Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:42 PM GMT

PDB ID	:	4MHX
Title	:	Crystal Structure of Sulfamidase
Authors	:	Sidhu, N.S.; Uson, I.; Schreiber, K.; Proepper, K.; Becker, S.; Gaertner, J.; Kraetzner, R.; Steinfeld, R.; Sheldrick, G.M.
Deposited on	:	2013-08-30
Resolution	:	2.00 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:

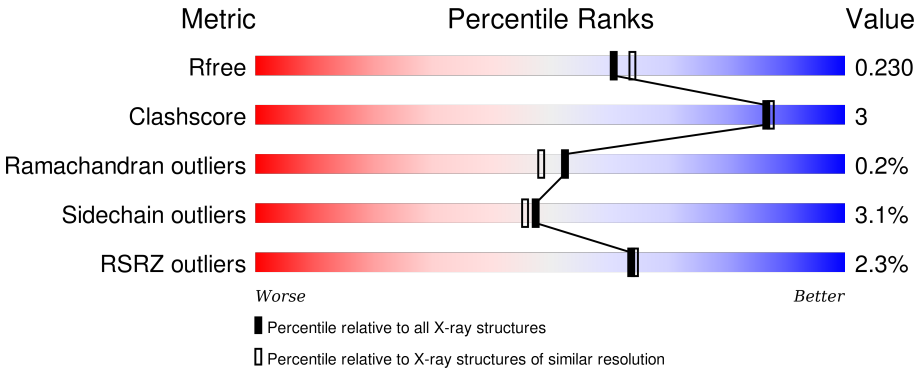
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	510	2% 87% 7% • 5%
1	B	510	2% 86% 7% • 5%

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
3	NAG	A	602	-	-	-	X
5	MG	B	608	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7975 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 N-sulphoglucosamine sulphohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	P	S	0	0	0
			3792	2441	655	684	1	11			
1	B	482	Total	C	N	O	P	S	0	2	0
			3806	2445	654	695	1	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	70	FGP	CYS	MODIFIED RESIDUE	UNP P51688
A	503	ARG	-	EXPRESSION TAG	UNP P51688
A	504	SER	-	EXPRESSION TAG	UNP P51688
A	505	HIS	-	EXPRESSION TAG	UNP P51688
A	506	HIS	-	EXPRESSION TAG	UNP P51688
A	507	HIS	-	EXPRESSION TAG	UNP P51688
A	508	HIS	-	EXPRESSION TAG	UNP P51688
A	509	HIS	-	EXPRESSION TAG	UNP P51688
A	510	HIS	-	EXPRESSION TAG	UNP P51688
B	70	FGP	CYS	MODIFIED RESIDUE	UNP P51688
B	503	ARG	-	EXPRESSION TAG	UNP P51688
B	504	SER	-	EXPRESSION TAG	UNP P51688
B	505	HIS	-	EXPRESSION TAG	UNP P51688
B	506	HIS	-	EXPRESSION TAG	UNP P51688
B	507	HIS	-	EXPRESSION TAG	UNP P51688
B	508	HIS	-	EXPRESSION TAG	UNP P51688
B	509	HIS	-	EXPRESSION TAG	UNP P51688
B	510	HIS	-	EXPRESSION TAG	UNP P51688

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		

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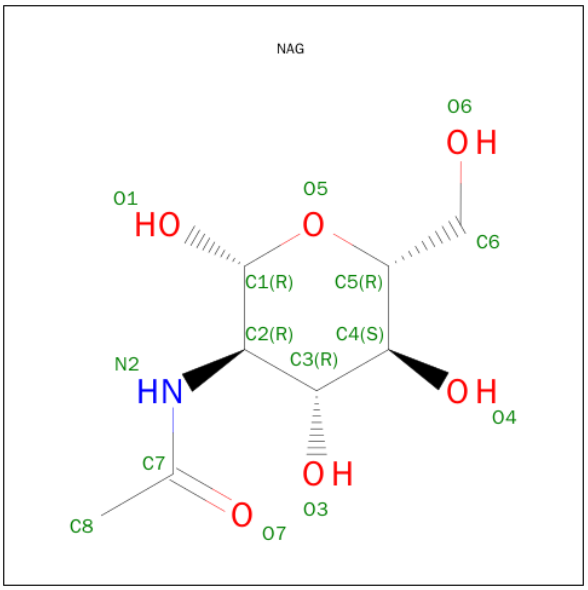
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0

- Molecule 3 is SUGAR (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 N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Mg 2 2	0	0

- Molecule 6 is water.

