



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:43 AM GMT

PDB ID : 1D5L  
Title : CRYSTAL STRUCTURE OF CYANIDE-BOUND HUMAN MYELOPER-  
OXIDASE ISOFORM C AT PH 5.5  
Authors : Fiedler, T.J.; Davey, C.A.; Fenna, R.E.  
Deposited on : 1999-10-07  
Resolution : 1.90 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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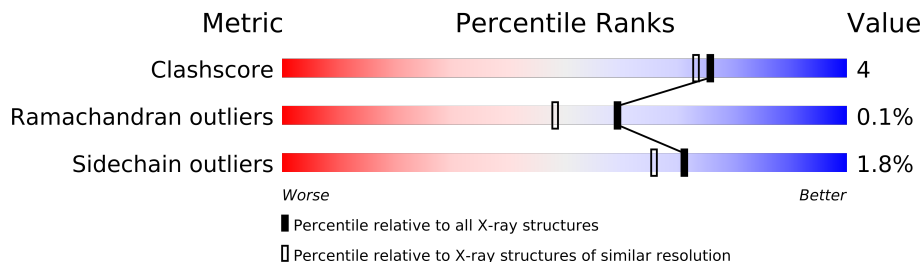
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
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 1.90 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	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	104	
1	B	104	
2	C	466	
2	D	466	

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 10347 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 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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	6	Total	C	N	O	0	0
			71	40	2	29		
4	D	6	Total	C	N	O	0	0
			71	40	2	29		

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

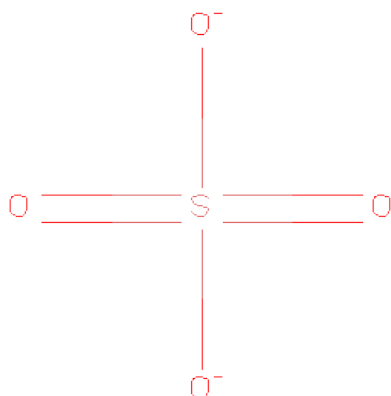
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

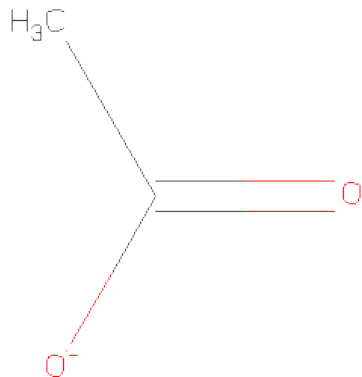
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



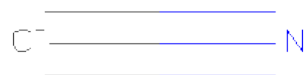
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



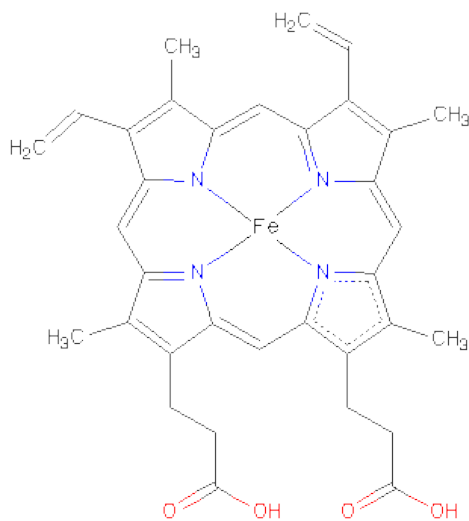
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	N	0	0
			2	1	1		
9	C	1	Total	C	N	0	0
			2	1	1		
9	B	1	Total	C	N	0	0
			2	1	1		
9	D	1	Total	C	N	0	0
			2	1	1		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	96	Total 96	O 96	0	0
11	B	105	Total 105	O 105	0	0
11	C	338	Total 338	O 338	0	0
11	D	327	Total 327	O 327	0	0

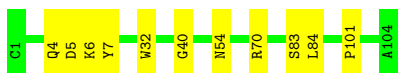
### 3 Residue-property plots

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.

