	2.26	0.51
2:C:521:SER:OG	2:C:523:GLN:HG2	2.10	0.51
2:C:114:ASN:HA	12:C:973(A):HOH:O	2.11	0.51
2:C:507:ARG:HG3	2:C:513:TRP:CE2	2.46	0.51
2:D:255:ARG:NH1	2:D:377:ILE:HD11	2.26	0.51
2:C:139:ASN:HB2	2:C:142:ASP:OD1	2.11	0.50
2:D:138:LYS:NZ	2:D:138:LYS:HA	2.25	0.50
2:D:328:PHE:CD1	2:D:502:GLN:HG2	2.46	0.50
2:D:244:PRO:HB2	2:D:343:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:605:HEM:HBC2	6:A:605:HEM:HMC2	1.94	0.49
2:C:465:MET:CE	2:C:471:PRO:HD3	2.42	0.49
2:D:116:GLU:OE1	2:D:411:MET:HE3	2.11	0.49
2:C:394:GLN:HB3	2:C:460:LEU:HD22	1.93	0.49
2:D:416:ASP:O	2:D:420:LEU:HG	2.11	0.49
2:C:548:LYS:HD2	2:C:560:ASP:HA	1.94	0.49
1:A:20:PRO:HG2	1:B:40:GLY:HA3	1.95	0.48
1:A:92:LEU:HD22	2:C:249:MET:HB3	1.96	0.48
1:A:17:ARG:HB3	12:A:915(B):HOH:O	2.13	0.48
2:D:416:ASP:OD2	2:D:418:PRO:HD2	2.13	0.48
2:C:549:ASN:HB3	12:C:1232(A):HOH:O	2.13	0.48
2:C:116:GLU:HG3	2:C:147:PHE:CZ	2.48	0.47
2:C:549:ASN:ND2	12:C:829(A):HOH:O	2.46	0.47
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.49	0.47
2:D:213:PHE:CD2	2:D:231:PRO:HG2	2.50	0.47
2:D:554:SER:HB3	2:D:560:ASP:HB3	1.95	0.47
2:C:173:ALA:HA	2:C:175:MET:SD	2.55	0.47
2:D:548:LYS:HG2	2:D:562:VAL:HG13	1.96	0.47
2:D:354:GLU:HB3	2:D:355:PRO:HA	1.97	0.47
2:C:123:PRO:CB	11:C:1606:ACT:H3	2.42	0.46
2:D:394:GLN:HG3	12:D:850(B):HOH:O	2.15	0.46
2:C:462:ARG:O	2:C:466:GLU:HG2	2.15	0.46
2:D:345:ARG:NH1	12:D:762(B):HOH:O	2.48	0.46
2:D:378:ASP:O	2:D:543:ILE:HD11	2.15	0.46
2:C:333:ARG:HD3	2:C:421:ASN:ND2	2.30	0.46
4:A:758:BR:BR	2:C:543:ILE:HG23	2.70	0.46
2:C:361:LEU:O	2:C:364:VAL:HG22	2.16	0.46
2:D:533:LEU:HB3	2:D:534:PRO:HD3	1.98	0.46
1:B:32:TRP:CE2	2:D:325:ALA:HB2	2.51	0.46
2:C:297:LEU:HD11	2:C:503:PHE:CD1	2.51	0.46
1:A:1:CYS:SG	1:A:20:PRO:HB3	2.56	0.45
2:C:181:GLU:HB2	2:C:182:PRO:HD3	1.98	0.45
2:C:200:ASN:ND2	2:C:202:ARG:H	2.14	0.45
2:D:260:LEU:O	2:D:264:LEU:HG	2.17	0.45
2:C:416:ASP:OD2	2:C:418:PRO:HD2	2.15	0.45
2:D:115:CYS:HB2	2:D:147:PHE:CZ	2.51	0.45
2:C:255:ARG:NH1	2:C:377:ILE:HD11	2.32	0.45
2:D:122:GLN:HE21	2:D:122:GLN:CA	2.25	0.45
2:D:123:PRO:HA	2:D:124:PRO:HA	1.83	0.45
2:C:199:VAL:HG12	2:C:254:LEU:HD21	1.99	0.45
2:D:223:LEU:HD22	2:D:226:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:491:VAL:HB	2:C:495:LEU:HB2	1.99	0.45