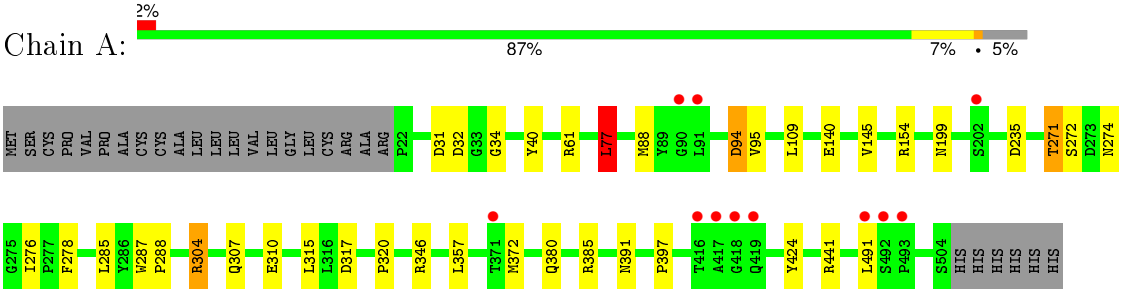
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	95	Total O 95 95	0	0
6	B	110	Total O 110 110	0	0

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.

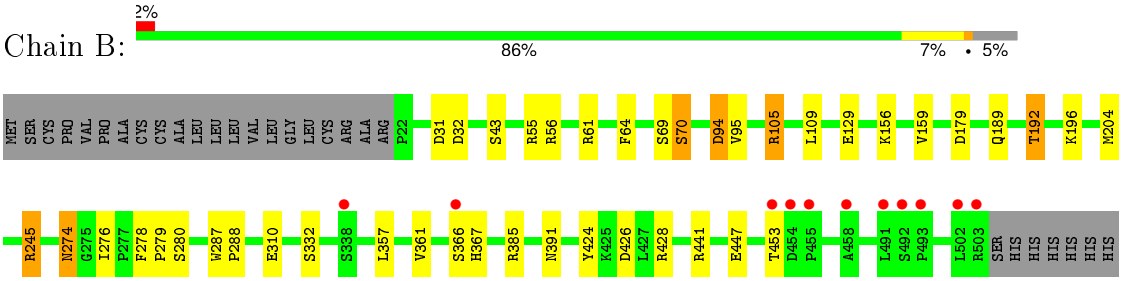
- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain A:



- Molecule 1: N-sulphoglucosamine sulphohydrolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.38Å 107.90Å 79.79Å 90.00° 104.07° 90.00°	Depositor
Resolution (Å)	44.30 – 2.00 44.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.30-2.00) 99.9 (44.26-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.230 0.197 , 0.230	Depositor DCC
R_{free} test set	3448 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 67884 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7975	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MG, FGP, CA, 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	0.62	0/3902	0.76	4/5334 (0.1%)
1	B	0.66	0/3922	0.74	2/5361 (0.0%)
All	All	0.64	0/7824	0.75	6/10695 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	MET	CG-SD-CE	-13.29	78.93	100.20
1	A	154	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	245	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	77	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	428	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	441	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	FGP	Mainchain

