Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2025 – 06:01 PM JST

PDB ID	:	9K1L
Title	:	Complex structure of CNK2 and SAMD12
Authors	:	Lin, Z.; Chen, K.; Zhang, M.
Deposited on	:	2024-10-16
Resolution	:	2.85 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

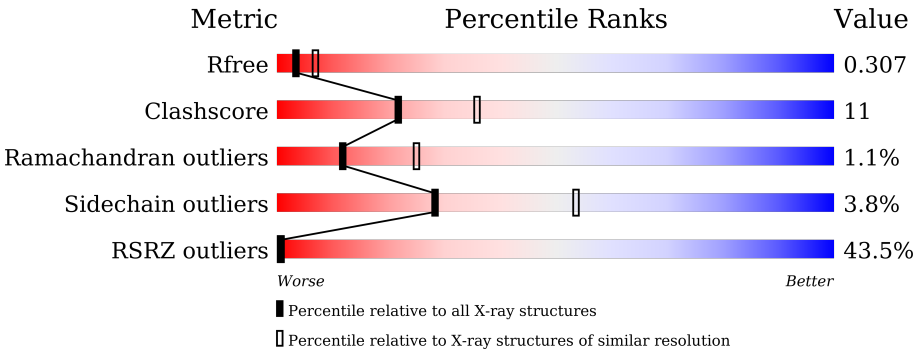
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 2.85 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}	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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	319	39% 68% 22% • 9%
2	B	98	41% 53% 33% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2901 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 Connector enhancer of kinase suppressor of ras 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2211	1384	384	432	11			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q80YA9
A	-3	GLY	-	expression tag	UNP Q80YA9
A	-2	SER	-	expression tag	UNP Q80YA9
A	-1	GLY	-	expression tag	UNP Q80YA9
A	0	SER	-	expression tag	UNP Q80YA9

- Molecule 2 is a protein called Sterile alpha motif domain-containing protein 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	84	Total	C	N	O	S	0	0	0
			673	424	124	122	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	74	GLY	-	expression tag	UNP Q0VE29
B	75	PRO	-	expression tag	UNP Q0VE29
B	76	GLY	-	expression tag	UNP Q0VE29
B	77	SER	-	expression tag	UNP Q0VE29
B	162	GLY	-	expression tag	UNP Q0VE29
B	163	SER	-	expression tag	UNP Q0VE29
B	164	GLY	-	expression tag	UNP Q0VE29
B	165	SER	-	expression tag	UNP Q0VE29
B	166	GLU	-	expression tag	UNP Q0VE29
B	167	ASN	-	expression tag	UNP Q0VE29
B	168	LEU	-	expression tag	UNP Q0VE29

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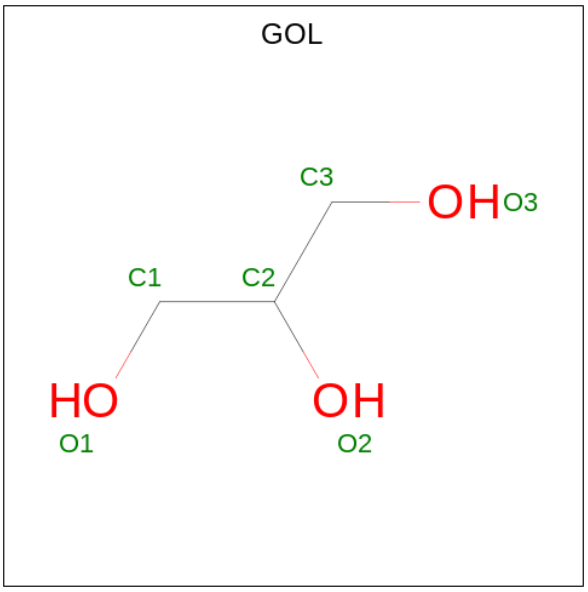
Chain	Residue	Modelled	Actual	Comment	Reference
B	169	TYR	-	expression tag	UNP Q0VE29
B	170	PHE	-	expression tag	UNP Q0VE29
B	171	GLN	-	expression tag	UNP Q0VE29

