



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:33 PM GMT

PDB ID : 3ZS0  
Title : Human Myeloperoxidase inactivated by TX2  
Authors : Tiden, A.K.; Sjogren, T.; Svensson, M.; Bernlind, A.; Senthilmohan, R.; Auchere, F.; Norman, H.; Markgren, P.O.; Gustavsson, S.; Schmidt, S.; Lundquist, S.; Forbes, L.V.; Magon, N.J.; Jameson, G.N.; Eriksson, H.; Kettle, A.J.  
Deposited on : 2011-06-21  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

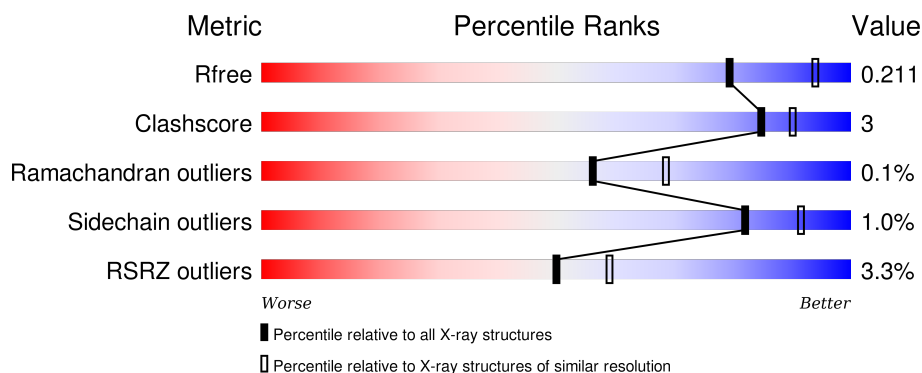
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	108	<div> <div>5%</div> <div>89%</div> <div>6%</div> <div>• •</div> </div>
1	B	108	<div> <div>2%</div> <div>93%</div> <div>• • •</div> </div>
2	C	467	<div> <div>2%</div> <div>94%</div> <div>5%</div> </div>
2	D	467	<div> <div>4%</div> <div>91%</div> <div>8%</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	BMA	D	1586	-	-	-	X
4	ZS0	C	1579	-	-	-	X
7	BMA	C	1586	-	-	-	X
7	MAN	C	1587	X	-	-	-

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 10054 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.

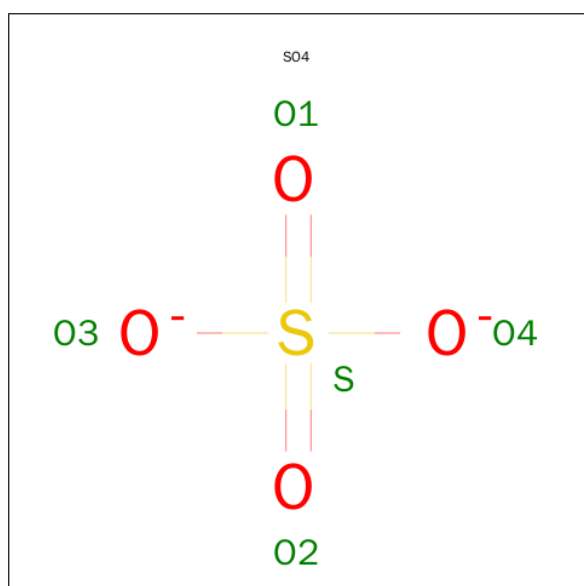
- Molecule 1 is a protein called MYELOPEROXIDASE LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			837	529	148	155	5			
1	B	104	Total	C	N	O	S	0	0	0
			837	529	148	155	5			

- Molecule 2 is a protein called MYELOPEROXIDASE HEAVY CHAIN.

