



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:52 AM GMT

PDB ID : 4C1M
Title : Myeloperoxidase in complex with the reversible inhibitor HX1
Authors : Forbes, L.V.; Sjogren, T.; Auchere, F.; Jenkins, D.W.; Thong, B.; Laughton, D.; Hemsley, P.; Pairaudeau, G.; Eriksson, H.; Unitt, J.F.; Kettle, A.J.
Deposited on : 2013-08-13
Resolution : 2.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

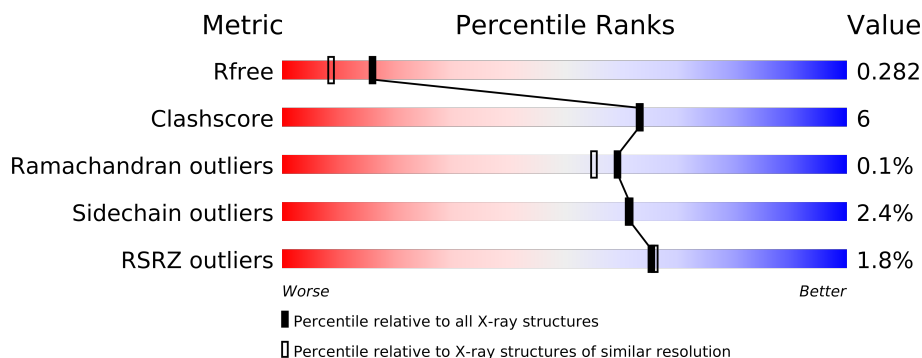
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	108	
1	B	108	
2	C	467	
2	D	467	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	NIH	A	606	-	X
4	NIH	B	606	-	X
5	SO4	B	1003	-	X
6	GOL	C	631	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	D	631	-	X
9	ACT	D	1581	-	X
9	ACT	D	1582	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10168 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.

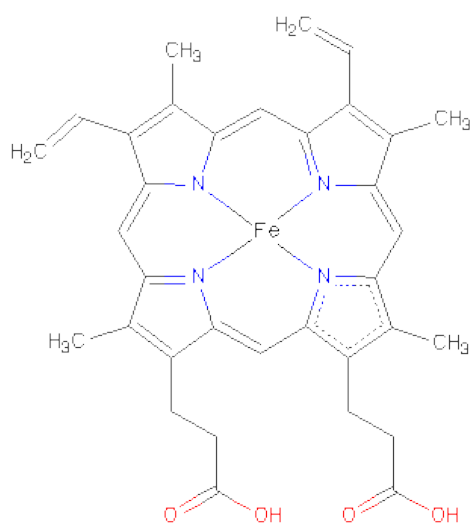
- Molecule 1 is a protein called MYELOPEROXIDASE LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	1
			816	516	146	150	4			
1	B	105	Total	C	N	O	S	0	0	1
			838	529	149	155	5			

- Molecule 2 is a protein called MYELOPEROXIDASE HEAVY CHAIN.

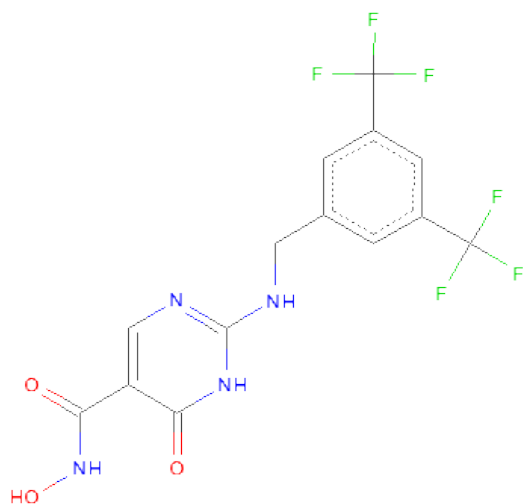
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			
2	D	467	Total	C	N	O	S	0	0	1
			3733	2351	688	667	27			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is 2-{[3,5-BIS(TRIFLUOROMETHYL)BENZYL]AMINO}-N-HYDROXY-6-OXO-1,6-DIHYDROPYRIMIDINE-5-CARBOXAMIDE (three-letter code: NIH) (formula: C₁₄H₁₀F₆N₄O₃).



