



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:11 PM GMT

PDB ID : 1DNU
Title : STRUCTURAL ANALYSES OF HUMAN MYELOPEROXIDASE-THIOCYANATE COMPLEX
Authors : Blair-Johnson, M.; Fiedler, T.J.; Fenna, R.E.
Deposited on : 1999-12-16
Resolution : 1.85 Å(reported)

This is a full wwPDB validation 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>

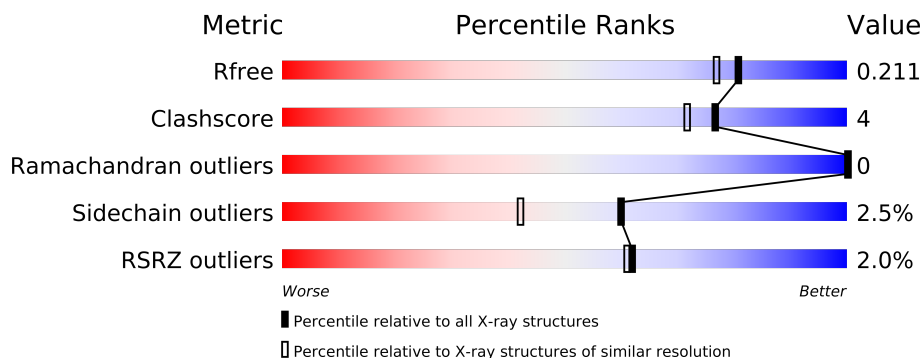
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.85 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	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

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	104	
1	B	104	
2	C	466	
2	D	466	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	D	630	-	X
7	SO4	D	7	-	X
9	ACY	C	15	-	X
9	ACY	C	16	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
9	ACY	D	13	-	X
9	ACY	D	14	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10318 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: C₈H₁₅NO₆).



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).

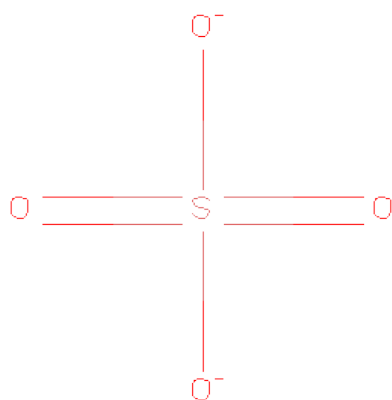
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



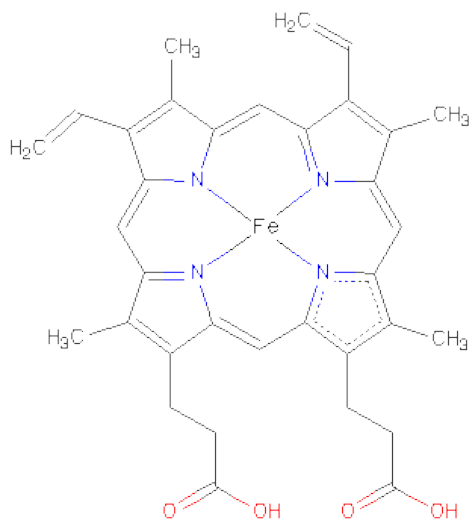
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N S 3 1 1 1	0	0
6	A	1	Total C N S 3 1 1 1	0	0
6	B	1	Total C N S 3 1 1 1	0	0
6	B	1	Total C N S 3 1 1 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



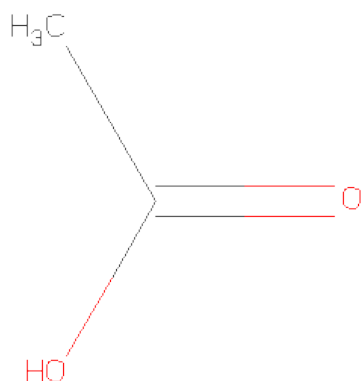
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 9 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	92	Total	O	0	0
			92	92		
10	B	103	Total	O	0	0
			103	103		

