



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2016 – 06:14 PM EDT

PDB ID : 5FNO
Title : Manganese Lipxygenase
Authors : Wennman, A.; Karkehabadi, S.; Oliw, E.H.; Chen, Y.
Deposited on : 2015-11-16
Resolution : 2.04 Å(reported)

This is a Full wwPDB X-ray Structure 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/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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
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) : rb-20027107

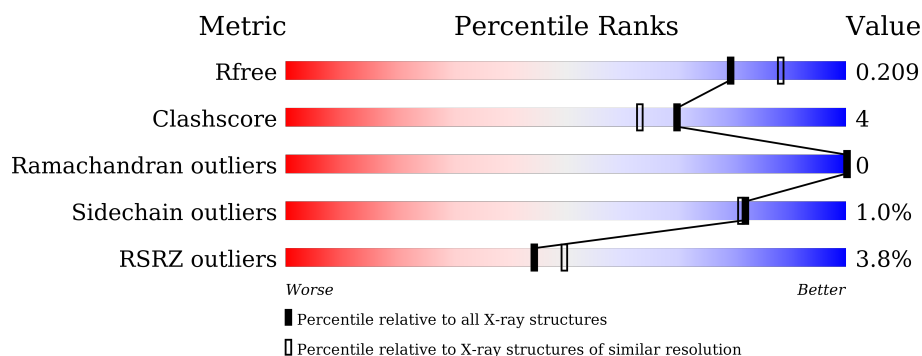
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	605	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	B	605	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </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
4	NAG	A	1011	-	-	-	X
4	NAG	B	1011	-	-	-	X
4	NAG	B	1021	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9741 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 MANGANESE LIPOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	568	Total	C	N	O	S	0	0	0
			4472	2845	788	824	15			
1	B	568	Total	C	N	O	S	0	0	0
			4472	2845	788	824	15			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	-	EXPRESSION TAG	UNP G4NAP4
A	2	PHE	-	EXPRESSION TAG	UNP G4NAP4
A	575	ALA	-	EXPRESSION TAG	UNP G4NAP4
A	576	ARG	-	EXPRESSION TAG	UNP G4NAP4
A	577	ARG	-	EXPRESSION TAG	UNP G4NAP4
A	578	PHE	-	EXPRESSION TAG	UNP G4NAP4
A	579	ASP	-	EXPRESSION TAG	UNP G4NAP4
A	580	ASP	-	EXPRESSION TAG	UNP G4NAP4
A	581	ARG	-	EXPRESSION TAG	UNP G4NAP4
A	582	GLY	-	EXPRESSION TAG	UNP G4NAP4
A	583	LEU	-	EXPRESSION TAG	UNP G4NAP4
A	584	SER	-	EXPRESSION TAG	UNP G4NAP4
A	585	GLN	-	EXPRESSION TAG	UNP G4NAP4
A	586	GLY	-	EXPRESSION TAG	UNP G4NAP4
A	587	MET	-	EXPRESSION TAG	UNP G4NAP4
A	588	PRO	-	EXPRESSION TAG	UNP G4NAP4
A	589	PHE	-	EXPRESSION TAG	UNP G4NAP4
A	590	ILE	-	EXPRESSION TAG	UNP G4NAP4