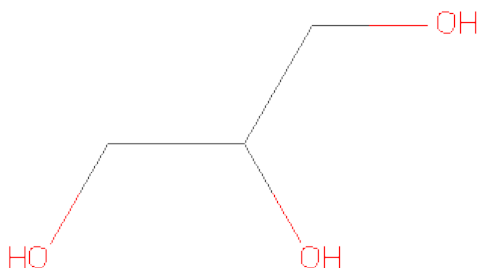
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			27	14	6	4	3		
4	B	1	Total	C	F	N	O	0	0
			27	14	6	4	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

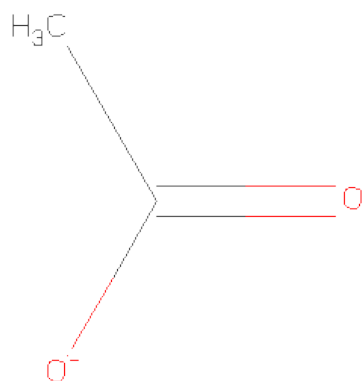
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

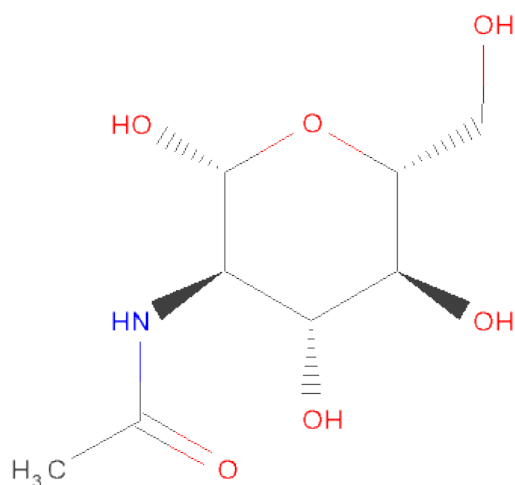
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total	Cl	0	0
			1	1		
8	C	1	Total	Cl	0	0
			1	1		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 11 is a polymer of unknown type called SUGAR (6-MER).

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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	103	Total	O	0	0
			103	103		
12	B	108	Total	O	0	0
			108	108		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	254	Total 254	O 254	0	0
12	D	199	Total 199	O 199	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.

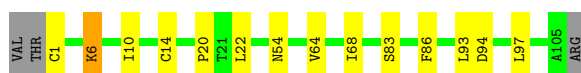
- Molecule 1: MYELOPEROXIDASE LIGHT CHAIN

Chain A: 



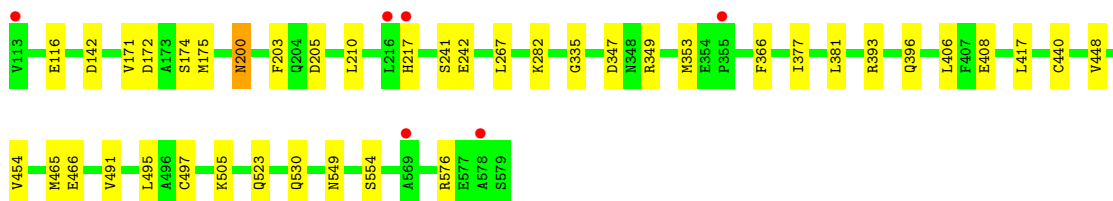
- Molecule 1: MYELOPEROXIDASE LIGHT CHAIN

Chain B: 



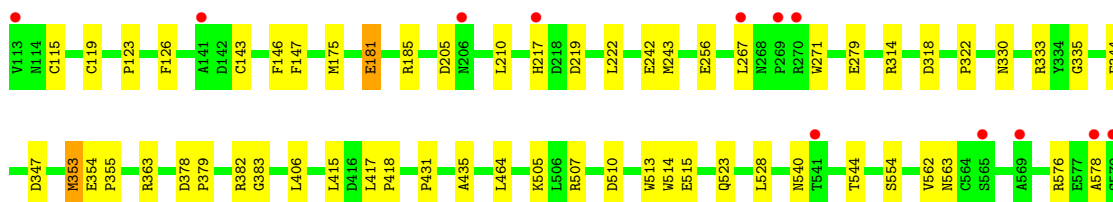
- Molecule 2: MYELOPEROXIDASE HEAVY CHAIN

Chain C: 



- Molecule 2: MYELOPEROXIDASE HEAVY CHAIN

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.28Å 63.44Å 92.38Å 90.00° 97.36° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 55.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-2.00) 94.0 (55.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.222 , 0.278 0.227 , 0.282	Depositor DCC
R_{free} test set	4064 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.945	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 25.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 81440 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	10168	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: GOL, CSO, BMA, NAG, CL, SO4, CA, NIH, FUC, ACT, HEM, 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	0.81	1/840 (0.1%)	0.87	1/1144 (0.1%)
1	B	0.73	0/863	0.82	0/1176
2	C	0.76	0/3811	0.79	0/5170
2	D	0.69	0/3811	0.74	1/5170 (0.0%)
All	All	0.73	1/9325 (0.0%)	0.78	2/12660 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	ALA	C-N	-5.02	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	510	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	94	ASP	CB-CG-OD2	-5.19	113.63	118.30

