Full wwPDB X-ray Structure Validation Report (i)

Mar 21, 2016 – 03:52 PM EDT

PDB ID	:	5FCA
Title	:	Murine SMPDL3A in presence of excess zinc
Authors	:	Gorelik, A.; Illes, K.; Superti-Furga, G.; Nagar, B.
Deposited on	:	2015-12-15
Resolution	:	1.92 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

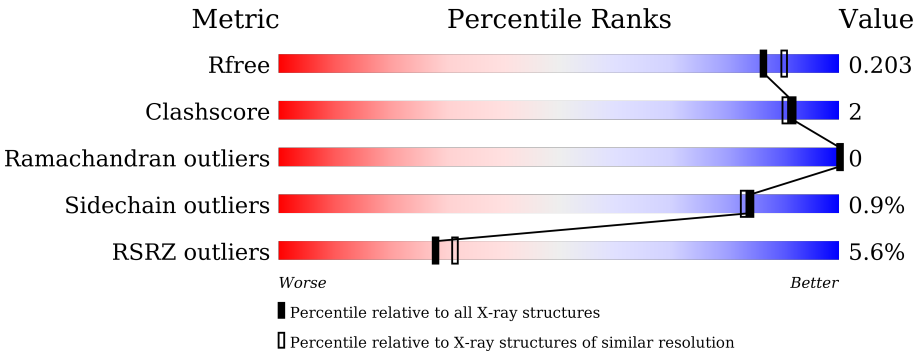
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	5832 (1.94-1.90)
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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 <=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	433	5% 93% 5% ·
1	B	433	6% 93% 6% ·

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
2	ZN	A	503	-	-	-	X
2	ZN	B	503	-	-	-	X
3	NAG	A	516	-	-	-	X
3	NAG	B	515	-	-	-	X
4	FUC	A	515	-	-	-	X
7	GOL	A	518	-	-	-	X
7	GOL	A	519	-	-	-	X
7	GOL	A	520	-	-	-	X
7	GOL	A	521	-	-	-	X
7	GOL	A	523	-	-	-	X
7	GOL	B	517	-	-	-	X
7	GOL	B	518	-	-	-	X
7	GOL	B	519	-	-	-	X
7	GOL	B	521	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15306 atoms, of which 7178 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 Acid sphingomyelinase-like phosphodiesterase 3a.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	426	Total	C	H	N	O	S	0	15	0
			6840	2233	3382	560	644	21			
1	B	426	Total	C	H	N	O	S	0	14	0
			6823	2229	3377	556	641	20			

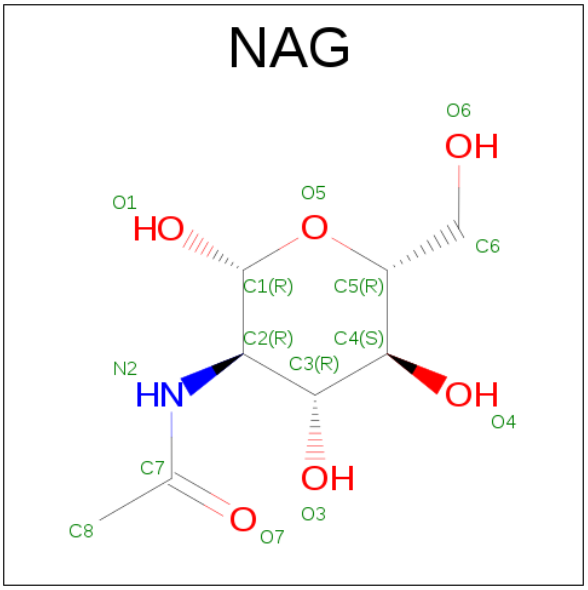
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASP	-	expression tag	UNP P70158
A	14	ARG	-	expression tag	UNP P70158
A	15	HIS	-	expression tag	UNP P70158
A	16	HIS	-	expression tag	UNP P70158
A	17	HIS	-	expression tag	UNP P70158
A	18	HIS	-	expression tag	UNP P70158
A	19	HIS	-	expression tag	UNP P70158
A	20	HIS	-	expression tag	UNP P70158
A	21	LYS	-	expression tag	UNP P70158
A	22	LEU	-	expression tag	UNP P70158
B	13	ASP	-	expression tag	UNP P70158
B	14	ARG	-	expression tag	UNP P70158
B	15	HIS	-	expression tag	UNP P70158
B	16	HIS	-	expression tag	UNP P70158
B	17	HIS	-	expression tag	UNP P70158
B	18	HIS	-	expression tag	UNP P70158
B	19	HIS	-	expression tag	UNP P70158
B	20	HIS	-	expression tag	UNP P70158
B	21	LYS	-	expression tag	UNP P70158
B	22	LEU	-	expression tag	UNP P70158