Note EDS failed to run properly.

- Molecule 1: MYELOPEROXIDASE

Chain A: 



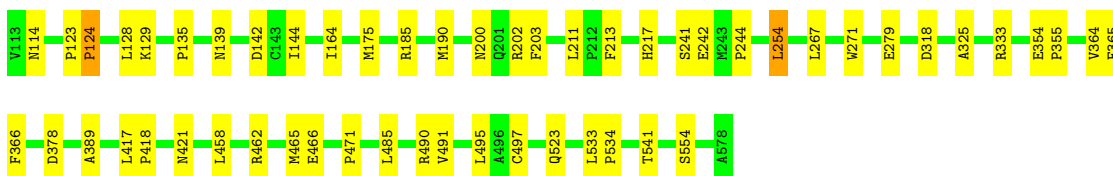
- Molecule 1: MYELOPEROXIDASE

Chain B: 



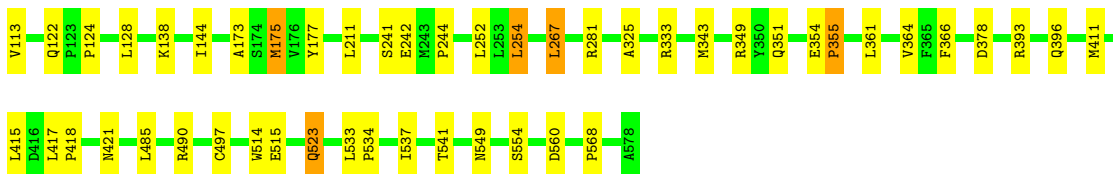
- Molecule 2: MYELOPEROXIDASE

Chain C: 



- Molecule 2: MYELOPEROXIDASE

Chain D: 



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.22Å 63.51Å 92.34Å 90.00° 97.43° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	91.3 (30.00-1.90)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.42 (at 1.91Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.172 , 0.215	Depositor
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.393	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 95626 reflections	Xtriage
Total number of atoms	10347	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: CSO, BMA, NAG, CL, SO4, CA, FUC, ACT, HEM, CYN, MAN

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	0.58	0/863	0.67	0/1174
1	B	0.57	0/863	0.66	0/1174
2	C	0.54	0/3811	0.59	0/5168
2	D	0.52	0/3811	0.57	0/5168
All	All	0.54	0/9348	0.60	0/12684

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	838	0	798	8	0
1	B	838	0	798	3	0
2	C	3733	0	3725	34	0
2	D	3733	0	3725	31	0
3	C	28	0	26	0	0
3	D	28	0	26	0	0
4	C	71	0	61	0	0
4	D	71	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
8	C	16	0	12	0	0
8	D	12	0	9	1	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	1	0
9	D	2	0	0	0	0
10	A	43	0	30	3	0
10	B	43	0	30	3	0
11	A	96	0	0	2	0
11	B	105	0	0	0	0
11	C	338	0	0	2	0
11	D	327	0	0	3	0
All	All	10347	0	9301	74	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 4.