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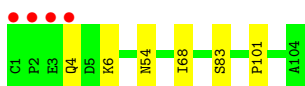
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	334	Total 334	O 334	0	0
10	D	310	Total 310	O 310	0	0

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

Chain A: 



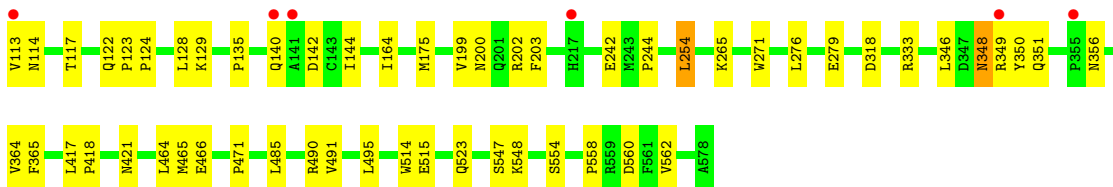
- Molecule 1: MYELOPEROXIDASE

Chain B: 



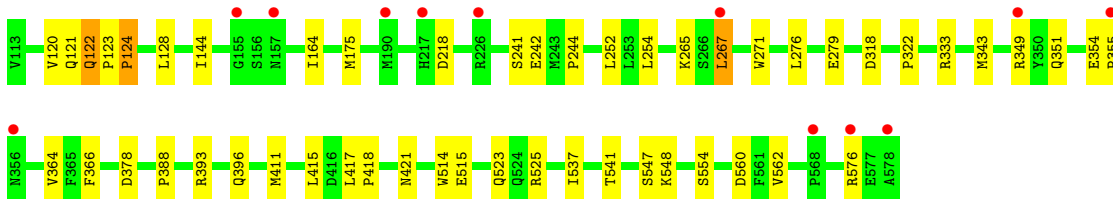
- Molecule 2: MYELOPEROXIDASE

Chain C: 



- Molecule 2: MYELOPEROXIDASE

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	111.24Å 63.87Å 92.62Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	10.00 – 1.85 48.79 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.7 (10.00-1.85) 98.1 (48.79-1.86)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.51 (at 1.86Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.178 , 0.210 0.179 , 0.211	Depositor DCC
R_{free} test set	5388 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.6	EDS
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 106892 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10318	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: CSO, SCN, NAG, CA, BMA, SO4, HEM, ACY, MAN, FUC