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

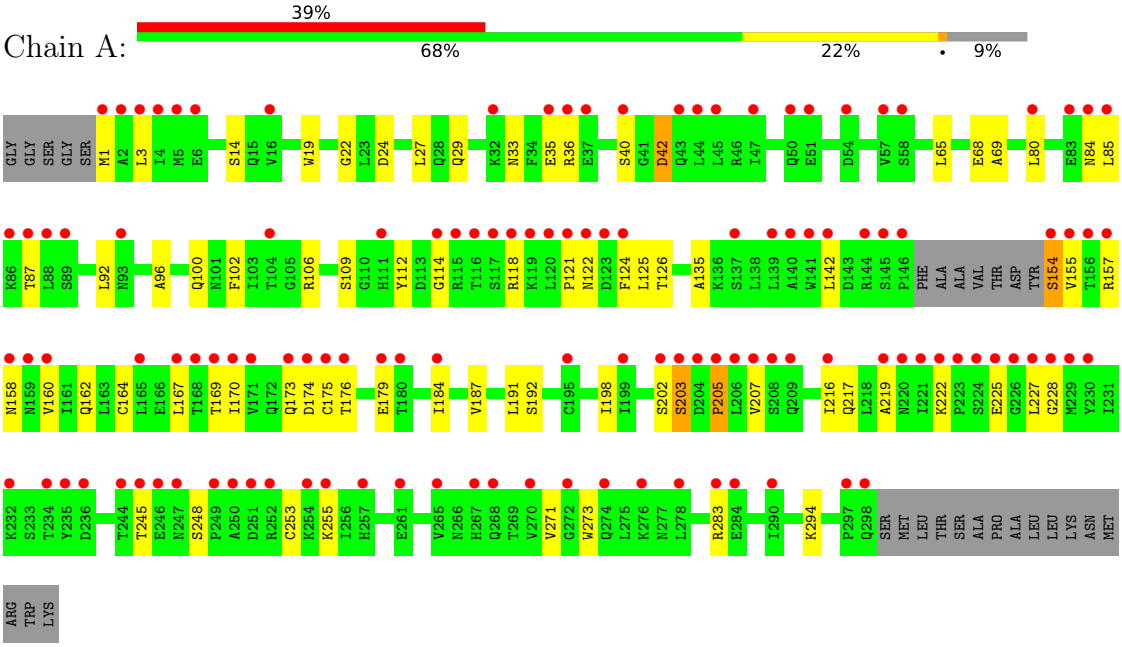
- Molecule 4 is water.

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

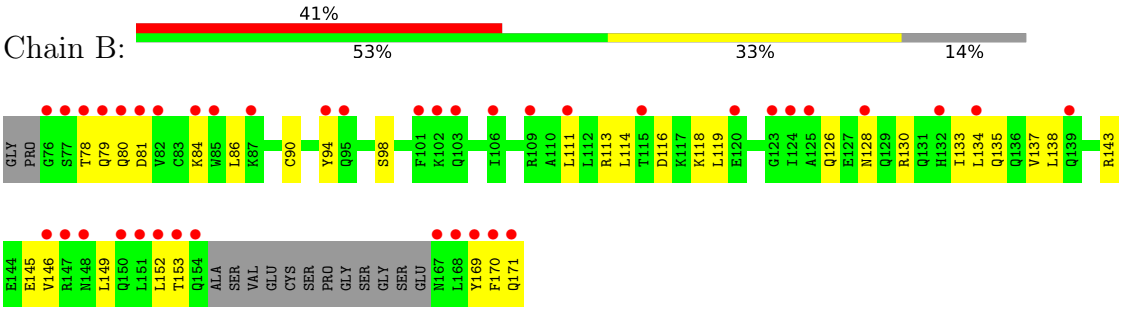
3 Residue-property plots (i)

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: Connector enhancer of kinase suppressor of ras 2



• Molecule 2: Sterile alpha motif domain-containing protein 12



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	109.31Å 109.31Å 203.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.15 – 2.85 48.15 – 2.85	Depositor EDS
% Data completeness (in resolution range)	95.4 (48.15-2.85) 98.8 (48.15-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.254 , 0.299 0.266 , 0.307	Depositor DCC
R_{free} test set	847 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	2901	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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

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	0.43	0/2243	0.62	1/3050 (0.0%)
2	B	0.45	0/682	0.65	0/917
All	All	0.44	0/2925	0.63	1/3967 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	271	VAL	C-N-CA	-5.28	111.22	122.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2211	0	2184	46	1
2	B	673	0	656	22	1
3	A	6	0	8	0	0
4	A	6	0	0	2	0
4	B	5	0	0	0	0
All	All	2901	0	2848	61	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 11.

