



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:01 PM UTC

PDB ID : 5GN6 / pdb_00005gn6
Title : Crystal structure of glycerol kinase from Trypanosoma brucei gambiense complexed with cumarin derivative-17b
Authors : Balogun, E.O.; Inaoka, D.K.; Shiba, T.; Tsuge, T.; May, B.; Sato, T.; Kido, Y.; Takeshi, N.; Aoki, T.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Michels, P.A.M.; Watanabe, Y.; Moore, A.L.; Harada, S.; Kita, K.
Deposited on : 2016-07-19
Resolution : 2.50 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

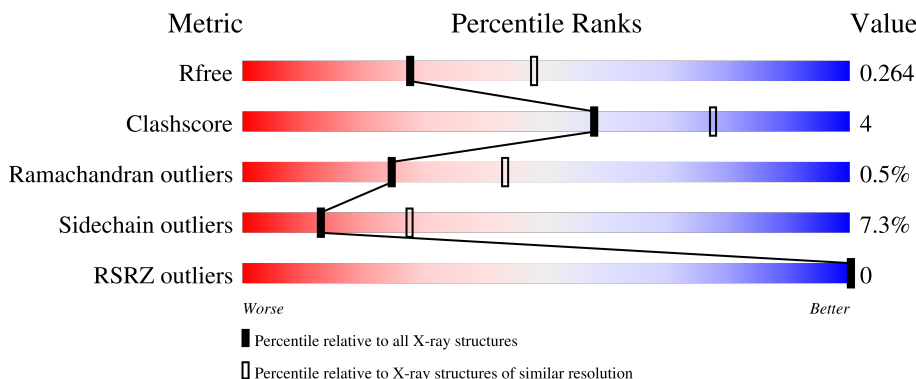
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	514	
1	B	514	
1	C	514	
1	D	514	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16091 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.

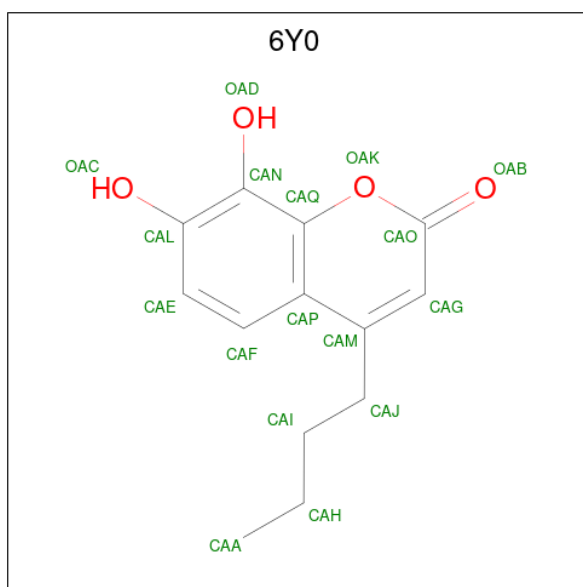
- Molecule 1 is a protein called Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3951	2493	694	731	33			
1	B	513	Total	C	N	O	S	0	1	0
			3959	2499	695	732	33			
1	C	513	Total	C	N	O	S	0	1	0
			3960	2498	695	734	33			
1	D	513	Total	C	N	O	S	0	1	0
			3960	2498	695	734	33			

There are 8 discrepancies between the modelled and reference sequences:

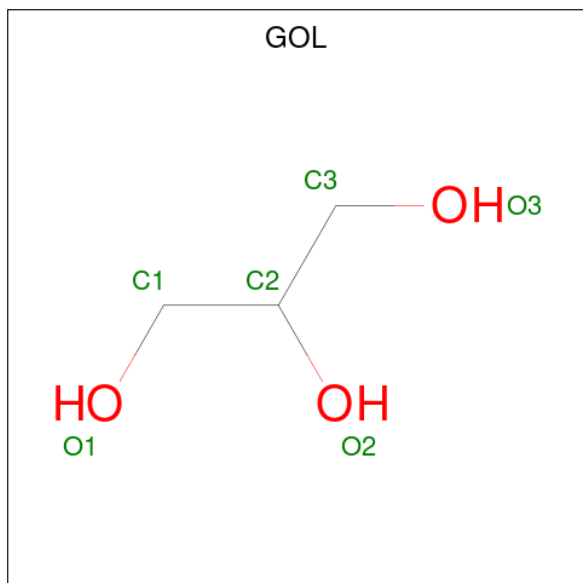
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
B	-1	ALA	-	expression tag	UNP D3KVM3
B	0	THR	-	expression tag	UNP D3KVM3
C	-1	ALA	-	expression tag	UNP D3KVM3
C	0	THR	-	expression tag	UNP D3KVM3
D	-1	ALA	-	expression tag	UNP D3KVM3
D	0	THR	-	expression tag	UNP D3KVM3