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	0.64	0/863	0.70	0/1174
1	B	0.60	0/863	0.73	0/1174
2	C	0.60	0/3811	0.63	0/5168
2	D	0.57	0/3811	0.61	0/5168
All	All	0.59	0/9348	0.64	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	4	0
1	B	838	0	798	5	0
2	C	3733	0	3725	37	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	6	0	0	0	0
6	B	6	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	B	43	0	30	2	0
8	C	43	0	30	2	0
9	C	12	0	9	2	0
9	D	12	0	9	1	0
10	A	92	0	0	1	0
10	B	103	0	0	0	0
10	C	334	0	0	2	0
10	D	310	0	0	0	0
All	All	10318	0	9298	72	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 (72) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:135:PRO:HG2	10:C:897:HOH:O	1.84	0.77
2:D:525:ARG:HH11	9:D:13:ACY:H2	1.48	0.75
2:C:348:ASN:H	2:C:348:ASN:HD22	1.37	0.71
2:D:349:ARG:HG3	2:D:351:GLN:HG2	1.77	0.66
2:C:271:TRP:CZ3	2:C:279:GLU:HG3	2.33	0.63
2:D:265:LYS:HD3	2:D:276:LEU:HD11	1.80	0.62
10:A:188:HOH:O	2:C:129:LYS:HD3	2.00	0.60
2:C:333:ARG:HH21	2:C:421:ASN:HD22	1.50	0.60
2:C:200:ASN:HD22	2:C:203:PHE:H	1.49	0.59
2:D:411:MET:HE2	2:D:415:LEU:HD21	1.85	0.58
2:C:200:ASN:ND2	2:C:202:ARG:H	2.01	0.58
2:C:128:LEU:HB2	2:C:144:ILE:HB	1.85	0.58
2:C:200:ASN:HD22	2:C:202:ARG:H	1.51	0.57
2:D:411:MET:CE	2:D:415:LEU:HD21	2.34	0.57
2:C:142:ASP:HB3	10:C:928:HOH:O	2.05	0.57
8:B:107:HEM:HMC2	8:B:107:HEM:HBC2	1.87	0.56
2:C:465:MET:HE1	2:C:471:PRO:HD3	1.90	0.55
2:D:354:GLU:HB3	2:D:355:PRO:HA	1.90	0.53
2:D:548:LYS:HG2	2:D:562:VAL:HG13	1.90	0.53
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:333:ARG:HH21	2:D:421:ASN:HD22	1.57	0.52
2:D:120:VAL:HG12	2:D:122:GLN:CG	2.41	0.51
2:D:244:PRO:HD3	2:D:364:VAL:O	2.09	0.51
2:C:348:ASN:ND2	2:C:348:ASN:H	2.06	0.50
1:A:101:PRO:HD2	2:C:164:ILE:O	2.12	0.50
2:C:548:LYS:HG2	2:C:562:VAL:HG13	1.93	0.50
2:C:265:LYS:HD3	2:C:276:LEU:HD11	1.94	0.49
2:C:333:ARG:HH21	2:C:421:ASN:ND2	2.11	0.48
8:B:107:HEM:HBB2	2:D:242:GLU:OE1	2.13	0.48
2:C:200:ASN:ND2	2:C:203:PHE:H	2.12	0.48
1:B:83:SER:HB3	2:D:554:SER:O	2.13	0.47
2:D:267:LEU:HD13	2:D:576:ARG:NE	2.29	0.47
1:B:1:CYS:SG	1:B:20:PRO:HB3	2.55	0.47
1:A:68:ILE:HD13	2:C:464:LEU:HD23	1.96	0.47
