Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:19 PM GMT

PDB ID	:	1X38
Title	:	crystal structure of barley beta-D-glucan glucohydrolase isoenzyme exo1 in complex with gluco-phenylimidazole
Authors	:	Hrmova, M.; Streltsov, V.A.; Smith, B.J.; Vasella, A.; Varghese, J.N.; Fincher, G.B.
Deposited on	:	2005-05-02
Resolution	:	1.70 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:

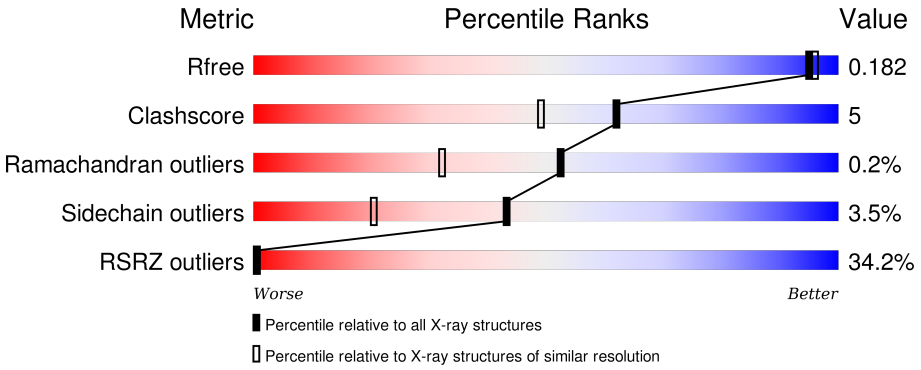
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	602	34% 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
2	NAG	A	2211	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	4981	-	-	-	X
3	NAG	A	4986	-	-	-	X
4	NAG	A	6001	-	-	-	X
7	GOL	A	2001[A]	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5721 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 beta-D-glucan exohydrolase isoenzyme ExoI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4566	2891	787	862	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	LYS	ASN	SEE REMARK 999	GB 4566505

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

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

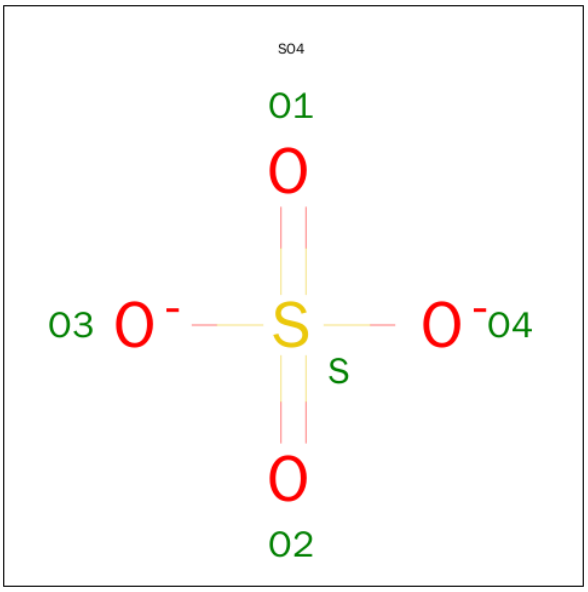
- Molecule 3 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	7	Total	C	N	O	0	0
			83	47	3	33		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

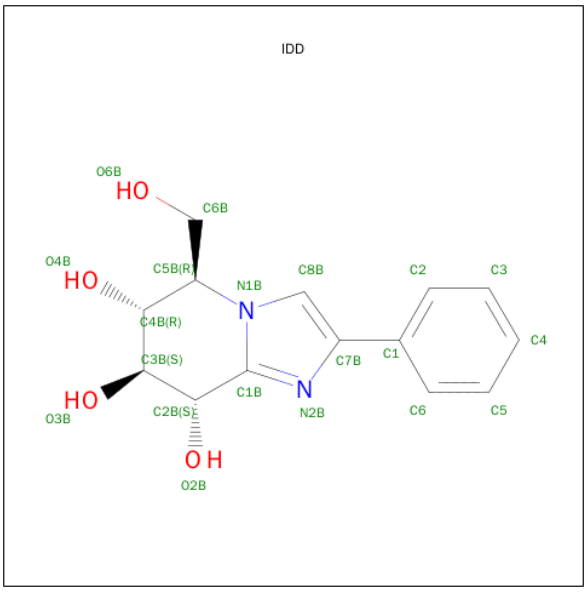
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			58	33	2	23		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