- Molecule 2 is 4-butyl-7,8-bis(oxidanyl)chromen-2-one (CCD ID: 6Y0) (formula: C₁₃H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	13	4		
2	B	1	Total	C	O	0	0
			17	13	4		
2	C	1	Total	C	O	0	0
			17	13	4		
2	D	1	Total	C	O	0	0
			17	13	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

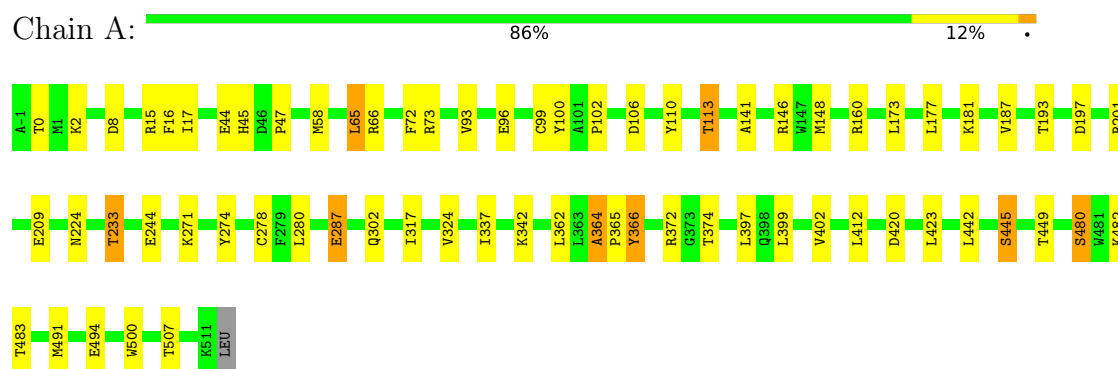
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	32	Total	O	0	0
			32	32		
4	C	44	Total	O	0	0
			44	44		
4	D	35	Total	O	0	0
			35	35		

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.

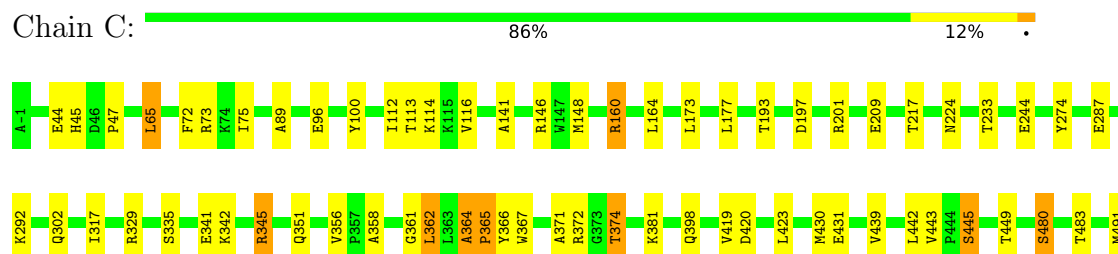
• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase

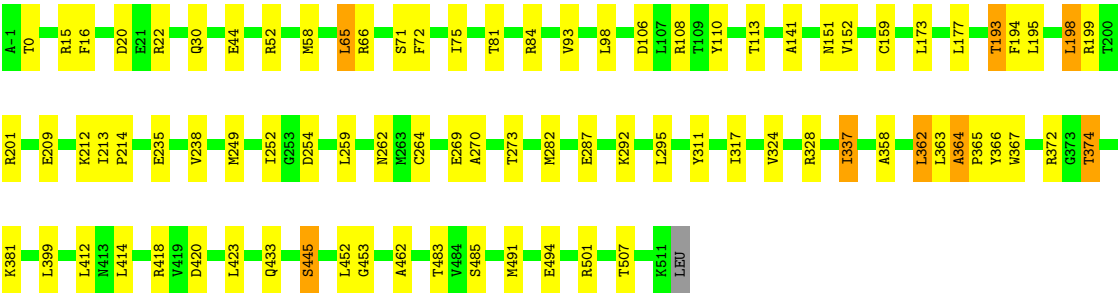
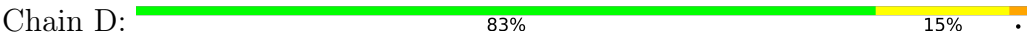