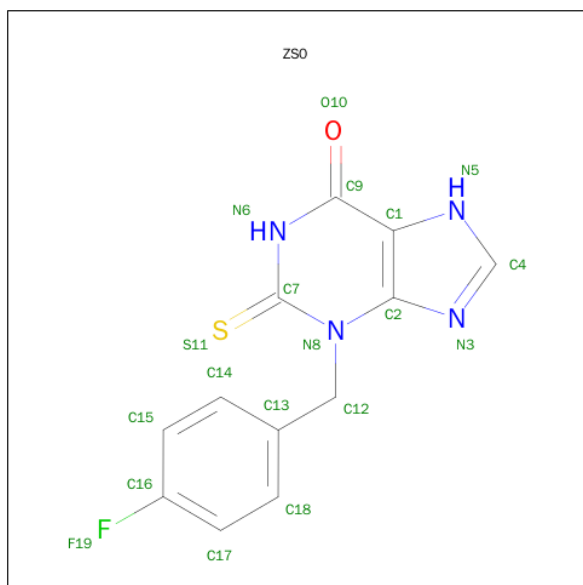
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	466	Total	C	N	O	S	0	0	0
			3732	2351	687	667	27			
2	D	466	Total	C	N	O	S	0	0	0
			3732	2351	687	667	27			

- Molecule 3 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



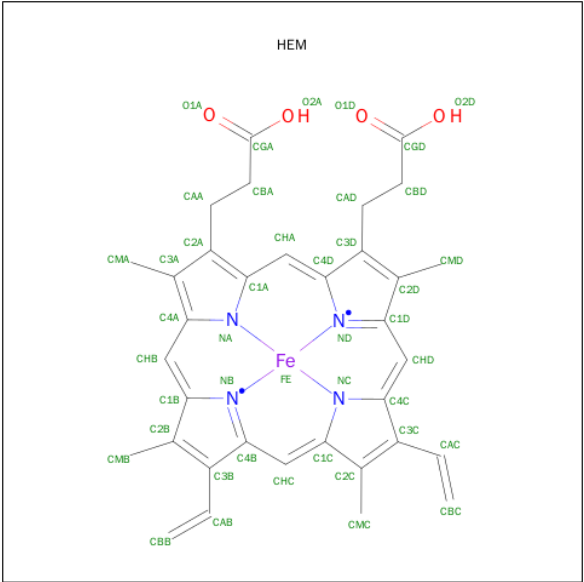
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is 3-(4-FLUOROBENZYL)-2-THIOXO-1,2,3,7-TETRAHYDRO-6H-PURIN-6-ONE (three-letter code: ZS0) (formula: C<sub>12</sub>H<sub>9</sub>FN<sub>4</sub>OS).



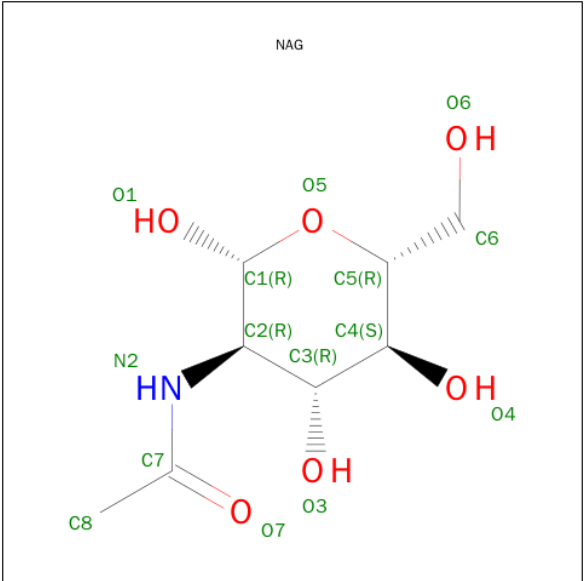
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C F N O S 19 12 1 4 1 1	0	0
4	D	1	Total C F N O S 19 12 1 4 1 1	0	0

- Molecule 5 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
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

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

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

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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 10 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
10	C	1	Total	C	O	0	0
			4	2	2		
10	C	1	Total	C	O	0	0
			4	2	2		
10	C	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		
10	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	99	Total	O	0	0
			99	99		
12	B	88	Total	O	0	0
			88	88		

