Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 10:02 PM JST

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PDB ID	:	5Y90
Title	:	MAP2K7 mutant -C218S
Authors	:	Kinoshita, T.; Hashimoto, T.; Sogabe, Y.; Matsumoto, T.; Sawa, M.; Fukada, H.
Deposited on	:	2017-08-22
Resolution	:	1.30 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.30 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	Percentile Ranks	Value
Rfree		0.170
Clashscore		15
Ramachandran outliers		1.7%
Sidechain outliers		3.8%
RSRZ outliers		8.2%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
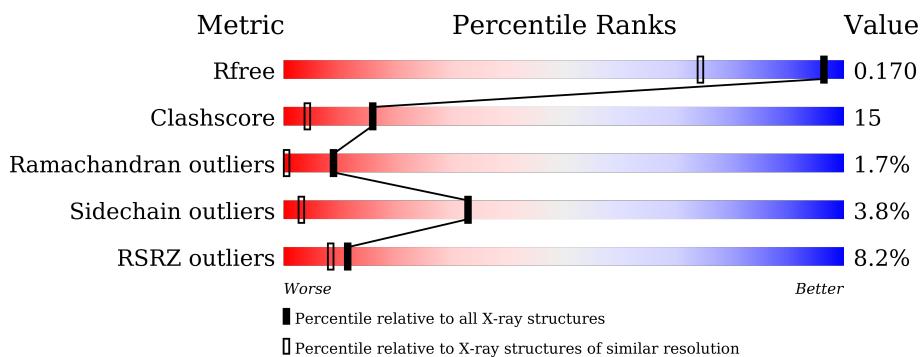
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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	323	8% 70% 19% · · 6%
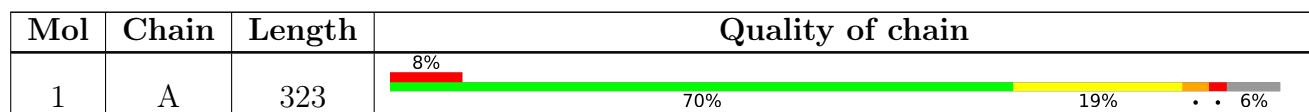
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	503	-	-	X	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2925 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 Dual specificity mitogen-activated protein kinase kinase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2560	1644	441	453	22	0	23	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	SER	CYS	engineered mutation	UNP O14733
A	436	HIS	-	expression tag	UNP O14733
A	437	HIS	-	expression tag	UNP O14733
A	438	HIS	-	expression tag	UNP O14733
A	439	HIS	-	expression tag	UNP O14733
A	440	HIS	-	expression tag	UNP O14733
A	441	HIS	-	expression tag	UNP O14733

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

GOL

C3 OH O3

C1 C2

HO OH

O1 O2
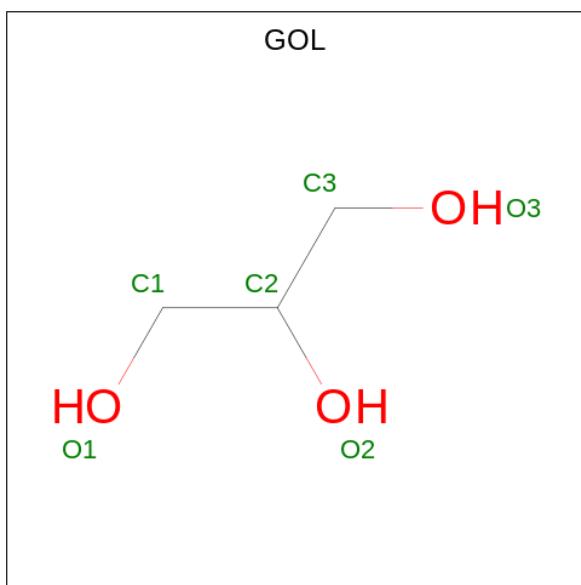
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	341	Total 341	O 341	0	0