2:D:393:ARG:HB2	2:D:396:GLN:HB2	1.97	0.47
2:D:378:ASP:OD1	2:D:541:THR:HB	2.15	0.46
2:D:333:ARG:HH21	2:D:421:ASN:ND2	2.12	0.46
2:D:271:TRP:CZ3	2:D:279:GLU:HG3	2.50	0.46
2:C:554:SER:HB3	2:C:560:ASP:HB3	1.97	0.46
1:A:83:SER:HB3	2:C:554:SER:O	2.15	0.46
8:C:10:HEM:HMC2	8:C:10:HEM:HBC2	1.98	0.46
2:C:514:TRP:CE2	2:C:515:GLU:HG3	2.50	0.46
2:C:199:VAL:HG12	2:C:254:LEU:HD21	1.97	0.46
2:C:123:PRO:HB3	9:C:15:ACY:H3	1.98	0.46
2:D:120:VAL:HG12	2:D:122:GLN:HG2	1.96	0.46
2:C:349:ARG:HG3	2:C:351:GLN:HG2	1.98	0.45
2:C:491:VAL:HB	2:C:495:LEU:HB2	1.98	0.44
2:C:485:LEU:HD13	2:C:490:ARG:HA	1.99	0.44
2:D:244:PRO:HB2	2:D:343:MET:SD	2.58	0.44
2:D:349:ARG:HG3	2:D:351:GLN:CG	2.46	0.43
2:C:124:PRO:HA	9:C:15:ACY:CH3	2.49	0.43
2:D:554:SER:HB3	2:D:560:ASP:HB3	2.01	0.43
2:D:514:TRP:CE2	2:D:515:GLU:HG3	2.54	0.43
2:D:252:LEU:HD11	2:D:537:ILE:HA	2.02	0.42
2:C:333:ARG:HD3	2:C:421:ASN:ND2	2.34	0.42
2:C:417:LEU:HB3	2:C:418:PRO:HD3	2.00	0.42
2:C:244:PRO:HD3	2:C:364:VAL:O	2.19	0.42
2:D:121:GLN:C	2:D:122:GLN:HG2	2.39	0.42
1:B:79:ASP:O	2:D:388:PRO:HB3	2.19	0.42
2:C:346:LEU:HB3	2:C:350:TYR:HA	2.02	0.42
1:A:68:ILE:CD1	2:C:464:LEU:HD23	2.50	0.42
2:C:123:PRO:HA	2:C:124:PRO:HA	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:101:PRO:HD2	2:D:164:ILE:O	2.19	0.42
2:D:123:PRO:HA	2:D:124:PRO:HA	1.89	0.41
2:D:120:VAL:HG12	2:D:122:GLN:HG3	2.03	0.41
2:C:242:GLU:OE1	8:C:10:HEM:HBB2	2.21	0.41
2:D:241:SER:O	2:D:366:PHE:HA	2.20	0.41
2:C:113:VAL:HG12	2:C:114:ASN:N	2.35	0.41
2:C:114:ASN:HB3	2:C:117:THR:OG1	2.20	0.41
1:B:6:LYS:HB2	1:B:6:LYS:HE2	1.99	0.41
2:D:128:LEU:HB2	2:D:144:ILE:HB	2.03	0.41
2:C:242:GLU:O	2:C:365:PHE:HA	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%)	99 (97%)	3 (3%)	0	100	100
1	B	102/104 (98%)	99 (97%)	3 (3%)	0	100	100
2	C	463/466 (99%)	450 (97%)	13 (3%)	0	100	100
2	D	463/466 (99%)	453 (98%)	10 (2%)	0	100	100
All	All	1130/1140 (99%)	1101 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	87 (97%)	3 (3%)	50	29
1	B	90/90 (100%)	89 (99%)	1 (1%)	84	77
2	C	410/410 (100%)	399 (97%)	11 (3%)	57	39
2	D	410/410 (100%)	400 (98%)	10 (2%)	61	44
All	All	1000/1000 (100%)	975 (98%)	25 (2%)	60	42