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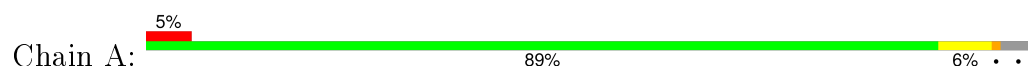
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	226	Total 226	O 226	0	0
12	D	149	Total 149	O 149	0	0

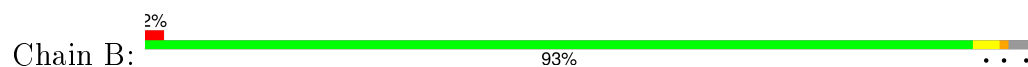
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

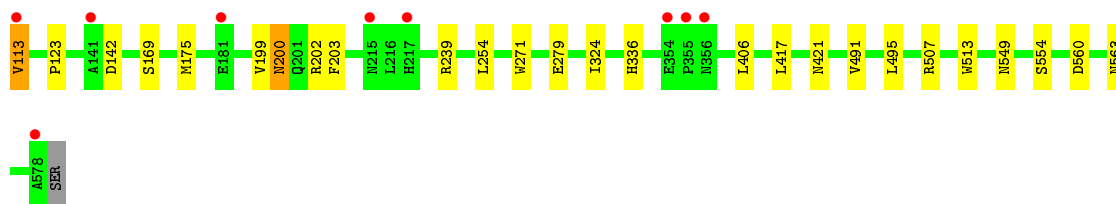
- Molecule 1: MYELOPEROXIDASE LIGHT CHAIN



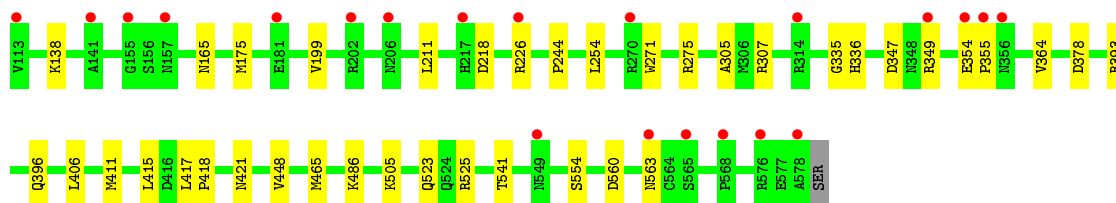
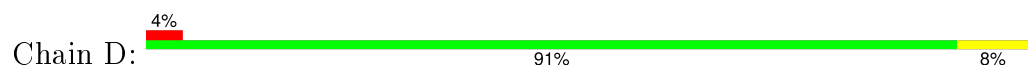
- Molecule 1: MYELOPEROXIDASE LIGHT CHAIN



- Molecule 2: MYELOPEROXIDASE HEAVY CHAIN



- Molecule 2: MYELOPEROXIDASE HEAVY CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.91Å 64.11Å 111.45Å 90.00° 97.12° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 32.71 – 2.21	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-2.30) 94.8 (32.71-2.21)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.170 , 0.207 0.174 , 0.211	Depositor DCC
$R_{free}$ test set	2878 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 62489 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, ZS0, NAG, CL, SO4, CA, 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	0.56	0/862	0.78	0/1174
1	B	0.53	0/862	0.76	0/1174
2	C	0.54	0/3810	0.69	1/5168 (0.0%)
2	D	0.54	0/3810	0.66	0/5168
All	All	0.54	0/9344	0.69	1/12684 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	1	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	C	142	ASP	CB-CG-OD1	5.82	123.54	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	1587	MAN	C1

There are no planarity outliers.

## 5.2 Too-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 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	837	0	798	8	0
1	B	837	0	798	4	0
2	C	3732	0	3725	17	0
2	D	3732	0	3725	27	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
4	C	19	0	9	1	0
4	D	19	0	9	0	0
5	C	43	0	30	5	0
5	D	43	0	30	1	0
6	C	28	0	26	0	0
6	D	28	0	26	0	0
7	C	71	0	61	1	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	C	12	0	9	0	0
10	D	12	0	9	2	0
11	D	60	0	52	0	0
12	A	99	0	0	1	0
12	B	88	0	0	0	0
12	C	226	0	0	3	0
12	D	149	0	0	5	0
All	All	10054	0	9307	53	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 3.

