



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:09 pm GMT

PDB ID : 3NIU
Title : Crystal structure of the complex of dimeric goat lactoperoxidase with diethylene glycol at 2.9 Å resolution
Authors : Vikram, G.; Singh, R.P.; Singh, A.K.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2010-06-16
Resolution : 2.94 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

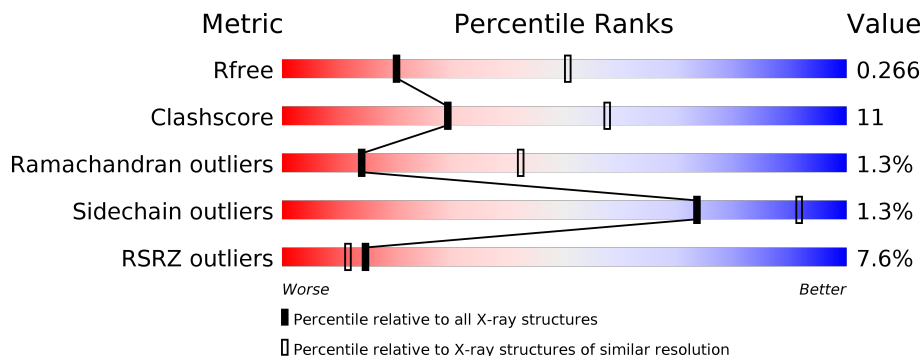
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	100719	2289 (2.98-2.90)
Clashscore	112137	2543 (2.98-2.90)
Ramachandran outliers	110173	2475 (2.98-2.90)
Sidechain outliers	110143	2477 (2.98-2.90)
RSRZ outliers	101464	2301 (2.98-2.90)

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 ≥ 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	595	<div> <div>7%</div> <div>86%</div> <div>13%</div> </div>
1	B	595	<div> <div>8%</div> <div>84%</div> <div>14%</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
5	PO4	A	2001	-	-	X	X
5	PO4	B	2004	-	-	X	X
7	HEM	A	1001	-	-	-	X
7	HEM	B	1021	-	-	X	X
8	PEG	A	5001	-	-	X	X
8	PEG	B	5001	-	-	X	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 10318 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 Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4757	3021	844	865	1	26			
1	B	595	Total	C	N	O	P	S	0	0	0
			4757	3021	844	865	1	26			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

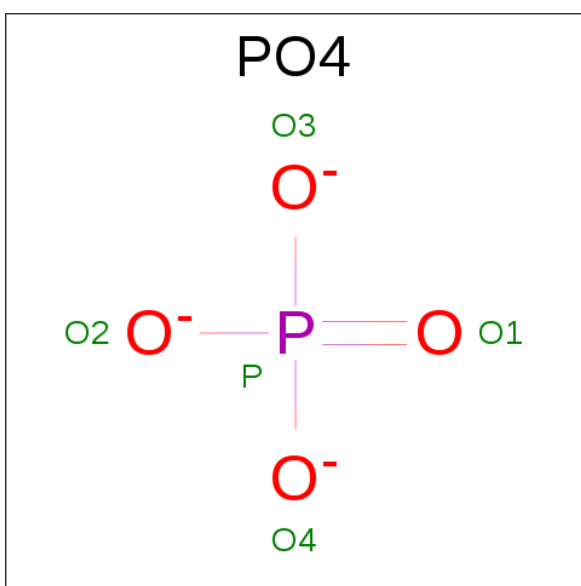
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		

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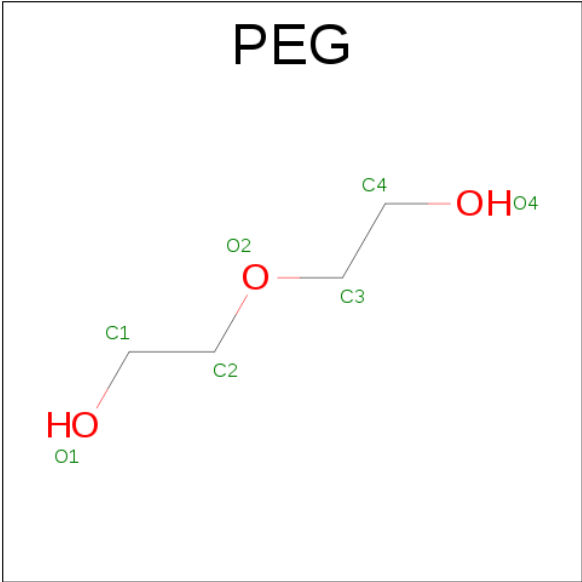
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 5	O 4	P 1	0	0
5	B	1	Total 5	O 4	P 1	0	0