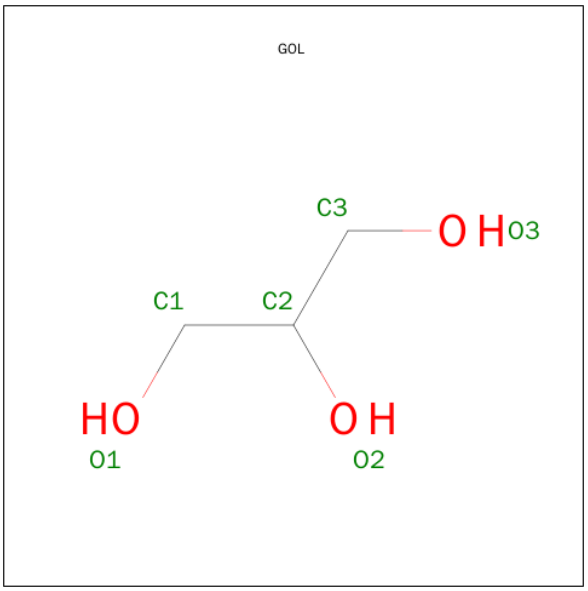
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0

- Molecule 6 is (5R,6R,7S,8S)-5-(HYDROXYMETHYL)-2-PHENYL-5,6,7,8-TETRAHYDRO IMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (three-letter code: IDD) (formula: $C_{14}H_{16}N_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 20 14 2 4	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	O	0	1
			7	3	4		
7	A	1	Total	C	O	0	1
			12	6	6		

- Molecule 8 is water.

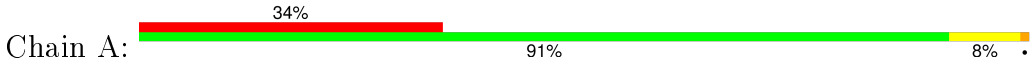
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	931	Total	O	0	0
			931	931		

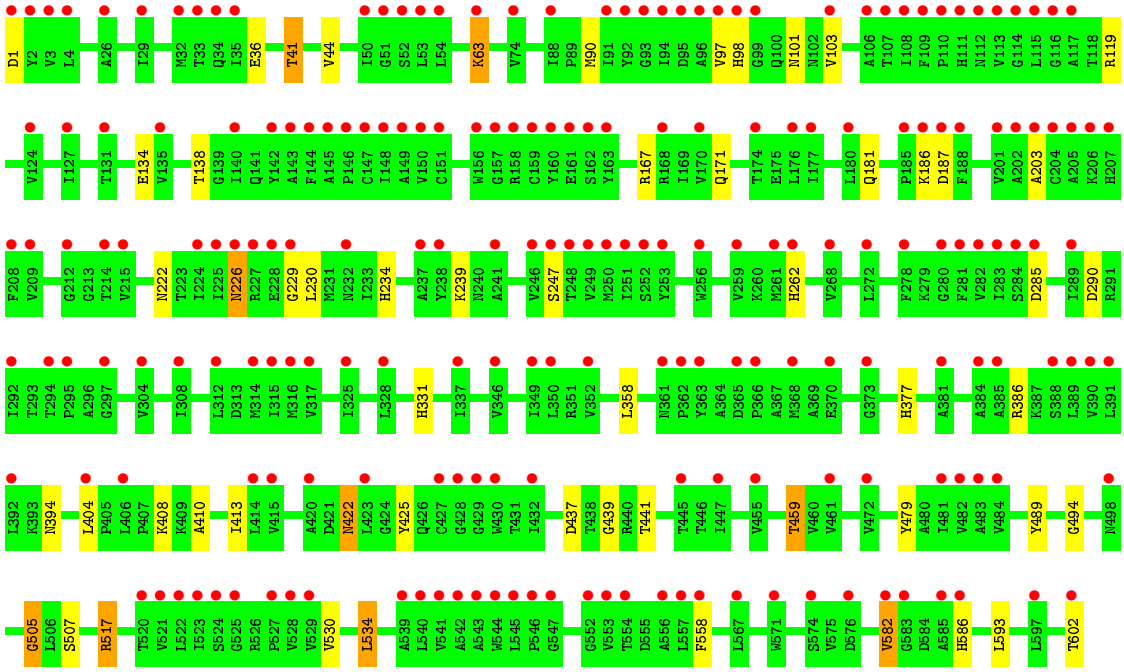
3 Residue-property plots (i)