A	591	TRP	-	EXPRESSION TAG	UNP G4NAP4
A	592	GLN	-	EXPRESSION TAG	UNP G4NAP4
A	593	ALA	-	EXPRESSION TAG	UNP G4NAP4
A	594	LEU	-	EXPRESSION TAG	UNP G4NAP4
A	595	ASP	-	EXPRESSION TAG	UNP G4NAP4
A	596	PRO	-	EXPRESSION TAG	UNP G4NAP4
A	597	GLY	-	EXPRESSION TAG	UNP G4NAP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	598	ASN	-	EXPRESSION TAG	UNP G4NAP4
A	599	ILE	-	EXPRESSION TAG	UNP G4NAP4
A	600	PRO	-	EXPRESSION TAG	UNP G4NAP4
A	601	PHE	-	EXPRESSION TAG	UNP G4NAP4
A	602	TYR	-	EXPRESSION TAG	UNP G4NAP4
A	603	LEU	-	EXPRESSION TAG	UNP G4NAP4
A	604	SER	-	EXPRESSION TAG	UNP G4NAP4
A	605	VAL	-	EXPRESSION TAG	UNP G4NAP4
B	1	GLU	-	EXPRESSION TAG	UNP G4NAP4
B	2	PHE	-	EXPRESSION TAG	UNP G4NAP4
B	575	ALA	-	EXPRESSION TAG	UNP G4NAP4
B	576	ARG	-	EXPRESSION TAG	UNP G4NAP4
B	577	ARG	-	EXPRESSION TAG	UNP G4NAP4
B	578	PHE	-	EXPRESSION TAG	UNP G4NAP4
B	579	ASP	-	EXPRESSION TAG	UNP G4NAP4
B	580	ASP	-	EXPRESSION TAG	UNP G4NAP4
B	581	ARG	-	EXPRESSION TAG	UNP G4NAP4
B	582	GLY	-	EXPRESSION TAG	UNP G4NAP4
B	583	LEU	-	EXPRESSION TAG	UNP G4NAP4
B	584	SER	-	EXPRESSION TAG	UNP G4NAP4
B	585	GLN	-	EXPRESSION TAG	UNP G4NAP4
B	586	GLY	-	EXPRESSION TAG	UNP G4NAP4
B	587	MET	-	EXPRESSION TAG	UNP G4NAP4
B	588	PRO	-	EXPRESSION TAG	UNP G4NAP4
B	589	PHE	-	EXPRESSION TAG	UNP G4NAP4
B	590	ILE	-	EXPRESSION TAG	UNP G4NAP4
B	591	TRP	-	EXPRESSION TAG	UNP G4NAP4
B	592	GLN	-	EXPRESSION TAG	UNP G4NAP4
B	593	ALA	-	EXPRESSION TAG	UNP G4NAP4
B	594	LEU	-	EXPRESSION TAG	UNP G4NAP4
B	595	ASP	-	EXPRESSION TAG	UNP G4NAP4
B	596	PRO	-	EXPRESSION TAG	UNP G4NAP4
B	597	GLY	-	EXPRESSION TAG	UNP G4NAP4
B	598	ASN	-	EXPRESSION TAG	UNP G4NAP4
B	599	ILE	-	EXPRESSION TAG	UNP G4NAP4
B	600	PRO	-	EXPRESSION TAG	UNP G4NAP4
B	601	PHE	-	EXPRESSION TAG	UNP G4NAP4
B	602	TYR	-	EXPRESSION TAG	UNP G4NAP4
B	603	LEU	-	EXPRESSION TAG	UNP G4NAP4
B	604	SER	-	EXPRESSION TAG	UNP G4NAP4
B	605	VAL	-	EXPRESSION TAG	UNP G4NAP4