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Zn 3 3	0	0
2	A	5	Total Zn 5 5	0	0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H N O 26 8 12 1 5	0	0
3	A	1	Total C H N O 28 8 14 1 5	0	0
3	A	1	Total C H N O 27 8 13 1 5	0	0
3	A	1	Total C H N O 28 8 14 1 5	0	0
3	A	1	Total C H N O 27 8 13 1 5	0	0
3	A	1	Total C H N O 27 8 13 1 5	0	0
3	A	1	Total C H N O 26 8 12 1 5	0	0
3	A	1	Total C H N O 28 8 14 1 5	0	0
3	B	1	Total C H N O 26 8 12 1 5	0	0
3	B	1	Total C H N O 28 8 14 1 5	0	0

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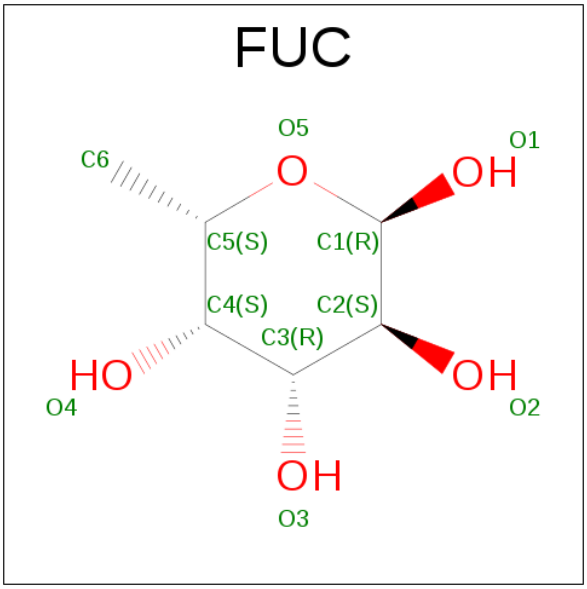
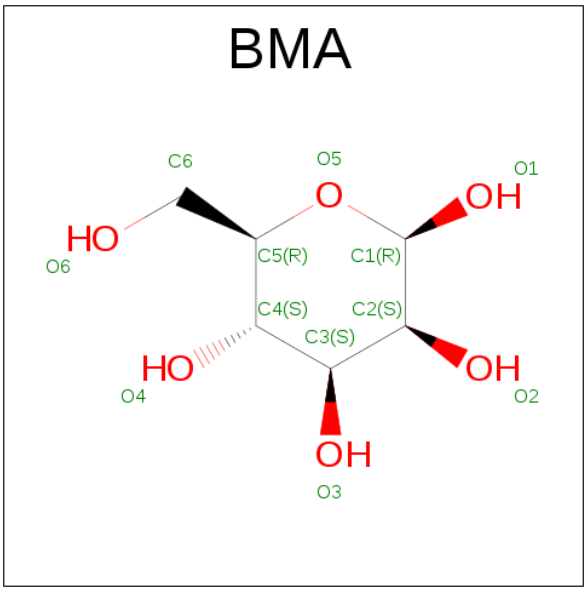
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	B	1	Total	C	H	N	O	0	0
			26	8	12	1	5		
3	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 4 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



