



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:54 PM UTC

PDB ID : 4JDY / pdb_00004jdy
Title : Crystal structure of Rv2606c
Authors : Kim, S.; Kim, K.-J.
Deposited on : 2013-02-25
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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

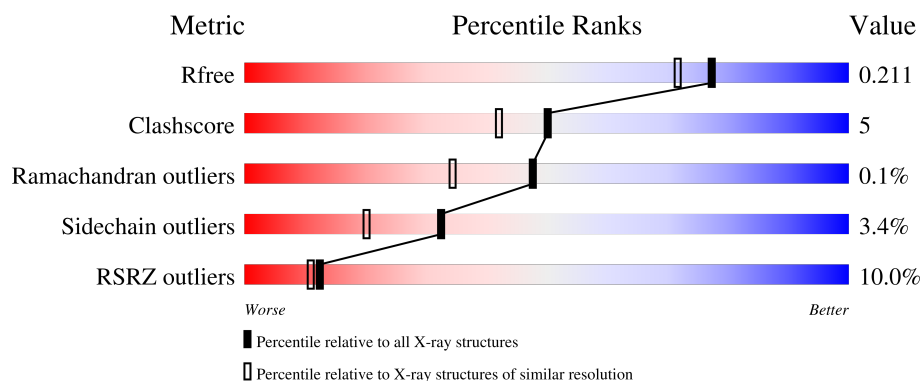
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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 $\leq 5\%$. 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	264	10% 84% 15% .
1	B	264	10% 80% 17% .
1	C	264	10% 78% 19% .

2 Entry composition [i](#)

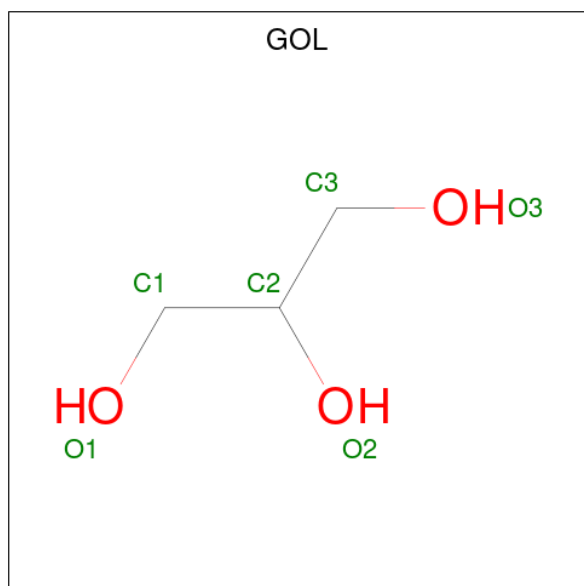
There are 3 unique types of molecules in this entry. The entry contains 6304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyridoxal biosynthesis lyase PdxS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			1947	1221	342	370	14			
1	B	264	Total	C	N	O	S	0	0	0
			1947	1221	342	370	14			
1	C	264	Total	C	N	O	S	0	0	0
			1947	1221	342	370	14			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

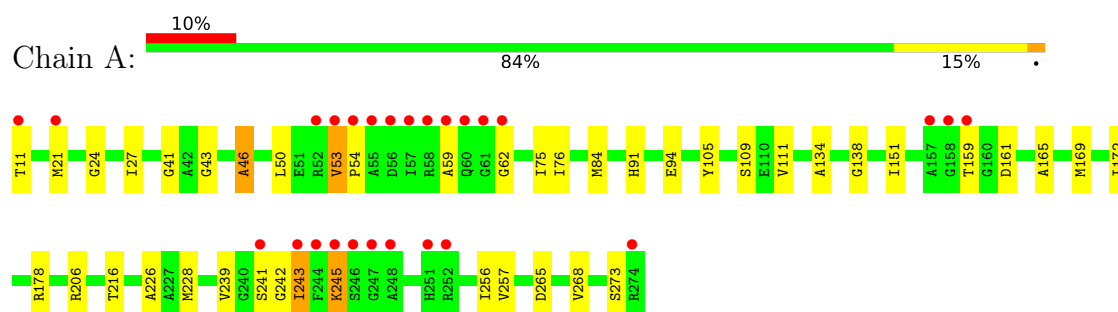
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total 138	O 138	0	0
3	B	153	Total 153	O 153	0	0
3	C	154	Total 154	O 154	0	0