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 6 | B | 1 | Total Ca
1 1 | 0 | 0 |
| 6 | A | 1 | Total Ca
1 1 | 0 | 0 |

- # HEM
-
- The diagram illustrates the chemical structure of Hemoglobin (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The iron atom is also coordinated by a proximal histidine residue (NA) and a distal water molecule (O1A). The porphyrin ring is substituted with various side chains, including vinyl groups (C1B, C2B, C3B, C4B), methyl groups (C1A, C2A, C3A, C4A), and other functional groups (C1C, C2C, C3C, C4C). The structure is labeled with various atoms and bonds, including O1A, O2A, O1D, O2D, C1A, C2A, C3A, C4A, C1B, C2B, C3B, C4B, C1C, C2C, C3C, C4C, C1D, C2D, C3D, C4D, C1E, C2E, C3E, C4E, C1F, C2F, C3F, C4F, C1G, C2G, C3G, C4G, C1H, C2H, C3H, C4H, C1I, C2I, C3I, C4I, C1J, C2J, C3J, C4J, C1K, C2K, C3K, C4K, C1L, C2L, C3L, C4L, C1M, C2M, C3M, C4M, C1N, C2N, C3N, C4N, C1O, C2O, C3O, C4O, C1P, C2P, C3P, C4P, C1Q, C2Q, C3Q, C4Q, C1R, C2R, C3R, C4R, C1S, C2S, C3S, C4S, C1T, C2T, C3T, C4T, C1U, C2U, C3U, C4U, C1V, C2V, C3V, C4V, C1W, C2W, C3W, C4W, C1X, C2X, C3X, C4X, C1Y, C2Y, C3Y, C4Y, C1Z, C2Z, C3Z, C4Z, C1AA, C2AA, C3AA, C4AA, C1AB, C2AB, C3AB, C4AB, C1AC, C2AC, C3AC, C4AC, C1AD, C2AD, C3AD, C4AD, C1AE, C2AE, C3AE, C4AE, C1AF, C2AF, C3AF, C4AF, C1AG, C2AG, C3AG, C4AG, C1AH, C2AH, C3AH, C4AH, C1AI, C2AI, C3AI, C4AI, C1AJ, C2AJ, C3AJ, C4AJ, C1AK, C2AK, C3AK, C4AK, C1AL, C2AL, C3AL, C4AL, C1AM, C2AM, C3AM, C4AM, C1AN, C2AN, C3AN, C4AN, C1AO, C2AO, C3AO, C4AO, C1AP, C2AP, C3AP, C4AP, C1AQ, C2AQ, C3AQ, C4AQ, C1AR, C2AR, C3AR, C4AR, C1AS, C2AS, C3AS, C4AS, C1AT, C2AT, C3AT, C4AT, C1AU, C2AU, C3AU, C4AU, C1AV, C2AV, C3AV, C4AV, C1AW, C2AW, C3AW, C4AW, C1AX, C2AX, C3AX, C4AX, C1AY, C2AY, C3AY, C4AY, C1AZ, C2AZ, C3AZ, C4AZ, C1BA, C2BA, C3BA, C4BA, C1BB, C2BB, C3BB, C4BB, C1BC, C2BC, C3BC, C4BC, C1BD, C2BD, C3BD, C4BD, C1BE, C2BE, C3BE, C4BE, C1BF, C2BF, C3BF, C4BF, C1BG, C2BG, C3BG, C4BG, C1BH, C2BH, C3BH, C4BH, C1BI, C2BI, C3BI, C4BI, C1BJ, C2BJ, C3BJ, C4BJ, C1BK, C2BK, C3BK, C4BK, C1BL, C2BL, C3BL, C4BL, C1BM, C2BM, C3BM, C4BM, C1BN, C2BN, C3BN, C4BN, C1BO, C2BO, C3BO, C4BO, C1BP, C2BP, C3BP, C4BP, C1BQ, C2BQ, C3BQ, C4BQ, C1BR, C2BR, C3BR, C4BR, C1BS, C2BS, C3BS, C4BS, C1BT, C2BT, C3BT, C4BT, C1BU, C2BU, C3BU, C4BU, C1BV, C2BV, C3BV, C4BV, C1BW, C2BW, C3BW, C4BW, C1BX, C2BX, C3BX, C4BX, C1BY, C2BY, C3BY, C4BY, C1BZ, C2BZ, C3BZ, C4BZ, C1CA, C2CA, C3CA, C4CA, C1CB, C2CB, C3CB, C4CB, C1CC, C2CC, C3CC, C4CC, C1CD, C2CD, C3CD, C4CD, C1CE, C2CE, C3CE, C4CE, C1CF, C2CF, C3CF, C4CF, 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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
7	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- WORLDWIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