3 Residue-property plots ⓘ

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: Dual specificity mitogen-activated protein kinase kinase 7
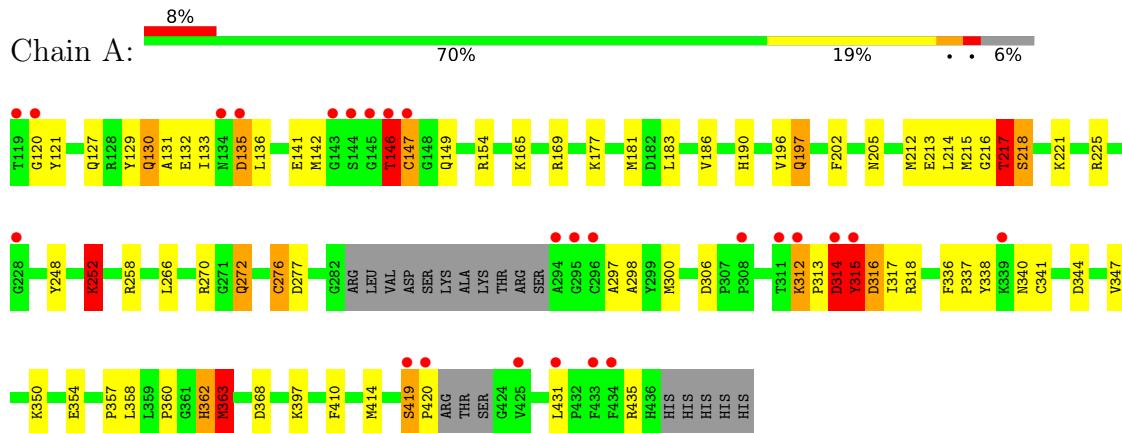
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.40Å 70.61Å 92.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.05 – 1.30 38.59 – 1.30	Depositor EDS
% Data completeness (in resolution range)	91.7 (56.05-1.30) 91.7 (38.59-1.30)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.61 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.127 , 0.167 0.128 , 0.170	Depositor DCC
R_{free} test set	3853 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	13.1	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 70.8	EDS
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	2925	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	1.19	7/2669 (0.3%)	1.11	13/3585 (0.4%)

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	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	CYS	CB-SG	-17.67	1.52	1.82
1	A	218	SER	CB-OG	15.85	1.62	1.42
1	A	121	TYR	CG-CD2	6.55	1.47	1.39
1	A	141	GLU	CD-OE1	5.80	1.32	1.25
1	A	197	GLN	CG-CD	5.35	1.63	1.51
1	A	435	ARG	CZ-NH1	-5.08	1.26	1.33
1	A	363	MET	CG-SD	5.01	1.94	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	MET	CA-CB-CG	6.74	124.76	113.30
1	A	368	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	217[A]	THR	CB-CA-C	-6.45	94.20	111.60
1	A	217[B]	THR	CB-CA-C	-6.45	94.20	111.60
1	A	225	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	344	ASP	CB-CG-OD2	-5.91	112.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	LYS	CD-CE-NZ	-5.84	98.26	111.70
1	A	344	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	306	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	130[A]	GLN	CB-CA-C	5.50	121.40	110.40
1	A	130[B]	GLN	CB-CA-C	5.50	121.40	110.40
1	A	318	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	A	154	ARG	NE-CZ-NH2	-5.33	117.63	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	THR	Peptide
1	A	147	CYS	Peptide
1	A	315	TYR	Peptide
1	A	362	HIS	Peptide

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	2560	0	2651	76	0
2	A	24	0	32	11	0
3	A	341	0	0	26	2
All	All	2925	0	2683	77	2

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 15.