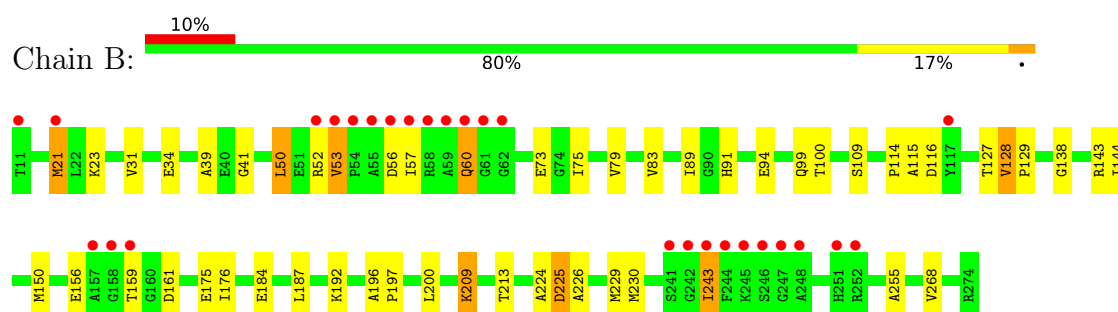
3 Residue-property plots [i](#)

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.

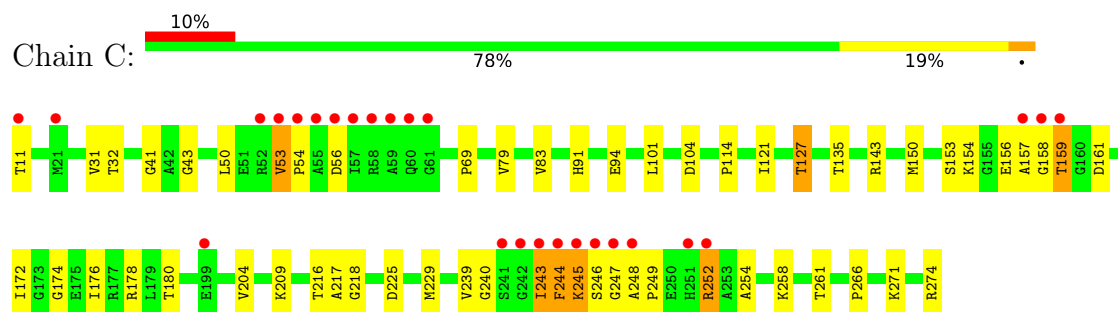
• Molecule 1: Pyridoxal biosynthesis lyase PdxS



• Molecule 1: Pyridoxal biosynthesis lyase PdxS



• Molecule 1: Pyridoxal biosynthesis lyase PdxS



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	110.75Å 126.08Å 180.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.80) 99.0 (50.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.211 0.184 , 0.211	Depositor DCC
R_{free} test set	5767 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6304	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.68	19/1976 (1.0%)	1.30	5/2672 (0.2%)
1	B	1.80	24/1976 (1.2%)	1.36	6/2672 (0.2%)
1	C	1.75	22/1976 (1.1%)	1.34	5/2672 (0.2%)
All	All	1.75	65/5928 (1.1%)	1.33	16/8016 (0.2%)