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	6	LYS
1	A	54	ASN
2	C	122	GLN
2	C	140	GLN
2	C	175	MET
2	C	254	LEU
2	C	318	ASP
2	C	348	ASN
2	C	356	ASN
2	C	466	GLU
2	C	523	GLN
2	C	547	SER
2	C	558	PRO
1	B	54	ASN
2	D	122	GLN
2	D	124	PRO
2	D	175	MET
2	D	218	ASP
2	D	254	LEU
2	D	267	LEU
2	D	318	ASP
2	D	322	PRO
2	D	523	GLN
2	D	547	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	200	ASN
2	C	348	ASN

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Mol	Chain	Res	Type
2	C	421	ASN
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	7.58	3 (50%)	3,6,8	2.15	2 (66%)
2	CSO	D	150	2	6,6,7	7.69	3 (50%)	3,6,8	1.36	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	-	0/2/5/7	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	18.29	1.24	1.11
2	C	150	CSO	O-C	18.00	1.23	1.11
2	D	150	CSO	OD-SG	-3.21	1.48	1.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	150	CSO	OD-SG	-3.17	1.49	1.62
2	C	150	CSO	CA-C	2.95	1.53	1.48
2	D	150	CSO	CA-C	2.64	1.53	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	150	CSO	C-CA-N	-2.82	111.02	113.83
2	C	150	CSO	CA-CB-SG	2.43	117.34	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	640	2,4	12,14,15	0.78	0	15,19,21	0.85	0
4	NAG	C	641	4	12,14,15	0.50	0	15,19,21	0.64	0
4	BMA	C	642	4	10,11,12	0.64	0	11,15,17	0.50	0
4	MAN	C	643	4	10,11,12	0.74	0	11,15,17	0.37	0
4	MAN	C	644	4	10,11,12	0.50	0	11,15,17	0.38	0
4	FUC	C	645	4	9,10,11	0.53	0	10,14,16	0.40	0
4	NAG	D	640	2,4	12,14,15	0.62	0	15,19,21	0.85	0
4	NAG	D	641	4	12,14,15	0.67	0	15,19,21	0.65	0
4	BMA	D	642	4	10,11,12	0.60	0	11,15,17	0.68	0
4	MAN	D	643	4	10,11,12	0.66	0	11,15,17	0.37	0
4	MAN	D	644	4	10,11,12	0.50	0	11,15,17	0.27	0
4	FUC	D	645	4	9,10,11	0.47	0	10,14,16	0.32	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	640	2,4	-	0/6/23/26	0/1/1/1
4	NAG	C	641	4	-	0/6/23/26	0/1/1/1
4	BMA	C	642	4	-	0/2/19/22	0/1/1/1
4	MAN	C	643	4	-	0/2/19/22	0/1/1/1
4	MAN	C	644	4	-	0/2/19/22	0/1/1/1
4	FUC	C	645	4	-	0/0/17/20	0/1/1/1
4	NAG	D	640	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	641	4	-	0/6/23/26	0/1/1/1
4	BMA	D	642	4	-	0/2/19/22	0/1/1/1
4	MAN	D	643	4	-	0/2/19/22	0/1/1/1
4	MAN	D	644	4	-	0/2/19/22	0/1/1/1
4	FUC	D	645	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 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	$\# Z > 2$
6	SCN	A	105	-	2,2,2	1.07	0	1,1,1	0.51	0
7	SO4	A	106	-	4,4,4	0.08	0	6,6,6	0.07	0
6	SCN	A	107	-	2,2,2	1.16	0	1,1,1	0.53	0
6	SCN	B	105	-	2,2,2	1.19	0	1,1,1	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SCN	B	106	-	2,2,2	1.09	0	1,1,1	0.53	0
8	HEM	B	107	1,10,2	49,50,50	1.96	11 (22%)	46,82,82	1.25	4 (8%)