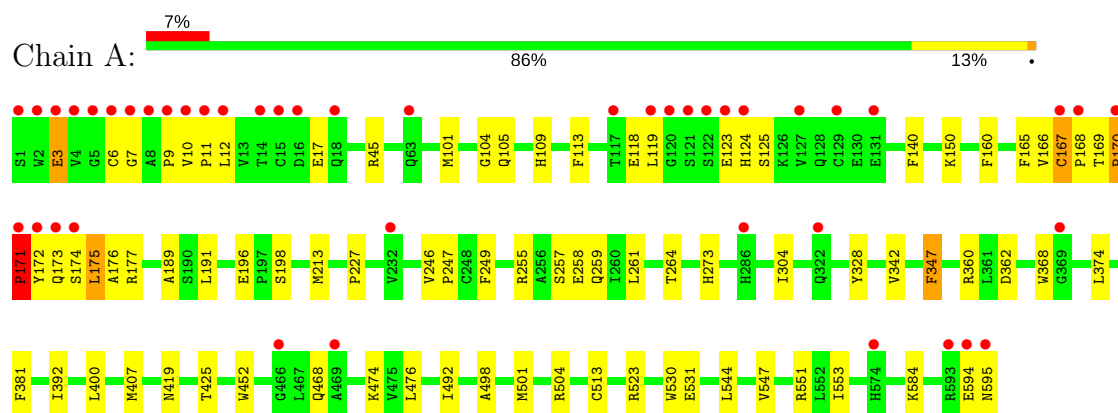
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	224	Total	O	0	0
			224	224		
9	B	240	Total	O	0	0
			240	240		

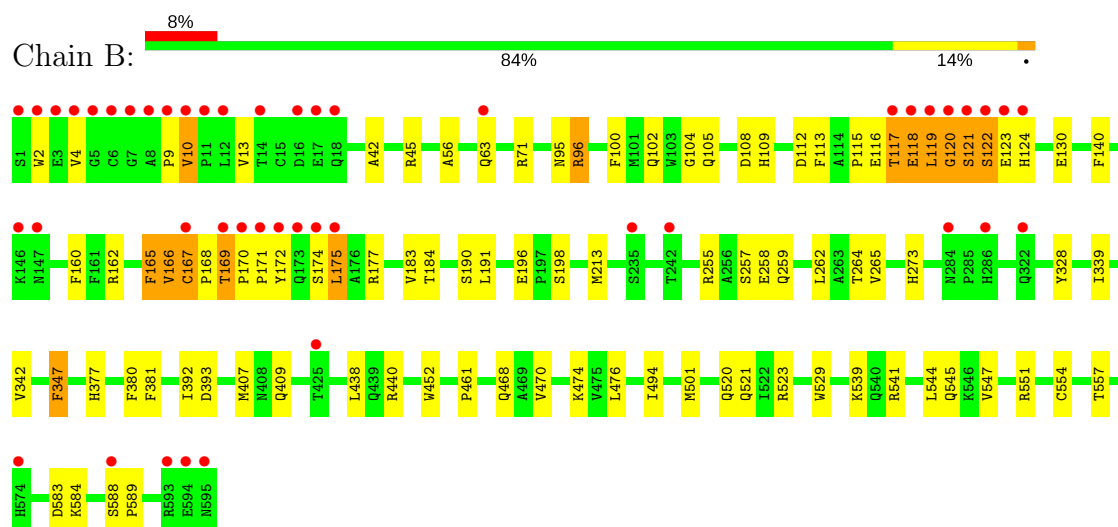
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lactoperoxidase