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	172	ILE	CA-CB	8.19	1.64	1.54
1	B	128	VAL	CA-C	7.69	1.59	1.52
1	B	89	ILE	CA-CB	7.62	1.63	1.54
1	B	144	ILE	CA-CB	7.61	1.64	1.54
1	A	268	VAL	CA-CB	7.36	1.63	1.54
1	B	79	VAL	CA-C	-7.33	1.45	1.52
1	A	265	ASP	C-O	-7.17	1.17	1.24
1	C	150	MET	SD-CE	-7.12	1.61	1.79
1	B	143	ARG	N-CA	6.89	1.54	1.46
1	C	154	LYS	C-O	-6.82	1.15	1.24
1	B	39	ALA	CA-CB	6.77	1.63	1.53
1	C	121	ILE	CA-CB	6.74	1.61	1.54
1	C	174	GLY	N-CA	6.69	1.54	1.45
1	C	261	THR	C-O	-6.58	1.16	1.24
1	A	84	MET	CA-C	-6.55	1.45	1.52
1	B	41	GLY	N-CA	6.40	1.54	1.45
1	B	129	PRO	N-CA	6.39	1.54	1.46
1	C	217	ALA	C-O	-6.37	1.16	1.23
1	B	138	GLY	N-CA	6.34	1.53	1.45
1	C	159	THR	CA-C	6.32	1.60	1.52
1	A	216	THR	CA-C	-6.24	1.45	1.52
1	C	218	GLY	C-O	-6.19	1.15	1.23
1	A	206	ARG	N-CA	6.14	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	258	LYS	C-O	-6.09	1.17	1.24
1	B	116	ASP	C-O	-6.07	1.17	1.23
1	A	105	TYR	N-CA	5.95	1.53	1.45
1	A	226	ALA	CA-CB	5.94	1.62	1.53
1	B	75	ILE	CA-CB	5.84	1.61	1.54
1	C	83	VAL	CA-CB	5.84	1.61	1.54
1	B	268	VAL	CA-CB	5.83	1.61	1.54
1	A	75	ILE	CA-CB	5.81	1.61	1.54
1	B	187	LEU	N-CA	5.80	1.53	1.46
1	C	178	ARG	C-O	-5.73	1.17	1.24
1	B	53	VAL	CA-C	5.68	1.58	1.52
1	A	178	ARG	C-O	-5.63	1.17	1.24
1	C	127	THR	CA-CB	5.59	1.62	1.53
1	B	229	MET	N-CA	5.56	1.53	1.46
1	C	143	ARG	N-CA	5.56	1.52	1.46
1	A	138	GLY	N-CA	5.54	1.52	1.45
1	B	83	VAL	N-CA	-5.51	1.39	1.46
1	C	204	VAL	CA-C	5.45	1.59	1.52
1	A	257	VAL	CA-CB	5.43	1.60	1.54
1	C	153	SER	N-CA	5.37	1.52	1.45
1	B	196	ALA	CA-CB	5.36	1.61	1.54
1	B	225	ASP	N-CA	5.35	1.52	1.46
1	A	41	GLY	N-CA	5.35	1.52	1.45
1	A	46	ALA	CA-C	-5.34	1.46	1.52
1	B	114	PRO	CA-CB	5.30	1.60	1.53
1	B	255	ALA	CA-CB	-5.30	1.45	1.53
1	C	79	VAL	CA-C	-5.29	1.46	1.52
1	C	114	PRO	C-O	5.28	1.30	1.23
1	B	109	SER	C-O	-5.26	1.17	1.24
1	A	134	ALA	C-O	5.21	1.30	1.23
1	B	226	ALA	CA-CB	5.20	1.61	1.53
1	A	151	ILE	N-CA	5.17	1.52	1.46
1	A	76	ILE	C-O	5.17	1.30	1.24
1	A	43	GLY	CA-C	5.17	1.58	1.51
1	B	150	MET	CG-SD	5.14	1.93	1.80
1	C	104	ASP	C-O	-5.13	1.17	1.24
1	A	172	ILE	CA-CB	5.11	1.60	1.54
1	C	43	GLY	CA-C	5.09	1.58	1.51
1	A	228	MET	C-O	-5.03	1.18	1.24
1	C	254	ALA	CA-CB	5.03	1.61	1.53
1	B	224	ALA	CA-C	5.02	1.59	1.52
1	C	53	VAL	CA-C	5.00	1.58	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	MET	CG-SD-CE	-8.37	82.49	100.90
1	A	59	ALA	N-CA-C	6.61	118.56	111.36
1	B	109	SER	N-CA-C	5.81	118.43	109.07
1	A	24	GLY	N-CA-C	-5.79	107.33	115.32
1	A	257	VAL	N-CA-C	5.66	115.85	110.42
1	B	230	MET	N-CA-C	5.52	117.30	111.28
1	C	244	PHE	N-CA-C	5.33	117.17	111.36
1	C	135	THR	N-CA-C	-5.32	106.73	114.12
1	C	41	GLY	N-CA-C	-5.29	107.76	114.16
1	A	109	SER	N-CA-C	5.21	117.47	109.07
1	A	62	GLY	CA-C-O	-5.19	116.55	122.78
1	B	115	ALA	N-CA-C	-5.15	107.16	113.50
1	B	176	ILE	N-CA-C	-5.12	105.51	110.42
1	B	184	GLU	CA-CB-CG	-5.09	103.92	114.10
1	C	158	GLY	N-CA-C	5.01	125.05	113.18
1	C	154	LYS	N-CA-C	-5.00	105.93	112.23