• Molecule 1: Glycerol kinase





• Molecule 1: Glycerol kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.42Å 122.04Å 154.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.50) 93.2 (20.00-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.195 , 0.260 0.202 , 0.264	Depositor DCC
R_{free} test set	3758 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 22.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16091	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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, 6Y0

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	0.99	0/4032	1.03	3/5456 (0.1%)
1	B	0.91	0/4040	1.03	2/5467 (0.0%)
1	C	0.99	0/4041	1.04	2/5468 (0.0%)
1	D	0.90	0/4041	1.03	3/5468 (0.1%)
All	All	0.95	0/16154	1.03	10/21859 (0.0%)

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	D	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	TYR	N-CA-C	-7.83	97.48	109.85
1	B	151	ASN	N-CA-C	6.18	120.53	112.92
1	D	151	ASN	N-CA-C	5.95	120.67	113.17
1	A	233	THR	N-CA-C	-5.88	100.41	109.52
1	A	181	LYS	N-CA-C	5.49	119.69	112.89
1	D	238	VAL	N-CA-C	5.38	115.59	110.53
1	B	74	LYS	N-CA-C	5.21	116.76	108.79
1	C	439	VAL	N-CA-C	-5.13	101.67	108.96
1	D	152	VAL	N-CA-C	5.04	113.14	108.15
1	C	356	VAL	CB-CA-C	-5.03	105.11	110.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	445	SER	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	3951	0	3966	30	0
1	B	3959	0	3976	46	0
1	C	3960	0	3971	28	0
1	D	3960	0	3971	39	0
2	A	17	0	0	0	0
2	B	17	0	0	0	0
2	C	17	0	0	0	0
2	D	17	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	2	0
4	A	58	0	0	0	0
4	B	32	0	0	1	0
4	C	44	0	0	1	0
4	D	35	0	0	0	0
All	All	16091	0	15916	142	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 4.