5.2 Too-close contacts (i)

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	3792	0	3594	19	0
1	B	3806	0	3584	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	26	1	0
3	B	28	0	26	0	0
4	A	56	0	50	0	0
4	B	56	0	50	0	0
5	B	2	0	0	0	0
6	A	95	0	0	1	0
6	B	110	0	0	4	0
All	All	7975	0	7330	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (41) 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:192:THR:HG22	6:B:809:HOH:O	1.95	0.67
1:A:61:ARG:HD2	1:A:310:GLU:OE2	1.99	0.63
1:B:385:ARG:HD3	1:B:447:GLU:OE2	2.00	0.61
1:B:43:SER:CB	6:B:765:HOH:O	2.50	0.60
1:B:61:ARG:HD2	1:B:310:GLU:OE2	2.03	0.58
1:B:357:LEU:O	1:B:357:LEU:HD12	2.04	0.57
1:B:179:ASP:OD2	1:B:245:ARG:HD2	2.05	0.57
1:B:366[B]:SER:OG	1:B:367:HIS:N	2.38	0.57
1:A:40:TYR:HA	3:A:602:NAG:H82	1.88	0.56
1:A:357:LEU:O	1:A:357:LEU:HD12	2.05	0.55
1:A:271:THR:HG21	1:A:315:LEU:HD11	1.89	0.54
1:B:156:LYS:O	1:B:159[A]:VAL:HG12	2.07	0.54
1:B:287:TRP:HB3	1:B:288:PRO:HD3	1.92	0.51
1:A:34:GLY:HA2	6:A:778:HOH:O	2.11	0.50
1:B:276:ILE:HD12	1:B:278:PHE:CD2	2.47	0.50
1:A:31:ASP:O	1:A:32:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ASP:O	1:B:32:ASP:HB2	2.12	0.49
1:A:285:LEU:O	1:A:385:ARG:NH2	2.47	0.48
1:A:276:ILE:HD12	1:A:278:PHE:CD2	2.49	0.47
1:B:105:ARG:N	1:B:105:ARG:HD2	2.30	0.47
1:A:140:GLU:HB3	1:A:145:VAL:HG12	1.97	0.47
1:B:189:GLN:OE1	1:B:189:GLN:N	2.44	0.46
1:A:304:ARG:HG3	1:A:307:GLN:CD	2.36	0.46
1:B:69:SER:O	1:B:70:FGP:C	2.64	0.46
1:B:32:ASP:OD1	1:B:274:ASN:ND2	2.44	0.44
1:A:271:THR:HG22	1:A:272:SER:H	1.83	0.44
1:A:77:LEU:C	1:A:77:LEU:CD2	2.86	0.43
1:A:287:TRP:HB3	1:A:288:PRO:HD3	2.00	0.43
1:B:279:PRO:O	1:B:280:SER:HB2	2.19	0.42
1:B:385:ARG:HD2	1:B:441:ARG:HD2	2.02	0.42
1:A:77:LEU:C	1:A:77:LEU:HD23	2.38	0.42
1:B:55:ARG:HD2	6:B:776:HOH:O	2.18	0.42
1:B:426:ASP:HB2	6:B:784:HOH:O	2.20	0.41
1:B:64:PHE:HB2	1:B:361:VAL:HG11	2.02	0.41
1:A:199:ASN:OD1	1:A:199:ASN:C	2.59	0.41
1:A:140:GLU:HB3	1:A:145:VAL:CG1	2.50	0.41
1:A:380:GLN:OE1	1:A:385:ARG:NH1	2.53	0.41
1:A:317:ASP:C	1:A:320:PRO:HD2	2.41	0.41
1:B:196:LYS:O	1:B:204:MET:HB3	2.22	0.40
1:B:287:TRP:N	1:B:288:PRO:CD	2.84	0.40
1:A:372:MET:HG2	1:A:397:PRO:HB2	2.03	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	480/510 (94%)	467 (97%)	12 (2%)	1 (0%)	52 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	481/510 (94%)	466 (97%)	14 (3%)	1 (0%)	52 48
All	All	961/1020 (94%)	933 (97%)	26 (3%)	2 (0%)	52 48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	B	94	ASP

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	391/442 (88%)	379 (97%)	12 (3%)	47 46
1	B	394/442 (89%)	382 (97%)	12 (3%)	48 47
All	All	785/884 (89%)	761 (97%)	24 (3%)	47 46

