Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 05:28 PM JST

PDB ID	:	5GN6
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 (i) 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 (i)) were used in the production of this report:

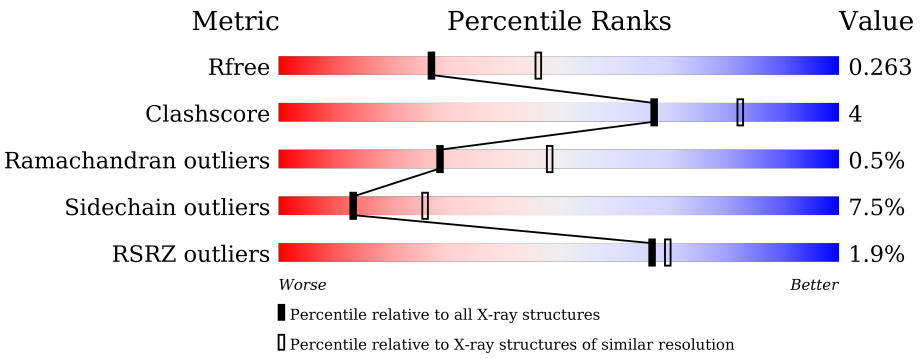
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	87% 11% •
1	B	514	5% 83% 15% •
1	C	514	87% 11% •
1	D	514	3% 84% 13% •

2 Entry composition (i)

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.

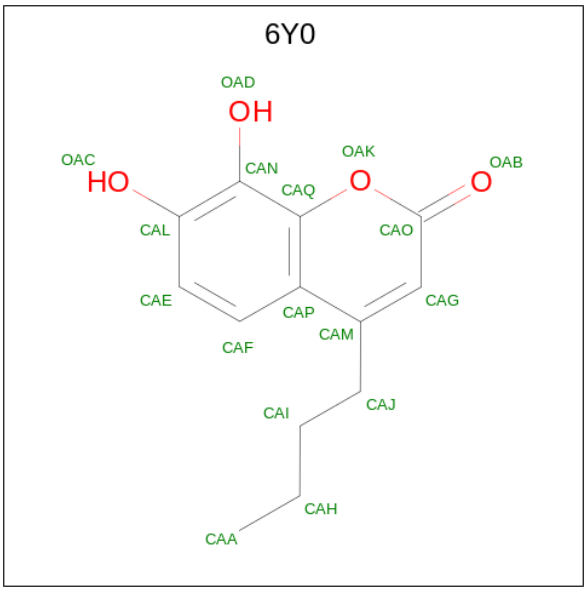
- Molecule 1 is a protein called Glycerol kinase.

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

There are 8 discrepancies between the modelled and reference sequences:

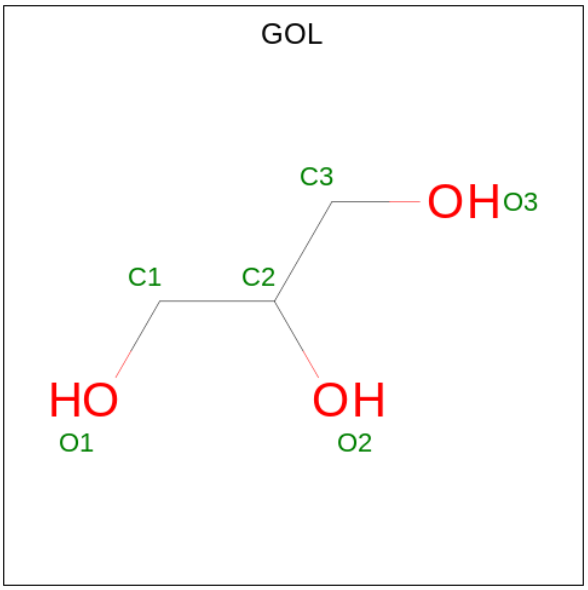
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
B	-1	ALA	-	expression tag	UNP D3KVM3
B	0	THR	-	expression tag	UNP D3KVM3
C	-1	ALA	-	expression tag	UNP D3KVM3
C	0	THR	-	expression tag	UNP D3KVM3
D	-1	ALA	-	expression tag	UNP D3KVM3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

- Molecule 2 is 4-butyl-7,8-bis(oxidanyl)chromen-2-one (three-letter code: 6Y0) (formula: $C_{13}H_{14}O_4$).



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

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



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

- Molecule 4 is water.

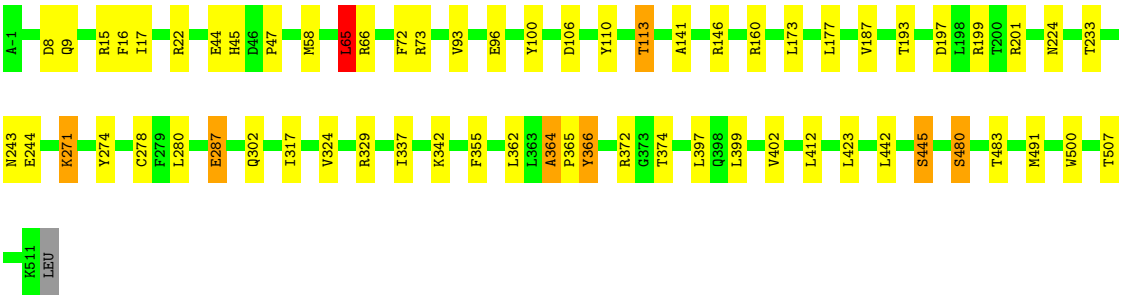
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	58	58	58	0	0
4	B	32	32	32	0	0
4	C	44	44	44	0	0
4	D	35	35	35	0	0

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.