All (142) 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:399[B]:LEU:HD12	1:B:399[B]:LEU:O	1.74	0.88
1:B:324:VAL:HG21	1:B:423:LEU:HD21	1.69	0.74
1:D:110:TYR:O	1:D:113:THR:HG22	1.87	0.74
1:B:364:ALA:HB1	1:B:365:PRO:CD	2.22	0.70
1:D:399:LEU:HB2	1:D:433:GLN:HE22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ALA:HB3	1:A:193:THR:HA	1.76	0.67
1:D:358:ALA:HB2	1:D:362:LEU:HD13	1.77	0.67
1:D:44:GLU:HG3	1:D:108:ARG:HH22	1.65	0.62
1:D:317:ILE:HD11	1:D:399:LEU:HG	1.81	0.62
1:A:224:ASN:HD22	1:A:302:GLN:H	1.46	0.62
1:A:99:CYS:SG	1:A:148:MET:HE2	2.40	0.62
1:B:399[B]:LEU:HD12	1:B:399[B]:LEU:C	2.23	0.62
1:D:141:ALA:HB3	1:D:193:THR:HA	1.81	0.61
1:C:65:LEU:HD13	1:C:72:PHE:CG	2.34	0.61
1:B:358:ALA:HB2	1:B:362:LEU:HD13	1.82	0.61
1:A:274:TYR:HB3	1:A:423:LEU:HB2	1.82	0.60
1:B:44:GLU:HG3	1:B:108:ARG:HH22	1.66	0.60
1:D:364:ALA:HB1	1:D:365:PRO:CD	2.32	0.59
1:A:65:LEU:HD13	1:A:72:PHE:CG	2.37	0.59
1:C:224:ASN:HD22	1:C:302:GLN:H	1.50	0.59
1:D:374:THR:HG21	1:D:507:THR:HA	1.83	0.59
1:B:263:MET:HE3	1:B:475:SER:HB2	1.85	0.58
1:C:364:ALA:HB1	1:C:365:PRO:CD	2.33	0.58
1:B:141:ALA:HB3	1:B:193:THR:HA	1.86	0.58
1:B:399[B]:LEU:HD11	1:B:403:VAL:HG23	1.85	0.58
1:B:20:ASP:OD2	1:B:22:ARG:NH1	2.36	0.57
1:A:364:ALA:HB1	1:A:365:PRO:CD	2.34	0.57
1:C:372:ARG:O	1:C:374:THR:HG22	2.05	0.57
1:C:364:ALA:O	1:C:367:TRP:CZ3	2.58	0.57
1:B:399[B]:LEU:HD23	1:B:433:GLN:CD	2.30	0.56
1:A:364:ALA:HB1	1:A:365:PRO:HD3	1.86	0.56
1:B:89:ALA:CB	1:B:148:MET:HE2	2.36	0.55
1:D:65:LEU:HD13	1:D:72:PHE:CD1	2.41	0.55
1:A:374:THR:HG21	1:A:507:THR:HA	1.89	0.55
1:B:364:ALA:HB1	1:B:365:PRO:HD2	1.89	0.54
1:C:445:SER:OG	1:C:480:SER:O	2.24	0.54
1:A:110:TYR:O	1:A:113:THR:HG22	2.06	0.54
1:B:89:ALA:HB2	1:B:148:MET:HE2	1.91	0.53
1:B:374:THR:HG21	1:B:507:THR:HA	1.90	0.53
1:A:45:HIS:O	1:A:47:PRO:HD3	2.09	0.53
1:B:99:CYS:SG	1:B:148:MET:HE3	2.49	0.53
1:C:420:ASP:OD1	1:C:449:THR:OG1	2.26	0.53
1:A:8:ASP:OD1	1:A:15:ARG:NH1	2.41	0.53
1:C:89:ALA:HB2	1:C:148:MET:HE2	1.91	0.53
1:D:20:ASP:OD2	1:D:22:ARG:NH1	2.42	0.52
1:D:364:ALA:O	1:D:367:TRP:CH2	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:712:HOH:O	1:D:374:THR:HG22	2.09	0.52
1:D:194:PHE:O	1:D:195:LEU:HD23	2.10	0.52
1:D:254:ASP:OD2	3:D:602:GOL:O2	2.27	0.51
1:D:324:VAL:HG21	1:D:423:LEU:HD21	1.92	0.51
1:D:198:LEU:HD22	1:D:311:TYR:CE1	2.45	0.51
1:B:42:TRP:HA	1:B:106:ASP:OD1	2.11	0.51
1:C:44:GLU:HG2	1:C:100:TYR:HB3	1.92	0.51
1:C:358:ALA:HB2	1:C:362:LEU:HD13	1.92	0.51
1:D:270:ALA:HB3	1:D:414:LEU:HD11	1.92	0.51
1:A:102:PRO:HD3	1:A:148:MET:HE3	1.91	0.51
1:A:397:LEU:HD13	1:A:500:TRP:HB2	1.93	0.51
1:D:159:CYS:SG	1:D:214:PRO:HG2	2.51	0.51
1:D:364:ALA:HB1	1:D:365:PRO:HD3	1.93	0.51
1:C:141:ALA:HB3	1:C:193:THR:HA	1.92	0.50
1:D:84:ARG:HH21	3:D:602:GOL:H31	1.76	0.50
1:B:175:TYR:CE1	1:B:180:GLY:HA2	2.47	0.50
1:C:419:VAL:CG2	1:C:443:VAL:HG22	2.42	0.50
1:B:399[B]:LEU:CD1	1:B:403:VAL:HG23	2.41	0.50
1:B:171:THR:HG23	1:B:184:VAL:O	2.12	0.50
1:A:44:GLU:HG2	1:A:100:TYR:HB3	1.93	0.49
1:A:445:SER:OG	1:A:480:SER:O	2.30	0.49
1:B:364:ALA:CB	1:B:365:PRO:CD	2.90	0.49
1:A:271:LYS:O	1:A:280:LEU:HD12	2.12	0.49
1:B:419:VAL:HG21	1:B:430:MET:SD	2.52	0.49
1:B:106:ASP:OD2	1:B:108:ARG:NE	2.47	0.48
1:D:65:LEU:HD13	1:D:72:PHE:CG	2.49	0.48
1:D:328:ARG:HH12	1:D:337:ILE:HD13	1.76	0.48
1:C:89:ALA:CB	1:C:148:MET:HE2	2.43	0.48