2:C:265:LYS:HD3	2:C:276:LEU:HD11	1.98	0.44
6:A:605:HEM:HBC2	6:A:605:HEM:CMC	2.46	0.44
2:C:135:PRO:CG	12:C:1204(A):HOH:O	2.63	0.44
1:A:45:TYR:CE1	1:A:53:ARG:HG3	2.53	0.44
2:D:241:SER:O	2:D:366:PHE:HA	2.18	0.44
2:C:259:ARG:O	2:C:263:GLU:HG3	2.17	0.44
2:C:378:ASP:HB2	2:C:379:PRO:HD3	2.00	0.44
2:C:513:TRP:CD1	2:C:515:GLU:HB2	2.53	0.43
2:D:533:LEU:N	2:D:534:PRO:CD	2.81	0.43
4:B:843:BR:BR	2:D:242:GLU:HG3	2.74	0.43
1:B:101:PRO:HD2	2:D:164:ILE:O	2.19	0.43
2:C:229:ARG:HG2	2:C:229:ARG:HH11	1.84	0.43
1:A:68:ILE:HD13	2:C:464:LEU:HD23	2.00	0.43
1:A:101:PRO:HD2	2:C:164:ILE:O	2.18	0.43
2:D:194:LEU:HD13	12:D:948(B):HOH:O	2.18	0.43
1:A:79:ASP:O	2:C:388:PRO:HB3	2.19	0.43
2:D:526:GLN:NE2	2:D:530:GLN:HE21	2.17	0.43
6:B:605:HEM:CBC	2:D:335:GLY:HA3	2.48	0.43
2:C:124:PRO:HA	11:C:1606:ACT:H1	2.00	0.43
2:C:244:PRO:HD3	2:C:364:VAL:O	2.18	0.43
1:B:23:GLY:HA2	2:D:169:SER:OG	2.19	0.42
2:C:533:LEU:HB3	2:C:534:PRO:HD3	2.01	0.42
2:C:501:THR:HA	12:C:814(A):HOH:O	2.19	0.42
1:A:45:TYR:CZ	1:A:53:ARG:HG3	2.55	0.42
2:C:282:LYS:HG2	2:C:520:PHE:CZ	2.54	0.42
2:D:344:PHE:CD1	2:D:387:THR:HG21	2.55	0.42
2:C:242:GLU:O	2:C:365:PHE:HA	2.20	0.42
2:C:526:GLN:NE2	2:C:530:GLN:NE2	2.68	0.42
2:D:313:TYR:CZ	2:D:315:SER:HA	2.54	0.42
2:D:116:GLU:OE2	2:D:411:MET:HB2	2.20	0.42
6:B:605:HEM:HBB2	2:D:242:GLU:OE1	2.20	0.42
11:C:1606:ACT:H2	12:C:1213(A):HOH:O	2.19	0.41
1:B:11:THR:O	2:D:168:THR:HG22	2.20	0.41
2:D:332:PHE:C	2:D:334:TYR:H	2.24	0.41
1:A:4:GLN:HG2	1:A:5:ASP:N	2.35	0.41
2:D:430:LEU:HA	2:D:431:PRO:HD3	1.97	0.41
2:C:547:SER:HB2	2:C:551:ILE:HG13	2.03	0.41
1:A:48:THR:HA	1:A:49:PRO:HD3	1.92	0.41
1:A:11:THR:O	1:A:24:ALA:HA	2.20	0.41
1:B:29:PHE:CZ	2:D:329:THR:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:309:TYR:CZ	2:D:497:CYS:HA	2.55	0.41
1:A:60:LEU:HD12	1:A:60:LEU:N	2.36	0.41
1:A:95:HIS:CD2	2:C:239:ARG:CZ	3.04	0.41
2:D:525:ARG:HH21	11:D:2604:ACT:CH3	2.33	0.41
2:C:309:TYR:CZ	2:C:497:CYS:HA	2.56	0.40
2:C:267:LEU:HD12	2:C:576:ARG:HB2	2.03	0.40
2:C:328:PHE:CD1	2:C:502:GLN:HG2	2.56	0.40
2:C:489:GLY:O	2:C:490:ARG:HD3	2.21	0.40
2:D:363:ARG:HG2	2:D:409:GLN:NE2	2.36	0.40
2:D:370:ARG:O	2:D:374:GLU:HB2	2.21	0.40