All (77) 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:270[B]:ARG:NH2	1:A:272[B]:GLN:NE2	1.61	1.46
1:A:357[B]:PRO:O	1:A:358[B]:LEU:HD23	1.58	1.03
1:A:216[A]:GLY:HA2	3:A:604:HOH:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LYS:HE2	3:A:612:HOH:O	1.68	0.94
1:A:132:GLU:O	1:A:135:ASP:HB3	1.74	0.86
1:A:135:ASP:CG	2:A:503:GOL:H2	1.99	0.83
1:A:270[B]:ARG:CZ	3:A:601:HOH:O	2.26	0.83
1:A:270[B]:ARG:NH2	3:A:601:HOH:O	2.11	0.82
1:A:133:ILE:HD12	1:A:136:LEU:HD12	1.67	0.76
1:A:190:HIS:HA	1:A:197:GLN:OE1	1.86	0.75
1:A:217[A]:THR:HG22	1:A:221:LYS:HB2	1.70	0.74
1:A:270[B]:ARG:CZ	1:A:272[B]:GLN:NE2	2.50	0.72
1:A:270[B]:ARG:NH1	3:A:601:HOH:O	2.24	0.68
1:A:135:ASP:OD1	3:A:602:HOH:O	2.14	0.65
1:A:217[A]:THR:CG2	1:A:221:LYS:HB2	2.27	0.65
1:A:135:ASP:HB2	2:A:503:GOL:C3	2.28	0.64
1:A:312:LYS:CE	3:A:612:HOH:O	2.34	0.62
1:A:314:ASP:O	1:A:316:ASP:N	2.33	0.61
1:A:337:PRO:HB2	1:A:357[A]:PRO:HB2	1.83	0.60
1:A:317:ILE:HA	3:A:633:HOH:O	2.01	0.60
1:A:146:THR:HB	3:A:810:HOH:O	2.00	0.60
1:A:120:GLY:HA3	1:A:202:PHE:CD2	2.36	0.59
1:A:181[A]:MET:CE	3:A:777:HOH:O	2.49	0.58
1:A:357[B]:PRO:O	1:A:358[B]:LEU:CD2	2.45	0.58
1:A:340:ASN:N	3:A:609:HOH:O	2.36	0.58
1:A:127[B]:GLN:NE2	3:A:610:HOH:O	2.37	0.57
1:A:135:ASP:HB2	2:A:503:GOL:H32	1.87	0.56
1:A:298:ALA:HB1	1:A:336:PHE:CZ	2.40	0.56
2:A:501:GOL:C3	3:A:660:HOH:O	2.54	0.55
1:A:165[B]:LYS:HE3	1:A:277:ASP:OD2	2.08	0.54
1:A:127[A]:GLN:NE2	3:A:610:HOH:O	2.41	0.54
1:A:312:LYS:HE2	3:A:887:HOH:O	2.07	0.53
1:A:419:SER:HB2	1:A:420:PRO:HD3	1.90	0.52
1:A:217[A]:THR:HG22	1:A:218:SER:N	2.25	0.52
1:A:135:ASP:CB	2:A:503:GOL:H2	2.39	0.52
1:A:131:ALA:HA	2:A:503:GOL:O2	2.10	0.51
1:A:183:LEU:HA	1:A:186[B]:VAL:HG22	1.93	0.50
1:A:297:ALA:HA	1:A:300[A]:MET:HE3	1.94	0.50
1:A:313:PRO:O	1:A:315:TYR:N	2.45	0.49
1:A:142[B]:MET:HE1	1:A:214:LEU:HD11	1.95	0.48
1:A:165[B]:LYS:HE2	1:A:212:MET:HG3	1.95	0.48
1:A:135:ASP:CG	3:A:602:HOH:O	2.50	0.48
1:A:312:LYS:NZ	3:A:612:HOH:O	2.38	0.48
1:A:165[A]:LYS:NZ	3:A:622:HOH:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:OD2	1:A:316:ASP:OD2	2.31	0.48
1:A:298:ALA:HA	1:A:347:VAL:HG11	1.95	0.47
1:A:338:TYR:O	3:A:603:HOH:O	2.20	0.47
1:A:165[B]:LYS:CE	1:A:277:ASP:OD2	2.62	0.47
1:A:169:ARG:NH1	1:A:205[B]:ASN:OD1	2.47	0.47
1:A:149:GLN:HB3	3:A:728:HOH:O	2.15	0.47
1:A:181[A]:MET:HE2	3:A:777:HOH:O	2.14	0.47
1:A:341:CYS:SG	1:A:350[A]:LYS:HD2	2.55	0.47
1:A:337:PRO:HB2	1:A:357[A]:PRO:CB	2.46	0.46
1:A:127[B]:GLN:HB2	1:A:129:TYR:CE2	2.51	0.46
1:A:196[B]:VAL:HG21	1:A:266:LEU:HD12	1.98	0.46
1:A:135:ASP:CB	2:A:503:GOL:H32	2.46	0.45
1:A:248:TYR:CE2	1:A:252:LYS:HG2	2.52	0.44
1:A:272[A]:GLN:NE2	3:A:626:HOH:O	2.50	0.44
1:A:120:GLY:HA3	1:A:202:PHE:CE2	2.52	0.44
1:A:258:ARG:HD2	3:A:736:HOH:O	2.18	0.44
1:A:132:GLU:HB2	2:A:503:GOL:H32	2.00	0.44
1:A:350[B]:LYS:HD2	1:A:354[B]:GLU:OE2	2.19	0.43
1:A:217[A]:THR:HG23	3:A:851:HOH:O	2.18	0.43
1:A:190:HIS:CD2	1:A:190:HIS:H	2.36	0.42
1:A:196[B]:VAL:HG13	1:A:213:GLU:HB3	2.01	0.42
1:A:276:CYS:SG	1:A:277:ASP:N	2.92	0.41
1:A:135:ASP:OD1	2:A:503:GOL:C1	2.67	0.41
1:A:215[A]:MET:O	3:A:604:HOH:O	2.22	0.41
1:A:360:PRO:HG2	1:A:363:MET:SD	2.60	0.41
1:A:337:PRO:O	2:A:504:GOL:C1	2.69	0.41
1:A:177:LYS:O	1:A:181[B]:MET:HG3	2.20	0.41
1:A:340:ASN:CA	3:A:609:HOH:O	2.69	0.41
1:A:362:HIS:CE1	1:A:363:MET:HG3	2.56	0.41
1:A:135:ASP:CG	2:A:503:GOL:C2	2.79	0.41
1:A:397:LYS:HA	1:A:397:LYS:HD3	1.92	0.40
1:A:410:PHE:CE1	1:A:414:MET:HG3	2.57	0.40