1:D:249:MET:CE	1:D:462:ALA:HB2	2.44	0.48
1:B:198:LEU:HD22	1:B:311:TYR:CE1	2.49	0.48
1:D:249:MET:HE1	1:D:462:ALA:HB2	1.96	0.48
1:D:358:ALA:CB	1:D:362:LEU:HD13	2.43	0.47
1:C:361:GLY:HA2	1:C:371:ALA:O	2.14	0.47
1:D:15:ARG:HG2	1:D:30:GLN:HG3	1.96	0.47
1:C:364:ALA:HB1	1:C:365:PRO:HD3	1.97	0.47
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.75	0.47
1:C:345:ARG:NH1	1:C:431:GLU:OE2	2.47	0.47
1:D:273:THR:HG23	1:D:420:ASP:OD2	2.15	0.47
1:A:287:GLU:HG2	1:C:160:ARG:HG2	1.98	0.46
1:B:22:ARG:NH2	1:B:24:ARG:HG3	2.31	0.46
1:C:374:THR:HG21	1:C:507:THR:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:CYS:SG	1:B:214:PRO:HG2	2.55	0.46
1:B:249:MET:SD	1:B:462:ALA:HB2	2.55	0.46
1:A:374:THR:HG22	4:B:714:HOH:O	2.15	0.46
1:C:341:GLU:OE2	1:C:345:ARG:NH2	2.49	0.46
1:D:262:ASN:HB3	1:D:418:ARG:HG3	1.97	0.45
1:B:152:VAL:O	1:B:153:PRO:C	2.59	0.45
1:C:164:LEU:HB3	1:C:217:THR:HG22	1.99	0.45
1:A:364:ALA:CB	1:A:365:PRO:CD	2.94	0.45
1:B:341:GLU:OE2	1:B:345:ARG:NH2	2.49	0.45
1:C:45:HIS:O	1:C:47:PRO:HD3	2.17	0.44
1:B:152:VAL:HB	1:B:155:VAL:HG12	1.99	0.44
1:C:364:ALA:CB	1:C:365:PRO:CD	2.94	0.44
1:C:112:ILE:O	1:C:116:VAL:HG23	2.17	0.44
1:C:274:TYR:HB3	1:C:423:LEU:HB2	1.99	0.44
1:A:372:ARG:O	1:A:374:THR:HG23	2.17	0.43
1:B:82:ASN:ND2	1:B:83:GLN:O	2.51	0.43
1:B:273:THR:HG23	1:B:420:ASP:OD2	2.18	0.43
1:D:452:LEU:O	1:D:453:GLY:C	2.60	0.43
1:B:192:ARG:NH1	1:B:314:GLU:OE1	2.51	0.43
1:B:17:ILE:HD12	1:B:451:ALA:CB	2.48	0.43
1:D:372:ARG:O	1:D:374:THR:HG23	2.19	0.43
1:D:364:ALA:O	1:D:367:TRP:CZ3	2.72	0.43
1:B:110:TYR:O	1:B:113:THR:HG22	2.19	0.43
1:D:16:PHE:CD2	1:D:58:MET:HA	2.53	0.43
1:B:81:THR:HA	1:B:252:ILE:O	2.18	0.43
1:B:148:MET:C	1:B:155:VAL:HG11	2.44	0.43
1:B:263:MET:HE3	1:B:475:SER:CB	2.47	0.42
1:A:280:LEU:HD23	1:A:402:VAL:HG12	2.01	0.42
1:D:270:ALA:CB	1:D:414:LEU:HD11	2.49	0.42
1:B:262:ASN:HB3	1:B:418:ARG:HG3	2.02	0.42
1:C:274:TYR:CZ	1:C:430:MET:HE1	2.55	0.42
1:C:364:ALA:O	1:C:367:TRP:CH2	2.73	0.42
1:A:324:VAL:HG21	1:A:423:LEU:HD21	2.02	0.42
1:A:420:ASP:OD1	1:A:449:THR:OG1	2.34	0.42
1:B:96:GLU:HG3	1:B:97:PRO:HD2	2.01	0.42
1:A:274:TYR:HB3	1:A:423:LEU:CB	2.47	0.42
1:B:399[B]:LEU:HB3	1:B:433:GLN:HE22	1.84	0.42
1:B:399[B]:LEU:HD23	1:B:433:GLN:NE2	2.34	0.41
1:A:16:PHE:CD2	1:A:58:MET:HA	2.55	0.41
1:D:81:THR:HA	1:D:252:ILE:O	2.18	0.41
1:D:199:ARG:O	1:D:201:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ASP:O	1:C:201:ARG:N	2.52	0.41
1:D:259:LEU:HD12	1:D:264:CYS:HB2	2.01	0.41
1:B:280:LEU:C	1:B:281:LEU:HD12	2.45	0.41
1:B:452:LEU:O	1:B:453:GLY:C	2.63	0.41
1:A:0:THR:O	1:A:2:LYS:NZ	2.53	0.41
1:A:15:ARG:NH2	1:A:17:ILE:HD11	2.36	0.41
1:D:269:GLU:OE1	1:D:418:ARG:NH2	2.54	0.41
1:D:106:ASP:OD2	1:D:108:ARG:NH2	2.54	0.40
1:A:197:ASP:O	1:A:201:ARG:N	2.52	0.40
1:A:278:CYS:HB2	1:A:317:ILE:HB	2.02	0.40
1:B:328:ARG:HH12	1:B:337:ILE:HD13	1.86	0.40
1:C:317:ILE:HD13	1:C:398:GLN:HB2	2.03	0.40
1:D:282:MET:HE2	1:D:414:LEU:HD13	2.02	0.40
1:B:14:THR:C	1:B:15:ARG:HG3	2.47	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	511/514 (99%)	488 (96%)	22 (4%)	1 (0%)	43	63
1	B	512/514 (100%)	461 (90%)	47 (9%)	4 (1%)	16	31
1	C	512/514 (100%)	483 (94%)	27 (5%)	2 (0%)	30	49
1	D	512/514 (100%)	468 (91%)	41 (8%)	3 (1%)	21	38
All	All	2047/2056 (100%)	1900 (93%)	137 (7%)	10 (0%)	24	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA

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Mol	Chain	Res	Type
1	B	295	LEU
1	B	364	ALA
1	C	364	ALA
1	B	448	GLU
1	D	235	GLU
1	D	295	LEU
1	D	364	ALA
1	B	346	SER
1	C	365	PRO

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	420/421 (100%)	392 (93%)	28 (7%)	15	31
1	B	421/421 (100%)	388 (92%)	33 (8%)	11	24
1	C	421/421 (100%)	390 (93%)	31 (7%)	13	27
1	D	421/421 (100%)	390 (93%)	31 (7%)	13	27
All	All	1683/1684 (100%)	1560 (93%)	123 (7%)	13	27

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	66	ARG
1	A	73	ARG
1	A	93	VAL
1	A	96	GLU
1	A	106	ASP
1	A	113	THR
1	A	146	ARG
1	A	160	ARG
1	A	173	LEU
1	A	177	LEU
1	A	187	VAL

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Mol	Chain	Res	Type
1	A	209	GLU
1	A	233	THR
1	A	244	GLU
1	A	287	GLU
1	A	337	ILE
1	A	342	LYS
1	A	362	LEU
1	A	366	TYR
1	A	412	LEU
1	A	442	LEU
1	A	445	SER
1	A	480	SER
1	A	482	LYS
1	A	483	THR
1	A	491	MET
1	A	494	GLU
1	B	65	LEU
1	B	66	ARG
1	B	73	ARG
1	B	75	ILE
1	B	80	ILE
1	B	93	VAL
1	B	94	THR
1	B	98	LEU
1	B	113	THR
1	B	163	THR
1	B	173	LEU
1	B	177	LEU
1	B	187	VAL
1	B	198	LEU
1	B	213	ILE
1	B	243	ASN
1	B	328	ARG
1	B	335	SER
1	B	337	ILE
1	B	342	LYS
1	B	362	LEU
1	B	363	LEU
1	B	366	TYR
1	B	374	THR
1	B	412	LEU
1	B	439	VAL