2:D:525:ARG:HH21	11:D:2604:ACT:C	2.34	0.40
2:D:466:GLU:HG2	2:D:466:GLU:O	2.22	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	102/104 (98%)	100 (98%)	1 (1%)	1 (1%)	18	4
1	B	102/104 (98%)	100 (98%)	2 (2%)	0	100	100
2	C	463/466 (99%)	445 (96%)	18 (4%)	0	100	100
2	D	463/466 (99%)	449 (97%)	14 (3%)	0	100	100
All	All	1130/1140 (99%)	1094 (97%)	35 (3%)	1 (0%)	55	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	SER

### 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	90/90 (100%)	89 (99%)	1 (1%)	78	64
1	B	90/90 (100%)	88 (98%)	2 (2%)	57	33
2	C	410/410 (100%)	401 (98%)	9 (2%)	57	33
2	D	410/410 (100%)	403 (98%)	7 (2%)	66	47
All	All	1000/1000 (100%)	981 (98%)	19 (2%)	62	41

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	122	GLN
2	C	175	MET
2	C	217	HIS
2	C	218	ASP
2	C	254	LEU
2	C	318	ASP
2	C	470	THR
2	C	497	CYS
2	C	523	GLN
1	B	54	ASN
1	B	81	GLU
2	D	124	PRO
2	D	138	LYS
2	D	175	MET
2	D	267	LEU
2	D	318	ASP
2	D	497	CYS
2	D	523	GLN

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	54	ASN
2	C	140	GLN
2	C	200	ASN
2	C	201	GLN
2	C	356	ASN
2	C	526	GLN
2	C	530	GLN
2	C	549	ASN
1	B	54	ASN
2	D	122	GLN
2	D	421	ASN
2	D	526	GLN
2	D	549	ASN

### 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	CSO	C	150	2	4,6,7	1.48	1 (25%)	1,6,8	1.69	0
2	CSO	D	150	2	4,6,7	1.15	0	1,6,8	1.66	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
2	CSO	C	150	2	-	0/1/5/7	0/0/0/0
2	CSO	D	150	2	-	0/1/5/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	150	CSO	CA-C	2.70	1.53	1.50

There are no bond angle outliers.

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 37 ligands modelled in this entry, 10 are monoatomic - leaving 27 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	SO4	A	1602	-	4,4,4	0.19	0	6,6,6	0.16	0
6	HEM	A	605	1,12,2	28,50,50	1.71	6 (21%)	17,82,82	1.19	1 (5%)
5	SO4	B	2602	-	4,4,4	0.36	0	6,6,6	0.06	0
6	HEM	B	605	1,12,2	28,50,50	1.67	7 (25%)	17,82,82	1.17	1 (5%)
5	SO4	C	1603	-	4,4,4	0.33	0	6,6,6	0.13	0
11	ACT	C	1604	-	1,3,3	3.43	1 (100%)	0,3,3	0.00	-
11	ACT	C	1606	-	1,3,3	2.68	1 (100%)	0,3,3	0.00	-
11	ACT	C	1607	-	1,3,3	3.86	1 (100%)	0,3,3	0.00	-
7	NAG	C	1620	2	14,14,15	0.65	0	15,19,21	1.10	1 (6%)