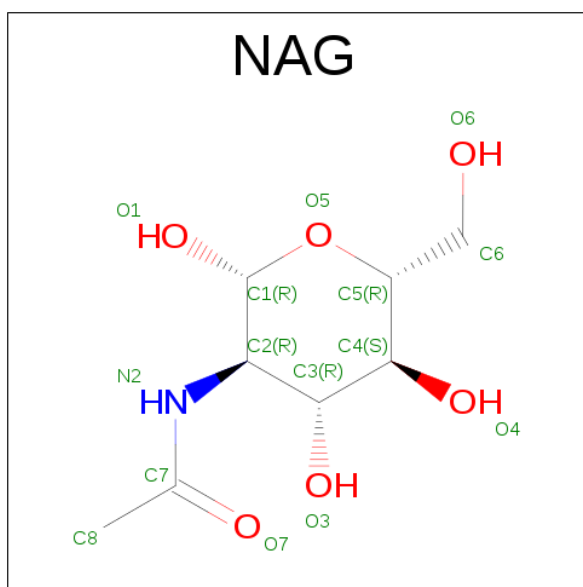
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- 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	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		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

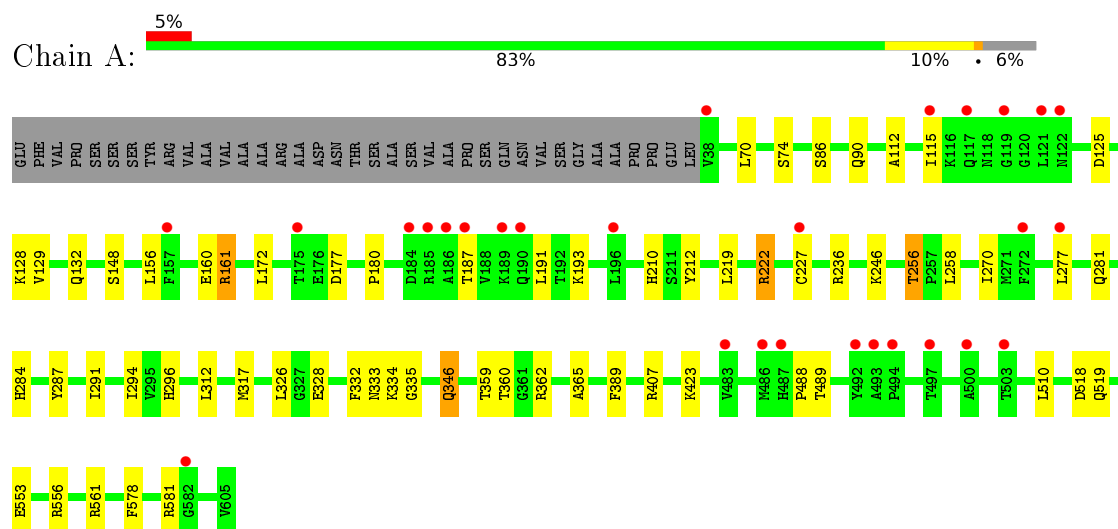
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	364	Total 364	O 364	0	0
5	B	319	Total 319	O 319	0	0

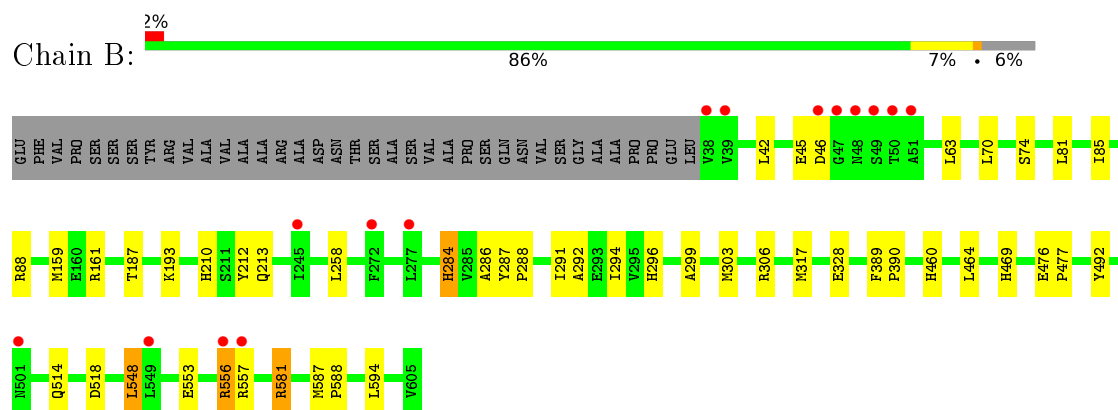
3 Residue-property plots [i](#)

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: MANGANESE LIPOXYGENASE



• Molecule 1: MANGANESE LIPOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.72Å 111.37Å 171.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 2.04 29.71 – 2.04	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.70-2.04) 96.8 (29.71-2.04)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.04Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.168 , 0.213 0.164 , 0.209	Depositor DCC
R_{free} test set	7983 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 84190 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9741	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MN, NAG

