Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 12:21 pm GMT

PDB ID	:	6SAV
Title	:	Structural and functional characterisation of three novel fungal amylases with enhanced stability and pH tolerance
Authors	:	Roth, C.; Moroz, O.V.; Turkenburg, J.P.; Blagova, E.; Waterman, J.; Ariza, A.; Ming, L.; Tianqi, S.; Andersen, C.; Davies, G.J.; Wilson, K.S.
Deposited on	:	2019-07-17
Resolution	:	1.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

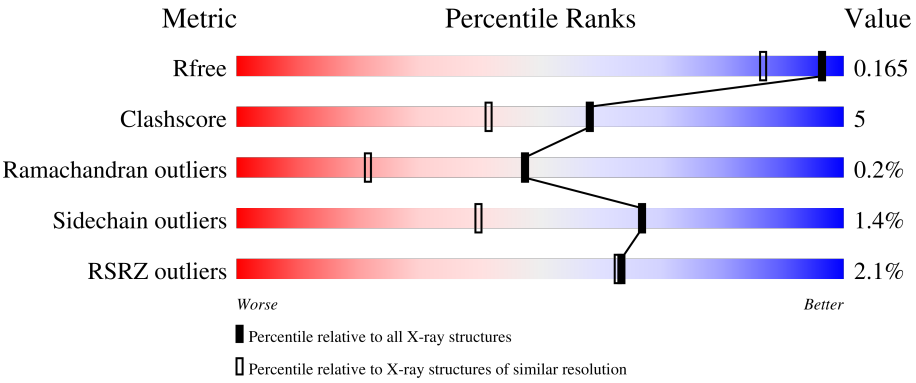
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.40 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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	438	3% 91% 8%
2	B	438	% 91% 8%

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	GOL	A	506	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8306 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 Alpha-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	438	3662	2303	592	753	14	0	35	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	THR	conflict	UNP M9TI89
A	103	ASP	GLY	conflict	UNP M9TI89
A	231	SER	PRO	conflict	UNP M9TI89
A	333	THR	ALA	conflict	UNP M9TI89
A	358	ALA	THR	conflict	UNP M9TI89

- Molecule 2 is a protein called Alpha-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	438	3600	2273	581	733	13	6	25	0

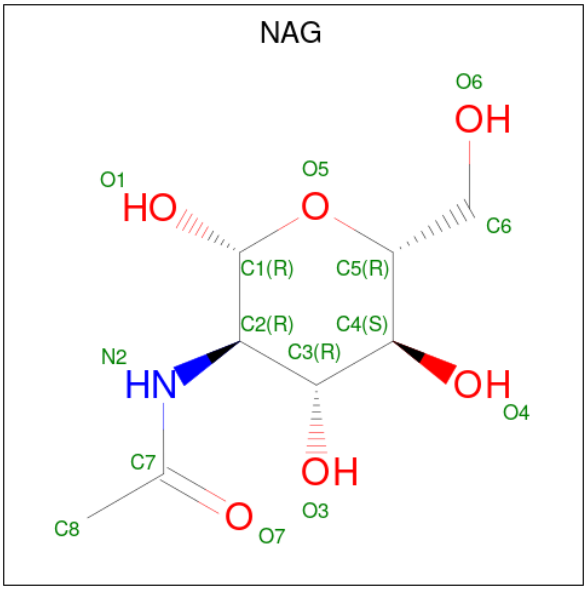
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	94	ALA	THR	conflict	UNP M9TI89
B	103	ASP	GLY	conflict	UNP M9TI89
B	120	IAS	ASN	conflict	UNP M9TI89
B	231	SER	PRO	conflict	UNP M9TI89
B	333	THR	ALA	conflict	UNP M9TI89
B	358	ALA	THR	conflict	UNP M9TI89