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	1947	0	1972	15	0
1	B	1947	0	1972	28	0
1	C	1947	0	1972	24	0
2	A	6	0	8	0	0
2	B	6	0	8	1	0
2	C	6	0	8	0	0
3	A	138	0	0	2	0
3	B	153	0	0	5	0
3	C	154	0	0	3	0
All	All	6304	0	5940	63	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 (63) 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:C:246:SER:HB3	1:C:252:ARG:HH11	1.18	1.02
1:B:159:THR:HG23	1:B:161:ASP:H	1.24	1.01
1:A:53:VAL:HG11	1:A:241:SER:OG	1.66	0.96
1:A:159:THR:HG23	1:A:161:ASP:H	1.31	0.95
1:C:159:THR:HG23	1:C:161:ASP:H	1.32	0.92
1:C:246:SER:HB3	1:C:252:ARG:NH1	1.93	0.84
1:C:246:SER:CB	1:C:252:ARG:HH11	1.96	0.78
1:B:21:MET:HE1	3:B:474:HOH:O	1.88	0.74
1:B:99:GLN:HE22	1:B:127:THR:H	1.42	0.68
1:B:99:GLN:HE21	1:B:128:VAL:H	1.42	0.66
1:A:53:VAL:CG1	1:A:241:SER:OG	2.44	0.66
1:A:54:PRO:HD2	3:A:490:HOH:O	1.97	0.65
1:A:245:LYS:HG2	1:A:245:LYS:O	1.98	0.64
1:B:213:THR:HG23	3:B:452:HOH:O	1.97	0.62
1:C:157:ALA:HB2	3:C:542:HOH:O	2.01	0.61
1:C:91:HIS:CD2	1:C:94:GLU:H	2.21	0.59
1:B:91:HIS:CD2	1:B:94:GLU:H	2.21	0.58
1:B:52:ARG:NH2	1:B:60:GLN:HG2	2.19	0.58
1:A:242:GLY:HA2	1:A:245:LYS:HE2	1.84	0.57
1:B:73:GLU:CD	1:C:274:ARG:HH11	2.13	0.57
1:C:247:GLY:O	1:C:249:PRO:HD3	2.06	0.56
1:A:91:HIS:CD2	1:A:94:GLU:H	2.23	0.56
1:B:156:GLU:O	1:B:159:THR:HG22	2.07	0.55
1:B:53:VAL:O	1:B:57:ILE:HG13	2.07	0.53
1:B:175:GLU:HG3	3:B:540:HOH:O	2.09	0.52
1:B:100:THR:HG21	1:C:266:PRO:HB2	1.91	0.52
1:B:197:PRO:HG2	1:B:200:LEU:HD12	1.92	0.51
1:C:209:LYS:HE2	3:C:527:HOH:O	2.10	0.51