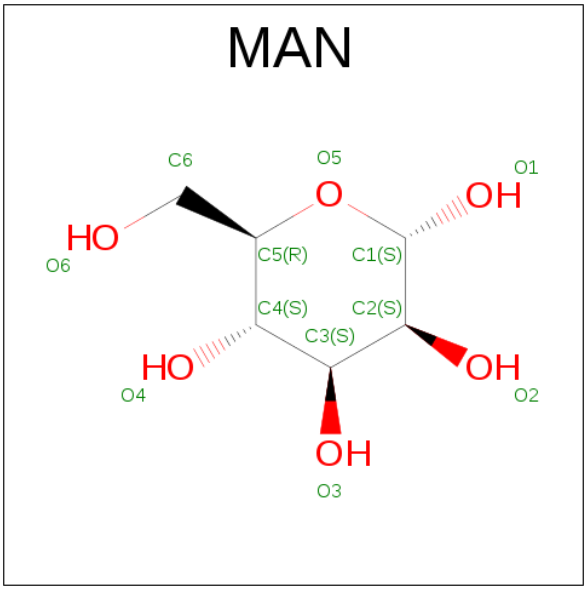
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	O		0	0
			21	6	11	4			
4	A	1	Total	C	H	O		0	0
			21	6	11	4			
4	B	1	Total	C	H	O		0	0
			21	6	11	4			
4	B	1	Total	C	H	O		0	0
			21	6	11	4			

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			20	6	9	5		
5	B	1	Total	C	H	O	0	0
			20	6	9	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			22	6	11	5		
6	A	1	Total	C	H	O	0	0
			22	6	11	5		

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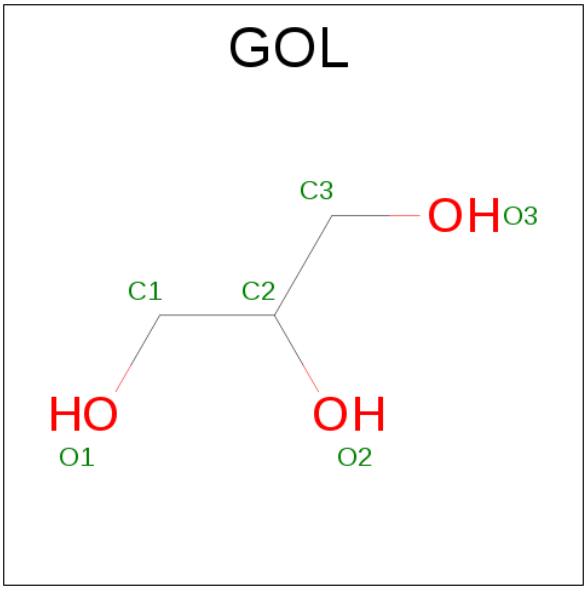
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C H O 22 6 11 5	0	0
6	B	1	Total C H O 22 6 11 5	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 14 3 8 3	0	0
7	A	1	Total C H O 14 3 8 3	0	0
7	A	1	Total C H O 14 3 8 3	0	0
7	A	1	Total C H O 14 3 8 3	0	0
7	A	1	Total C H O 14 3 8 3	0	0
7	A	1	Total C H O 14 3 8 3	0	0
7	B	1	Total C H O 14 3 8 3	0	0
7	B	1	Total C H O 14 3 8 3	0	0
7	B	1	Total C H O 14 3 8 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is water.

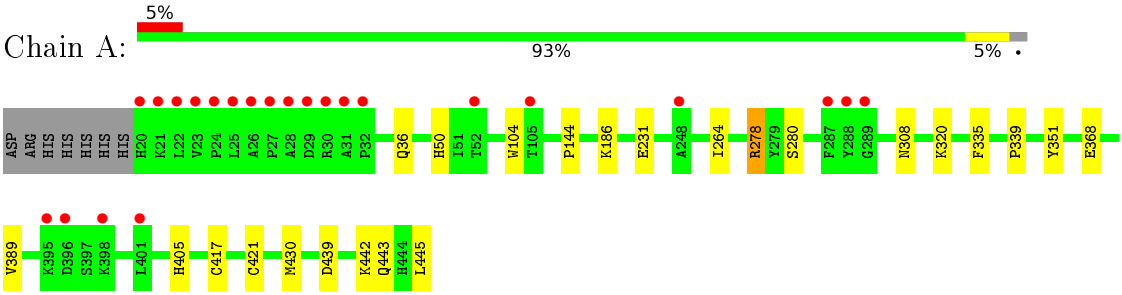
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	419	Total	O	0	0
			419	419		
8	B	389	Total	O	0	0
			389	389		

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.