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	94	ASP
1	A	95	VAL
1	A	109	LEU
1	A	235	ASP
1	A	271	THR
1	A	274	ASN
1	A	304	ARG
1	A	346	ARG
1	A	391	ASN
1	A	424	TYR
1	A	491	LEU
1	B	56	ARG
1	B	94	ASP

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Mol	Chain	Res	Type
1	B	95	VAL
1	B	105	ARG
1	B	109	LEU
1	B	129	GLU
1	B	192	THR
1	B	274	ASN
1	B	332	SER
1	B	391	ASN
1	B	424	TYR
1	B	453	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	FGP	A	70	1,2	7,10,11	0.75	0	7,14,16	2.62	1 (14%)
1	FGP	B	70	1,2	7,10,11	0.86	0	7,14,16	2.96	3 (42%)

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	FGP	A	70	1,2	-	0/5/11/13	0/0/0/0
1	FGP	B	70	1,2	-	0/5/11/13	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	70	FGP	O-C-CA	-6.88	107.28	125.44
1	A	70	FGP	O-C-CA	-6.13	109.25	125.44
1	B	70	FGP	P-OG2-CB	-2.06	116.61	121.56
1	B	70	FGP	O3P-P-O2P	2.90	118.41	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	70	FGP	1	0

5.5 Carbohydrates (i)

8 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	A	603	1,4	14,14,15	0.71	0	15,19,21	1.11	1 (6%)
4	NAG	A	604	4	14,14,15	0.55	0	15,19,21	1.39	3 (20%)
4	NAG	A	605	1,4	14,14,15	0.49	0	15,19,21	1.16	1 (6%)
4	NAG	A	606	4	14,14,15	0.57	0	15,19,21	1.51	3 (20%)
4	NAG	B	603	1,4	14,14,15	0.81	0	15,19,21	1.66	2 (13%)
4	NAG	B	604	4	14,14,15	0.65	0	15,19,21	0.97	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	605	1,4	14,14,15	0.74	1 (7%)	15,19,21	1.80	3 (20%)
4	NAG	B	606	4	14,14,15	0.66	0	15,19,21	1.73	2 (13%)