7	NAG	C	1630	2	14,14,15	0.53	0	15,19,21	0.84	0
7	NAG	C	1640	10,2,7	14,14,15	0.84	0	15,19,21	1.01	1 (6%)
7	NAG	C	1641	8,7	14,14,15	0.74	0	15,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	BMA	C	1642	9,7	11,11,12	0.71	0	13,15,17	0.60	0
9	MAN	C	1643	8	11,11,12	0.67	0	13,15,17	0.86	0
9	MAN	C	1644	8	11,11,12	0.56	0	13,15,17	0.75	0
10	FUC	C	1645	7	9,10,11	0.64	0	13,14,16	0.66	0
11	ACT	D	2604	-	1,3,3	3.38	1 (100%)	0,3,3	0.00	-
11	ACT	D	2606	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-
11	ACT	D	2607	-	1,3,3	3.42	1 (100%)	0,3,3	0.00	-
7	NAG	D	2620	2	14,14,15	0.52	0	15,19,21	0.77	0
7	NAG	D	2630	2	14,14,15	0.79	0	15,19,21	1.09	2 (13%)
7	NAG	D	2640	10,2,7	14,14,15	0.70	0	15,19,21	1.24	2 (13%)
7	NAG	D	2641	8,7	14,14,15	0.86	0	15,19,21	0.97	1 (6%)
8	BMA	D	2642	9,7	11,11,12	0.87	1 (9%)	13,15,17	0.66	0
9	MAN	D	2643	8	11,11,12	0.78	0	13,15,17	1.04	1 (7%)
9	MAN	D	2644	8	11,11,12	0.75	0	13,15,17	0.64	0
10	FUC	D	2645	7	9,10,11	0.95	0	13,14,16	0.71	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	SO4	A	1602	-	-	0/0/0/0	0/0/0/0
6	HEM	A	605	1,12,2	-	0/6/54/54	0/0/8/8
5	SO4	B	2602	-	-	0/0/0/0	0/0/0/0
6	HEM	B	605	1,12,2	-	0/6/54/54	0/0/8/8
5	SO4	C	1603	-	-	0/0/0/0	0/0/0/0
11	ACT	C	1604	-	-	0/0/0/0	0/0/0/0
11	ACT	C	1606	-	-	0/0/0/0	0/0/0/0
11	ACT	C	1607	-	-	0/0/0/0	0/0/0/0
7	NAG	C	1620	2	-	0/6/23/26	0/1/1/1
7	NAG	C	1630	2	-	0/6/23/26	0/1/1/1
7	NAG	C	1640	10,2,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1641	8,7	-	0/6/23/26	0/1/1/1
8	BMA	C	1642	9,7	-	0/2/19/22	0/1/1/1
9	MAN	C	1643	8	-	0/2/19/22	0/1/1/1
9	MAN	C	1644	8	-	0/2/19/22	0/1/1/1
10	FUC	C	1645	7	-	0/0/17/20	0/1/1/1
11	ACT	D	2604	-	-	0/0/0/0	0/0/0/0
11	ACT	D	2606	-	-	0/0/0/0	0/0/0/0
11	ACT	D	2607	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	D	2620	2	-	0/6/23/26	0/1/1/1
7	NAG	D	2630	2	-	0/6/23/26	0/1/1/1
7	NAG	D	2640	10,2,7	-	0/6/23/26	0/1/1/1
7	NAG	D	2641	8,7	-	0/6/23/26	0/1/1/1
8	BMA	D	2642	9,7	-	0/2/19/22	0/1/1/1
9	MAN	D	2643	8	-	0/2/19/22	0/1/1/1
9	MAN	D	2644	8	-	0/2/19/22	0/1/1/1
10	FUC	D	2645	7	-	0/0/17/20	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	HEM	C3C-CAC	-4.22	1.39	1.47
6	B	605	HEM	C3B-C2B	-4.12	1.34	1.40
6	A	605	HEM	C3B-CAB	-3.79	1.40	1.47