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: beta-D-glucan exohydrolase isoenzyme ExoI

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	100.56Å 100.56Å 182.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.30 – 1.70 34.30 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.30-1.70) 99.8 (34.30-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0011	Depositor
R, R_{free}	0.160 , 0.183 0.158 , 0.182	Depositor DCC
R_{free} test set	5168 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 35.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 103323 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5721	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: XYP, GOL, BMA, NAG, FUC, IDD, MAN, 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	0.54	0/4663	0.61	0/6334

There are no bond length outliers.

There are no bond angle outliers.

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	4566	0	4550	49	1
2	A	39	0	34	1	0
3	A	83	0	71	2	0
4	A	58	0	50	0	0
5	A	5	0	0	0	0
6	A	20	0	16	0	0
7	A	19	0	22	1	0
8	A	931	0	0	11	1
All	All	5721	0	4743	51	1

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 (51) 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:517:ARG:HB2	1:A:517:ARG:NH1	1.41	1.34
1:A:517:ARG:CB	1:A:517:ARG:HH11	1.47	1.27
1:A:41:THR:HG22	1:A:44:VAL:H	1.39	0.86
1:A:394:ASN:HD21	1:A:404:LEU:H	1.18	0.86
1:A:410:ALA:O	1:A:459:THR:HB	1.78	0.83
1:A:41:THR:HG21	8:A:6671:HOH:O	1.84	0.78
1:A:97:VAL:H	1:A:101:ASN:HD21	1.34	0.75
1:A:181:GLN:HE21	1:A:203:ALA:H	1.37	0.72
1:A:422:ASN:HD21	1:A:439:GLY:H	1.37	0.72
1:A:167:ARG:HH11	1:A:171:GLN:HE22	1.39	0.70
1:A:239:LYS:HE2	8:A:6936:HOH:O	1.91	0.70
1:A:505:GLY:N	8:A:6932:HOH:O	2.28	0.65
1:A:422:ASN:ND2	1:A:439:GLY:H	1.95	0.65
1:A:262:HIS:HE1	1:A:285:ASP:H	1.43	0.64
1:A:97:VAL:H	1:A:101:ASN:ND2	1.96	0.63
1:A:119:ARG:HE	7:A:2002[A]:GOL:H2	1.63	0.62
1:A:517:ARG:HB2	1:A:517:ARG:HH11	0.58	0.62
3:A:4984:FUC:H63	8:A:6766:HOH:O	2.01	0.60
1:A:479:TYR:HB3	1:A:517:ARG:HH12	1.68	0.59
1:A:234:HIS:HE1	8:A:6196:HOH:O	1.86	0.58
1:A:408:LYS:O	1:A:459:THR:HG21	2.04	0.57
1:A:386:ARG:NH1	8:A:6930:HOH:O	2.33	0.57
1:A:167:ARG:NH1	1:A:171:GLN:HE22	2.02	0.56
1:A:167:ARG:HH11	1:A:171:GLN:NE2	2.01	0.56
1:A:234:HIS:HD2	8:A:6027:HOH:O	1.88	0.56
1:A:262:HIS:CE1	1:A:285:ASP:H	2.23	0.56
1:A:226:ASN:ND2	1:A:229:GLY:H	2.03	0.55
1:A:331:HIS:HD2	8:A:6340:HOH:O	1.90	0.55
1:A:507:SER:OG	8:A:6932:HOH:O	2.18	0.54
1:A:582:VAL:HG11	1:A:593:LEU:HB3	1.89	0.54
1:A:181:GLN:HE22	1:A:247:SER:H	1.57	0.53
1:A:186:LYS:HD3	1:A:186:LYS:H	1.75	0.52
1:A:134:GLU:OE2	1:A:377:HIS:HD2	1.94	0.51
1:A:530:VAL:HG13	1:A:534:LEU:HD22	1.92	0.51
1:A:41:THR:CG2	1:A:44:VAL:H	2.19	0.50
1:A:422:ASN:C	1:A:422:ASN:HD22	2.16	0.49
1:A:222:ASN:HB2	2:A:2211:NAG:H82	1.96	0.48
1:A:226:ASN:C	1:A:226:ASN:HD22	2.19	0.46
1:A:437:ASP:HB3	1:A:441:THR:HG21	1.98	0.46
1:A:186:LYS:N	1:A:186:LYS:HD3	2.30	0.46
1:A:422:ASN:ND2	1:A:425:TYR:H	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4982:NAG:H82	3:A:4985:MAN:O3	2.18	0.43
1:A:602:THR:HG21	8:A:6307:HOH:O	2.18	0.43
1:A:489:TYR:CD2	1:A:494:GLY:HA3	2.55	0.42
1:A:181:GLN:HE22	1:A:247:SER:N	2.18	0.42
1:A:63:LYS:N	1:A:63:LYS:HE3	2.35	0.42
1:A:558:PHE:HB2	8:A:6652:HOH:O	2.21	0.41
1:A:413:ILE:HG21	1:A:479:TYR:CZ	2.55	0.41
1:A:63:LYS:H	1:A:63:LYS:HE3	1.86	0.41
1:A:103:VAL:HG21	1:A:138:THR:HG21	2.03	0.40
1:A:186:LYS:H	1:A:186:LYS:CD	2.33	0.40