All (74) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:411:MET:HE2	2:D:415:LEU:HD21	1.76	0.68
2:D:113:VAL:HG21	2:D:122:GLN:HB2	1.81	0.62
2:C:465:MET:HE1	2:C:471:PRO:HG3	1.81	0.62
11:A:1243(A):HOH:O	2:C:129:LYS:HD3	1.99	0.61
2:C:333:ARG:HH11	2:C:421:ASN:HD22	1.48	0.60
2:D:568:PRO:HG2	11:D:996(B):HOH:O	2.00	0.59
10:B:605:HEM:HMC2	10:B:605:HEM:HBC2	1.83	0.59
2:C:333:ARG:HH11	2:C:421:ASN:ND2	1.99	0.59
2:D:411:MET:CE	2:D:415:LEU:HD21	2.34	0.57
2:C:271:TRP:CZ3	2:C:279:GLU:HG3	2.41	0.56
2:C:135:PRO:HG2	11:C:1204(A):HOH:O	2.06	0.55
1:A:4:GLN:HG2	1:A:5:ASP:N	2.20	0.55
10:A:605:HEM:HMC2	10:A:605:HEM:HBC2	1.89	0.55
2:D:241:SER:O	2:D:366:PHE:HA	2.07	0.54
2:D:349:ARG:HG3	2:D:351:GLN:HG2	1.89	0.54
2:C:213:PHE:H	9:C:1889:CYN:C	2.20	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:333:ARG:HH11	2:D:421:ASN:ND2	2.04	0.54
10:B:605:HEM:HBB2	2:D:242:GLU:OE1	2.08	0.54
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.91	0.53
10:A:605:HEM:HBB2	2:C:242:GLU:OE1	2.09	0.52
2:C:491:VAL:HB	2:C:495:LEU:HB2	1.92	0.52
2:C:200:ASN:ND2	2:C:202:ARG:H	2.08	0.51
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.93	0.51
2:C:200:ASN:HD22	2:C:203:PHE:H	1.57	0.51
2:D:554:SER:HB3	2:D:560:ASP:HB3	1.93	0.51
1:A:70:ARG:HD2	11:A:650(A):HOH:O	2.10	0.50
8:D:2606:ACT:H1	11:D:981(B):HOH:O	2.11	0.50
2:D:244:PRO:HB2	2:D:343:MET:SD	2.52	0.50
2:D:534:PRO:HG2	2:D:549:ASN:ND2	2.26	0.50
2:C:465:MET:HE1	2:C:471:PRO:CG	2.41	0.49
1:A:83:SER:HB3	2:C:554:SER:O	2.12	0.49
2:C:211:LEU:HD23	2:C:254:LEU:HD13	1.93	0.49
2:D:378:ASP:OD1	2:D:541:THR:HB	2.13	0.48
2:C:417:LEU:HB3	2:C:418:PRO:HD3	1.95	0.48
2:C:200:ASN:HD22	2:C:202:ARG:H	1.59	0.48
2:D:333:ARG:HH11	2:D:421:ASN:HD22	1.61	0.48
1:B:83:SER:HB3	2:D:554:SER:O	2.13	0.47
2:C:354:GLU:HB3	2:C:355:PRO:HA	1.96	0.47
2:D:349:ARG:HE	2:D:351:GLN:HG3	1.80	0.47
2:C:242:GLU:O	2:C:365:PHE:HA	2.15	0.46
1:A:32:TRP:CE2	2:C:325:ALA:HB2	2.52	0.45
1:A:101:PRO:HD2	2:C:164:ILE:O	2.17	0.45
2:C:142:ASP:HB3	11:C:1239(A):HOH:O	2.17	0.45
1:B:32:TRP:CE2	2:D:325:ALA:HB2	2.52	0.44
2:C:462:ARG:O	2:C:466:GLU:HG2	2.18	0.44
2:C:458:LEU:O	2:C:462:ARG:HG3	2.18	0.44
1:A:84:LEU:HD13	2:C:389:ALA:HA	2.00	0.44
2:D:533:LEU:HB3	2:D:534:PRO:HD3	2.00	0.44
2:C:485:LEU:HD13	2:C:490:ARG:HA	2.00	0.43
2:D:173:ALA:HA	2:D:175:MET:SD	2.58	0.43
2:D:523:GLN:H	2:D:523:GLN:CD	2.22	0.43
2:C:123:PRO:HA	2:C:124:PRO:HA	1.78	0.43
2:C:533:LEU:N	2:C:534:PRO:CD	2.81	0.43
2:D:354:GLU:HB3	2:D:355:PRO:HA	2.00	0.42
2:C:139:ASN:HB2	2:C:142:ASP:OD1	2.18	0.42
2:C:378:ASP:OD1	2:C:541:THR:HB	2.19	0.42
10:A:605:HEM:HBC2	10:A:605:HEM:CMC	2.49	0.42
2:C:185:ARG:HG3	2:C:190:MET:CE	2.50	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:B:605:HEM:CMC	10:B:605:HEM:HBC2	2.50	0.42
2:D:211:LEU:HD23	2:D:254:LEU:HD13	2.01	0.42
1:A:40:GLY:HA2	1:B:20:PRO:HD2	2.02	0.41
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.55	0.41
2:D:177:TYR:OH	2:D:281:ARG:HA	2.20	0.41
2:C:244:PRO:HD3	2:C:364:VAL:O	2.21	0.41
2:D:549:ASN:ND2	11:D:829(B):HOH:O	2.53	0.41
2:D:485:LEU:HD13	2:D:490:ARG:HA	2.03	0.41
2:C:241:SER:O	2:C:366:PHE:HA	2.21	0.41
2:D:393:ARG:HB2	2:D:396:GLN:HB2	2.03	0.41
1:A:6:LYS:HE3	1:A:7:TYR:CZ	2.57	0.40
2:C:129:LYS:HB3	2:C:129:LYS:HE2	1.78	0.40
2:D:128:LEU:HB2	2:D:144:ILE:HB	2.03	0.40
2:D:252:LEU:HD11	2:D:537:ILE:HA	2.03	0.40
2:D:361:LEU:O	2:D:364:VAL:HG22	2.22	0.40
2:D:267:LEU:HD22	2:D:267:LEU:HA	1.84	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%)	2 (2%)	0	100	100
1	B	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	C	463/466 (99%)	453 (98%)	9 (2%)	1 (0%)	56	44
2	D	463/466 (99%)	453 (98%)	10 (2%)	0	100	100
All	All	1130/1140 (99%)	1105 (98%)	24 (2%)	1 (0%)	59	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	114	ASN