6	A	605	HEM	C3B-C2B	-3.17	1.36	1.40
6	B	605	HEM	C3B-CAB	-3.07	1.41	1.47
6	B	605	HEM	C3C-CAC	-2.51	1.42	1.47
6	B	605	HEM	C3C-C2C	-2.06	1.37	1.40
8	D	2642	BMA	C2-C3	2.06	1.55	1.52
6	A	605	HEM	CBC-CAC	2.14	1.43	1.28
11	D	2606	ACT	CH3-C	2.26	1.51	1.48
6	A	605	HEM	CBB-CAB	2.39	1.45	1.28
6	B	605	HEM	CBC-CAC	2.43	1.46	1.28
6	B	605	HEM	CBB-CAB	2.46	1.46	1.28
6	A	605	HEM	C1B-NB	2.49	1.39	1.36
11	C	1606	ACT	CH3-C	2.68	1.52	1.48
6	B	605	HEM	C4D-ND	2.84	1.40	1.36
11	D	2604	ACT	CH3-C	3.38	1.53	1.48
11	D	2607	ACT	CH3-C	3.42	1.53	1.48
11	C	1604	ACT	CH3-C	3.43	1.53	1.48
11	C	1607	ACT	CH3-C	3.86	1.53	1.48

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	2640	NAG	C2-N2-C7	-3.06	118.48	122.94
7	D	2641	NAG	C2-N2-C7	-2.64	119.09	122.94
7	D	2630	NAG	C1-C2-N2	-2.56	106.12	110.49
7	C	1620	NAG	C2-N2-C7	-2.43	119.39	122.94
7	D	2630	NAG	C1-O5-C5	-2.22	109.10	112.17
7	D	2640	NAG	O5-C1-C2	-2.05	108.62	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1640	NAG	O5-C1-C2	-2.05	108.63	111.47
6	B	605	HEM	C3B-C4B-NB	2.19	112.03	109.21
6	A	605	HEM	C3B-C4B-NB	2.46	112.38	109.21
9	D	2643	MAN	C1-O5-C5	2.99	116.28	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	605	HEM	3	0
6	B	605	HEM	2	0
11	C	1606	ACT	4	0
7	C	1620	NAG	1	0
11	D	2604	ACT	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	114:ASN	C	115:CYS	N	1.19

## 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	104/104 (100%)	1.39	19 (18%) 1 2	2, 6, 17, 43	0
1	B	104/104 (100%)	1.44	27 (25%) 1 1	3, 7, 15, 23	0
2	C	465/466 (99%)	1.47	105 (22%) 1 1	2, 7, 19, 35	0
2	D	465/466 (99%)	1.64	140 (30%) 1 1	3, 9, 24, 41	0
All	All	1138/1140 (99%)	1.53	291 (25%) 1 1	2, 8, 22, 43	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	14.8
2	D	355	PRO	8.9
2	D	568	PRO	6.2
1	A	4	GLN	5.8
2	D	578	ALA	5.2
1	A	2	PRO	5.2
2	C	353	MET	5.1
2	D	218	ASP	5.0
2	C	223	LEU	4.9
2	D	543	ILE	4.9
2	C	355	PRO	4.8
2	D	562	VAL	4.6
2	D	217	HIS	4.5
2	C	190	MET	4.5
2	C	157	ASN	4.4
2	C	212	PRO	4.2
2	D	529	ALA	4.2
2	C	158	ILE	4.2
2	C	199	VAL	4.1
2	D	575	TRP	4.1
2	D	113	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1	CYS	4.0
1	B	1	CYS	4.0
2	D	261	ALA	4.0
2	D	315	SER	3.9
2	C	351	GLN	3.9
2	C	155	GLY	3.7