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	0.37	0/4585	0.56	1/6243 (0.0%)
1	B	0.41	1/4585 (0.0%)	0.58	5/6243 (0.1%)
All	All	0.39	1/9170 (0.0%)	0.57	6/12486 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	556	ARG	CB-CG	-8.14	1.30	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	581	ARG	NE-CZ-NH1	-8.41	116.10	120.30
1	B	556	ARG	CG-CD-NE	-7.82	95.38	111.80
1	A	312	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	556	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	548	LEU	CB-CG-CD2	5.25	119.93	111.00
1	B	581	ARG	NE-CZ-NH2	5.08	122.84	120.30

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	4472	0	4385	44	0
1	B	4472	0	4384	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	25	1	0
3	B	28	0	25	1	0
4	A	28	0	26	0	0
4	B	28	0	25	0	0
5	A	364	0	0	5	0
5	B	319	0	0	2	0
All	All	9741	0	8870	80	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 4.

All (80) 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:129:VAL:HA	1:A:132:GLN:HG2	1.60	0.84
1:A:581:ARG:NH1	1:B:581:ARG:HH12	1.75	0.84
1:B:556:ARG:HD2	1:B:556:ARG:N	1.93	0.82
1:B:548:LEU:O	1:B:556:ARG:NH2	2.15	0.79
1:A:128:LYS:HD3	1:A:148:SER:HB3	1.67	0.77
1:B:548:LEU:O	1:B:556:ARG:NH1	2.20	0.73
1:A:187:THR:HG23	1:A:258:LEU:HD12	1.68	0.73
1:B:296:HIS:CG	1:B:317:MET:HG3	2.27	0.69
1:B:548:LEU:C	1:B:556:ARG:HH22	1.98	0.66
1:B:556:ARG:N	1:B:556:ARG:CD	2.61	0.62
1:B:514:GLN:NE2	1:B:518:ASP:OD1	2.33	0.62
1:A:553:GLU:OE1	1:A:556:ARG:NH1	2.33	0.61
1:A:407:ARG:NH1	5:A:2261:HOH:O	2.23	0.61
1:A:219:LEU:HB2	1:A:222:ARG:HG3	1.84	0.60
1:A:128:LYS:CD	1:A:148:SER:HB3	2.33	0.58
1:A:129:VAL:HA	1:A:132:GLN:CG	2.33	0.57
1:A:561:ARG:NH2	5:A:2330:HOH:O	2.37	0.56
1:A:256:THR:HG22	1:A:258:LEU:H	1.70	0.56
1:B:284:HIS:HA	1:B:287:TYR:O	2.05	0.56
1:B:548:LEU:O	1:B:556:ARG:CZ	2.53	0.56
1:B:390:PRO:HG2	1:B:587:MET:SD	2.46	0.56
1:A:581:ARG:HH11	1:B:581:ARG:HH12	1.49	0.56
1:B:161:ARG:HD3	5:B:2073:HOH:O	2.08	0.54
1:A:333:ASN:O	1:A:335:GLY:HA2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ALA:HB1	1:B:317:MET:HE3	1.90	0.53
1:A:210:HIS:HA	1:A:212:TYR:CE2	2.44	0.52
1:B:210:HIS:HA	1:B:212:TYR:CE2	2.44	0.52
1:A:281:GLN:O	1:A:284:HIS:ND1	2.40	0.52
1:A:284:HIS:HA	1:A:287:TYR:O	2.10	0.52
1:A:193:LYS:HG2	1:A:236:ARG:HH11	1.75	0.51
1:A:112:ALA:O	1:A:115:ILE:HG13	2.11	0.50
1:A:332:PHE:O	1:A:346:GLN:NE2	2.43	0.50
1:B:286:ALA:O	1:B:291:ILE:HG13	2.12	0.50
1:A:222:ARG:NH1	5:A:2150:HOH:O	2.40	0.49
1:A:74:SER:HB2	1:A:294:ILE:HB	1.94	0.49
1:B:212:TYR:CE1	1:B:213:GLN:HG3	2.48	0.49
1:A:291:ILE:HD11	1:A:360:THR:O	2.14	0.48