All (61) 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:122:ASN:OD1	2:B:135:GLN:NE2	2.13	0.81
2:B:143:ARG:O	2:B:146:VAL:HG12	1.93	0.69
1:A:222:LYS:HG2	1:A:225:GLU:HB2	1.74	0.67
2:B:78:THR:HG23	2:B:81:ASP:H	1.60	0.67
1:A:160:VAL:HG13	1:A:191:LEU:HD11	1.76	0.67
1:A:118:ARG:HG2	1:A:176:THR:HA	1.78	0.65
1:A:33:ASN:OD1	1:A:36:ARG:NH1	2.32	0.62
1:A:216:ILE:HD13	1:A:255:LYS:HB3	1.84	0.60
1:A:80:LEU:HG	1:A:294:LYS:HE2	1.85	0.58
1:A:154:SER:OG	1:A:155:VAL:N	2.36	0.58
1:A:227:LEU:O	1:A:248:SER:OG	2.23	0.57
1:A:112:TYR:CZ	1:A:114:GLY:HA3	2.40	0.56
1:A:203:SER:HB2	1:A:205:PRO:HD2	1.88	0.55
2:B:80:GLN:O	2:B:84:LYS:HG3	2.06	0.55
1:A:22:GLY:HA3	1:A:273:TRP:CE2	2.43	0.54
1:A:227:LEU:N	2:B:171:GLN:O	2.41	0.54
1:A:245:THR:O	1:A:248:SER:HB3	2.09	0.53
1:A:157:ARG:NH1	2:B:152:LEU:O	2.41	0.52
1:A:122:ASN:O	1:A:126:THR:HG23	2.10	0.52
2:B:86:LEU:HG	2:B:90:CYS:HB2	1.92	0.52
1:A:169:THR:O	1:A:173:GLN:HG2	2.10	0.51
1:A:228:GLY:HA3	1:A:248:SER:OG	2.11	0.50
1:A:40:SER:OG	1:A:42:ASP:HB2	2.12	0.50
1:A:142:LEU:HD11	1:A:198:ILE:HG21	1.95	0.49
1:A:222:LYS:HE3	1:A:225:GLU:HG3	1.95	0.49
1:A:27:LEU:HD11	1:A:65:LEU:HB3	1.94	0.49
2:B:133:ILE:O	2:B:137:VAL:HG23	2.12	0.49
1:A:106:ARG:HD2	4:A:503:HOH:O	2.13	0.47
2:B:111:LEU:O	2:B:114:LEU:HB2	2.14	0.47
1:A:167:LEU:HG	1:A:187:VAL:HG11	1.96	0.47
2:B:145:GLU:O	2:B:149:LEU:HG	2.15	0.47
1:A:170:ILE:HG21	1:A:184:ILE:HG13	1.95	0.47
1:A:1:MET:HG3	1:A:3:LEU:H	1.80	0.47
2:B:78:THR:O	2:B:81:ASP:HB2	2.15	0.46
1:A:125:LEU:HB3	2:B:138:LEU:HB3	1.98	0.46
2:B:126:GLN:HG2	2:B:128:ASN:HB3	1.98	0.45
1:A:68:GLU:HG3	2:B:113:ARG:NH1	2.31	0.45
1:A:22:GLY:HA3	1:A:273:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ASP:OD1	2:B:130:ARG:HD2	2.17	0.45
2:B:113:ARG:O	2:B:118:LYS:NZ	2.37	0.44
1:A:84:ASN:O	1:A:87:THR:HB	2.17	0.44
1:A:125:LEU:HB2	2:B:138:LEU:HD13	1.99	0.43
1:A:102:PHE:CZ	1:A:106:ARG:HD3	2.53	0.43
2:B:94:TYR:O	2:B:98:SER:HB3	2.19	0.43
2:B:119:LEU:HD23	2:B:119:LEU:HA	1.87	0.43
1:A:176:THR:CG2	1:A:179:GLU:H	2.31	0.43
1:A:176:THR:HG23	1:A:179:GLU:H	1.82	0.43
1:A:92:LEU:CD1	1:A:135:ALA:HA	2.48	0.43
1:A:96:ALA:O	1:A:100:GLN:HG3	2.19	0.43
1:A:219:ALA:HB1	4:A:506:HOH:O	2.19	0.42
1:A:85:LEU:HD23	1:A:207:VAL:HG23	2.01	0.42
1:A:158:ASN:HD21	1:A:162:GLN:HE21	1.68	0.42
1:A:19:TRP:CZ2	1:A:69:ALA:HB1	2.55	0.42
2:B:119:LEU:HD12	2:B:134:LEU:CD1	2.49	0.42
1:A:222:LYS:HG2	1:A:225:GLU:CB	2.47	0.41
1:A:173:GLN:O	1:A:175:CYS:N	2.53	0.41
1:A:164:CYS:O	1:A:167:LEU:HB2	2.21	0.41
2:B:169:TYR:CG	2:B:170:PHE:N	2.88	0.41
1:A:121:PRO:O	1:A:124:PHE:HB2	2.21	0.40
1:A:164:CYS:HB3	2:B:149:LEU:HD11	2.03	0.40
1:A:176:THR:HG22	1:A:179:GLU:OE2	2.21	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:283:ARG:NH2	2:B:169:TYR:OH[10_555]	2.13	0.07