1:B:73:GLU:OE2	1:C:274:ARG:NH1	2.44	0.50
1:C:176:ILE:O	1:C:180:THR:HG23	2.10	0.50
1:C:243:ILE:HG22	1:C:244:PHE:CD2	2.47	0.49
1:C:91:HIS:HD2	1:C:94:GLU:H	1.58	0.48
1:C:245:LYS:O	1:C:245:LYS:HD3	2.13	0.48
1:B:23:LYS:HE2	1:B:213:THR:HG22	1.94	0.48
1:B:31:VAL:HG12	1:B:50:LEU:HD13	1.94	0.48
1:B:91:HIS:HD2	1:B:94:GLU:H	1.61	0.48
1:A:27:ILE:HG12	1:A:46:ALA:HB3	1.96	0.48
1:B:99:GLN:NE2	1:B:127:THR:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:HIS:HE1	1:B:225:ASP:OD1	1.97	0.47
1:C:69:PRO:HB3	1:C:101:LEU:HD11	1.96	0.46
1:A:239:VAL:HG21	1:A:256:ILE:HG21	1.98	0.46
1:B:192:LYS:HD3	3:B:543:HOH:O	2.16	0.46
1:C:31:VAL:HG23	1:C:32:THR:HG23	1.98	0.46
1:A:54:PRO:HG3	1:A:111:VAL:HG11	1.97	0.45
1:B:50:LEU:HD12	1:B:50:LEU:N	2.31	0.45
1:B:23:LYS:CE	1:B:213:THR:HG22	2.46	0.45
1:B:56:ASP:O	1:B:60:GLN:HB3	2.17	0.45
1:B:91:HIS:HE1	1:C:225:ASP:OD1	2.00	0.44
1:C:216:THR:HG21	1:C:229:MET:HG3	2.00	0.43
1:C:159:THR:HG23	1:C:161:ASP:N	2.16	0.43
1:C:11:THR:HG23	1:C:11:THR:O	2.19	0.42
1:B:209:LYS:HB3	1:B:209:LYS:HE3	1.44	0.41
1:C:54:PRO:HD2	3:C:537:HOH:O	2.19	0.41
1:C:156:GLU:O	1:C:159:THR:HG22	2.19	0.41
1:A:243:ILE:HD13	1:A:243:ILE:HG21	1.85	0.41
1:A:159:THR:CG2	1:A:161:ASP:H	2.16	0.41
1:B:50:LEU:HD12	1:B:50:LEU:H	1.86	0.41
1:B:99:GLN:HE22	1:B:127:THR:N	2.13	0.41
1:A:21:MET:HE1	3:A:471:HOH:O	2.20	0.41
1:B:243:ILE:HD13	1:B:243:ILE:HG21	1.72	0.41
1:C:239:VAL:HG12	1:C:240:GLY:N	2.35	0.41
2:B:301:GOL:H32	3:B:478:HOH:O	2.21	0.40
1:A:165:ALA:O	1:A:169:MET:HG2	2.22	0.40