1:B:548:LEU:C	1:B:556:ARG:NH2	2.63	0.48
1:A:270:ILE:HD13	1:A:510:LEU:HD21	1.96	0.48
1:B:588:PRO:HB3	3:B:1001:NAG:H82	1.96	0.48
1:B:492:TYR:OH	5:B:2176:HOH:O	2.20	0.47
1:B:46:ASP:OD2	1:B:306:ARG:NH1	2.45	0.47
1:A:172:LEU:HD11	1:A:180:PRO:HD3	1.96	0.47
1:B:42:LEU:HB2	1:B:45:GLU:HG3	1.97	0.47
1:B:193:LYS:HD3	1:B:193:LYS:HA	1.59	0.46
1:A:578:PHE:CE2	3:A:1001:NAG:H5	2.50	0.46
1:A:86:SER:O	1:A:90:GLN:HG3	2.15	0.46
1:A:256:THR:CG2	1:A:258:LEU:H	2.29	0.46
1:B:553:GLU:O	1:B:557:ARG:HG3	2.15	0.46
1:A:359:THR:O	1:A:362:ARG:HG3	2.16	0.45
1:A:161:ARG:HA	1:A:161:ARG:HD3	1.77	0.45
1:B:187:THR:HG23	1:B:258:LEU:HD12	1.99	0.45
1:B:159:MET:HB3	1:B:587:MET:HG2	1.97	0.45
1:B:74:SER:HB2	1:B:294:ILE:HB	1.99	0.45
1:A:129:VAL:HG13	1:A:132:GLN:NE2	2.32	0.45
1:A:172:LEU:HD22	1:A:177:ASP:HB3	1.99	0.45
1:A:70:LEU:HD23	1:A:328:GLU:HG2	1.98	0.44
1:A:191:LEU:HD11	1:A:256:THR:HG23	1.98	0.44
1:A:334:LYS:NZ	5:A:2194:HOH:O	2.41	0.44
1:B:288:PRO:HG3	1:B:469:HIS:HB2	1.99	0.44
1:B:460:HIS:O	1:B:464:LEU:HG	2.18	0.44
1:B:556:ARG:CD	1:B:556:ARG:H	2.28	0.44
1:B:299:ALA:HB1	1:B:303:MET:HE1	1.99	0.43
1:B:70:LEU:HD23	1:B:328:GLU:HG2	2.00	0.43
1:A:423:LYS:HA	1:A:423:LYS:HD3	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:HB2	1:B:81:LEU:HD23	2.01	0.43
1:B:594:LEU:HA	1:B:594:LEU:HD23	1.89	0.43
1:B:476:GLU:HB3	1:B:477:PRO:HD3	2.01	0.42
1:A:296:HIS:CG	1:A:317:MET:HG3	2.54	0.42
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.83	0.42
1:A:227:CYS:HA	1:A:246:LYS:O	2.20	0.42
1:B:299:ALA:HB1	1:B:303:MET:CE	2.49	0.42
1:A:193:LYS:N	1:A:193:LYS:HD3	2.35	0.42
1:A:362:ARG:HB2	1:A:365:ALA:HB3	2.02	0.41
1:A:156:LEU:O	1:A:160:GLU:HG3	2.20	0.41
1:A:222:ARG:HD2	5:A:2150:HOH:O	2.20	0.41
1:A:277:LEU:HD21	1:A:489:THR:HG22	2.02	0.41
1:B:85:ILE:HG23	1:B:88:ARG:NH2	2.37	0.40
1:A:488:PRO:HA	1:A:519:GLN:HE22	1.86	0.40
1:B:303:MET:HE2	1:B:303:MET:HB2	1.91	0.40

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	566/605 (94%)	547 (97%)	19 (3%)	0	100	100
1	B	566/605 (94%)	547 (97%)	19 (3%)	0	100	100
All	All	1132/1210 (94%)	1094 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	468/496 (94%)	461 (98%)	7 (2%)	72	70
1	B	468/496 (94%)	466 (100%)	2 (0%)	93	94
All	All	936/992 (94%)	927 (99%)	9 (1%)	82	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ASP
1	A	161	ARG
1	A	222	ARG
1	A	256	THR
1	A	346	GLN
1	A	389	PHE
1	A	518	ASP
1	B	284	HIS
1	B	389	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	100	GLN
1	A	132	GLN
1	A	519	GLN
1	B	190	GLN
1	B	213	GLN
1	B	514	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

