Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:57 am BST

PDB ID	:	5FKY
Title	:	Structure of a hydrolase bound with an inhibitor
Authors	:	Cekic, N.; Heinonen, J.E.; Stubbs, K.A.; Roth, C.; McEachern, E.J.; Davies, G.J.; Vocadlo, D.J.
Deposited on	:	2015-10-20
Resolution	:	1.80 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 ⓘ symbol.

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

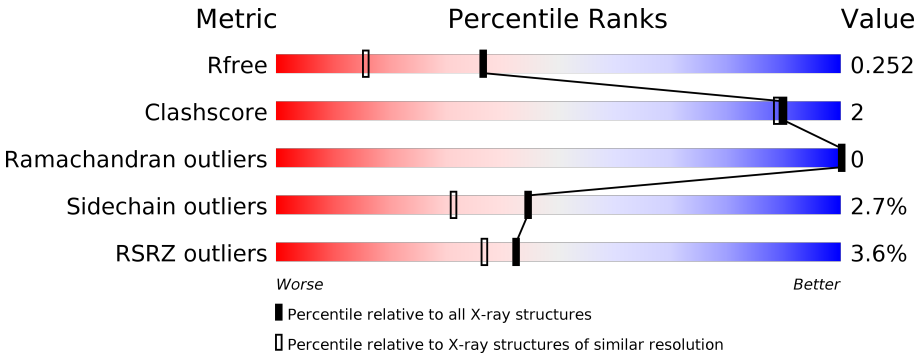
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	716	5%, 84%, 5% •, 10%
1	B	716	2%, 81%, 8%, 10%

2 Entry composition

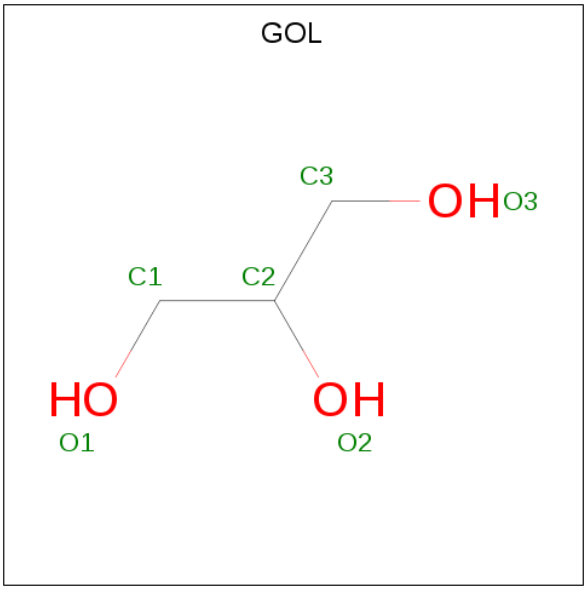
There are 4 unique types of molecules in this entry. The entry contains 11469 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 O-GLCNACASE BT_4395.

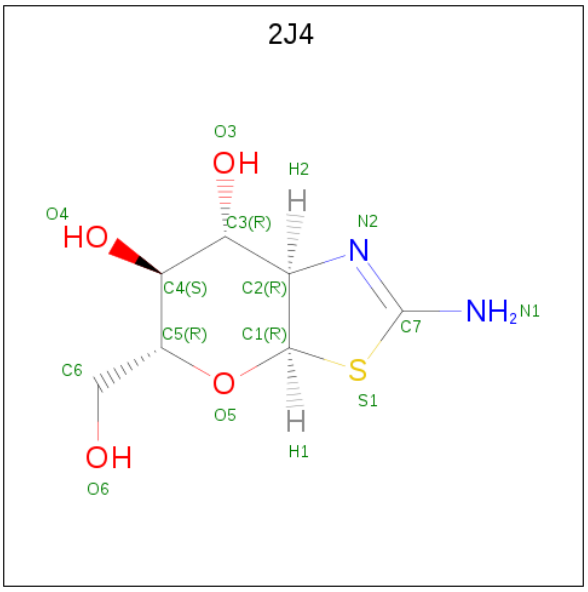
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	6	0
			5263	3382	882	980	19			
1	B	645	Total	C	N	O	S	0	5	0
			5267	3379	889	980	19			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is (3aR,5R,6S,7R,7aR)-2-amino-5-(hydroxymethyl)-5,6,7,7a-tetrahydro-3aH-pyrano[3,2-d][1,3]thiazole-6,7-diol (three-letter code: 2J4) (formula: $C_7H_{12}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	7	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			14	7	2	4	1		

- Molecule 4 is water.