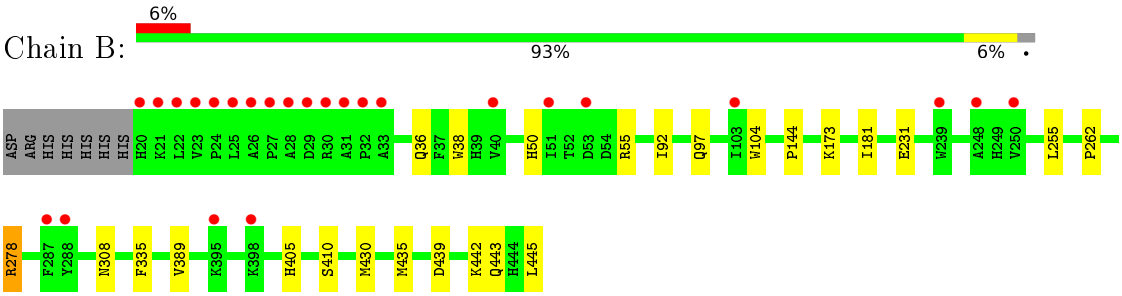
- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a

Chain A:



- Molecule 1: Acid sphingomyelinase-like phosphodiesterase 3a

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.14Å 123.59Å 131.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.31 – 1.92 39.31 – 1.92	Depositor EDS
% Data completeness (in resolution range)	91.1 (39.31-1.92) 83.8 (39.31-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.175 , 0.204 0.174 , 0.203	Depositor DCC
R_{free} test set	3753 reflections (2.15%)	DCC
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 52.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 91444 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15306	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.82 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.3099e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, ZN, BMA, NAG, FUC, 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	0.52	0/3604	0.62	1/4917 (0.0%)
1	B	0.52	0/3586	0.63	1/4894 (0.0%)
All	All	0.52	0/7190	0.63	2/9811 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	278	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	278	ARG	NE-CZ-NH2	-5.32	117.64	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	3458	3382	3412	17	0
1	B	3446	3377	3404	14	0
2	A	5	0	0	0	0
2	B	3	0	0	0	0
3	A	112	105	97	0	0
3	B	112	104	97	1	0
4	A	20	22	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	20	22	20	0	0
5	A	11	9	8	0	0
5	B	11	9	8	0	0
6	A	22	22	20	0	0
6	B	22	22	20	0	0
7	A	36	48	48	0	0
7	B	42	56	56	2	0
8	A	419	0	0	7	2
8	B	389	0	0	3	2
All	All	8128	7178	7210	31	2

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 2.

All (31) 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:435[B]:MET:SD	8:B:977:HOH:O	2.18	1.01
1:B:231:GLU:OE2	1:B:278:ARG:NH2	2.11	0.83
1:A:439[A]:ASP:OD1	8:A:601:HOH:O	1.98	0.80
1:B:97:GLN:O	7:B:523:GOL:O1	2.16	0.63
7:B:521:GOL:O3	8:B:601:HOH:O	2.16	0.63
1:A:439[B]:ASP:OD2	1:A:443:GLN:NE2	2.35	0.60
1:A:430[A]:MET:HE3	8:A:906:HOH:O	2.05	0.56
1:B:439:ASP:OD2	1:B:443:GLN:NE2	2.42	0.51
1:A:231:GLU:OE2	1:A:278:ARG:NH2	2.32	0.51
1:A:320[A]:LYS:NZ	8:A:606:HOH:O	2.30	0.51
1:A:339:PRO:O	8:A:602:HOH:O	2.20	0.51
1:A:36:GLN:HA	1:A:335:PHE:O	2.12	0.49
1:A:389:VAL:HG11	1:A:430[A]:MET:HG3	1.96	0.47
1:B:389:VAL:HG11	1:B:430[A]:MET:HG3	1.96	0.47
1:A:104:TRP:O	1:A:144:PRO:HA	2.16	0.46
3:B:506:NAG:H3	3:B:506:NAG:O7	2.16	0.44
1:A:405:HIS:HE1	8:A:877:HOH:O	2.01	0.43
1:A:389:VAL:HG11	1:A:430[B]:MET:HG2	2.00	0.43
1:B:173:LYS:HA	1:B:181:ILE:HD11	2.01	0.42
1:B:38:TRP:CE2	1:B:92:ILE:HG23	2.54	0.42
1:B:389:VAL:HG11	1:B:430[B]:MET:HG2	2.02	0.41
1:B:405:HIS:CE1	1:B:410:SER:HA	2.55	0.41
1:A:445:LEU:O	1:B:442:LYS:HD2	2.19	0.41
1:A:442:LYS:HD2	1:B:445:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HE2	8:A:982:HOH:O	2.21	0.41
1:B:104:TRP:O	1:B:144:PRO:HA	2.21	0.41
1:A:351:TYR:CD1	1:A:368:GLU:HB2	2.56	0.41
1:B:255:LEU:HD23	8:B:924:HOH:O	2.21	0.41
1:B:36:GLN:HA	1:B:335:PHE:O	2.20	0.40
1:A:264:ILE:HG12	8:A:719:HOH:O	2.20	0.40
1:A:417:CYS:SG	1:A:421[C]:CYS:HB3	2.61	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:967:HOH:O	8:B:939:HOH:O[4_545]	2.15	0.05
8:A:940:HOH:O	8:B:838:HOH:O[3_554]	2.17	0.03