There are no symmetry-related clashes.

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	262/264 (99%)	258 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	262/264 (99%)	257 (98%)	5 (2%)	0	100	100
1	C	262/264 (99%)	258 (98%)	3 (1%)	1 (0%)	30	19
All	All	786/792 (99%)	773 (98%)	12 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	248	ALA

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	197/197 (100%)	191 (97%)	6 (3%)	36	24
1	B	197/197 (100%)	191 (97%)	6 (3%)	36	24
1	C	197/197 (100%)	189 (96%)	8 (4%)	27	15
All	All	591/591 (100%)	571 (97%)	20 (3%)	32	20

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	50	LEU
1	A	53	VAL
1	A	243	ILE
1	A	245	LYS
1	A	273	SER
1	B	21	MET
1	B	34	GLU
1	B	50	LEU
1	B	60	GLN
1	B	209	LYS
1	B	243	ILE
1	C	50	LEU

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Mol	Chain	Res	Type
1	C	53	VAL
1	C	56	ASP
1	C	127	THR
1	C	243	ILE
1	C	245	LYS
1	C	252	ARG
1	C	271	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	119	HIS
1	B	91	HIS
1	B	99	GLN
1	B	119	HIS
1	C	91	HIS

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](#)

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	$\# Z > 2$
2	GOL	A	301	-	5,5,5	0.15	0	5,5,5	0.56	0
2	GOL	B	301	-	5,5,5	0.27	0	5,5,5	1.19	0
2	GOL	C	301	-	5,5,5	0.25	0	5,5,5	0.49	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	301	-	-	1/4/4/4	-
2	GOL	B	301	-	-	4/4/4/4	-
2	GOL	C	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	GOL	O1-C1-C2-C3
2	B	301	GOL	C1-C2-C3-O3
2	C	301	GOL	O1-C1-C2-C3
2	B	301	GOL	O1-C1-C2-O2
2	B	301	GOL	O2-C2-C3-O3
2	C	301	GOL	O1-C1-C2-O2
2	A	301	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	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, 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	264/264 (100%)	0.17	26 (9%)	13 11	12, 21, 50, 75	0
1	B	264/264 (100%)	-0.08	27 (10%)	12 10	10, 18, 51, 70	0
1	C	264/264 (100%)	0.01	26 (9%)	13 11	11, 18, 49, 77	0
All	All	792/792 (100%)	0.04	79 (9%)	12 11	10, 19, 53, 77	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	ALA	10.1
1	A	55	ALA	7.8
1	A	61	GLY	7.4
1	A	54	PRO	7.3
1	B	55	ALA	7.2
1	C	59	ALA	6.6
1	C	54	PRO	6.5
1	A	59	ALA	6.5
1	B	59	ALA	6.4
1	A	57	ILE	5.9
1	C	57	ILE	5.9
1	C	61	GLY	5.5
1	B	61	GLY	5.5
1	A	53	VAL	5.4
1	B	54	PRO	5.3
1	A	157	ALA	5.1
1	B	248	ALA	5.1
1	B	57	ILE	5.0
1	C	247	GLY	5.0
1	C	53	VAL	4.7
1	B	53	VAL	4.6
1	C	246	SER	4.6
1	C	245	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	56	ASP	4.4
1	B	245	LYS	4.3
1	A	58	ARG	4.3
1	B	117	TYR	4.3
1	B	247	GLY	4.2
1	A	248	ALA	4.1
1	B	11	THR	4.1
1	C	58	ARG	4.0
1	A	245	LYS	3.9
1	B	246	SER	3.8
1	A	56	ASP	3.6
1	C	248	ALA	3.5
1	A	21	MET	3.5
1	B	244	PHE	3.4
1	A	247	GLY	3.4
1	B	62	GLY	3.4
1	B	58	ARG	3.4
1	B	159	THR	3.4
1	A	243	ILE	3.3
1	B	243	ILE	3.3
1	C	60	GLN	3.3
1	C	157	ALA	3.3
1	A	246	SER	3.2
1	A	52	ARG	3.1
1	B	56	ASP	3.0
1	A	11	THR	3.0
1	C	243	ILE	2.9
1	A	62	GLY	2.9
1	C	52	ARG	2.8
1	C	158	GLY	2.8
1	C	241	SER	2.8
1	B	60	GLN	2.8
1	A	158	GLY	2.8
1	B	251	HIS	2.7
1	A	60	GLN	2.6
1	C	11	THR	2.6
1	B	52	ARG	2.6
1	C	159	THR	2.6
1	B	252	ARG	2.6
1	B	157	ALA	2.6
1	A	244	PHE	2.5
1	C	244	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	252	ARG	2.4
1	A	251	HIS	2.4
1	C	199	GLU	2.4
1	B	158	GLY	2.3
1	C	252	ARG	2.3
1	A	241	SER	2.2
1	B	21	MET	2.2
1	C	242	GLY	2.2
1	B	241	SER	2.2
1	C	251	HIS	2.1
1	A	159	THR	2.1
1	B	242	GLY	2.1
1	C	21	MET	2.1
1	A	274	ARG	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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
2	GOL	A	301	6/6	0.91	0.12	32,40,45,46	0
2	GOL	B	301	6/6	0.91	0.12	29,37,41,47	0
2	GOL	C	301	6/6	0.94	0.10	30,35,39,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.