1	A	3	GLU	3.7
2	D	351	GLN	3.7
2	D	216	LEU	3.6
2	D	222	LEU	3.6
2	D	269	PRO	3.6
2	C	217	HIS	3.6
2	D	406	LEU	3.6
2	D	417	LEU	3.6
2	D	572	LEU	3.6
2	D	190	MET	3.5
2	D	227	SER	3.5
1	B	89	TRP	3.5
2	D	226	ARG	3.5
1	A	97	LEU	3.5
2	C	452	GLY	3.5
1	B	60	LEU	3.5
2	D	157	ASN	3.4
2	C	147	PHE	3.4
2	D	202	ARG	3.4
2	D	538	CYS	3.4
2	D	124	PRO	3.4
2	D	407	PHE	3.4
2	D	527	ALA	3.4
2	D	303	PRO	3.4
1	B	47	TRP	3.4
2	C	436	TRP	3.4
2	D	352	PRO	3.3
2	C	141	ALA	3.3
2	C	578	ALA	3.3
2	D	267	LEU	3.3
2	D	253	LEU	3.3
2	D	117	THR	3.2
2	D	328	PHE	3.2
2	C	379	PRO	3.2
1	B	51	VAL	3.2
2	C	128	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	357	PRO	3.1
2	D	185	ARG	3.1
2	C	324	ILE	3.1
2	D	567	LEU	3.1
2	D	471	PRO	3.0
2	D	173	ALA	3.0
2	C	369	TRP	3.0
2	D	360	PRO	3.0
2	C	561	PHE	3.0
2	D	557	TYR	3.0
2	D	302	GLY	3.0
2	D	357	PRO	2.9
2	C	557	TYR	2.9
2	D	271	TRP	2.9
1	B	33	LEU	2.9
2	D	264	LEU	2.9
2	D	410	VAL	2.9
2	C	133	ASN	2.9
2	C	327	VAL	2.9
2	C	359	VAL	2.9
1	B	63	ALA	2.9
2	D	272	ASP	2.9
2	D	348	ASN	2.9
2	D	576	ARG	2.9
1	B	92	LEU	2.9
2	D	499	ILE	2.9
2	D	309	TYR	2.9
2	C	216	LEU	2.8
2	C	543	ILE	2.8
2	D	296	TYR	2.8
2	D	542	GLY	2.8
1	A	30	VAL	2.8
2	D	546	VAL	2.8
2	C	462	ARG	2.8
2	D	212	PRO	2.8
2	C	140	GLN	2.8
2	C	114	ASN	2.8
2	D	356	ASN	2.8
2	D	566	THR	2.8
2	C	417	LEU	2.8
2	D	561	PHE	2.8
2	C	139	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	164	ILE	2.7
2	D	359	VAL	2.7
2	C	440	CYS	2.7
1	A	47	TRP	2.7
2	C	519	VAL	2.7
2	D	494	LEU	2.7
2	C	328	PHE	2.7
2	C	354	GLU	2.7
2	D	419	ALA	2.7
2	C	506	LEU	2.7
2	C	320	VAL	2.7
1	A	89	TRP	2.7
2	C	211	LEU	2.7
2	D	120	VAL	2.7
2	C	352	PRO	2.7
2	D	574	SER	2.7
2	D	353	MET	2.6
1	A	76	LEU	2.6
2	C	171	VAL	2.6
2	D	350	TYR	2.6
2	D	485	LEU	2.6
2	C	283	ILE	2.6
2	D	397	ILE	2.6
2	D	544	THR	2.6
2	D	220	PRO	2.6
2	C	313	TYR	2.6
2	D	147	PHE	2.6
2	D	176	VAL	2.6
2	C	461	ALA	2.6
2	D	221	CYS	2.6
2	C	220	PRO	2.6
1	B	100	THR	2.6
1	A	93	LEU	2.6
2	C	253	LEU	2.6
2	C	386	ALA	2.6
2	C	430	LEU	2.6
2	C	485	LEU	2.6
2	D	280	ALA	2.6
1	A	99	PHE	2.5
2	C	419	ALA	2.5
2	C	334	TYR	2.5
2	D	548	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	156	SER	2.5
2	D	565	SER	2.5
2	D	496	ALA	2.5
2	C	477	TRP	2.5
2	D	558	PRO	2.5
2	C	264	LEU	2.5
2	C	325	ALA	2.5