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

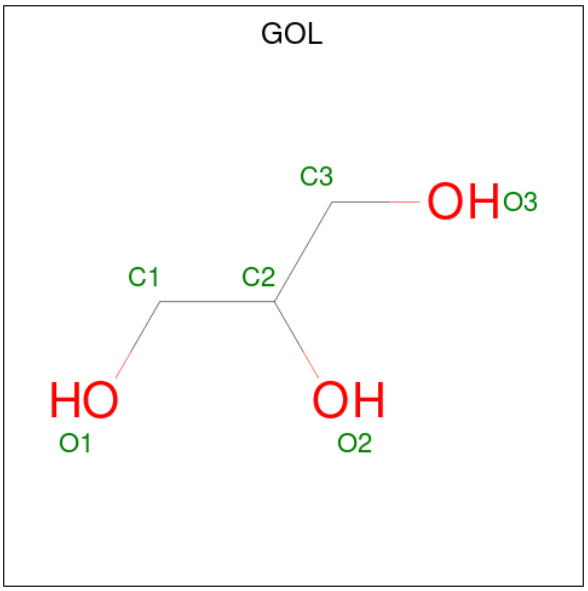
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



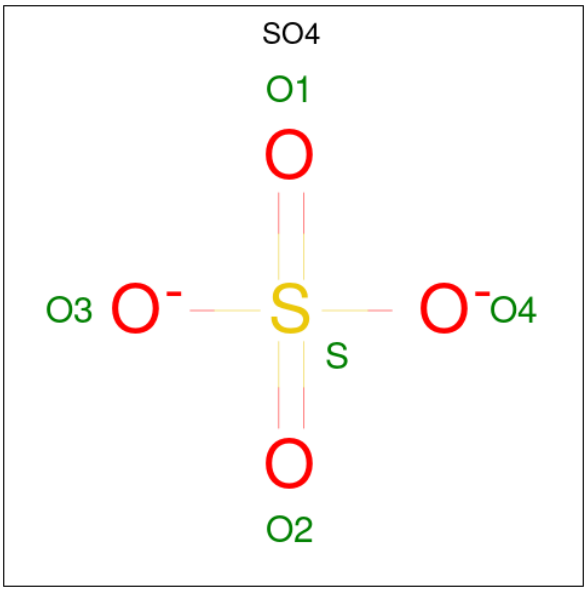
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

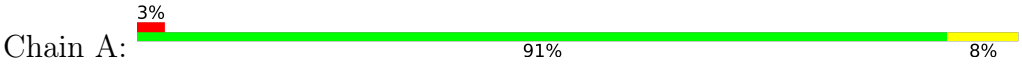
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	492	Total O 492 492	0	0
7	B	451	Total O 451 451	0	0

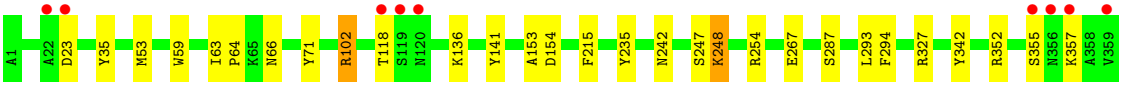
3 Residue-property plots (i)

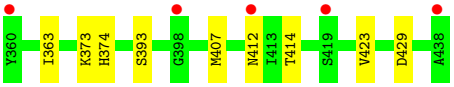
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha-amylase

Chain A:

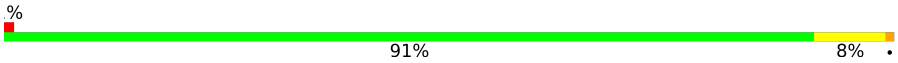


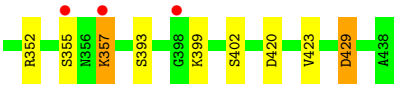




• Molecule 2: Alpha-amylase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.22Å 62.60Å 66.81Å 77.03° 81.04° 89.62°	Depositor
Resolution (Å)	39.99 – 1.40 43.21 – 1.40	Depositor EDS
% Data completeness (in resolution range)	92.9 (39.99-1.40) 92.9 (43.21-1.40)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.136 , 0.164 0.137 , 0.165	Depositor DCC
R_{free} test set	7328 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	11.6	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8306	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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, 0.333 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: IAS, CA, NAG, GOL, SO4