The worst 5 of 53 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASP:CG	5:C:1580:HEM:HMD1	1.77	1.04
1:A:94:ASP:OD2	5:C:1580:HEM:HMD1	0.68	0.85
1:B:6:LYS:H	1:B:6:LYS:HD2	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LYS:N	1:B:6:LYS:HD2	2.00	0.76
2:C:113:VAL:HG21	2:C:123:PRO:O	1.87	0.72

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	102/108 (94%)	98 (96%)	3 (3%)	1 (1%)	19	21
1	B	102/108 (94%)	100 (98%)	2 (2%)	0	100	100
2	C	463/467 (99%)	448 (97%)	15 (3%)	0	100	100
2	D	463/467 (99%)	452 (98%)	11 (2%)	0	100	100
All	All	1130/1150 (98%)	1098 (97%)	31 (3%)	1 (0%)	56	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO

### 5.3.2 Protein sidechains [i](#)

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	90/93 (97%)	88 (98%)	2 (2%)	60	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	90/93 (97%)	88 (98%)	2 (2%)	60	77
2	C	410/411 (100%)	407 (99%)	3 (1%)	88	95
2	D	410/411 (100%)	407 (99%)	3 (1%)	88	95
All	All	1000/1008 (99%)	990 (99%)	10 (1%)	82	91

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	113	VAL
2	C	175	MET
2	D	175	MET
1	B	54	ASN
2	C	200	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	200	ASN
2	D	549	ASN
2	C	549	ASN
1	B	54	ASN
2	C	467	GLN

### 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	3,6,7	0.42	0	1,6,8	2.09	1 (100%)
2	CSO	D	150	2	3,6,7	0.59	0	1,6,8	1.99	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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	150	CSO	O-C-CA	-2.09	120.04	125.49

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

11 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
7	NAG	C	1584	2,7	14,14,15	0.63	0	15,19,21	1.73	1 (6%)
7	NAG	C	1585	7	14,14,15	0.56	0	15,19,21	1.11	1 (6%)
7	BMA	C	1586	7	11,11,12	0.62	0	14,15,17	1.96	3 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	C	1587	7	11,11,12	0.71	0	14,15,17	3.34	4 (28%)
7	MAN	C	1588	7	11,11,12	0.49	0	14,15,17	1.29	1 (7%)
7	FUC	C	1589	7	10,10,11	0.59	0	14,14,16	1.10	1 (7%)
11	NAG	D	1584	11,2	14,14,15	0.53	0	15,19,21	1.56	1 (6%)
11	NAG	D	1585	11	14,14,15	0.60	0	15,19,21	0.86	0
11	BMA	D	1586	11	11,11,12	0.74	0	14,15,17	1.10	1 (7%)
11	FUC	D	1588	11	10,10,11	0.62	0	14,14,16	1.37	2 (14%)
11	MAN	D	1590	11	11,11,12	0.53	0	14,15,17	1.01	1 (7%)

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	NAG	C	1584	2,7	-	0/6/23/26	0/1/1/1
7	NAG	C	1585	7	-	0/6/23/26	0/1/1/1
7	BMA	C	1586	7	-	0/2/19/22	0/1/1/1
7	MAN	C	1587	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	C	1588	7	-	0/2/19/22	0/1/1/1
7	FUC	C	1589	7	-	0/0/17/20	0/1/1/1
11	NAG	D	1584	11,2	-	0/6/23/26	0/1/1/1
11	NAG	D	1585	11	-	0/6/23/26	0/1/1/1
11	BMA	D	1586	11	-	0/2/19/22	0/1/1/1
11	FUC	D	1588	11	-	0/0/17/20	0/1/1/1
11	MAN	D	1590	11	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1587	MAN	C1-C2-C3	-9.31	98.53	109.54
7	C	1587	MAN	C1-O5-C5	-6.70	103.74	112.25
7	C	1586	BMA	O3-C3-C4	-4.51	100.17	110.34
11	D	1588	FUC	O2-C2-C1	2.16	113.53	109.21
7	C	1587	MAN	C3-C4-C5	2.17	113.99	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	1587	MAN	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1588	MAN	1	0