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	287/319 (90%)	268 (93%)	15 (5%)	4 (1%)	9 20
2	B	80/98 (82%)	78 (98%)	2 (2%)	0	100 100
All	All	367/417 (88%)	346 (94%)	17 (5%)	4 (1%)	12 25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	174	ASP
1	A	29	GLN
1	A	205	PRO

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	245/282 (87%)	235 (96%)	10 (4%)	26 50
2	B	70/89 (79%)	68 (97%)	2 (3%)	37 63
All	All	315/371 (85%)	303 (96%)	12 (4%)	28 54

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	24	ASP
1	A	35	GLU
1	A	109	SER
1	A	154	SER
1	A	192	SER
1	A	202	SER
1	A	203	SER
1	A	217	GLN
1	A	253	CYS
2	B	79	GLN
2	B	153	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
2	B	89	HIS
2	B	135	GLN
2	B	139	GLN
2	B	150	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)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand 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	$\#\|Z\| > 2$
3	GOL	A	401	-	5,5,5	1.40	1 (20%)	5,5,5	1.07	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	GOL	A	401	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	GOL	C3-C2	2.67	1.62	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	C1-C2-C3-O3
3	A	401	GOL	O2-C2-C3-O3
3	A	401	GOL	O1-C1-C2-C3

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	291/319 (91%)	2.02	123 (42%)	1	0	32, 46, 75, 92	0
2	B	84/98 (85%)	2.20	40 (47%)	0	0	39, 54, 77, 90	0
All	All	375/417 (89%)	2.06	163 (43%)	1	0	32, 48, 77, 92	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	167	ASN	8.8
1	A	226	GLY	8.2
1	A	207	VAL	7.3
1	A	89	SER	7.3
2	B	154	GLN	6.4
1	A	228	GLY	6.3
1	A	2	ALA	5.8
2	B	77	SER	5.8
1	A	206	LEU	5.7
1	A	219	ALA	5.3
1	A	235	TYR	5.3
1	A	225	GLU	5.3
1	A	204	ASP	5.0
1	A	205	PRO	4.9
2	B	76	GLY	4.9
1	A	247	ASN	4.9
1	A	58	SER	4.8
1	A	199	ILE	4.7
1	A	223	PRO	4.7
2	B	168	LEU	4.7
2	B	169	TYR	4.7
1	A	227	LEU	4.5
1	A	168	THR	4.5
1	A	1	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	87	THR	4.4
1	A	203	SER	4.4
1	A	208	SER	4.3
1	A	43	GLN	4.2
2	B	128	ASN	4.1
1	A	224	SER	4.1
1	A	6	GLU	4.1
1	A	230	TYR	4.0
1	A	155	VAL	4.0
1	A	145	SER	4.0
1	A	221	ILE	3.9
1	A	158	ASN	3.9
2	B	81	ASP	3.8
1	A	220	ASN	3.8
1	A	3	LEU	3.8
1	A	156	THR	3.8
2	B	139	GLN	3.8
1	A	119	LYS	3.7
2	B	80	GLN	3.6
1	A	179	GLU	3.5