All (2) 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)
3:A:886:HOH:O	3:A:901:HOH:O[4_455]	1.97	0.23
3:A:619:HOH:O	3:A:658:HOH:O[1_565]	2.12	0.08

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	321/323 (99%)	308 (96%)	8 (2%)	5 (2%)	9	0

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	THR
1	A	314	ASP
1	A	316	ASP
1	A	419	SER
1	A	315	TYR

5.3.2 Protein sidechains ⓘ

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	288/284 (101%)	275 (96%)	13 (4%)	27	2

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

Mol	Chain	Res	Type
1	A	130[A]	GLN
1	A	130[B]	GLN
1	A	135	ASP
1	A	147	CYS
1	A	217[A]	THR
1	A	217[B]	THR

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Mol	Chain	Res	Type
1	A	252	LYS
1	A	272[A]	GLN
1	A	272[B]	GLN
1	A	312	LYS
1	A	314	ASP
1	A	363	MET
1	A	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	190	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	#$\|Z\| > 2$
2	GOL	A	503	-	5,5,5	0.74	0	5,5,5	1.39	1 (20%)
2	GOL	A	501	-	5,5,5	0.57	0	5,5,5	0.65	0
2	GOL	A	502	-	5,5,5	0.79	0	5,5,5	0.73	0
2	GOL	A	504	-	5,5,5	1.48	0	5,5,5	0.93	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
2	GOL	A	503	-	-	3/4/4/4	-
2	GOL	A	501	-	-	1/4/4/4	-
2	GOL	A	502	-	-	2/4/4/4	-
2	GOL	A	504	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	503	GOL	O3-C3-C2	2.48	122.08	110.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	GOL	C1-C2-C3-O3
2	A	503	GOL	O2-C2-C3-O3
2	A	502	GOL	C1-C2-C3-O3
2	A	504	GOL	O1-C1-C2-C3
2	A	502	GOL	O2-C2-C3-O3
2	A	504	GOL	O1-C1-C2-O2
2	A	501	GOL	O2-C2-C3-O3
2	A	503	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	GOL	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	1	0
2	A	504	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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	304/323 (94%)	0.31	25 (8%)	11	8	10, 22, 75, 181	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	TYR	12.1
1	A	146	THR	10.0
1	A	294	ALA	7.2
1	A	145	GLY	7.0
1	A	143	GLY	6.9
1	A	144	SER	6.5
1	A	433	PHE	5.7
1	A	419	SER	5.4
1	A	147	CYS	5.4
1	A	314	ASP	5.2
1	A	420	PRO	5.0
1	A	296	CYS	4.9
1	A	295	GLY	4.2
1	A	120	GLY	3.6
1	A	312	LYS	3.6
1	A	431	LEU	3.5
1	A	434	PHE	3.3
1	A	135	ASP	2.9
1	A	119	THR	2.7
1	A	308	PRO	2.5
1	A	339	LYS	2.5
1	A	134	ASN	2.2
1	A	425	VAL	2.2
1	A	228	GLY	2.1
1	A	311	THR	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th 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	GOL	A	504	6/6	0.63	0.39	39,59,81,92	0
2	GOL	A	503	6/6	0.80	0.41	58,70,91,248	0
2	GOL	A	502	6/6	0.88	0.19	39,78,89,101	0
2	GOL	A	501	6/6	0.91	0.12	56,63,82,102	0

6.5 Other polymers ⓘ

There are no such residues in this entry.