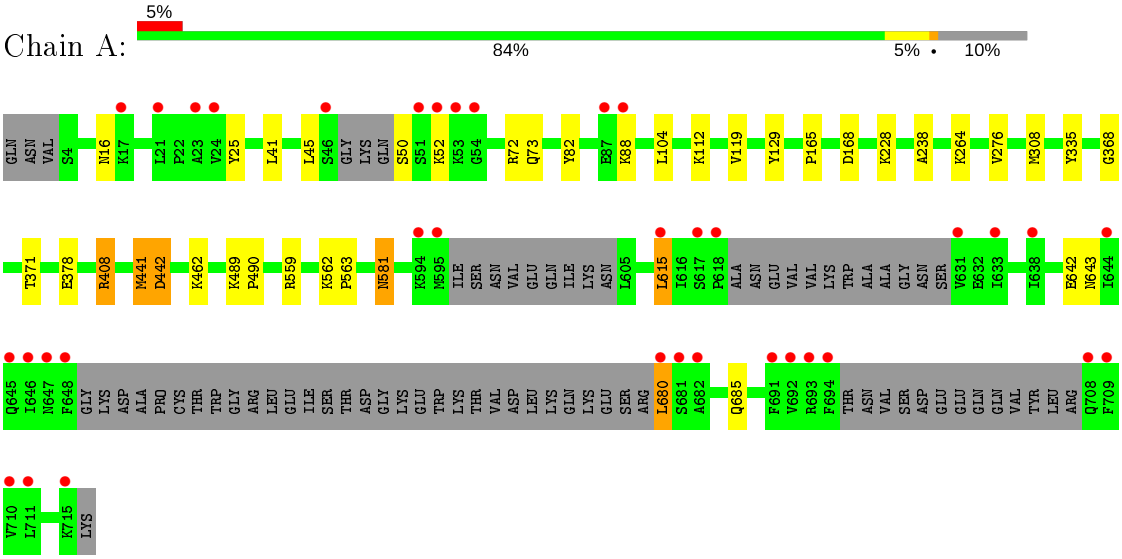
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	428	Total	O	0	0
			428	428		
4	B	477	Total	O	0	0
			477	477		

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 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.

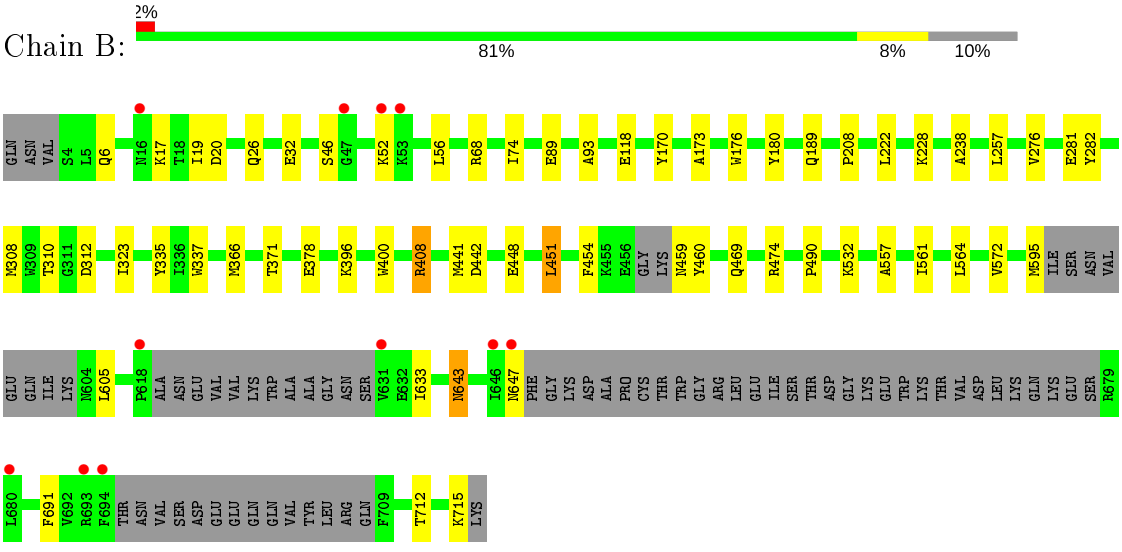
- Molecule 1: O-GLCNACASE BT_4395

Chain A:



- Molecule 1: O-GLCNACASE BT_4395

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.44Å 93.69Å 99.02Å 104.07° 94.18° 102.97°	Depositor
Resolution (Å)	95.17 – 1.80 33.83 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.8 (95.17-1.80) 95.8 (33.83-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.211 , 0.249 0.217 , 0.252	Depositor DCC
R_{free} test set	7706 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	12.4	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 30.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11469	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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: GOL, 2J4