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	440/433 (102%)	419 (95%)	21 (5%)	0	100	100
1	B	438/433 (101%)	418 (95%)	20 (5%)	0	100	100
All	All	878/866 (101%)	837 (95%)	41 (5%)	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	393/384 (102%)	390 (99%)	3 (1%)	86 85
1	B	391/384 (102%)	387 (99%)	4 (1%)	82 80
All	All	784/768 (102%)	777 (99%)	7 (1%)	84 83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	280	SER
1	A	308	ASN
1	B	50	HIS
1	B	55	ARG
1	B	262	PRO
1	B	308	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 47 ligands modelled in this entry, 8 are monoatomic - leaving 39 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	NAG	A	505	1,3,4	14,14,15	0.58	0	15,19,21	0.81	0
4	FUC	A	506	3	10,10,11	1.47	2 (20%)	13,14,16	1.25	1 (7%)
3	NAG	A	507	3	14,14,15	0.69	0	15,19,21	1.59	4 (26%)
3	NAG	A	508	1,3	14,14,15	0.60	0	15,19,21	0.73	0
3	NAG	A	509	3	14,14,15	0.75	0	15,19,21	1.34	3 (20%)
5	BMA	A	510	3,6	11,11,12	0.80	0	15,15,17	1.25	2 (13%)
6	MAN	A	511	5	11,11,12	1.12	1 (9%)	15,15,17	1.37	1 (6%)
6	MAN	A	512	5	11,11,12	1.33	2 (18%)	15,15,17	1.89	4 (26%)
3	NAG	A	513	1,3	14,14,15	0.36	0	15,19,21	0.53	0
3	NAG	A	514	3,5	14,14,15	0.47	0	15,19,21	0.61	0
4	FUC	A	515	3	10,10,11	1.40	2 (20%)	13,14,16	1.13	1 (7%)
3	NAG	A	516	1,3,4	14,14,15	0.95	1 (7%)	15,19,21	0.42	0
3	NAG	A	517	3	14,14,15	0.32	0	15,19,21	0.51	0
7	GOL	A	518	-	5,5,5	0.28	0	5,5,5	0.49	0
7	GOL	A	519	-	5,5,5	0.27	0	5,5,5	0.28	0
7	GOL	A	520	-	5,5,5	0.40	0	5,5,5	0.42	0
7	GOL	A	521	-	5,5,5	0.41	0	5,5,5	0.27	0
7	GOL	A	522	-	5,5,5	0.30	0	5,5,5	0.30	0
7	GOL	A	523	-	5,5,5	0.42	0	5,5,5	0.21	0
4	FUC	B	504	3	10,10,11	1.33	1 (10%)	13,14,16	1.40	2 (15%)
3	NAG	B	505	1,3,4	14,14,15	0.74	1 (7%)	15,19,21	0.88	1 (6%)
3	NAG	B	506	3	14,14,15	0.62	0	15,19,21	1.49	3 (20%)
3	NAG	B	507	1,3	14,14,15	0.31	0	15,19,21	0.61	0
3	NAG	B	508	3	14,14,15	0.28	0	15,19,21	0.37	0
5	BMA	B	509	3,6	11,11,12	0.66	0	15,15,17	0.68	0
6	MAN	B	510	5	11,11,12	1.15	1 (9%)	15,15,17	1.33	1 (6%)
6	MAN	B	511	5	11,11,12	1.32	2 (18%)	15,15,17	1.46	2 (13%)
3	NAG	B	512	1,3	14,14,15	0.29	0	15,19,21	0.53	0
3	NAG	B	513	3,5	14,14,15	0.45	0	15,19,21	0.47	0
4	FUC	B	514	3	10,10,11	1.51	1 (10%)	13,14,16	1.11	1 (7%)
3	NAG	B	515	1,3,4	14,14,15	1.13	1 (7%)	15,19,21	0.77	1 (6%)
3	NAG	B	516	3	14,14,15	0.32	0	15,19,21	0.39	0
7	GOL	B	517	-	5,5,5	0.46	0	5,5,5	0.35	0
7	GOL	B	518	-	5,5,5	0.32	0	5,5,5	0.38	0
7	GOL	B	519	-	5,5,5	0.40	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GOL	B	520	-	5,5,5	0.55	0	5,5,5	0.44	0
7	GOL	B	521	-	5,5,5	0.29	0	5,5,5	0.58	0
7	GOL	B	522	-	5,5,5	0.23	0	5,5,5	0.46	0
7	GOL	B	523	-	5,5,5	0.23	0	5,5,5	0.56	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	505	1,3,4	-	0/6/23/26	0/1/1/1
4	FUC	A	506	3	-	0/0/17/20	0/1/1/1
3	NAG	A	507	3	-	0/6/23/26	0/1/1/1
3	NAG	A	508	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	509	3	-	0/6/23/26	0/1/1/1
5	BMA	A	510	3,6	-	0/2/19/22	0/1/1/1
6	MAN	A	511	5	-	0/2/19/22	1/1/1/1
6	MAN	A	512	5	-	0/2/19/22	0/1/1/1