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	603	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	604	4	-	0/6/23/26	0/1/1/1
4	NAG	A	605	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	606	4	-	0/6/23/26	0/1/1/1
4	NAG	B	603	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	604	4	-	0/6/23/26	0/1/1/1
4	NAG	B	605	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	606	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	605	NAG	O5-C5	-2.05	1.38	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	605	NAG	O3-C3-C2	-3.58	102.03	109.11
4	A	604	NAG	C2-N2-C7	-2.66	119.62	123.04
4	A	606	NAG	C3-C4-C5	-2.41	106.00	110.20
4	A	603	NAG	O7-C7-C8	-2.33	117.78	122.06
4	B	604	NAG	O7-C7-C8	-2.31	117.83	122.06
4	A	604	NAG	C4-C3-C2	-2.06	108.03	111.23
4	A	604	NAG	C1-O5-C5	2.09	114.90	112.25
4	B	603	NAG	O7-C7-N2	2.15	126.26	121.86
4	A	606	NAG	C2-N2-C7	2.81	126.65	123.04
4	A	606	NAG	O4-C4-C5	2.89	116.89	109.24
4	B	605	NAG	C1-O5-C5	3.10	116.19	112.25
4	B	606	NAG	C4-C3-C2	3.28	116.33	111.23
4	A	605	NAG	C1-O5-C5	3.64	116.86	112.25
4	B	605	NAG	C3-C4-C5	3.81	116.84	110.20
4	B	606	NAG	C3-C4-C5	4.55	118.13	110.20
4	B	603	NAG	C1-O5-C5	5.20	118.85	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
3	NAG	A	602	1	14,14,15	0.62	0	15,19,21	2.01	5 (33%)
3	NAG	A	607	1	14,14,15	0.77	1 (7%)	15,19,21	1.67	5 (33%)
3	NAG	B	602	1	14,14,15	0.64	0	15,19,21	1.10	1 (6%)
3	NAG	B	607	1	14,14,15	0.53	0	15,19,21	1.75	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
3	NAG	A	602	1	-	0/6/23/26	0/1/1/1
3	NAG	A	607	1	-	0/6/23/26	0/1/1/1
3	NAG	B	602	1	-	0/6/23/26	0/1/1/1
3	NAG	B	607	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	607	NAG	C1-C2	2.21	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	NAG	O7-C7-C8	-3.29	116.03	122.06
3	B	602	NAG	C2-N2-C7	-2.70	119.58	123.04
3	A	607	NAG	O7-C7-C8	-2.41	117.65	122.06
3	A	607	NAG	C3-C4-C5	-2.08	106.57	110.20
3	A	602	NAG	C3-C2-N2	2.01	115.38	110.56
3	A	607	NAG	O4-C4-C5	2.07	114.74	109.24
3	A	607	NAG	C1-O5-C5	2.77	115.76	112.25
3	A	602	NAG	O7-C7-N2	2.81	127.59	121.86
3	A	607	NAG	O3-C3-C2	3.29	115.63	109.11
3	A	602	NAG	C1-O5-C5	3.64	116.87	112.25
3	A	602	NAG	C2-N2-C7	4.05	128.25	123.04
3	B	607	NAG	C1-O5-C5	5.45	119.16	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NAG	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	482/510 (94%)	0.02	11 (2%)	64	64	23, 44, 65, 92	0
1	B	481/510 (94%)	0.00	11 (2%)	64	64	22, 42, 65, 107	0
All	All	963/1020 (94%)	0.01	22 (2%)	64	64	22, 43, 65, 107	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	SER	6.8
1	B	492	SER	6.1
1	A	418	GLY	4.9
1	B	493	PRO	4.5
1	A	491	LEU	3.8
1	B	338	SER	3.6
1	B	491	LEU	3.2
1	B	455	PRO	3.2
1	B	454	ASP	3.1
1	A	202	SER	3.0
1	B	458	ALA	3.0
1	B	453	THR	3.0
1	A	419	GLN	2.9
1	A	493	PRO	2.9
1	A	416	THR	2.8
1	B	503	ARG	2.6
1	B	502	LEU	2.6
1	A	371	THR	2.3
1	A	417	ALA	2.3
1	A	90	GLY	2.2
1	A	91	LEU	2.1
1	B	366[A]	SER	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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
1	FGP	A	70	11/12	0.92	0.14	-	29,40,76,84	0
1	FGP	B	70	11/12	0.93	0.13	-	24,35,69,75	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, 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
4	NAG	A	603	14/15	0.96	0.11	-0.04	37,43,47,61	0
4	NAG	B	605	14/15	0.92	0.10	-0.68	48,56,64,66	0
4	NAG	B	603	14/15	0.97	0.09	-0.91	34,41,48,55	0
4	NAG	A	605	14/15	0.82	0.29	-	65,75,79,80	0
4	NAG	B	606	14/15	0.90	0.22	-	77,79,85,86	0
4	NAG	A	606	14/15	0.79	0.29	-	62,75,77,77	0
4	NAG	B	604	14/15	0.88	0.26	-	59,72,80,82	0
4	NAG	A	604	14/15	0.79	0.28	-	50,72,78,81	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, 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
5	MG	B	608	1/1	0.87	0.36	7.02	72,72,72,72	0
3	NAG	A	602	14/15	0.82	0.17	4.79	52,60,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	B	602	14/15	0.83	0.14	1.47	51,71,79,80	0
5	MG	B	609	1/1	0.98	0.07	-1.31	53,53,53,53	0
2	CA	B	601	1/1	0.99	0.07	-1.71	43,43,43,43	0
2	CA	A	601	1/1	0.99	0.05	-3.76	46,46,46,46	0
3	NAG	B	607	14/15	0.89	0.21	-	46,55,67,68	0
3	NAG	A	607	14/15	0.87	0.21	-	64,73,81,83	0

6.5 Other polymers

There are no such residues in this entry.