All (1) 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)
1:A:63:LYS:NZ	8:A:6243:HOH:O[3_554]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	600/602 (100%)	584 (97%)	15 (2%)	1 (0%)	52 32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	505	GLY

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	485/485 (100%)	468 (96%)	17 (4%)	43 20

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	36	GLU
1	A	41	THR
1	A	63	LYS
1	A	90	MET
1	A	98	HIS
1	A	187	ASP
1	A	226	ASN
1	A	230	LEU
1	A	290	ASP
1	A	358	LEU
1	A	422	ASN
1	A	459	THR
1	A	517	ARG
1	A	534	LEU
1	A	582	VAL
1	A	586	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	112	ASN
1	A	171	GLN
1	A	181	GLN
1	A	199	ASN
1	A	226	ASN
1	A	234	HIS
1	A	240	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	257	ASN
1	A	262	HIS
1	A	265	GLN
1	A	331	HIS
1	A	333	ASN
1	A	377	HIS
1	A	394	ASN
1	A	422	ASN
1	A	581	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)

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

5.5 Carbohydrates (i)

15 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	2211	1,2	14,14,15	0.62	0	15,19,21	0.99	1 (6%)
2	NAG	A	2212	2	14,14,15	0.48	0	15,19,21	0.79	0
2	BMA	A	2213	2	11,11,12	0.63	0	14,15,17	1.02	1 (7%)
3	NAG	A	4981	1,3	14,14,15	0.55	0	15,19,21	0.79	1 (6%)
3	NAG	A	4982	3	14,14,15	0.55	0	15,19,21	1.09	1 (6%)
3	BMA	A	4983	3	11,11,12	0.57	0	14,15,17	0.68	0
3	FUC	A	4984	3	10,10,11	0.60	0	14,14,16	1.16	1 (7%)
3	MAN	A	4985	3	11,11,12	0.55	0	14,15,17	0.87	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	4986	3	14,14,15	0.41	0	15,19,21	0.98	1 (6%)
3	XYP	A	4987	3	9,9,10	1.20	1 (11%)	12,12,14	0.66	0
4	NAG	A	6001	1,4	14,14,15	0.55	0	15,19,21	0.72	0
4	NAG	A	6002	4	14,14,15	0.46	0	15,19,21	0.56	0
4	BMA	A	6003	4	11,11,12	0.54	0	14,15,17	0.72	0
4	FUC	A	6004	4	10,10,11	0.56	0	14,14,16	0.98	1 (7%)
4	XYP	A	6005	4	9,9,10	1.19	1 (11%)	12,12,14	1.02	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2211	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2212	2	-	0/6/23/26	0/1/1/1
2	BMA	A	2213	2	-	0/2/19/22	0/1/1/1