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Mol	Chain	Res	Type
1	B	476	ARG
1	B	480	SER
1	B	483	THR
1	B	485	SER
1	B	489	SER
1	B	491	MET
1	B	511	LYS
1	C	65	LEU
1	C	73	ARG
1	C	75	ILE
1	C	96	GLU
1	C	113	THR
1	C	114	LYS
1	C	146	ARG
1	C	160	ARG
1	C	173	LEU
1	C	177	LEU
1	C	209	GLU
1	C	233	THR
1	C	244	GLU
1	C	287	GLU
1	C	292	LYS
1	C	329	ARG
1	C	335	SER
1	C	342	LYS
1	C	345	ARG
1	C	351	GLN
1	C	362	LEU
1	C	366	TYR
1	C	374	THR
1	C	381	LYS
1	C	442	LEU
1	C	445	SER
1	C	480	SER
1	C	483	THR
1	C	491	MET
1	C	494	GLU
1	C	511	LYS
1	D	0	THR
1	D	52	ARG
1	D	65	LEU
1	D	66	ARG

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Mol	Chain	Res	Type
1	D	71	SER
1	D	75	ILE
1	D	93	VAL
1	D	98	LEU
1	D	173	LEU
1	D	177	LEU
1	D	193	THR
1	D	198	LEU
1	D	209	GLU
1	D	212	LYS
1	D	213	ILE
1	D	287[A]	GLU
1	D	287[B]	GLU
1	D	292	LYS
1	D	337	ILE
1	D	362	LEU
1	D	363	LEU
1	D	366	TYR
1	D	374	THR
1	D	381	LYS
1	D	412	LEU
1	D	445	SER
1	D	483	THR
1	D	485	SER
1	D	491	MET
1	D	494	GLU
1	D	501	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	36	HIS
1	A	224	ASN
1	A	243	ASN
1	A	336	HIS
1	A	400	ASN
1	B	224	ASN
1	B	272	ASN
1	B	336	HIS
1	B	413	ASN
1	C	23	GLN

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Mol	Chain	Res	Type
1	C	224	ASN
1	C	243	ASN
1	C	336	HIS
1	C	351	GLN
1	C	400	ASN
1	D	23	GLN
1	D	29	HIS
1	D	224	ASN
1	D	243	ASN
1	D	262	ASN
1	D	336	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](#)

8 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	GOL	A	602	-	5,5,5	0.51	0	5,5,5	0.63	0
3	GOL	B	602	-	5,5,5	0.57	0	5,5,5	0.46	0
2	6Y0	A	601	-	18,18,18	1.63	2 (11%)	25,25,25	1.94	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	602	-	5,5,5	0.46	0	5,5,5	0.80	0
3	GOL	C	602	-	5,5,5	0.59	0	5,5,5	1.13	0
2	6Y0	C	601	-	18,18,18	1.70	3 (16%)	25,25,25	1.95	7 (28%)
2	6Y0	D	601	-	18,18,18	1.58	3 (16%)	25,25,25	1.85	6 (24%)
2	6Y0	B	601	-	18,18,18	1.55	4 (22%)	25,25,25	2.05	6 (24%)