8	HEM	C	10	1,2	49,50,50	2.40	12 (24%)	46,82,82	1.30	5 (10%)
9	ACY	C	15	-	3,3,3	0.92	0	3,3,3	1.42	0
9	ACY	C	16	-	3,3,3	1.14	0	3,3,3	1.44	0
9	ACY	C	17	-	3,3,3	0.87	0	3,3,3	1.50	1 (33%)
3	NAG	C	620	2	12,14,15	0.54	0	15,19,21	0.80	0
3	NAG	C	630	2	12,14,15	0.73	0	15,19,21	0.58	0
7	SO4	C	9	-	4,4,4	0.51	0	6,6,6	0.18	0
9	ACY	D	12	-	3,3,3	1.03	0	3,3,3	1.48	1 (33%)
9	ACY	D	13	-	3,3,3	1.13	0	3,3,3	1.51	1 (33%)
9	ACY	D	14	-	3,3,3	1.05	0	3,3,3	1.44	0
3	NAG	D	620	2	12,14,15	0.55	0	15,19,21	0.73	0
3	NAG	D	630	2	12,14,15	0.56	0	15,19,21	0.72	0
7	SO4	D	7	-	4,4,4	0.41	0	6,6,6	0.11	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
6	SCN	A	105	-	-	0/0/0/0	0/0/0/0
7	SO4	A	106	-	-	0/0/0/0	0/0/0/0
6	SCN	A	107	-	-	0/0/0/0	0/0/0/0
6	SCN	B	105	-	-	0/0/0/0	0/0/0/0
6	SCN	B	106	-	-	0/0/0/0	0/0/0/0
8	HEM	B	107	1,10,2	-	0/14/114/114	0/0/8/8
8	HEM	C	10	1,2	-	0/14/114/114	0/0/8/8
9	ACY	C	15	-	-	0/0/0/0	0/0/0/0
9	ACY	C	16	-	-	0/0/0/0	0/0/0/0
9	ACY	C	17	-	-	0/0/0/0	0/0/0/0
3	NAG	C	620	2	-	0/6/23/26	0/1/1/1
3	NAG	C	630	2	-	0/6/23/26	0/1/1/1
7	SO4	C	9	-	-	0/0/0/0	0/0/0/0
9	ACY	D	12	-	-	0/0/0/0	0/0/0/0
9	ACY	D	13	-	-	0/0/0/0	0/0/0/0
9	ACY	D	14	-	-	0/0/0/0	0/0/0/0
3	NAG	D	620	2	-	0/6/23/26	0/1/1/1
3	NAG	D	630	2	-	0/6/23/26	0/1/1/1
7	SO4	D	7	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	10	HEM	C3D-C4D	8.32	1.46	1.44
8	C	10	HEM	C2D-C1D	6.56	1.46	1.44
8	C	10	HEM	C4A-C3A	5.27	1.46	1.40
8	B	107	HEM	C2D-C1D	5.26	1.45	1.44
8	C	10	HEM	C3D-C2D	-5.16	1.34	1.43
8	B	107	HEM	C3D-C2D	-4.70	1.35	1.43
8	C	10	HEM	C2B-C1B	4.57	1.45	1.44
8	B	107	HEM	C4A-C3A	4.46	1.45	1.40
8	B	107	HEM	C3B-C2B	-4.42	1.36	1.43
8	B	107	HEM	C2B-C1B	4.38	1.45	1.44
8	C	10	HEM	C3C-C2C	-3.67	1.37	1.43
8	C	10	HEM	C3B-C2B	-3.64	1.37	1.43
8	B	107	HEM	CBB-CAB	3.01	1.46	1.28
8	C	10	HEM	CBB-CAB	2.95	1.46	1.28
8	B	107	HEM	CHB-C1B	2.82	1.39	1.35
8	B	107	HEM	C3C-C2C	-2.82	1.38	1.43
8	C	10	HEM	CBC-CAC	2.74	1.44	1.28
8	B	107	HEM	C3D-C4D	2.63	1.45	1.44
8	B	107	HEM	CBC-CAC	2.59	1.43	1.28
8	C	10	HEM	C3B-C4B	2.35	1.47	1.44
8	C	10	HEM	CHB-C1B	2.25	1.39	1.35
8	B	107	HEM	CMC-C2C	2.04	1.53	1.47
8	C	10	HEM	CMB-C2B	2.02	1.53	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	107	HEM	C3A-C4A-NA	3.63	112.15	109.41
8	C	10	HEM	C3A-C4A-NA	3.57	112.11	109.41
8	B	107	HEM	C4A-NA-C1A	-3.04	102.75	106.76
8	C	10	HEM	C3B-C4B-NB	-2.83	111.97	114.00
8	C	10	HEM	C4A-NA-C1A	-2.71	103.19	106.76
8	B	107	HEM	C3B-C4B-NB	-2.17	112.44	114.00
8	C	10	HEM	C4C-NC-C1C	-2.17	103.28	105.53
8	C	10	HEM	C4A-CHB-C1B	-2.16	124.62	127.47
8	B	107	HEM	C1A-CHA-C4D	-2.09	124.72	127.47
9	D	13	ACY	O-C-CH3	-2.05	113.11	122.06
9	C	17	ACY	O-C-CH3	-2.05	113.13	122.06
9	D	12	ACY	O-C-CH3	-2.02	113.26	122.06