3	NAG	A	4981	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	4982	3	-	0/6/23/26	0/1/1/1
3	BMA	A	4983	3	-	0/2/19/22	0/1/1/1
3	FUC	A	4984	3	-	0/0/17/20	0/1/1/1
3	MAN	A	4985	3	-	0/2/19/22	0/1/1/1
3	NAG	A	4986	3	-	0/6/23/26	0/1/1/1
3	XYP	A	4987	3	-	0/0/14/17	0/1/1/1
4	NAG	A	6001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	6002	4	-	0/6/23/26	0/1/1/1
4	BMA	A	6003	4	-	0/2/19/22	0/1/1/1
4	FUC	A	6004	4	-	0/0/17/20	0/1/1/1
4	XYP	A	6005	4	-	0/0/14/17	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	6005	XYP	O5B-C1B	-3.21	1.36	1.42
3	A	4987	XYP	O5B-C1B	-3.17	1.36	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4981	NAG	C1-O5-C5	2.01	114.79	112.25
3	A	4982	NAG	C1-O5-C5	2.05	114.85	112.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4985	MAN	C1-O5-C5	2.25	115.10	112.25
2	A	2213	BMA	C3-C4-C5	2.28	114.17	110.20
4	A	6004	FUC	O5-C5-C6	2.31	109.95	106.13
4	A	6005	XYP	C5B-O5B-C1B	2.72	115.96	111.57
3	A	4986	NAG	C1-O5-C5	2.84	115.85	112.25
2	A	2211	NAG	C1-O5-C5	2.90	115.93	112.25
3	A	4984	FUC	O5-C5-C6	3.84	112.49	106.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2211	NAG	1	0
3	A	4982	NAG	1	0
3	A	4984	FUC	1	0
3	A	4985	MAN	1	0

5.6 Ligand geometry (i)

6 ligands 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	$\#\|Z\| > 2$
6	IDD	A	1001	-	17,22,22	0.83	0	21,32,32	1.49	4 (19%)
7	GOL	A	2001[A]	-	5,5,5	0.49	0	5,5,5	0.29	0
7	GOL	A	2001[B]	-	5,5,5	0.50	0	5,5,5	0.19	0
7	GOL	A	2002[A]	-	5,5,5	0.42	0	5,5,5	0.19	0
7	GOL	A	2002[B]	-	5,5,5	0.31	0	5,5,5	0.41	0
5	SO4	A	3001	-	4,4,4	0.05	0	6,6,6	0.15	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
6	IDD	A	1001	-	-	0/6/26/26	0/2/3/3
7	GOL	A	2001[A]	-	-	0/4/4/4	0/0/0/0
7	GOL	A	2001[B]	-	-	0/4/4/4	0/0/0/0
7	GOL	A	2002[A]	-	-	0/4/4/4	0/0/0/0
7	GOL	A	2002[B]	-	-	0/4/4/4	0/0/0/0
5	SO4	A	3001	-	-	0/0/0/0	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})
6	A	1001	IDD	C8B-C7B-C1	-3.86	124.07	129.44
6	A	1001	IDD	C2-C1-C7B	-2.36	117.39	121.24
6	A	1001	IDD	O2B-C2B-C3B	2.02	112.85	108.63
6	A	1001	IDD	C1-C7B-N2B	3.23	125.03	120.62