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	0.84	1/5413 (0.0%)	0.84	6/7334 (0.1%)
1	B	0.89	3/5413 (0.1%)	0.89	7/7332 (0.1%)
All	All	0.86	4/10826 (0.0%)	0.86	13/14666 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	GLU	CD-OE2	6.25	1.32	1.25
1	A	378	GLU	CD-OE2	6.08	1.32	1.25
1	B	282	TYR	CE1-CZ	5.11	1.45	1.38
1	B	32	GLU	CG-CD	5.03	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	68	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	408	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	474	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	408	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	312	ASP	CB-CG-OD1	6.45	124.11	118.30
1	B	474	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	B	442	ASP	CB-CG-OD1	6.36	124.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	559	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	442	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	168	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	B	366	MET	CG-SD-CE	5.41	108.86	100.20
1	A	72	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	615	LEU	CA-CB-CG	5.21	127.28	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	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	5263	0	5194	13	0
1	B	5267	0	5195	24	0
2	A	6	0	8	0	0
3	A	14	0	12	0	0
3	B	14	0	12	0	0
4	A	428	0	0	2	0
4	B	477	0	0	3	0
All	All	11469	0	10421	37	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 2.

All (37) 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:26:GLN:NE2	1:B:52:LYS:O	2.24	0.70
1:B:308:MET:HA	1:B:335:TYR:O	2.04	0.58
1:A:441[A]:MET:HG2	4:A:2336:HOH:O	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:PHE:HZ	1:B:572:VAL:HG12	1.70	0.56
1:B:19:ILE:HD12	1:B:20:ASP:O	2.06	0.55
1:B:557:ALA:HB1	1:B:561:ILE:HB	1.90	0.54
1:A:680:LEU:N	1:A:680:LEU:HD12	2.23	0.53
1:B:459:ASN:OD1	1:B:460:TYR:N	2.44	0.51
1:A:25:TYR:CE2	1:A:45:LEU:HD13	2.47	0.50
1:A:238:ALA:HA	1:A:276:VAL:O	2.11	0.49
1:B:396:LYS:HE2	4:B:2013:HOH:O	2.11	0.49
1:B:189:GLN:NE2	4:B:2190:HOH:O	2.38	0.49
1:B:454:PHE:CZ	1:B:572:VAL:HG12	2.48	0.49
1:B:56:LEU:HD23	1:B:89:GLU:OE1	2.14	0.46
1:A:41:LEU:HB2	1:A:104:LEU:HD11	1.97	0.46
1:B:17:LYS:HG2	1:B:118:GLU:OE1	2.15	0.46
1:A:442:ASP:HB2	4:A:2340:HOH:O	2.17	0.44
1:B:378:GLU:HG3	1:B:490:PRO:HB2	2.00	0.43
1:A:562:LYS:HB3	1:A:563:PRO:HD3	2.01	0.43
1:A:308:MET:HA	1:A:335:TYR:O	2.19	0.43
1:A:581:ASN:OD1	1:A:581:ASN:N	2.51	0.43
1:A:489:LYS:N	1:A:490:PRO:CD	2.83	0.42
1:B:173:ALA:HB2	4:B:2158:HOH:O	2.19	0.42
1:B:643:ASN:HD22	1:B:712:THR:HB	1.83	0.42
1:A:129:TYR:O	1:A:368:GLY:HA2	2.21	0.41
1:B:400:TRP:CH2	1:B:441[A]:MET:HE1	2.54	0.41
1:A:228:LYS:HD2	1:A:228:LYS:HA	1.90	0.41
1:B:170:TYR:HB2	1:B:180:TYR:CE2	2.56	0.41
1:B:176:TRP:CD1	1:B:208:PRO:HA	2.56	0.41
1:B:633:ILE:O	1:B:691:PHE:HA	2.21	0.41
1:B:222:LEU:HD13	1:B:257:LEU:HD21	2.02	0.41
1:B:74:ILE:HD11	1:B:93:ALA:HB1	2.03	0.40
1:A:73:GLN:HB3	1:A:82:TYR:CD1	2.57	0.40
1:B:532:LYS:HD2	1:B:532:LYS:HA	1.93	0.40
1:B:238:ALA:HA	1:B:276:VAL:O	2.21	0.40
1:B:310:THR:HA	1:B:337:TRP:O	2.22	0.40
1:B:451:LEU:HD22	1:B:564:LEU:HD12	2.04	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	638/716 (89%)	615 (96%)	23 (4%)	0	100	100
1	B	638/716 (89%)	620 (97%)	18 (3%)	0	100	100
All	All	1276/1432 (89%)	1235 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	573/630 (91%)	555 (97%)	18 (3%)	40	25
1	B	572/630 (91%)	558 (98%)	14 (2%)	49	36
All	All	1145/1260 (91%)	1113 (97%)	32 (3%)	44	30