3	NAG	A	513	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	514	3,5	-	0/6/23/26	0/1/1/1
4	FUC	A	515	3	-	0/0/17/20	0/1/1/1
3	NAG	A	516	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	517	3	-	0/6/23/26	0/1/1/1
7	GOL	A	518	-	-	0/4/4/4	0/0/0/0
7	GOL	A	519	-	-	0/4/4/4	0/0/0/0
7	GOL	A	520	-	-	0/4/4/4	0/0/0/0
7	GOL	A	521	-	-	0/4/4/4	0/0/0/0
7	GOL	A	522	-	-	0/4/4/4	0/0/0/0
7	GOL	A	523	-	-	0/4/4/4	0/0/0/0
4	FUC	B	504	3	-	0/0/17/20	0/1/1/1
3	NAG	B	505	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	506	3	-	0/6/23/26	0/1/1/1
3	NAG	B	507	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	508	3	-	0/6/23/26	0/1/1/1
5	BMA	B	509	3,6	-	0/2/19/22	0/1/1/1
6	MAN	B	510	5	-	0/2/19/22	0/1/1/1
6	MAN	B	511	5	-	0/2/19/22	0/1/1/1
3	NAG	B	512	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	513	3,5	-	0/6/23/26	0/1/1/1
4	FUC	B	514	3	-	0/0/17/20	0/1/1/1
3	NAG	B	515	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	516	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	517	-	-	0/4/4/4	0/0/0/0
7	GOL	B	518	-	-	0/4/4/4	0/0/0/0
7	GOL	B	519	-	-	0/4/4/4	0/0/0/0
7	GOL	B	520	-	-	0/4/4/4	0/0/0/0
7	GOL	B	521	-	-	0/4/4/4	0/0/0/0
7	GOL	B	522	-	-	0/4/4/4	0/0/0/0
7	GOL	B	523	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	515	NAG	O5-C1	-4.03	1.37	1.43
3	A	516	NAG	O5-C1	-3.40	1.38	1.43
3	B	505	NAG	O5-C1	-2.57	1.39	1.43
4	A	506	FUC	C2-C3	2.02	1.55	1.52
6	B	511	MAN	C2-C3	2.16	1.55	1.52
6	A	511	MAN	C4-C5	2.16	1.57	1.53
4	A	515	FUC	C6-C5	2.17	1.56	1.51
6	B	510	MAN	C1-C2	2.23	1.57	1.52
4	A	515	FUC	C1-C2	2.30	1.57	1.52
6	A	512	MAN	C2-C3	2.52	1.55	1.52
6	B	511	MAN	C1-C2	2.99	1.59	1.52
4	B	504	FUC	C1-C2	3.09	1.59	1.52
6	A	512	MAN	C1-C2	3.17	1.59	1.52
4	A	506	FUC	C1-C2	3.20	1.60	1.52
4	B	514	FUC	C1-C2	3.22	1.60	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	512	MAN	O2-C2-C3	-2.52	105.11	110.19
5	A	510	BMA	O5-C1-C2	-2.19	107.39	110.89
3	A	509	NAG	C4-C3-C2	-2.16	107.99	111.34
3	A	507	NAG	C2-N2-C7	2.05	125.77	123.11
4	A	515	FUC	O2-C2-C1	2.09	113.43	109.23
6	B	511	MAN	O5-C1-C2	2.16	114.35	110.89
3	B	506	NAG	C3-C4-C5	2.27	114.27	110.23
3	B	505	NAG	C1-O5-C5	2.44	115.73	112.14
3	B	515	NAG	C1-O5-C5	2.46	115.76	112.14
4	B	514	FUC	O2-C2-C1	2.48	114.19	109.23
5	A	510	BMA	C3-C4-C5	2.54	114.76	110.23
4	B	504	FUC	O5-C1-C2	2.63	115.09	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	507	NAG	C3-C4-C5	2.67	114.99	110.23
6	A	512	MAN	O5-C1-C2	2.69	115.19	110.89
3	B	506	NAG	O5-C5-C4	2.69	114.60	110.13
3	A	509	NAG	O5-C5-C4	2.70	114.60	110.13
3	A	509	NAG	C1-O5-C5	2.84	116.32	112.14
3	A	507	NAG	C1-O5-C5	2.93	116.45	112.14
4	B	504	FUC	C1-C2-C3	2.95	113.13	109.55
3	A	507	NAG	O5-C5-C4	3.21	115.45	110.13
4	A	506	FUC	C1-C2-C3	3.26	113.50	109.55
6	B	510	MAN	C1-O5-C5	3.60	117.44	112.14
6	B	511	MAN	C1-O5-C5	3.70	117.58	112.14
6	A	512	MAN	C1-O5-C5	3.77	117.68	112.14
3	B	506	NAG	C1-O5-C5	3.96	117.96	112.14
6	A	511	MAN	C1-O5-C5	4.15	118.24	112.14
6	A	512	MAN	C1-C2-C3	4.45	114.94	109.55