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	816	0	779	13	0
1	B	838	0	800	15	0
2	C	3733	0	3727	31	0
2	D	3733	0	3729	41	0
3	A	43	0	30	10	0
3	B	43	0	30	17	0
4	A	27	0	10	1	0
4	B	27	0	10	1	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	C	8	0	6	0	0
9	D	12	0	9	0	0
10	C	28	0	26	0	0
10	D	28	0	26	0	0
11	C	71	0	61	6	0
11	D	71	0	61	4	0
12	A	103	0	0	4	0
12	B	108	0	0	2	0
12	C	254	0	0	10	0
12	D	199	0	0	7	0
All	All	10168	0	9320	104	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 6.

The worst 5 of 104 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:605:HEM:HBB1	2:D:243:MET:SD	1.57	1.44
1:A:94:ASP:OD2	3:A:605:HEM:CMD	1.64	1.44
3:A:605:HEM:CMB	2:C:242:GLU:OE2	1.69	1.37
3:B:605:HEM:CBB	2:D:243:MET:SD	2.13	1.35
3:A:605:HEM:HMB1	2:C:242:GLU:OE2	1.17	1.33

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	100/108 (93%)	97 (97%)	3 (3%)	0	100	100
1	B	103/108 (95%)	100 (97%)	3 (3%)	0	100	100
2	C	464/467 (99%)	449 (97%)	15 (3%)	0	100	100
2	D	464/467 (99%)	452 (97%)	11 (2%)	1 (0%)	56	51
All	All	1131/1150 (98%)	1098 (97%)	32 (3%)	1 (0%)	59	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	578	ALA

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	87/93 (94%)	86 (99%)	1 (1%)	84	86
1	B	90/93 (97%)	88 (98%)	2 (2%)	64	65
2	C	410/411 (100%)	400 (98%)	10 (2%)	61	61
2	D	410/411 (100%)	399 (97%)	11 (3%)	57	56
All	All	997/1008 (99%)	973 (98%)	24 (2%)	61	61

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	466	GLU
2	D	175	MET
2	D	544	THR

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Mol	Chain	Res	Type
2	C	523	GLN
2	C	576	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	B	80	GLN
2	C	200	ASN
2	C	421	ASN
2	C	530	GLN

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	7.34	3 (50%)	3,6,8	2.16	1 (33%)
2	CSO	D	150	2	6,6,7	7.53	2 (33%)	3,6,8	2.48	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSO	D	150	2	-	0/2/5/7	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	150	CSO	O-C	17.90	1.23	1.11
2	C	150	CSO	O-C	17.30	1.23	1.11
2	D	150	CSO	CB-SG	-3.69	1.78	1.82
2	C	150	CSO	CB-SG	-3.66	1.78	1.82
2	C	150	CSO	CA-C	2.48	1.52	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	150	CSO	C-CA-N	-4.23	109.60	113.83
2	C	150	CSO	C-CA-N	-3.42	110.41	113.83

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
11	NAG	C	1640	11,2	12,14,15	0.95	0	15,19,21	2.05	4 (26%)
11	NAG	C	1641	11	12,14,15	1.59	2 (16%)	15,19,21	1.60	4 (26%)
11	BMA	C	1642	11	10,11,12	0.62	0	11,15,17	1.94	3 (27%)
11	MAN	C	1643	11	10,11,12	0.67	0	11,15,17	1.44	1 (9%)
11	MAN	C	1644	11	10,11,12	1.16	1 (10%)	11,15,17	1.21	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	FUC	C	1645	11	9,10,11	0.87	0	10,14,16	2.19	4 (40%)
11	NAG	D	2640	11,2	12,14,15	0.78	1 (8%)	15,19,21	1.65	3 (20%)
11	NAG	D	2641	11	12,14,15	1.31	2 (16%)	15,19,21	1.66	3 (20%)
11	BMA	D	2642	11	10,11,12	1.26	1 (10%)	11,15,17	2.76	6 (54%)
11	MAN	D	2643	11	10,11,12	0.63	0	11,15,17	3.58	3 (27%)
11	MAN	D	2644	11	10,11,12	0.65	0	11,15,17	1.13	2 (18%)
11	FUC	D	2645	11	9,10,11	0.94	1 (11%)	10,14,16	1.51	2 (20%)