• Molecule 1: Lactoperoxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.20Å 75.59Å 83.81Å 79.93° 77.86° 72.50°	Depositor
Resolution (Å)	25.00 – 2.94 24.51 – 2.94	Depositor EDS
% Data completeness (in resolution range)	95.0 (25.00-2.94) 91.8 (24.51-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.94Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.232 0.202 , 0.266	Depositor DCC
R_{free} test set	1366 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10318	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, SEP, PO4, HEM, PEG, CA

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	0.40	0/4875	0.58	3/6621 (0.0%)
1	B	0.48	2/4875 (0.0%)	0.58	2/6621 (0.0%)
All	All	0.44	2/9750 (0.0%)	0.58	5/13242 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165	PHE	CD2-CE2	-5.17	1.28	1.39
1	B	166	VAL	CB-CG1	-5.05	1.42	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	PRO	CA-N-CD	-9.73	97.87	111.50
1	B	124	HIS	CA-CB-CG	5.73	123.34	113.60
1	B	120	GLY	N-CA-C	-5.29	99.87	113.10
1	A	191	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	119	LEU	N-CA-C	5.17	124.96	111.00

There are no chirality outliers.

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	4757	0	4644	87	0
1	B	4757	0	4644	109	0
2	A	56	0	50	1	0
2	B	56	0	50	2	0
3	A	39	0	34	0	0
3	B	39	0	34	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	10	0	0	3	0
5	B	10	0	0	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	43	0	30	15	0
7	B	43	0	30	21	0
8	A	7	0	10	4	0
8	B	7	0	10	9	0
9	A	224	0	0	1	0
9	B	240	0	0	0	0
All	All	10318	0	9562	209	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 11.

The worst 5 of 209 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:B:108:ASP:OD1	7:B:1021:HEM:CMD	1.66	1.43
1:B:167:CYS:HB3	1:B:168:PRO:HD3	1.25	1.17
1:B:108:ASP:OD1	7:B:1021:HEM:HMD1	0.99	1.15
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.17	1.10
1:B:167:CYS:CB	1:B:168:PRO:CD	2.30	1.09

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	592/595 (100%)	568 (96%)	17 (3%)	7 (1%)	15	45
1	B	592/595 (100%)	561 (95%)	23 (4%)	8 (1%)	13	40
All	All	1184/1190 (100%)	1129 (95%)	40 (3%)	15 (1%)	14	42

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	CYS
1	A	171	PRO
1	B	9	PRO
1	B	121	SER
1	B	167	CYS

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	516/516 (100%)	512 (99%)	4 (1%)	85	95
1	B	516/516 (100%)	507 (98%)	9 (2%)	66	88
All	All	1032/1032 (100%)	1019 (99%)	13 (1%)	73	91

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	117	THR
1	B	118	GLU
1	B	191	LEU
1	B	96	ARG
1	B	190	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	497	ASN
1	A	520	GLN
1	B	423	GLN
1	A	468	GLN
1	B	437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	A	198	1	9,9,10	1.80	2 (22%)	9,12,14	1.43	1 (11%)
1	SEP	B	198	1	9,9,10	1.76	2 (22%)	9,12,14	1.28	1 (11%)

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
1	SEP	A	198	1	-	0/5/8/10	0/0/0/0
1	SEP	B	198	1	-	0/5/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	SEP	CA-C	2.64	1.53	1.50
1	A	198	SEP	CA-C	2.92	1.54	1.50
1	A	198	SEP	P-O1P	3.36	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	SEP	P-O1P	3.45	1.62	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	SEP	OG-CB-CA	2.36	110.50	108.17
1	A	198	SEP	OG-CB-CA	2.87	110.99	108.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	1	0
1	B	198	SEP	1	0