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	511	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	506	NAG	1	0
7	B	521	GOL	1	0
7	B	523	GOL	1	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

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, 95^{th} 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	426/433 (98%)	0.48	23 (5%)	29	33	28, 41, 63, 146	0
1	B	426/433 (98%)	0.54	25 (5%)	26	29	27, 43, 72, 150	0
All	All	852/866 (98%)	0.51	48 (5%)	28	31	27, 42, 67, 150	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	ASP	13.5
1	A	31	ALA	13.0
1	A	25	LEU	12.6
1	A	26	ALA	12.5
1	A	28	ALA	10.5
1	A	30	ARG	10.4
1	B	28	ALA	10.4
1	B	31	ALA	10.3
1	B	20	HIS	10.0
1	A	29	ASP	9.8
1	A	20	HIS	9.4
1	A	32	PRO	9.0
1	A	23	VAL	9.0
1	B	23	VAL	8.6
1	B	26	ALA	8.6
1	B	27	PRO	7.8
1	A	21	LYS	7.6
1	A	22	LEU	7.3
1	B	25	LEU	6.7
1	B	30	ARG	6.6
1	A	27	PRO	5.8
1	B	32	PRO	5.7
1	B	33	ALA	5.2
1	B	21	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	24	PRO	4.1
1	B	22	LEU	3.9
1	B	24	PRO	3.4
1	B	51	ILE	3.3
1	B	53	ASP	3.0
1	B	398	LYS	2.8
1	A	395	LYS	2.8
1	A	288	TYR	2.7
1	A	289	GLY	2.7
1	B	250	VAL	2.6
1	B	248	ALA	2.6
1	B	395	LYS	2.5
1	B	287	PHE	2.4
1	B	239	TRP	2.4
1	A	396	ASP	2.4
1	B	288	TYR	2.3
1	A	398	LYS	2.3
1	B	103	ILE	2.2
1	A	401	LEU	2.2
1	A	52	THR	2.2
1	A	287	PHE	2.1
1	B	40	VAL	2.0
1	A	248	ALA	2.0
1	A	105	THR	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)

There are no carbohydrates in this entry.