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
11	NAG	C	1640	11,2	-	0/6/23/26	0/1/1/1
11	NAG	C	1641	11	-	0/6/23/26	0/1/1/1
11	BMA	C	1642	11	-	0/2/19/22	0/1/1/1
11	MAN	C	1643	11	-	0/2/19/22	0/1/1/1
11	MAN	C	1644	11	-	0/2/19/22	0/1/1/1
11	FUC	C	1645	11	-	0/0/17/20	0/1/1/1
11	NAG	D	2640	11,2	-	0/6/23/26	0/1/1/1
11	NAG	D	2641	11	-	0/6/23/26	0/1/1/1
11	BMA	D	2642	11	-	0/2/19/22	0/1/1/1
11	MAN	D	2643	11	-	0/2/19/22	0/1/1/1
11	MAN	D	2644	11	-	0/2/19/22	0/1/1/1
11	FUC	D	2645	11	-	0/0/17/20	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1641	NAG	C2-N2	-4.43	1.41	1.46
11	D	2641	NAG	C2-N2	-3.46	1.42	1.46
11	D	2642	BMA	C4-C5	3.05	1.59	1.53
11	C	1644	MAN	O5-C5	-2.96	1.39	1.45
11	C	1641	NAG	O5-C5	-2.55	1.40	1.45

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	2643	MAN	O5-C5-C6	10.42	117.92	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1640	NAG	C3-C2-N2	-5.94	102.71	111.76
11	D	2642	BMA	O5-C5-C4	4.11	115.86	110.65
11	C	1643	MAN	O5-C5-C6	4.07	111.25	106.98
11	C	1645	FUC	O5-C5-C4	4.04	116.32	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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
3	HEM	A	605	2	49,50,50	4.47	27 (55%)	46,82,82	2.21	16 (34%)
4	NIH	A	606	-	28,28,28	1.37	3 (10%)	39,42,42	1.38	4 (10%)
5	SO4	B	1003	-	4,4,4	0.51	0	6,6,6	0.32	0
3	HEM	B	605	2	49,50,50	5.46	27 (55%)	46,82,82	2.08	16 (34%)
4	NIH	B	606	-	28,28,28	1.36	3 (10%)	39,42,42	1.55	6 (15%)
5	SO4	C	1581	-	4,4,4	0.42	0	6,6,6	0.42	0
9	ACT	C	1582	-	1,3,3	1.67	0	0,3,3	0.00	-
9	ACT	C	1583	-	1,3,3	1.36	0	0,3,3	0.00	-
10	NAG	C	1620	2	12,14,15	0.89	1 (8%)	15,19,21	1.37	2 (13%)
10	NAG	C	1630	2	12,14,15	0.78	0	15,19,21	1.81	4 (26%)
6	GOL	C	631	-	5,5,5	0.29	0	5,5,5	0.42	0
9	ACT	D	1581	-	1,3,3	1.71	0	0,3,3	0.00	-
9	ACT	D	1582	-	1,3,3	0.97	0	0,3,3	0.00	-
9	ACT	D	1583	-	1,3,3	1.38	0	0,3,3	0.00	-
10	NAG	D	2620	2	12,14,15	0.67	0	15,19,21	1.40	1 (6%)
10	NAG	D	2630	2	12,14,15	0.66	0	15,19,21	1.50	3 (20%)
6	GOL	D	631	-	5,5,5	0.35	0	5,5,5	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	605	2	-	0/14/114/114	0/0/8/8
4	NIH	A	606	-	-	0/23/23/23	0/2/2/2
5	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
3	HEM	B	605	2	-	0/14/114/114	0/0/8/8
4	NIH	B	606	-	-	0/23/23/23	0/2/2/2
5	SO4	C	1581	-	-	0/0/0/0	0/0/0/0
9	ACT	C	1582	-	-	0/0/0/0	0/0/0/0
9	ACT	C	1583	-	-	0/0/0/0	0/0/0/0
10	NAG	C	1620	2	-	0/6/23/26	0/1/1/1
10	NAG	C	1630	2	-	0/6/23/26	0/1/1/1
6	GOL	C	631	-	-	0/4/4/4	0/0/0/0
9	ACT	D	1581	-	-	0/0/0/0	0/0/0/0
9	ACT	D	1582	-	-	0/0/0/0	0/0/0/0
9	ACT	D	1583	-	-	0/0/0/0	0/0/0/0
10	NAG	D	2620	2	-	0/6/23/26	0/1/1/1
10	NAG	D	2630	2	-	0/6/23/26	0/1/1/1
6	GOL	D	631	-	-	0/4/4/4	0/0/0/0