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	0.79	1/3755 (0.0%)	0.99	6/5103 (0.1%)
2	B	0.80	1/3691 (0.0%)	0.99	6/5013 (0.1%)
All	All	0.79	2/7446 (0.0%)	0.99	12/10116 (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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	429	ASP	CG-OD2	5.99	1.39	1.25
1	A	429	ASP	CG-OD2	5.07	1.36	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	352	ARG	NE-CZ-NH2	-6.79	116.90	120.30
2	B	254	ARG	CG-CD-NE	-6.59	97.97	111.80
1	A	352	ARG	NE-CZ-NH1	6.49	123.54	120.30
2	B	352	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	B	181	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	A	294	PHE	CB-CG-CD1	6.16	125.11	120.80
1	A	429	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	102	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	B	228	TYR	CB-CG-CD2	5.18	124.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	181	TYR	CB-CG-CD2	5.15	124.09	121.00
2	B	71	TYR	CB-CG-CD2	5.06	124.04	121.00
1	A	235	TYR	CB-CG-CD2	5.05	124.03	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	ASN	Peptide

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	3662	0	3389	32	0
2	B	3600	0	3345	34	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	14	0	13	0	0
4	B	28	0	26	0	0
5	A	18	0	24	9	0
5	B	24	0	32	5	0
6	A	5	0	0	1	0
6	B	10	0	0	1	0
7	A	492	0	0	11	0
7	B	451	0	0	12	0
All	All	8306	0	6829	69	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 5.