2	D	155	GLY	2.5
2	D	325	ALA	2.5
1	A	41	PHE	2.5
2	D	192	ASN	2.5
2	C	558	PRO	2.5
2	C	203	PHE	2.5
2	C	332	PHE	2.5
1	B	97	LEU	2.5
2	D	246	LEU	2.5
2	D	193	GLN	2.5
2	D	545	THR	2.4
2	D	233	PHE	2.4
2	C	246	LEU	2.4
2	D	455	LEU	2.4
1	B	28	ALA	2.4
2	D	191	SER	2.4
2	D	292	THR	2.4
2	D	522	MET	2.4
1	A	29	PHE	2.4
1	A	71	PHE	2.4
1	A	92	LEU	2.4
2	D	339	ILE	2.4
2	D	169	SER	2.4
2	C	329	THR	2.4
1	A	32	TRP	2.4
2	D	207	GLY	2.4
2	D	436	TRP	2.4
2	D	266	SER	2.4
2	D	125	CYS	2.4
2	C	458	LEU	2.4
2	D	211	LEU	2.4
2	D	254	LEU	2.4
2	D	337	THR	2.4
2	C	127	PRO	2.4
2	C	349	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	513	TRP	2.4
2	D	369	TRP	2.4
2	D	349	ARG	2.3
2	D	399	VAL	2.3
2	D	290	ILE	2.3
2	D	498	ILE	2.3
2	C	542	GLY	2.3
1	B	32	TRP	2.3
2	C	514	TRP	2.3
2	D	379	PRO	2.3
1	B	83	SER	2.3
2	C	176	VAL	2.3
2	C	576	ARG	2.3
2	D	300	VAL	2.3
1	B	84	LEU	2.3
2	C	125	CYS	2.3
2	C	170	PHE	2.3
2	C	304	THR	2.3
2	D	354	GLU	2.3
2	D	310	LEU	2.3
2	C	130	ILE	2.3
2	C	227	SER	2.3
2	C	552	PHE	2.3
2	D	520	PHE	2.3
2	D	314	ARG	2.2
2	C	448	VAL	2.2
2	C	276	LEU	2.2
2	D	234	LEU	2.2
2	C	476	ILE	2.2
2	D	476	ILE	2.2
2	C	213	PHE	2.2
2	C	409	GLN	2.2
1	B	30	VAL	2.2
2	D	492	GLY	2.2
2	C	537	ILE	2.2
1	B	99	PHE	2.2
2	C	221	CYS	2.2
2	C	538	CYS	2.2
2	C	173	ALA	2.2
2	D	225	ASN	2.2
1	B	64	VAL	2.2
2	D	223	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	78	PRO	2.2
1	A	86	PHE	2.2
2	C	365	PHE	2.2
1	B	14	CYS	2.2
1	B	49	PRO	2.2
2	C	568	PRO	2.2
2	C	285	GLY	2.2
1	B	45	TYR	2.1
2	D	201	GLN	2.1
1	B	43	LEU	2.1
2	C	391	LEU	2.1
2	D	373	LEU	2.1
2	D	381	LEU	2.1
2	D	262	THR	2.1
2	C	228	ALA	2.1
2	C	398	ALA	2.1
2	D	182	PRO	2.1
2	C	512	PHE	2.1
2	D	203	PHE	2.1
2	C	284	VAL	2.1
2	C	331	ALA	2.1
2	D	331	ALA	2.1
2	D	563	ASN	2.1
2	D	154	PRO	2.1
2	D	270	ARG	2.1
2	C	366	PHE	2.1
2	C	545	THR	2.1
2	C	218	ASP	2.1
1	B	93	LEU	2.1
2	C	196	LEU	2.1
2	C	529	ALA	2.1
2	D	430	LEU	2.1
2	D	402	ILE	2.1
2	D	174	SER	2.1
2	D	547	SER	2.1
2	C	350	TYR	2.1
2	D	559	ARG	2.1
2	C	198	ALA	2.1
2	D	287	MET	2.1
2	C	194	LEU	2.1
2	D	252	LEU	2.1
2	D	338	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	209	ALA	2.0
2	C	309	TYR	2.0
2	C	316	TYR	2.0
2	D	284	VAL	2.0
2	D	555	ASN	2.0
1	B	71	PHE	2.0
2	C	344	PHE	2.0
2	D	366	PHE	2.0