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	605	HEM	C2D-C1D	24.15	1.50	1.44
3	B	605	HEM	C2B-C1B	18.98	1.49	1.44
3	A	605	HEM	C2D-C1D	18.68	1.49	1.44
3	A	605	HEM	C3D-C4D	15.39	1.48	1.44
3	B	605	HEM	C3D-C4D	11.35	1.47	1.44

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	HEM	C3B-C4B-NB	-7.07	108.94	114.00
4	A	606	NIH	C4-N3-C2	5.40	121.79	117.03
3	A	605	HEM	C3A-C4A-NA	4.75	113.00	109.41
3	B	605	HEM	CHC-C4B-NB	4.69	128.48	124.58
4	B	606	NIH	C4-N3-C2	4.68	121.16	117.03

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	102/108 (94%)	0.02	2 (1%) 62 62	4, 8, 21, 44	0
1	B	105/108 (97%)	-0.01	0 100 100	6, 11, 26, 35	0
2	C	467/467 (100%)	0.01	6 (1%) 74 74	3, 10, 24, 37	0
2	D	467/467 (100%)	0.17	12 (2%) 53 53	4, 15, 32, 42	0
All	All	1141/1150 (99%)	0.07	20 (1%) 65 66	3, 12, 29, 44	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ALA	11.4
2	D	578	ALA	5.0
2	C	113	VAL	3.9
2	D	113	VAL	3.9
2	D	269	PRO	3.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CSO	D	150	7/8	0.11	0.04	8,10,16,19	0
2	CSO	C	150	7/8	0.09	-1.44	5,6,10,12	0

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
11	MAN	D	2643	11/12	0.31	30.04	36,43,46,46	0
11	MAN	D	2644	11/12	0.21	18.15	21,24,25,29	0
11	BMA	C	1642	11/12	0.26	8.41	19,23,28,32	0
11	BMA	D	2642	11/12	0.19	6.68	24,27,36,41	0
11	MAN	C	1643	11/12	0.25	6.16	36,42,46,48	0
11	FUC	D	2645	10/11	0.21	5.09	23,25,28,30	0
11	FUC	C	1645	10/11	0.18	2.83	17,20,21,22	0
11	NAG	C	1641	14/15	0.13	1.12	8,10,12,15	0
11	NAG	C	1640	14/15	0.13	0.54	10,11,14,15	0
11	MAN	C	1644	11/12	0.12	0.32	24,25,27,28	0
11	NAG	D	2641	14/15	0.12	0.00	9,11,13,17	0
11	NAG	D	2640	14/15	0.13	-0.21	10,12,13,17	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	B	1003	5/5	0.36	19.61	29,29,31,31	5
9	ACT	D	1582	4/4	0.24	12.57	39,39,40,40	0
4	NIH	B	606	27/27	0.33	8.00	10,12,13,14	27
4	NIH	A	606	27/27	0.26	6.94	4,6,7,8	27
6	GOL	C	631	6/6	0.20	6.04	35,39,41,46	0
9	ACT	D	1581	4/4	0.19	3.06	22,27,27,28	0
6	GOL	D	631	6/6	0.20	2.65	32,34,36,37	0
3	HEM	A	605	43/43	0.13	0.88	4,5,7,10	0
8	CL	D	1580	1/1	0.13	0.88	6,6,6,6	0
9	ACT	C	1582	4/4	0.16	0.69	35,37,38,38	0
10	NAG	C	1620	14/15	0.13	0.43	15,17,19,20	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HEM	B	605	43/43	0.12	0.30	5,7,9,12	0
10	NAG	C	1630	14/15	0.14	0.06	19,21,24,25	0
5	SO4	C	1581	5/5	0.12	0.01	34,34,36,37	0
10	NAG	D	2620	14/15	0.15	-0.08	22,23,25,27	0
10	NAG	D	2630	14/15	0.15	-0.52	31,34,36,37	0
9	ACT	C	1583	4/4	0.11	-0.99	25,26,27,27	0
9	ACT	D	1583	4/4	0.09	-1.51	34,34,34,36	0
8	CL	C	1580	1/1	0.10	-1.97	4,4,4,4	0
7	CA	D	1579	1/1	0.06	-3.00	7,7,7,7	0
7	CA	C	1579	1/1	0.03	-12.06	4,4,4,4	0

6.5 Other polymers ⓘ

There are no such residues in this entry.