4 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	$\# Z > 2$
3	NAG	A	1001	1,3	14,14,15	0.34	0	15,19,21	0.68	0
3	NAG	A	1002	3	14,14,15	0.32	0	15,19,21	0.63	1 (6%)
3	NAG	B	1001	1,3	14,14,15	0.62	0	15,19,21	0.67	1 (6%)
3	NAG	B	1002	3	14,14,15	0.25	0	15,19,21	0.48	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	NAG	A	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1002	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1002	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	NAG	C1-O5-C5	2.11	115.24	112.14
3	A	1002	NAG	C1-O5-C5	2.17	115.33	112.14

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
3	A	1001	NAG	1	0
3	B	1001	NAG	1	0

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
4	NAG	A	1011	1	14,14,15	0.47	0	15,19,21	0.85	0
4	NAG	A	1021	1	14,14,15	0.45	0	15,19,21	0.67	0
4	NAG	B	1011	1	14,14,15	0.40	0	15,19,21	0.39	0
4	NAG	B	1021	1	14,14,15	0.38	0	15,19,21	0.64	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
4	NAG	A	1011	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1021	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1021	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1021	NAG	C1-O5-C5	2.23	115.43	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	568/605 (93%)	0.09	28 (4%) 33 38	22, 40, 71, 99	0
1	B	568/605 (93%)	-0.10	15 (2%) 59 65	25, 40, 62, 96	0
All	All	1136/1210 (93%)	-0.00	43 (3%) 44 50	22, 40, 67, 99	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	VAL	4.1
1	A	500	ALA	4.1
1	A	121	LEU	4.0
1	A	272	PHE	4.0
1	A	186	ALA	4.0
1	B	48	ASN	3.6
1	B	39	VAL	3.5
1	A	117	GLN	3.5
1	A	190	GLN	3.1
1	B	549	LEU	3.1
1	A	483	VAL	3.1
1	A	187	THR	3.0
1	B	50	THR	3.0
1	B	277	LEU	3.0
1	A	122	ASN	2.9
1	A	175	THR	2.9
1	A	494	PRO	2.7
1	A	115	ILE	2.7
1	A	227	CYS	2.6
1	B	47	GLY	2.6
1	B	51	ALA	2.6
1	A	157	PHE	2.6
1	A	185	ARG	2.5
1	A	277	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	46	ASP	2.4
1	A	184	ASP	2.4
1	B	38	VAL	2.3
1	B	556	ARG	2.3
1	A	119	GLY	2.3
1	A	582	GLY	2.3
1	A	189	LYS	2.3
1	B	501	ASN	2.3
1	B	557	ARG	2.3
1	A	493	ALA	2.2
1	A	196	LEU	2.2
1	B	49	SER	2.2
1	A	497	THR	2.1
1	A	487	HIS	2.1
1	B	272	PHE	2.1
1	A	486	MET	2.1
1	A	503	THR	2.1
1	A	492	TYR	2.0
1	B	245	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
3	NAG	A	1002	14/15	0.91	0.27	1.36	57,66,76,76	0
3	NAG	A	1001	14/15	0.86	0.22	0.83	45,54,83,97	0
3	NAG	B	1001	14/15	0.91	0.14	0.23	38,44,58,76	0
3	NAG	B	1002	14/15	0.86	0.36	-	52,59,65,68	0

6.4 Ligands [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
4	NAG	B	1011	14/15	0.78	0.28	11.92	72,78,81,83	0
4	NAG	A	1011	14/15	0.86	0.24	5.90	63,67,72,72	0
4	NAG	B	1021	14/15	0.91	0.25	2.83	54,73,82,84	0
4	NAG	A	1021	14/15	0.80	0.16	1.23	61,65,69,72	0
2	MN	A	606	1/1	0.99	0.10	-0.92	33,33,33,33	0
2	MN	B	606	1/1	1.00	0.08	-0.96	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.