5.5 Carbohydrates [i](#)

14 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	$\# Z > 2$
2	NAG	A	596	1,2	14,14,15	0.58	0	15,19,21	1.33	1 (6%)
2	NAG	A	597	2	14,14,15	0.49	0	15,19,21	0.80	1 (6%)
3	NAG	A	599	1,3	14,14,15	0.54	0	15,19,21	0.84	1 (6%)
3	NAG	A	600	3	14,14,15	0.63	0	15,19,21	1.49	1 (6%)
3	BMA	A	601	3	11,11,12	0.63	0	13,15,17	1.04	0
2	NAG	A	602	1,2	14,14,15	0.54	0	15,19,21	1.35	2 (13%)
2	NAG	A	603	2	14,14,15	0.42	0	15,19,21	1.47	1 (6%)
2	NAG	B	596	1,2	14,14,15	0.55	0	15,19,21	1.00	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	597	2	14,14,15	0.59	0	15,19,21	1.12	1 (6%)
2	NAG	B	602	1,2	14,14,15	0.54	0	15,19,21	1.21	2 (13%)
2	NAG	B	603	2	14,14,15	0.43	0	15,19,21	1.50	2 (13%)
3	NAG	B	604	1,3	14,14,15	0.57	0	15,19,21	1.23	3 (20%)
3	NAG	B	605	3	14,14,15	0.45	0	15,19,21	1.17	1 (6%)
3	BMA	B	606	3	11,11,12	0.60	0	13,15,17	1.03	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	NAG	A	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	597	2	-	0/6/23/26	0/1/1/1
3	NAG	A	599	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	600	3	-	0/6/23/26	0/1/1/1
3	BMA	A	601	3	-	0/2/19/22	0/1/1/1
2	NAG	A	602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	603	2	-	0/6/23/26	0/1/1/1
2	NAG	B	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	597	2	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	603	2	-	0/6/23/26	0/1/1/1
3	NAG	B	604	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	605	3	-	0/6/23/26	0/1/1/1
3	BMA	B	606	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	603	NAG	O5-C1-C2	-2.49	108.01	111.47
3	B	604	NAG	O5-C1-C2	-2.36	108.19	111.47
3	B	604	NAG	C1-O5-C5	2.11	115.08	112.17
3	A	599	NAG	C4-C3-C2	2.12	114.13	111.02
2	B	602	NAG	C4-C3-C2	2.17	114.20	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	597	NAG	1	0
2	B	602	NAG	2	0
2	B	603	NAG	2	0

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	HEM	A	1001	1	28,50,50	2.18	6 (21%)	17,82,82	1.35	2 (11%)
5	PO4	A	2001	-	4,4,4	0.83	0	6,6,6	0.44	0
5	PO4	A	2002	-	4,4,4	0.68	0	6,6,6	0.38	0
8	PEG	A	5001	-	6,6,6	0.67	0	5,5,5	3.03	2 (40%)
4	NAG	A	604	1	14,14,15	0.48	0	15,19,21	0.83	0
7	HEM	B	1021	1	28,50,50	2.16	6 (21%)	17,82,82	1.38	1 (5%)
5	PO4	B	2003	-	4,4,4	0.75	0	6,6,6	0.39	0
5	PO4	B	2004	-	4,4,4	0.82	0	6,6,6	0.45	0
8	PEG	B	5001	-	6,6,6	0.69	0	5,5,5	5.10	3 (60%)
4	NAG	B	607	1	14,14,15	0.60	0	15,19,21	1.03	1 (6%)