## 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	SO4	B	1105	-	4,4,4	0.15	0	6,6,6	0.06	0
4	ZS0	C	1579	5	15,21,21	1.57	3 (20%)	16,30,30	2.34	5 (31%)
5	HEM	C	1580	1,2,4	30,50,50	2.53	15 (50%)	24,82,82	2.59	6 (25%)
6	NAG	C	1582	2	14,14,15	0.47	0	15,19,21	1.03	1 (6%)
6	NAG	C	1583	2	14,14,15	0.49	0	15,19,21	1.48	1 (6%)
3	SO4	C	1593	-	4,4,4	0.17	0	6,6,6	0.13	0
3	SO4	C	1594	-	4,4,4	0.16	0	6,6,6	0.09	0
10	ACT	C	1595	-	1,3,3	1.25	0	0,3,3	0.00	-
10	ACT	C	1596	-	1,3,3	1.70	0	0,3,3	0.00	-
10	ACT	C	1597	-	1,3,3	1.23	0	0,3,3	0.00	-
4	ZS0	D	1579	5	15,21,21	1.35	2 (13%)	16,30,30	2.34	5 (31%)
5	HEM	D	1580	1,2,4	30,50,50	2.50	15 (50%)	24,82,82	2.59	9 (37%)
6	NAG	D	1582	2	14,14,15	0.50	0	15,19,21	1.25	1 (6%)
6	NAG	D	1583	2	14,14,15	0.44	0	15,19,21	1.33	1 (6%)
10	ACT	D	1591	-	1,3,3	1.43	0	0,3,3	0.00	-
10	ACT	D	1592	-	1,3,3	1.41	0	0,3,3	0.00	-
10	ACT	D	1593	-	1,3,3	0.96	0	0,3,3	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
3	SO4	B	1105	-	-	0/0/0/0	0/0/0/0
4	ZS0	C	1579	5	-	0/4/4/4	0/3/3/3
5	HEM	C	1580	1,2,4	-	0/10/54/54	0/0/8/8
6	NAG	C	1582	2	-	0/6/23/26	0/1/1/1
6	NAG	C	1583	2	-	0/6/23/26	0/1/1/1
3	SO4	C	1593	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1594	-	-	0/0/0/0	0/0/0/0
10	ACT	C	1595	-	-	0/0/0/0	0/0/0/0
10	ACT	C	1596	-	-	0/0/0/0	0/0/0/0
10	ACT	C	1597	-	-	0/0/0/0	0/0/0/0
4	ZS0	D	1579	5	-	0/4/4/4	0/3/3/3
5	HEM	D	1580	1,2,4	-	0/10/54/54	0/0/8/8
6	NAG	D	1582	2	-	0/6/23/26	0/1/1/1
6	NAG	D	1583	2	-	0/6/23/26	0/1/1/1
10	ACT	D	1591	-	-	0/0/0/0	0/0/0/0
10	ACT	D	1592	-	-	0/0/0/0	0/0/0/0
10	ACT	D	1593	-	-	0/0/0/0	0/0/0/0

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1580	HEM	C2D-C3D	-5.21	1.38	1.54
5	D	1580	HEM	C3B-C4B	-4.63	1.47	1.51
5	D	1580	HEM	C2D-C3D	-4.58	1.40	1.54
5	C	1580	HEM	C3B-C4B	-4.45	1.47	1.51
5	C	1580	HEM	C4C-NC	-2.35	1.33	1.36