All (69) 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:242[A]:ASN:ND2	5:A:506:GOL:H31	1.70	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242[A]:ASN:HD22	5:A:506:GOL:H31	1.18	1.06
1:A:287[A]:SER:HB2	7:A:601:HOH:O	1.65	0.97
2:B:141[A]:TYR:OH	6:B:505:SO4:O3	1.86	0.94
1:A:141[A]:TYR:OH	6:A:504:SO4:O2	1.85	0.93
1:A:242[A]:ASN:ND2	5:A:506:GOL:C3	2.32	0.93
2:B:97[A]:GLN:HG2	7:B:745:HOH:O	1.72	0.90
2:B:254:ARG:HH22	2:B:258:MET:CE	1.87	0.87
1:A:242[A]:ASN:HD22	5:A:506:GOL:C3	1.91	0.83
1:A:254:ARG:HD3	7:A:956:HOH:O	1.80	0.81
2:B:254:ARG:HH22	2:B:258:MET:HE2	1.46	0.80
1:A:363[B]:ILE:CD1	1:A:373:LYS:HG3	2.12	0.80
2:B:242:ASN:OD1	5:B:509:GOL:H31	1.82	0.80
1:A:363[B]:ILE:HD11	1:A:373:LYS:HG3	1.64	0.78
2:B:21[B]:ARG:NH2	2:B:25:SER:OG	2.18	0.76
2:B:305[A]:GLU:OE2	7:B:601:HOH:O	2.04	0.75
1:A:154[B]:ASP:OD1	7:A:602:HOH:O	2.09	0.71
1:A:327:ARG:HH12	5:A:505:GOL:H11	1.55	0.70
1:A:136:LYS:HE3	1:A:154[A]:ASP:O	1.94	0.67
2:B:197[A]:ASP:OD1	7:B:602:HOH:O	2.13	0.67
2:B:305[A]:GLU:CD	7:B:601:HOH:O	2.35	0.65
2:B:347[B]:THR:HG22	7:B:686:HOH:O	1.98	0.63
2:B:254:ARG:HH22	2:B:258:MET:HE1	1.63	0.63
2:B:305[A]:GLU:OE1	7:B:601:HOH:O	2.15	0.60
2:B:347[B]:THR:HG21	7:B:970:HOH:O	2.01	0.59
2:B:327:ARG:HH22	5:B:506:GOL:H11	1.68	0.58
2:B:355:SER:HA	2:B:357:LYS:HE2	1.85	0.58
1:A:242[A]:ASN:ND2	5:A:506:GOL:H32	2.18	0.57
1:A:407[A]:MET:HE2	7:A:752:HOH:O	2.05	0.57
1:A:287[A]:SER:CB	7:A:601:HOH:O	2.36	0.57
1:A:407[A]:MET:CE	7:A:752:HOH:O	2.52	0.57
2:B:65[A]:LYS:HE3	7:B:633:HOH:O	2.05	0.56
2:B:242:ASN:OD1	5:B:509:GOL:C3	2.52	0.55
5:B:507:GOL:O2	7:B:603:HOH:O	2.17	0.55
1:A:407[A]:MET:HG3	1:A:414[A]:THR:HG22	1.88	0.54
2:B:355:SER:HA	2:B:357:LYS:CE	2.39	0.52
1:A:53:MET:HG3	1:A:342:TYR:CE2	2.44	0.51
2:B:69:GLY:H	5:B:507:GOL:C1	2.24	0.51
1:A:327:ARG:HH12	5:A:505:GOL:C1	2.22	0.50
2:B:197[A]:ASP:CG	7:B:602:HOH:O	2.50	0.50
1:A:248[A]:LYS:HE3	1:A:293:LEU:HD11	1.94	0.49
2:B:97[A]:GLN:NE2	7:B:611:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247[B]:SER:HB3	7:A:644:HOH:O	2.13	0.49
2:B:343:GLN:O	2:B:347[B]:THR:HG23	2.12	0.49
2:B:65[B]:LYS:HD2	2:B:81:GLN:CD	2.34	0.48
1:A:53:MET:HG3	1:A:342:TYR:CZ	2.49	0.48
2:B:35:TYR:CE1	2:B:71:TYR:HA	2.48	0.48
5:A:506:GOL:O1	7:A:601:HOH:O	1.94	0.47
1:A:35:TYR:CE1	1:A:71:TYR:HA	2.49	0.47
1:A:393:SER:HA	1:A:423:VAL:O	2.16	0.46
1:A:355[B]:SER:OG	1:A:374:HIS:CD2	2.69	0.46
1:A:254:ARG:CD	7:A:956:HOH:O	2.53	0.46
2:B:344:PHE:O	2:B:347[B]:THR:OG1	2.27	0.46
5:A:506:GOL:C1	7:A:601:HOH:O	2.56	0.46
2:B:254:ARG:NH2	2:B:258:MET:HE2	2.22	0.45
2:B:194:ILE:HD12	2:B:199:TRP:CZ2	2.52	0.44
2:B:53:MET:HG3	2:B:342:TYR:CE2	2.53	0.43
2:B:429:ASP:CG	2:B:429:ASP:O	2.57	0.43
2:B:393:SER:HA	2:B:423:VAL:O	2.19	0.43
1:A:23:ASP:OD1	1:A:23:ASP:C	2.58	0.43
1:A:267[B]:GLU:HG3	7:A:697:HOH:O	2.19	0.43
2:B:283:ARG:HG2	7:B:747:HOH:O	2.20	0.42
2:B:22:ALA:HA	2:B:41[B]:GLU:OE1	2.20	0.41
1:A:153:ALA:O	1:A:154[A]:ASP:HB2	2.21	0.41
1:A:363[B]:ILE:HD11	1:A:373:LYS:CG	2.45	0.41
2:B:420:ASP:C	2:B:420:ASP:OD1	2.58	0.41
2:B:53:MET:HG3	2:B:342:TYR:CZ	2.57	0.40
1:A:63:ILE:N	1:A:64:PRO:CD	2.85	0.40
1:A:102:ARG:HH11	1:A:102:ARG:HG3	1.86	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	471/438 (108%)	456 (97%)	13 (3%)	2 (0%)	34 12
2	B	459/438 (105%)	448 (98%)	9 (2%)	2 (0%)	34 12
All	All	930/876 (106%)	904 (97%)	22 (2%)	4 (0%)	47 12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	154[A]	ASP
2	B	154[B]	ASP
1	A	118[A]	THR
1	A	118[B]	THR