### 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%)	84	82
1	B	90/90 (100%)	89 (99%)	1 (1%)	84	82
2	C	410/410 (100%)	402 (98%)	8 (2%)	68	61
2	D	410/410 (100%)	402 (98%)	8 (2%)	68	61
All	All	1000/1000 (100%)	982 (98%)	18 (2%)	71	66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	124	PRO
2	C	175	MET
2	C	217	HIS
2	C	254	LEU
2	C	267	LEU
2	C	318	ASP
2	C	497	CYS
2	C	523	GLN
1	B	54	ASN
2	D	124	PRO
2	D	138	LYS
2	D	175	MET
2	D	254	LEU
2	D	267	LEU
2	D	355	PRO
2	D	497	CYS
2	D	523	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
2	C	122	GLN
2	C	200	ASN

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Mol	Chain	Res	Type
2	C	421	ASN
2	C	526	GLN
1	B	54	ASN
2	D	421	ASN
2	D	549	ASN

### 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	$\# Z  > 2$
2	CSO	C	150	2	6,6,7	7.42	3 (50%)	3,6,8	2.11	2 (66%)
2	CSO	D	150	2	6,6,7	8.32	3 (50%)	3,6,8	1.65	1 (33%)

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	-	0/2/5/7	0/0/0/0
2	CSO	D	150	2	-	0/2/5/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	150	CSO	O-C	19.79	1.25	1.11
2	C	150	CSO	O-C	17.54	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	150	CSO	CA-C	3.55	1.55	1.48
2	C	150	CSO	OD-SG	-3.23	1.48	1.62
2	C	150	CSO	CA-C	2.92	1.53	1.48
2	D	150	CSO	OD-SG	-2.82	1.50	1.62

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	150	CSO	C-CA-N	-2.58	111.25	113.83
2	C	150	CSO	CA-CB-SG	2.52	117.50	113.01
2	D	150	CSO	CA-CB-SG	2.21	116.93	113.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