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1579	ZS0	C1-C9-N6	-4.55	117.37	123.59
5	C	1580	HEM	CBA-CAA-C2A	-4.37	104.69	112.53
4	C	1579	ZS0	C1-C9-N6	-4.11	117.97	123.59
4	C	1579	ZS0	C1-C2-N3	-2.74	105.52	110.83
5	D	1580	HEM	CBA-CAA-C2A	-2.49	108.07	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1579	ZS0	1	0
5	C	1580	HEM	5	0
5	D	1580	HEM	1	0
10	D	1592	ACT	1	0
10	D	1593	ACT	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	104/108 (96%)	-0.24	5 (4%) 34 43	10, 14, 26, 49	0
1	B	104/108 (96%)	-0.19	2 (1%) 70 76	12, 18, 30, 36	0
2	C	465/467 (99%)	-0.29	9 (1%) 70 76	6, 16, 29, 43	0
2	D	465/467 (99%)	0.05	21 (4%) 37 46	10, 22, 37, 46	0
All	All	1138/1150 (98%)	-0.14	37 (3%) 50 59	6, 19, 35, 49	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	355	PRO	7.0
2	C	355	PRO	6.5
2	D	217	HIS	5.0
2	C	217	HIS	4.8
1	A	3	GLU	4.3

### 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	0.94	0.13	-	18,18,26,26	0
2	CSO	C	150	7/8	0.96	0.11	-	15,16,22,23	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, 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	BMA	D	1586	11/12	0.91	0.16	3.98	28,30,32,33	0
7	BMA	C	1586	11/12	0.89	0.16	3.82	27,28,33,40	0
11	NAG	D	1585	14/15	0.96	0.11	1.67	16,20,22,25	0
7	NAG	C	1585	14/15	0.97	0.11	0.47	14,19,21,24	0
7	FUC	C	1589	10/11	0.90	0.17	-	34,36,37,38	0
11	FUC	D	1588	10/11	0.83	0.34	-	37,40,41,43	0
7	NAG	C	1584	14/15	0.94	0.11	-	18,20,25,28	0
11	MAN	D	1590	11/12	0.81	0.17	-	36,37,37,38	0
7	MAN	C	1587	11/12	0.74	0.28	-	45,48,50,50	0
7	MAN	C	1588	11/12	0.89	0.20	-	27,28,29,29	0
11	NAG	D	1584	14/15	0.95	0.12	-	22,24,31,31	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, 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
4	ZS0	C	1579	19/19	0.90	0.16	2.24	27,31,35,35	0
4	ZS0	D	1579	19/19	0.87	0.19	0.87	35,44,45,46	0
6	NAG	D	1582	14/15	0.91	0.16	0.42	30,32,35,35	0
5	HEM	C	1580	43/43	0.96	0.15	0.39	7,12,18,25	0
5	HEM	D	1580	43/43	0.97	0.17	0.36	13,17,23,27	0
6	NAG	C	1582	14/15	0.93	0.14	0.31	24,30,33,33	0
9	CL	D	1595	1/1	1.00	0.12	0.08	12,12,12,12	0
8	CA	D	1594	1/1	0.99	0.08	-1.45	14,14,14,14	0
9	CL	C	1592	1/1	1.00	0.09	-1.48	8,8,8,8	0
8	CA	C	1591	1/1	0.99	0.09	-1.85	11,11,11,11	0
6	NAG	C	1583	14/15	0.93	0.14	-	29,31,33,34	0
10	ACT	C	1597	4/4	0.96	0.16	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	1105	5/5	0.71	0.35	-	48,49,49,50	5
3	SO4	C	1594	5/5	0.97	0.19	-	44,45,45,46	0
10	ACT	D	1593	4/4	0.90	0.17	-	38,38,38,38	0
3	SO4	C	1593	5/5	0.93	0.25	-	76,76,76,76	0
10	ACT	D	1591	4/4	0.76	0.25	-	50,51,51,51	0
6	NAG	D	1583	14/15	0.84	0.22	-	43,45,46,47	0
10	ACT	D	1592	4/4	0.72	0.38	-	63,63,63,63	0
10	ACT	C	1596	4/4	0.70	0.23	-	55,56,56,56	0
10	ACT	C	1595	4/4	0.92	0.20	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.