2	B	151	LEU	3.5
1	A	146	PRO	3.5
1	A	298	GLN	3.4
1	A	222	LYS	3.4
2	B	95	GLN	3.4
1	A	111	HIS	3.4
2	B	94	TYR	3.4
1	A	169	THR	3.4
1	A	45	LEU	3.3
1	A	32	LYS	3.3
1	A	159	ASN	3.3
2	B	78	THR	3.2
2	B	111	LEU	3.2
1	A	83	GLU	3.2
1	A	4	ILE	3.2
2	B	171	GLN	3.2
1	A	139	LEU	3.2
1	A	142	LEU	3.2
1	A	124	PHE	3.1
1	A	84	ASN	3.1
2	B	84	LYS	3.1
1	A	195	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	209	GLN	3.0
1	A	252	ARG	3.0
1	A	249	PRO	3.0
1	A	270	VAL	3.0
1	A	250	ALA	3.0
1	A	154	SER	3.0
1	A	268	GLN	2.9
2	B	79	GLN	2.9
1	A	173	GLN	2.9
1	A	40	SER	2.9
1	A	184	ILE	2.9
2	B	147	ARG	2.9
1	A	118	ARG	2.8
1	A	88	LEU	2.8
1	A	120	LEU	2.8
1	A	283	ARG	2.8
1	A	116	THR	2.8
1	A	121	PRO	2.8
1	A	160	VAL	2.8
2	B	124	ILE	2.7
2	B	123	GLY	2.7
1	A	284	GLU	2.7
1	A	36	ARG	2.7
1	A	157	ARG	2.7
1	A	117	SER	2.7
1	A	202	SER	2.7
2	B	103	GLN	2.6
1	A	5	MET	2.6
1	A	137	SER	2.6
1	A	123	ASP	2.6
2	B	153	THR	2.6
1	A	114	GLY	2.6
1	A	140	ALA	2.6
2	B	87	LYS	2.6
1	A	234	THR	2.6
1	A	265	VAL	2.6
2	B	170	PHE	2.5
1	A	257	HIS	2.5
2	B	148	ASN	2.5
1	A	278	LEU	2.5
1	A	51	GLU	2.5
1	A	80	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	276	LYS	2.4
1	A	47	ILE	2.4
1	A	170	ILE	2.4
2	B	152	LEU	2.4
1	A	50	GLN	2.4
2	B	85	TRP	2.4
1	A	141	TRP	2.4
1	A	236	ASP	2.4
1	A	290	ILE	2.4
1	A	175	CYS	2.4
1	A	216	ILE	2.3
1	A	144	ARG	2.3
1	A	44	LEU	2.3
1	A	165	LEU	2.3
1	A	267	HIS	2.3
1	A	57	VAL	2.3
1	A	171	VAL	2.3
1	A	104	THR	2.3
1	A	180	THR	2.3
2	B	115	THR	2.3
1	A	255	LYS	2.3
2	B	109	ARG	2.3
1	A	232	LYS	2.3
2	B	146	VAL	2.3
1	A	54	ASP	2.3
2	B	134	LEU	2.3
1	A	254	LYS	2.3
2	B	120	GLU	2.2
1	A	176	THR	2.2
2	B	82	VAL	2.2
1	A	115	ARG	2.2
2	B	101	PHE	2.2
1	A	244	THR	2.2
1	A	122	ASN	2.2
1	A	85	LEU	2.2
1	A	297	PRO	2.2
1	A	93	ASN	2.2
1	A	261	GLU	2.2
1	A	174	ASP	2.2
1	A	35	GLU	2.1
1	A	37	GLU	2.1
1	A	246	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	245	THR	2.1
1	A	86	LYS	2.1
2	B	125	ALA	2.1
1	A	272	GLY	2.1
1	A	167	LEU	2.1
1	A	16	VAL	2.1
2	B	102	LYS	2.0
1	A	274	GLN	2.0
2	B	150	GLN	2.0
1	A	251	ASP	2.0
2	B	106	ILE	2.0
1	A	229	MET	2.0
2	B	132	HIS	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 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
3	GOL	A	401	6/6	0.67	0.25	46,47,50,53	0

6.5 Other polymers (i)

There are no such residues in this entry.