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
7	A	2002[A]	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	602/602 (100%)	1.76	206 (34%)	0	0	22, 36, 43, 54	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	586	HIS	10.8
1	A	585	ALA	8.9
1	A	283	ILE	8.6
1	A	113	VAL	7.8
1	A	249	VAL	7.1
1	A	251	ILE	7.0
1	A	523	ILE	6.8
1	A	144	PHE	6.7
1	A	282	VAL	6.6
1	A	97	VAL	6.6
1	A	147	CYS	6.5
1	A	148	ILE	5.9
1	A	145	ALA	5.9
1	A	163	TYR	5.8
1	A	187	ASP	5.7
1	A	545	LEU	5.5
1	A	160	TYR	5.5
1	A	543	ALA	5.4
1	A	204	CYS	5.4
1	A	143	ALA	5.3
1	A	186	LYS	5.3
1	A	544	TRP	5.2
1	A	250	MET	5.2
1	A	447	ILE	5.2
1	A	146	PRO	5.2
1	A	246	VAL	5.1
1	A	553	VAL	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	159	CYS	5.1
1	A	142	TYR	5.1
1	A	115	LEU	5.0
1	A	281	PHE	4.8
1	A	349	ILE	4.8
1	A	150	VAL	4.8
1	A	203	ALA	4.7
1	A	521	VAL	4.7
1	A	248	THR	4.6
1	A	206	LYS	4.6
1	A	94	ILE	4.5
1	A	557	LEU	4.5
1	A	149	ALA	4.5
1	A	312	LEU	4.5
1	A	91	ILE	4.4
1	A	546	PRO	4.4
1	A	205	ALA	4.3
1	A	541	VAL	4.3
1	A	522	LEU	4.2
1	A	54	LEU	4.2
1	A	430	TRP	4.1
1	A	390	VAL	4.1
1	A	238	TYR	4.1
1	A	208	PHE	4.1
1	A	542	ALA	4.1
1	A	389	LEU	4.1
1	A	140	ILE	4.0
1	A	202	ALA	4.0
1	A	162	SER	3.9
1	A	96	ALA	3.9
1	A	315	ILE	3.9
1	A	108	ILE	3.8
1	A	547	GLY	3.8
1	A	540	LEU	3.8
1	A	427	CYS	3.8
1	A	109	PHE	3.7
1	A	176	LEU	3.7
1	A	170	VAL	3.7
1	A	99	GLY	3.7
1	A	268	VAL	3.7
1	A	93	GLY	3.6
1	A	602	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	528	VAL	3.6
1	A	582	VAL	3.6
1	A	2	TYR	3.5
1	A	201	VAL	3.5
1	A	207	HIS	3.5
1	A	406	LEU	3.5
1	A	177	ILE	3.4
1	A	481	ILE	3.4
1	A	352	VAL	3.4
1	A	391	LEU	3.3
1	A	232	ASN	3.3
1	A	151	CYS	3.3
1	A	158	ARG	3.3
1	A	314	MET	3.3
1	A	278	PHE	3.3
1	A	385	ALA	3.2
1	A	156	TRP	3.2
1	A	127	ILE	3.2
1	A	525	GLY	3.2
1	A	363	TYR	3.2
1	A	226	ASN	3.2
1	A	110	PRO	3.2
1	A	112	ASN	3.1
1	A	103	VAL	3.1
1	A	63	LYS	3.1
1	A	520	THR	3.1
1	A	209	VAL	3.1
1	A	247	SER	3.1
1	A	111	HIS	3.0
1	A	284	SER	3.0
1	A	346	VAL	3.0
1	A	1	ASP	2.9
1	A	308	ILE	2.9
1	A	188	PHE	2.9
1	A	92	TYR	2.9
1	A	429	GLY	2.9
1	A	368	MET	2.9
1	A	180	LEU	2.9
1	A	524	SER	2.9
1	A	124	VAL	2.9
1	A	114	GLY	2.9
1	A	228	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	317	VAL	2.9
1	A	482	VAL	2.8
1	A	272	LEU	2.8
1	A	316	MET	2.8
1	A	554	THR	2.8
1	A	161	GLU	2.8
1	A	135	VAL	2.8
1	A	289	ILE	2.8
1	A	32	MET	2.8
1	A	107	THR	2.7
1	A	252	SER	2.7
1	A	212	GLY	2.7
1	A	131	THR	2.7
1	A	241	ALA	2.7
1	A	292	ILE	2.7
1	A	571	TRP	2.7
1	A	392	LEU	2.7
1	A	370	GLU	2.7
1	A	484	VAL	2.6
1	A	229	GLY	2.6