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	SER
1	A	52	LYS
1	A	88	LYS
1	A	112	LYS
1	A	119	VAL
1	A	165	PRO
1	A	264	LYS
1	A	371	THR

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Mol	Chain	Res	Type
1	A	408	ARG
1	A	441[A]	MET
1	A	441[B]	MET
1	A	462	LYS
1	A	581	ASN
1	A	615	LEU
1	A	642	GLU
1	A	643	ASN
1	A	680	LEU
1	A	685	GLN
1	B	6	GLN
1	B	46	SER
1	B	228	LYS
1	B	323	ILE
1	B	371	THR
1	B	408	ARG
1	B	448	GLU
1	B	451	LEU
1	B	469	GLN
1	B	595	MET
1	B	605	LEU
1	B	643	ASN
1	B	647	ASN
1	B	715	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	ASN
1	B	6	GLN
1	B	254	GLN
1	B	273	ASN
1	B	274	GLN
1	B	306	GLN
1	B	543	GLN
1	B	604	ASN
1	B	643	ASN

5.3.3 RNA

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)

3 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	$\#\|Z\| > 2$
3	2J4	B	1716	-	13,15,15	2.41	2 (15%)	13,22,22	2.14	1 (7%)
3	2J4	A	1717	-	13,15,15	2.55	3 (23%)	13,22,22	2.49	3 (23%)
2	GOL	A	1716	-	5,5,5	0.40	0	5,5,5	0.44	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	2J4	B	1716	-	-	0/2/30/30	0/2/2/2
3	2J4	A	1717	-	-	0/2/30/30	0/2/2/2
2	GOL	A	1716	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1716	2J4	C7-N2	6.45	1.35	1.29
3	A	1717	2J4	C7-N2	6.34	1.35	1.29
3	A	1717	2J4	C7-N1	5.42	1.45	1.34
3	B	1716	2J4	C7-N1	4.85	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1717	2J4	C7-S1	-2.34	1.72	1.77

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1717	2J4	S1-C7-N1	7.60	128.00	118.83
3	B	1716	2J4	S1-C7-N1	6.91	127.17	118.83
3	A	1717	2J4	O3-C3-C2	2.57	115.03	109.14
3	A	1717	2J4	C1-O5-C5	2.46	117.12	112.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1716	GOL	C1-C2-C3-O3
2	A	1716	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	644/716 (89%)	-0.14	36 (5%)	24	19	8, 21, 65, 93	0
1	B	645/716 (90%)	-0.36	11 (1%)	70	66	7, 19, 55, 78	0
All	All	1289/1432 (90%)	-0.25	47 (3%)	42	37	7, 20, 61, 93	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	648	PHE	6.6
1	A	631	VAL	6.3
1	A	694	PHE	6.0
1	A	709	PHE	5.0
1	A	680	LEU	5.0
1	A	24	VAL	5.0
1	B	693	ARG	4.6
1	B	631	VAL	4.4
1	B	680	LEU	4.1
1	B	646	ILE	3.8
1	B	694	PHE	3.8
1	A	638	ILE	3.7
1	A	691	PHE	3.7
1	A	54	GLY	3.6
1	A	23	ALA	3.6
1	B	647	ASN	3.4
1	A	711	LEU	3.4
1	A	52	LYS	3.4
1	A	708	GLN	3.3
1	A	682	ALA	3.2
1	A	681	SER	3.2
1	A	710	VAL	3.2
1	A	633	ILE	3.1
1	B	618	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	53	LYS	2.9
1	A	715	LYS	2.9
1	A	647	ASN	2.9
1	A	594	LYS	2.9
1	A	692	VAL	2.9
1	A	46	SER	2.8
1	A	617	SER	2.8
1	A	693	ARG	2.7
1	A	51	SER	2.6
1	B	16	ASN	2.5
1	A	618	PRO	2.5
1	A	646	ILE	2.5
1	A	615	LEU	2.3
1	B	53	LYS	2.3
1	B	47	GLY	2.2
1	A	21	LEU	2.2
1	A	644	ILE	2.2
1	B	52	LYS	2.2
1	A	88	LYS	2.1
1	A	595	MET	2.1
1	A	645	GLN	2.1
1	A	87	GLU	2.0
1	A	17	LYS	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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	1716	6/6	0.91	0.15	30,35,36,40	0
3	2J4	A	1717	14/14	0.99	0.08	8,10,11,12	0
3	2J4	B	1716	14/14	0.99	0.08	8,9,10,11	0

6.5 Other polymers

There are no such residues in this entry.