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, 95^{th} 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
7	GOL	B	517	6/6	0.68	0.51	12.72	65,80,96,96	0
4	FUC	A	515	10/11	0.71	0.38	9.57	93,118,140,143	0
7	GOL	B	518	6/6	0.76	0.32	7.21	65,78,89,91	0
7	GOL	B	519	6/6	0.88	0.29	5.85	59,71,82,82	0
7	GOL	A	521	6/6	0.86	0.35	5.78	57,70,84,84	0
3	NAG	A	516	14/15	0.81	0.28	4.48	66,91,111,119	0
7	GOL	A	520	6/6	0.66	0.28	4.47	68,82,93,96	0
2	ZN	A	503	1/1	0.80	0.26	4.46	74,74,74,74	0
7	GOL	A	519	6/6	0.90	0.34	3.93	70,88,97,105	0
7	GOL	A	518	6/6	0.90	0.15	3.73	51,62,70,85	0
3	NAG	B	515	14/15	0.83	0.23	3.32	71,95,116,123	0
7	GOL	B	521	6/6	0.73	0.21	2.50	56,67,74,79	0
7	GOL	A	523	6/6	0.91	0.21	2.48	58,71,96,106	0
2	ZN	B	503	1/1	0.89	0.21	2.16	74,74,74,74	0
7	GOL	B	520	6/6	0.86	0.34	1.91	58,74,87,105	0
7	GOL	B	523	6/6	0.88	0.16	1.08	55,67,83,84	0
3	NAG	A	505	14/15	0.86	0.17	0.88	67,85,108,108	0
7	GOL	A	522	6/6	0.86	0.17	0.82	54,76,134,134	0
3	NAG	B	507	14/15	0.87	0.13	0.74	68,84,103,108	0
3	NAG	B	513	14/15	0.90	0.12	0.71	67,87,104,107	0
3	NAG	B	505	14/15	0.88	0.19	0.70	83,102,125,129	0
3	NAG	A	508	14/15	0.88	0.11	0.49	55,70,87,93	0
7	GOL	B	522	6/6	0.89	0.12	0.38	61,73,86,86	0
3	NAG	A	513	14/15	0.91	0.11	0.34	52,65,79,85	0
2	ZN	A	524	1/1	0.95	0.11	0.19	44,44,44,44	1
2	ZN	A	501	1/1	0.99	0.13	-0.70	42,42,42,42	0
2	ZN	B	501	1/1	0.99	0.12	-0.97	47,47,47,47	0
3	NAG	B	512	14/15	0.95	0.07	-1.75	50,61,76,80	0
2	ZN	A	504	1/1	0.96	0.07	-2.00	44,44,44,44	1
2	ZN	B	502	1/1	0.99	0.10	-2.01	48,48,48,48	0
2	ZN	A	502	1/1	0.99	0.10	-2.33	48,48,48,48	0
5	BMA	B	509	11/12	0.85	0.29	-	97,109,128,131	0
3	NAG	A	517	14/15	0.66	0.47	-	85,113,138,144	0
4	FUC	B	504	10/11	0.84	0.41	-	119,125,149,150	0
5	BMA	A	510	11/12	0.79	0.29	-	117,138,162,166	0
3	NAG	A	514	14/15	0.89	0.16	-	78,95,118,125	0
6	MAN	B	511	11/12	0.62	0.44	-	100,122,141,146	0
3	NAG	A	509	14/15	0.72	0.37	-	70,111,136,149	0
6	MAN	A	511	11/12	0.59	0.41	-	102,137,158,166	0
6	MAN	A	512	11/12	0.65	0.51	-	111,137,156,167	0
6	MAN	B	510	11/12	0.66	0.41	-	94,113,130,138	0
4	FUC	A	506	10/11	0.87	0.29	-	95,108,127,129	0
4	FUC	B	514	10/11	0.50	0.47	-	106,128,160,167	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	B	508	14/15	0.61	0.33	-	76,112,140,143	0
3	NAG	A	507	14/15	0.79	0.36	-	89,117,142,145	0
3	NAG	B	506	14/15	0.83	0.36	-	102,125,150,152	0
3	NAG	B	516	14/15	0.60	0.49	-	95,123,150,156	0

6.5 Other polymers (i)

There are no such residues in this entry.