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	HEM	A	1001	1	-	0/6/54/54	0/0/8/8
5	PO4	A	2001	-	-	0/0/0/0	0/0/0/0
5	PO4	A	2002	-	-	0/0/0/0	0/0/0/0
8	PEG	A	5001	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	604	1	-	0/6/23/26	0/1/1/1
7	HEM	B	1021	1	-	0/6/54/54	0/0/8/8
5	PO4	B	2003	-	-	0/0/0/0	0/0/0/0
5	PO4	B	2004	-	-	0/0/0/0	0/0/0/0
8	PEG	B	5001	-	-	0/4/4/4	0/0/0/0
4	NAG	B	607	1	-	0/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1021	HEM	C3B-C2B	-4.65	1.34	1.40
7	A	1001	HEM	C3B-C2B	-4.60	1.34	1.40
7	B	1021	HEM	C3C-C2C	-4.02	1.35	1.40
7	A	1001	HEM	C3C-C2C	-3.94	1.35	1.40
7	B	1021	HEM	C4D-ND	2.35	1.39	1.36

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1001	HEM	CBD-CAD-C3D	-2.50	107.70	112.47
7	B	1021	HEM	CBD-CAD-C3D	-2.44	107.82	112.47
7	A	1001	HEM	CBA-CAA-C2A	-2.18	108.31	112.48
8	B	5001	PEG	O2-C3-C4	2.43	121.35	110.15
4	B	607	NAG	C4-C3-C2	3.20	115.71	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1001	HEM	15	0
5	A	2001	PO4	3	0
8	A	5001	PEG	4	0
7	B	1021	HEM	21	0
5	B	2004	PO4	3	0
8	B	5001	PEG	9	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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, 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	594/595 (99%)	0.12	44 (7%) 15 12	4, 17, 43, 67	0
1	B	594/595 (99%)	0.19	46 (7%) 14 11	6, 17, 44, 70	0
All	All	1188/1190 (99%)	0.15	90 (7%) 15 12	4, 17, 43, 70	0

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	SER	11.4
1	B	6	CYS	9.5
1	A	5	GLY	9.1
1	A	2	TRP	8.5
1	A	4	VAL	8.3

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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SEP	B	198	10/11	0.66	0.49	-	24,26,32,32	0
1	SEP	A	198	10/11	0.77	0.36	-	22,23,29,29	0

6.3 Carbohydrates [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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	B	604	14/15	0.90	0.19	0.94	29,31,33,36	0
3	NAG	A	599	14/15	0.91	0.18	0.37	31,34,37,42	0
2	NAG	A	602	14/15	0.90	0.17	-0.22	29,31,33,36	0
2	NAG	B	602	14/15	0.91	0.20	-0.45	33,35,37,40	0
3	NAG	B	605	14/15	0.82	0.32	-	39,40,42,44	0
3	BMA	A	601	11/12	0.66	0.74	-	55,57,57,57	0
3	BMA	B	606	11/12	0.70	0.64	-	46,47,47,48	0
2	NAG	A	603	14/15	0.74	0.42	-	39,41,42,42	0
3	NAG	A	600	14/15	0.84	0.49	-	46,49,50,53	0
2	NAG	A	596	14/15	0.81	0.49	-	35,40,42,46	0
2	NAG	A	597	14/15	0.77	0.56	-	49,52,52,53	0
2	NAG	B	603	14/15	0.68	0.57	-	43,45,45,45	0
2	NAG	B	597	14/15	0.46	0.57	-	51,53,54,55	0
2	NAG	B	596	14/15	0.86	0.35	-	37,42,44,48	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	PEG	B	5001	7/7	0.78	0.50	9.16	30,31,31,31	0
5	PO4	A	2001	5/5	0.91	0.37	8.77	63,63,63,63	0
8	PEG	A	5001	7/7	0.80	0.38	5.76	30,30,31,31	0
5	PO4	B	2004	5/5	0.93	0.33	5.70	56,56,56,56	0
7	HEM	A	1001	43/43	0.78	0.30	5.48	15,16,17,18	0
7	HEM	B	1021	43/43	0.80	0.28	3.09	12,14,15,16	0
6	CA	A	1000	1/1	0.98	0.08	-2.79	13,13,13,13	0
6	CA	B	1000	1/1	0.87	0.09	-2.96	22,22,22,22	0
5	PO4	A	2002	5/5	0.95	0.21	-	53,53,53,53	0
4	NAG	B	607	14/15	0.73	0.45	-	34,37,37,37	0
4	NAG	A	604	14/15	0.84	0.38	-	27,29,32,32	0
5	PO4	B	2003	5/5	0.91	0.30	-	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.