12 carbohydrates 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	$\# Z  > 2$
4	NAG	C	1640	2,4	12,14,15	0.73	0	15,19,21	0.89	0
4	NAG	C	1641	4	12,14,15	0.52	0	15,19,21	0.65	0
4	BMA	C	1642	4	10,11,12	0.56	0	11,15,17	0.49	0
4	MAN	C	1643	4	10,11,12	0.36	0	11,15,17	0.37	0
4	MAN	C	1644	4	10,11,12	0.40	0	11,15,17	0.59	0
4	FUC	C	1645	4	9,10,11	0.46	0	10,14,16	0.55	0
4	NAG	D	2640	2,4	12,14,15	0.46	0	15,19,21	0.89	0
4	NAG	D	2641	4	12,14,15	0.41	0	15,19,21	0.64	0
4	BMA	D	2642	4	10,11,12	0.57	0	11,15,17	0.68	0
4	MAN	D	2643	4	10,11,12	0.49	0	11,15,17	0.63	0
4	MAN	D	2644	4	10,11,12	0.49	0	11,15,17	0.46	0
4	FUC	D	2645	4	9,10,11	0.55	0	10,14,16	0.33	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
4	NAG	C	1640	2,4	-	0/6/23/26	0/1/1/1
4	NAG	C	1641	4	-	0/6/23/26	0/1/1/1
4	BMA	C	1642	4	-	0/2/19/22	0/1/1/1
4	MAN	C	1643	4	-	0/2/19/22	0/1/1/1
4	MAN	C	1644	4	-	0/2/19/22	0/1/1/1
4	FUC	C	1645	4	-	0/0/17/20	0/1/1/1
4	NAG	D	2640	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2641	4	-	0/6/23/26	0/1/1/1
4	BMA	D	2642	4	-	0/2/19/22	0/1/1/1
4	MAN	D	2643	4	-	0/2/19/22	0/1/1/1
4	MAN	D	2644	4	-	0/2/19/22	0/1/1/1
4	FUC	D	2645	4	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	$\# Z  > 2$
7	SO4	A	1602	-	4,4,4	0.18	0	6,6,6	0.11	0
9	CYN	A	1844	10	1,1,1	0.44	0	0,0,0	0.00	-
10	HEM	A	605	1,9,2	49,50,50	2.34	12 (24%)	46,82,82	1.17	4 (8%)
9	CYN	B	2844	10	1,1,1	0.33	0	0,0,0	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	HEM	B	605	1,9,2	49,50,50	2.21	9 (18%)	46,82,82	1.12	3 (6%)
7	SO4	C	1603	-	4,4,4	0.17	0	6,6,6	0.10	0
8	ACT	C	1604	-	1,3,3	2.08	1 (100%)	0,3,3	0.00	-
8	ACT	C	1606	-	1,3,3	1.98	0	0,3,3	0.00	-
8	ACT	C	1607	-	1,3,3	2.98	1 (100%)	0,3,3	0.00	-
8	ACT	C	1612	-	1,3,3	2.71	1 (100%)	0,3,3	0.00	-
3	NAG	C	1620	2	12,14,15	0.44	0	15,19,21	0.84	0
3	NAG	C	1630	2	12,14,15	0.54	0	15,19,21	0.65	0
9	CYN	C	1889	-	1,1,1	0.43	0	0,0,0	0.00	-
7	SO4	D	2602	-	4,4,4	0.24	0	6,6,6	0.06	0
8	ACT	D	2604	-	1,3,3	2.57	1 (100%)	0,3,3	0.00	-
8	ACT	D	2606	-	1,3,3	2.00	0	0,3,3	0.00	-
8	ACT	D	2607	-	1,3,3	2.45	1 (100%)	0,3,3	0.00	-
3	NAG	D	2620	2	12,14,15	0.33	0	15,19,21	0.74	0
3	NAG	D	2630	2	12,14,15	0.57	0	15,19,21	0.90	0
9	CYN	D	2889	-	1,1,1	0.41	0	0,0,0	0.00	-