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	104/104 (100%)	-0.15	4 (3%) 38 36	6, 9, 23, 46	0
1	B	104/104 (100%)	-0.24	0 100 100	6, 10, 19, 24	0
2	C	466/466 (100%)	-0.27	6 (1%) 74 72	5, 10, 24, 39	0
2	D	466/466 (100%)	-0.08	12 (2%) 53 50	6, 12, 27, 43	0
All	All	1140/1140 (100%)	-0.18	22 (1%) 62 63	5, 11, 25, 46	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	113	VAL	12.4
1	A	3	GLU	5.4
2	D	217	HIS	5.1
2	D	578	ALA	4.6
2	D	355	PRO	4.4
1	A	4	GLN	4.2
2	C	217	HIS	3.9
1	A	1	CYS	3.8
2	C	355	PRO	3.7
2	C	140	GLN	3.2
2	D	576	ARG	2.9
2	D	267	LEU	2.7
2	D	568	PRO	2.7
2	C	141	ALA	2.7
1	A	2	PRO	2.6
2	D	190	MET	2.5
2	D	155	GLY	2.5
2	D	349	ARG	2.4
2	D	356	ASN	2.3
2	C	349	ARG	2.2
2	D	157	ASN	2.2
2	D	226	ARG	2.0

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	C	150	7/8	0.08	0.74	8,10,11,15	0
2	CSO	D	150	7/8	0.09	-0.42	6,8,10,14	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
4	BMA	C	642	11/12	0.11	0.43	11,13,16,21	0
4	MAN	D	644	11/12	0.10	0.12	13,14,16,17	0
4	BMA	D	642	11/12	0.08	0.10	10,12,15,19	0
4	NAG	C	641	14/15	0.09	0.07	8,10,11,11	0
4	FUC	C	645	10/11	0.08	0.01	15,16,18,19	0
4	NAG	D	641	14/15	0.09	-0.11	8,11,12,13	0
4	NAG	C	640	14/15	0.09	-0.32	8,12,16,17	0
4	NAG	D	640	14/15	0.09	-0.60	10,12,17,20	0
4	MAN	C	644	11/12	0.12	-0.92	13,15,17,18	0
4	FUC	D	645	10/11	0.08	-1.40	14,15,17,18	0
4	MAN	D	643	11/12	0.12	-	22,24,28,30	0
4	MAN	C	643	11/12	0.10	-	24,26,27,27	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(\AA^2)	Q<0.9
7	SO4	D	7	5/5	0.36	23.30	46,47,47,47	5
9	ACY	C	16	4/4	0.14	8.26	27,28,29,29	0
9	ACY	C	15	4/4	0.15	6.82	27,28,29,30	0
9	ACY	D	13	4/4	0.42	6.66	38,38,38,39	0
9	ACY	D	14	4/4	0.13	3.09	20,21,21,24	0
3	NAG	D	630	14/15	0.19	2.98	32,34,37,38	0
3	NAG	D	620	14/15	0.17	1.44	17,24,28,29	0
3	NAG	C	620	14/15	0.10	1.31	15,17,21,22	0
9	ACY	C	17	4/4	0.21	1.21	17,20,20,21	0
8	HEM	C	10	43/43	0.09	0.97	4,8,9,10	0
6	SCN	B	105	3/3	0.14	0.96	11,11,16,17	0
6	SCN	A	105	3/3	0.12	0.58	12,12,12,17	0
3	NAG	C	630	14/15	0.14	0.57	23,28,36,36	0
6	SCN	B	106	3/3	0.08	0.56	19,19,19,19	0
7	SO4	C	9	5/5	0.14	0.40	27,29,31,33	0
6	SCN	A	107	3/3	0.08	0.21	15,15,18,20	0
8	HEM	B	107	43/43	0.09	0.08	5,8,10,12	0
5	CA	D	2	1/1	0.09	-0.30	9,9,9,9	0
5	CA	C	1	1/1	0.07	-0.51	10,10,10,10	0
9	ACY	D	12	4/4	0.11	-0.53	30,31,31,32	0
7	SO4	A	106	5/5	0.08	-0.56	25,25,28,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.