2	D	210	LEU	2.0
1	A	68	ILE	2.0
1	B	73	THR	2.0
1	B	69	VAL	2.0
1	B	56	PHE	2.0
2	D	276	LEU	2.0
2	D	332	PHE	2.0
2	D	342	PHE	2.0
1	A	5	ASP	2.0
2	D	268	ASN	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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CSO	D	150	7/8	0.91	0.13	-	5,6,8,10	0
2	CSO	C	150	7/8	0.94	0.10	-	2,5,7,9	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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	ACT	C	1606	4/4	0.47	0.27	6.80	22,23,24,25	0
8	BMA	C	1642	11/12	0.84	0.22	2.73	9,14,15,18	0
7	NAG	C	1630	14/15	0.74	0.23	1.85	18,22,27,28	0
7	NAG	D	2620	14/15	0.79	0.24	1.44	16,21,26,28	0
7	NAG	D	2630	14/15	0.75	0.26	1.37	26,30,34,35	0
7	NAG	C	1620	14/15	0.86	0.21	1.18	9,14,20,24	0
8	BMA	D	2642	11/12	0.87	0.17	1.17	9,12,14,18	0
7	NAG	C	1641	14/15	0.88	0.17	0.47	5,8,11,12	0
6	HEM	A	605	43/43	0.94	0.17	-0.16	2,5,8,8	0
7	NAG	D	2641	14/15	0.91	0.13	-0.32	6,8,10,11	0
6	HEM	B	605	43/43	0.93	0.16	-0.51	2,5,8,9	0
11	ACT	D	2606	4/4	0.91	0.12	-0.58	13,14,14,18	0
3	CA	B	600	1/1	1.00	0.13	-2.06	7,7,7,7	0
4	BR	B	889	1/1	0.98	0.06	-2.13	23,23,23,23	1
3	CA	A	600	1/1	1.00	0.10	-2.83	5,5,5,5	0
4	BR	A	889	1/1	0.99	0.06	-2.96	24,24,24,24	1
4	BR	B	758	1/1	0.94	0.12	-3.01	18,18,18,18	1
4	BR	B	601	1/1	1.00	0.10	-3.83	6,6,6,6	0
4	BR	A	758	1/1	0.98	0.07	-5.09	16,16,16,16	1
4	BR	A	601	1/1	1.00	0.09	-5.68	6,6,6,6	0
5	SO4	B	2602	5/5	0.48	0.33	-	42,42,43,44	5
9	MAN	D	2644	11/12	0.82	0.22	-	9,14,18,23	0
4	BR	A	843	1/1	0.97	0.14	-	12,12,12,12	1
5	SO4	C	1603	5/5	0.93	0.12	-	20,21,23,25	0
10	FUC	D	2645	10/11	0.80	0.22	-	10,14,16,19	0
5	SO4	A	1602	5/5	0.96	0.10	-	19,19,21,22	0
9	MAN	D	2643	11/12	0.68	0.26	-	17,20,22,23	0
11	ACT	D	2604	4/4	0.64	0.43	-	32,34,34,34	0
7	NAG	D	2640	14/15	0.88	0.15	-	9,10,15,16	0
9	MAN	C	1643	11/12	0.80	0.23	-	21,25,26,28	0
10	FUC	C	1645	10/11	0.85	0.14	-	9,13,15,17	0
7	NAG	C	1640	14/15	0.89	0.13	-	6,8,11,13	0
11	ACT	C	1607	4/4	0.79	0.26	-	22,23,23,25	0
11	ACT	C	1604	4/4	0.73	0.23	-	17,17,20,22	0
9	MAN	C	1644	11/12	0.86	0.18	-	13,15,17,18	0
4	BR	B	843	1/1	0.99	0.06	-	12,12,12,12	1
11	ACT	D	2607	4/4	0.48	0.29	-	29,30,30,31	0

## 6.5 Other polymers

There are no such residues in this entry.