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	403/369 (109%)	397 (98%)	6 (2%)	65 37
2	B	393/368 (107%)	386 (98%)	7 (2%)	59 28
All	All	796/737 (108%)	783 (98%)	13 (2%)	67 33

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TRP
1	A	66	ASN
1	A	215	PHE
1	A	248[A]	LYS
1	A	248[B]	LYS
1	A	357	LYS
2	B	215[A]	PHE
2	B	215[B]	PHE
2	B	235	TYR
2	B	357	LYS
2	B	399	LYS
2	B	402[A]	SER

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Mol	Chain	Res	Type
2	B	402[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	ASN
1	A	390	ASN
1	A	426	ASN
2	B	426	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	IAS	B	120	2	6,7,8	1.19	1 (16%)	6,8,10	1.39	1 (16%)

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	IAS	B	120	2	-	0/7/7/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	120	IAS	O-C	2.01	1.28	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	120	IAS	O-C-CA	-2.36	113.81	122.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	B	508	-	4,4,4	0.34	0	6,6,6	0.16	0
6	SO4	B	505	-	4,4,4	0.74	0	6,6,6	0.58	0
6	SO4	A	504	-	4,4,4	0.49	0	6,6,6	0.69	0
5	GOL	B	509	-	5,5,5	0.22	0	5,5,5	0.32	0
5	GOL	A	503	-	5,5,5	0.50	0	5,5,5	0.97	0
5	GOL	B	504	-	5,5,5	0.75	0	5,5,5	1.71	2 (40%)
4	NAG	B	502	2	14,14,15	0.94	1 (7%)	17,19,21	2.01	5 (29%)
5	GOL	A	505	-	5,5,5	0.27	0	5,5,5	0.66	0
4	NAG	B	503	2	14,14,15	0.96	1 (7%)	17,19,21	1.83	6 (35%)
5	GOL	A	506	-	5,5,5	0.33	0	5,5,5	0.41	0
5	GOL	B	506	-	5,5,5	0.37	0	5,5,5	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	502	1	14,14,15	1.38	3 (21%)	17,19,21	1.37	2 (11%)
5	GOL	B	507	-	5,5,5	0.23	0	5,5,5	1.33	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
5	GOL	B	509	-	-	1/4/4/4	-
5	GOL	A	503	-	-	2/4/4/4	-
5	GOL	B	504	-	-	2/4/4/4	-
4	NAG	B	502	2	-	0/6/23/26	0/1/1/1
5	GOL	A	505	-	-	2/4/4/4	-
4	NAG	B	503	2	-	2/6/23/26	0/1/1/1
5	GOL	A	506	-	-	0/4/4/4	-
5	GOL	B	506	-	-	2/4/4/4	-
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1
5	GOL	B	507	-	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	NAG	C2-N2	2.78	1.51	1.46
4	B	503	NAG	C1-C2	-2.43	1.48	1.52
4	A	502	NAG	O5-C1	2.36	1.47	1.43
4	A	502	NAG	C1-C2	-2.35	1.48	1.52
4	B	502	NAG	C6-C5	2.09	1.58	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	502	NAG	O5-C1-C2	-5.39	102.78	111.29
4	A	502	NAG	O5-C5-C6	-3.22	102.16	107.20
4	B	503	NAG	O5-C1-C2	-3.13	106.34	111.29
4	B	502	NAG	O4-C4-C3	-3.13	103.11	110.35
4	B	503	NAG	O5-C5-C6	-3.11	102.32	107.20
4	B	503	NAG	C6-C5-C4	-2.83	106.38	113.00
5	B	504	GOL	C3-C2-C1	-2.78	100.90	111.70
4	B	502	NAG	C4-C3-C2	-2.76	106.97	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	502	NAG	O5-C5-C4	-2.54	104.66	110.83
4	B	503	NAG	O3-C3-C2	-2.44	104.42	109.47
4	B	503	NAG	O6-C6-C5	-2.39	103.08	111.29
4	B	503	NAG	C1-O5-C5	2.39	115.42	112.19
5	B	504	GOL	O2-C2-C1	2.36	119.51	109.12
4	A	502	NAG	O5-C1-C2	-2.16	107.88	111.29
4	B	502	NAG	O7-C7-C8	-2.06	118.23	122.06