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
7	SO4	A	1602	-	-	0/0/0/0	0/0/0/0
9	CYN	A	1844	10	-	0/0/0/0	0/0/0/0
10	HEM	A	605	1,9,2	-	0/14/114/114	0/0/8/8
9	CYN	B	2844	10	-	0/0/0/0	0/0/0/0
10	HEM	B	605	1,9,2	-	0/14/114/114	0/0/8/8
7	SO4	C	1603	-	-	0/0/0/0	0/0/0/0
8	ACT	C	1604	-	-	0/0/0/0	0/0/0/0
8	ACT	C	1606	-	-	0/0/0/0	0/0/0/0
8	ACT	C	1607	-	-	0/0/0/0	0/0/0/0
8	ACT	C	1612	-	-	0/0/0/0	0/0/0/0
3	NAG	C	1620	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1630	2	-	0/6/23/26	0/1/1/1
9	CYN	C	1889	-	-	0/0/0/0	0/0/0/0
7	SO4	D	2602	-	-	0/0/0/0	0/0/0/0
8	ACT	D	2604	-	-	0/0/0/0	0/0/0/0
8	ACT	D	2606	-	-	0/0/0/0	0/0/0/0
8	ACT	D	2607	-	-	0/0/0/0	0/0/0/0
3	NAG	D	2620	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	2630	2	-	0/6/23/26	0/1/1/1
9	CYN	D	2889	-	-	0/0/0/0	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	605	HEM	C3D-C4D	9.21	1.46	1.44
10	B	605	HEM	C2B-C1B	8.28	1.46	1.44
10	A	605	HEM	C2D-C1D	6.95	1.46	1.44
10	B	605	HEM	C2D-C1D	6.54	1.46	1.44
10	B	605	HEM	C4A-C3A	4.70	1.46	1.40
10	B	605	HEM	C3D-C2D	-4.60	1.35	1.43
10	A	605	HEM	C3D-C2D	-4.37	1.36	1.43
10	B	605	HEM	C3B-C2B	-4.21	1.36	1.43
10	A	605	HEM	C2B-C1B	4.13	1.45	1.44
10	A	605	HEM	C3B-C2B	-3.92	1.36	1.43
10	A	605	HEM	C4A-C3A	3.51	1.44	1.40
10	A	605	HEM	C3C-C2C	-3.12	1.38	1.43
10	B	605	HEM	C3C-C2C	-3.02	1.38	1.43
10	B	605	HEM	CBB-CAB	2.99	1.46	1.28
8	C	1607	ACT	CH3-C	2.98	1.53	1.48
10	A	605	HEM	CBB-CAB	2.93	1.45	1.28
10	B	605	HEM	CBC-CAC	2.73	1.44	1.28
10	A	605	HEM	CBC-CAC	2.72	1.44	1.28
8	C	1612	ACT	CH3-C	2.71	1.52	1.48
8	D	2604	ACT	CH3-C	2.57	1.52	1.48
10	A	605	HEM	CHA-C4D	2.56	1.39	1.35
10	B	605	HEM	CHB-C1B	2.54	1.39	1.35
8	D	2607	ACT	CH3-C	2.45	1.52	1.48
10	A	605	HEM	C3B-C4B	2.18	1.47	1.44
8	C	1604	ACT	CH3-C	2.08	1.51	1.48
10	A	605	HEM	CMB-C2B	2.04	1.53	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	605	HEM	C3B-C4B-NB	-3.18	111.72	114.00
10	A	605	HEM	C3A-C4A-NA	2.80	111.52	109.41
10	B	605	HEM	C3A-C4A-NA	2.79	111.52	109.41
10	B	605	HEM	C4A-NA-C1A	-2.47	103.51	106.76
10	B	605	HEM	C3B-C4B-NB	-2.37	112.31	114.00
10	A	605	HEM	C1A-CHA-C4D	-2.35	124.37	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	605	HEM	C4A-NA-C1A	-2.29	103.75	106.76

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.