1	A	33	THR	2.6
1	A	583	GLY	2.6
1	A	384	ALA	2.6
1	A	455	VAL	2.6
1	A	558	PHE	2.6
1	A	498	ASN	2.6
1	A	52	SER	2.6
1	A	50	ILE	2.6
1	A	328	LEU	2.6
1	A	117	ALA	2.5
1	A	304	VAL	2.5
1	A	337	ILE	2.5
1	A	381	ALA	2.5
1	A	415	VAL	2.5
1	A	29	ILE	2.5
1	A	428	GLY	2.5
1	A	529	VAL	2.5
1	A	256	TRP	2.5
1	A	215	VAL	2.5
1	A	53	LEU	2.5
1	A	297	GLY	2.5
1	A	414	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	539	ALA	2.5
1	A	365	ASP	2.4
1	A	366	PRO	2.4
1	A	552	GLY	2.4
1	A	237	ALA	2.4
1	A	483	ALA	2.4
1	A	116	GLY	2.4
1	A	51	GLY	2.4
1	A	95	ASP	2.4
1	A	574	SER	2.4
1	A	576	ASP	2.4
1	A	350	LEU	2.3
1	A	361	ASN	2.3
1	A	285	ASP	2.3
1	A	567	LEU	2.3
1	A	432	ILE	2.3
1	A	227	ARG	2.3
1	A	106	ALA	2.3
1	A	404	LEU	2.3
1	A	262	HIS	2.3
1	A	259	VAL	2.3
1	A	295	PRO	2.3
1	A	98	HIS	2.2
1	A	261	MET	2.2
1	A	26	ALA	2.2
1	A	4	LEU	2.2
1	A	34	GLN	2.2
1	A	373	GLY	2.2
1	A	74	VAL	2.2
1	A	157	GLY	2.2
1	A	362	PRO	2.2
1	A	423	LEU	2.2
1	A	325	ILE	2.2
1	A	253	TYR	2.2
1	A	445	THR	2.2
1	A	185	PRO	2.2
1	A	35	ILE	2.2
1	A	225	ILE	2.2
1	A	597	LEU	2.1
1	A	294	THR	2.1
1	A	527	PRO	2.1
1	A	168	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	388	SER	2.1
1	A	556	ALA	2.1
1	A	88	ILE	2.1
1	A	461	VAL	2.1
1	A	214	THR	2.1
1	A	3	VAL	2.1
1	A	224	ILE	2.1
1	A	174	THR	2.0
1	A	472	VAL	2.0
1	A	280	GLY	2.0
1	A	420	ALA	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, 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	6001	14/15	0.65	0.46	18.63	44,50,54,55	0
3	NAG	A	4986	14/15	0.61	0.49	11.15	42,49,50,50	0
2	NAG	A	2211	14/15	0.83	0.30	8.15	38,41,46,51	0
3	NAG	A	4981	14/15	0.70	0.46	6.62	51,54,56,56	0
3	XYP	A	4987	9/10	0.20	0.67	-	67,68,70,70	0
4	BMA	A	6003	11/12	0.74	0.56	-	47,52,54,55	0
4	NAG	A	6002	14/15	0.81	0.47	-	50,51,53,53	0
3	MAN	A	4985	11/12	0.55	0.48	-	50,51,53,53	0
4	FUC	A	6004	10/11	0.76	0.45	-	57,58,60,60	0
4	XYP	A	6005	9/10	0.88	0.48	-	42,44,45,46	0
3	FUC	A	4984	10/11	0.65	0.62	-	58,59,59,59	0
3	NAG	A	4982	14/15	0.66	0.60	-	58,59,60,61	0
3	BMA	A	4983	11/12	0.28	0.74	-	56,61,63,65	0
2	NAG	A	2212	14/15	0.81	0.45	-	56,60,61,65	0
2	BMA	A	2213	11/12	0.38	0.61	-	67,69,70,70	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	A	2001[A]	6/6	0.85	0.26	8.38	25,32,37,40	1
6	IDD	A	1001	20/20	0.96	0.12	-1.22	17,20,25,26	0
7	GOL	A	2001[B]	6/6	0.85	0.26	-	32,33,37,40	1
7	GOL	A	2002[A]	6/6	0.79	0.31	-	37,40,40,40	6
5	SO4	A	3001	5/5	0.88	0.47	-	61,62,63,63	0
7	GOL	A	2002[B]	6/6	0.79	0.31	-	39,39,39,41	6

6.5 Other polymers

There are no such residues in this entry.