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	504	GOL	O1-C1-C2-C3
5	B	507	GOL	C1-C2-C3-O3
5	B	507	GOL	O2-C2-C3-O3
5	B	506	GOL	O2-C2-C3-O3
4	B	503	NAG	O5-C5-C6-O6
5	A	503	GOL	O1-C1-C2-C3
5	A	505	GOL	C1-C2-C3-O3
5	B	506	GOL	C1-C2-C3-O3
5	B	504	GOL	O1-C1-C2-O2
5	A	503	GOL	O1-C1-C2-O2
5	A	505	GOL	O2-C2-C3-O3
5	B	507	GOL	O1-C1-C2-O2
4	B	503	NAG	C4-C5-C6-O6
5	B	507	GOL	O1-C1-C2-C3
5	B	509	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	505	SO4	1	0
6	A	504	SO4	1	0
5	B	509	GOL	2	0
5	A	505	GOL	2	0
5	A	506	GOL	7	0
5	B	506	GOL	1	0
5	B	507	GOL	2	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	438/438 (100%)	-0.10	14 (3%) 47 46	7, 11, 25, 56	2 (0%)
2	B	437/438 (99%)	-0.16	4 (0%) 84 82	7, 11, 21, 44	1 (0%)
All	All	875/876 (99%)	-0.13	18 (2%) 63 63	7, 11, 23, 56	3 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	ASN	7.2
1	A	438	ALA	6.4
1	A	120	ASN	5.6
2	B	355	SER	4.1
2	B	398	GLY	4.0
1	A	357	LYS	3.9
1	A	412	ASN	3.5
1	A	355[A]	SER	3.3
1	A	359[A]	VAL	3.2
1	A	419	SER	3.0
2	B	22	ALA	2.8
1	A	22	ALA	2.6
1	A	119	SER	2.5
2	B	357	LYS	2.4
1	A	118[A]	THR	2.3
1	A	398	GLY	2.3
1	A	360[A]	TYR	2.3
1	A	23	ASP	2.2

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å^2)	Q<0.9
2	IAS	B	120	8/9	0.93	0.10	16,17,19,20	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
5	GOL	B	506	6/6	0.76	0.18	30,33,35,50	0
5	GOL	A	505	6/6	0.78	0.18	27,34,35,47	0
5	GOL	B	507	6/6	0.79	0.21	24,26,30,36	0
4	NAG	B	503	14/15	0.87	0.23	22,26,34,37	0
4	NAG	B	502	14/15	0.87	0.12	13,17,22,23	0
5	GOL	A	506	6/6	0.89	0.15	19,22,23,25	0
5	GOL	B	504	6/6	0.90	0.13	12,20,24,30	0
5	GOL	B	509	6/6	0.90	0.14	23,25,30,33	0
6	SO4	B	505	5/5	0.90	0.15	18,22,23,29	5
6	SO4	B	508	5/5	0.90	0.23	32,48,52,53	0
4	NAG	A	502	14/15	0.91	0.10	14,18,24,24	0
6	SO4	A	504	5/5	0.95	0.13	16,16,18,22	5
5	GOL	A	503	6/6	0.96	0.09	12,14,20,24	0
3	CA	B	501	1/1	1.00	0.08	7,7,7,7	0
3	CA	A	501	1/1	1.00	0.08	7,7,7,7	0

6.5 Other polymers (i)

There are no such residues in this entry.