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	602	-	-	1/4/4/4	-
3	GOL	B	602	-	-	0/4/4/4	-
2	6Y0	A	601	-	-	0/4/4/4	0/2/2/2
3	GOL	D	602	-	-	0/4/4/4	-
3	GOL	C	602	-	-	1/4/4/4	-
2	6Y0	C	601	-	-	0/4/4/4	0/2/2/2
2	6Y0	D	601	-	-	2/4/4/4	0/2/2/2
2	6Y0	B	601	-	-	2/4/4/4	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	6Y0	CAJ-CAM	-4.61	1.42	1.50
2	D	601	6Y0	CAJ-CAM	-4.42	1.43	1.50
2	A	601	6Y0	CAJ-CAM	-4.28	1.43	1.50
2	B	601	6Y0	CAJ-CAM	-3.98	1.43	1.50
2	A	601	6Y0	CAG-CAM	3.25	1.41	1.35
2	C	601	6Y0	CAG-CAM	3.17	1.41	1.35
2	B	601	6Y0	CAG-CAM	2.80	1.40	1.35
2	D	601	6Y0	CAG-CAM	2.75	1.40	1.35
2	D	601	6Y0	CAP-CAM	-2.32	1.41	1.46
2	B	601	6Y0	CAP-CAM	-2.13	1.42	1.46
2	B	601	6Y0	CAG-CAO	-2.08	1.40	1.44
2	C	601	6Y0	CAP-CAM	-2.06	1.42	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	6Y0	CAJ-CAM-CAP	5.44	124.69	118.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	6Y0	CAJ-CAM-CAP	5.28	124.52	118.68
2	A	601	6Y0	CAJ-CAM-CAP	5.07	124.28	118.68
2	D	601	6Y0	CAJ-CAM-CAP	4.96	124.16	118.68
2	B	601	6Y0	OAK-CAO-OAB	4.47	122.21	116.40
2	A	601	6Y0	OAB-CAO-CAG	-3.87	118.14	125.92
2	A	601	6Y0	CAQ-OAK-CAO	-3.86	118.78	121.97
2	B	601	6Y0	OAB-CAO-CAG	-3.82	118.23	125.92
2	D	601	6Y0	OAK-CAO-OAB	3.45	120.88	116.40
2	D	601	6Y0	CAL-CAN-CAQ	3.39	123.09	118.50
2	A	601	6Y0	OAK-CAO-OAB	3.35	120.75	116.40
2	C	601	6Y0	OAB-CAO-CAG	-3.15	119.58	125.92
2	A	601	6Y0	OAK-CAO-CAG	3.15	120.99	117.16
2	B	601	6Y0	CAE-CAL-CAN	-3.08	116.89	120.09
2	C	601	6Y0	OAK-CAO-CAG	2.82	120.58	117.16
2	B	601	6Y0	CAL-CAN-CAQ	2.80	122.30	118.50
2	C	601	6Y0	CAQ-OAK-CAO	-2.60	119.83	121.97
2	C	601	6Y0	CAE-CAL-CAN	-2.58	117.41	120.09
2	D	601	6Y0	OAB-CAO-CAG	-2.57	120.75	125.92
2	C	601	6Y0	OAK-CAO-OAB	2.57	119.74	116.40
2	D	601	6Y0	CAE-CAL-CAN	-2.49	117.50	120.09
2	C	601	6Y0	CAF-CAE-CAL	2.17	122.67	120.50
2	B	601	6Y0	CAQ-OAK-CAO	-2.11	120.23	121.97
2	D	601	6Y0	CAQ-OAK-CAO	-2.03	120.29	121.97

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	6Y0	CAI-CAJ-CAM-CAP
3	A	602	GOL	O1-C1-C2-C3
2	D	601	6Y0	CAH-CAI-CAJ-CAM
2	B	601	6Y0	CAI-CAJ-CAM-CAP
3	C	602	GOL	O1-C1-C2-C3
2	B	601	6Y0	CAH-CAI-CAJ-CAM

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	GOL	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	513/514 (99%)	-1.56	0 100 100	16, 33, 53, 75	1 (0%)
1	B	513/514 (99%)	-1.42	0 100 100	18, 48, 74, 110	2 (0%)
1	C	513/514 (99%)	-1.56	0 100 100	15, 33, 54, 79	2 (0%)
1	D	513/514 (99%)	-1.44	0 100 100	20, 47, 73, 98	2 (0%)
All	All	2052/2056 (99%)	-1.50	0 100 100	15, 39, 69, 110	7 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	6Y0	D	601	17/17	0.98	0.04	68,80,86,87	0
2	6Y0	B	601	17/17	0.99	0.04	55,81,88,91	0
2	6Y0	C	601	17/17	0.99	0.03	37,42,47,47	0
2	6Y0	A	601	17/17	0.99	0.03	38,44,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	602	6/6	0.99	0.03	41,47,48,51	0
3	GOL	B	602	6/6	0.99	0.04	22,24,26,28	0
3	GOL	C	602	6/6	0.99	0.04	40,43,48,57	0
3	GOL	D	602	6/6	0.99	0.04	24,28,33,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.