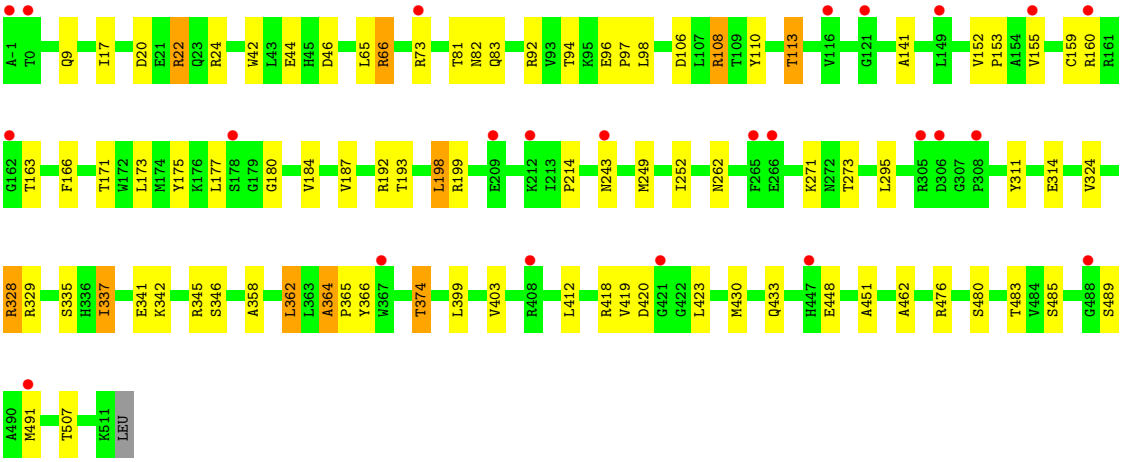
- Molecule 1: Glycerol kinase

Chain A:



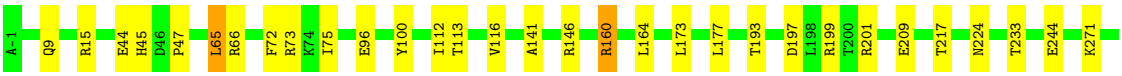
- Molecule 1: Glycerol kinase

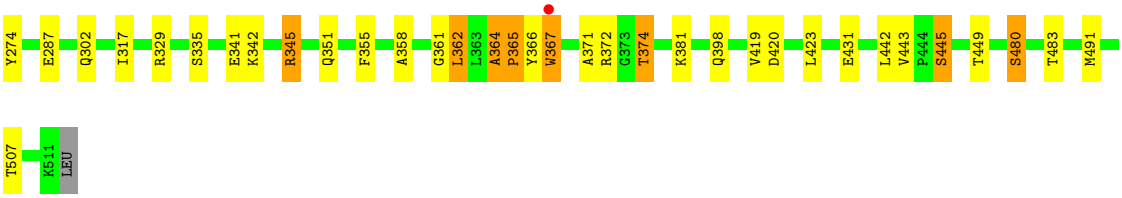
Chain B:



- Molecule 1: Glycerol kinase

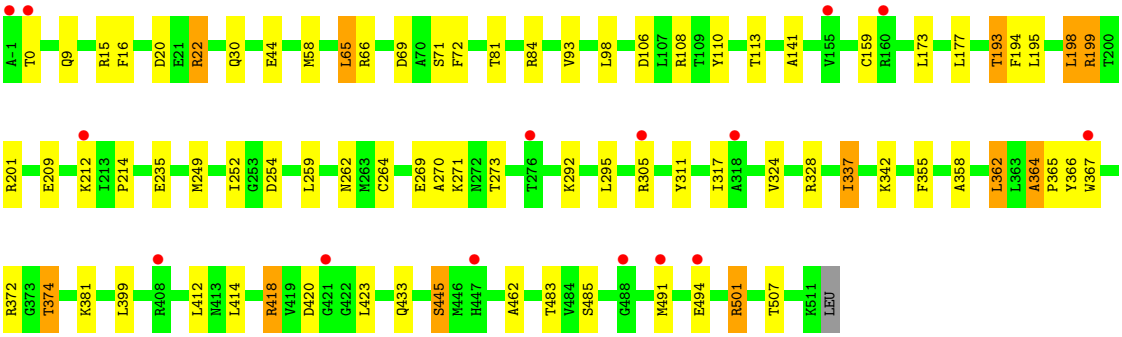
Chain C:





- Molecule 1: Glycerol kinase

Chain D:



4 Data and refinement statistics (i)

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 19.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.0 (20.00-2.50) 93.2 (19.88-2.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.195 , 0.260 0.202 , 0.263	Depositor DCC
R_{free} test set	3758 reflections (5.04%)	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)	0.35 , 21.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	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.*

[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 (i)

5.1 Standard geometry (i)

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	0.69	0/4032	0.87	4/5456 (0.1%)
1	B	0.65	0/4040	0.86	6/5467 (0.1%)
1	C	0.71	0/4041	0.86	1/5468 (0.0%)
1	D	0.65	0/4041	0.87	4/5468 (0.1%)
All	All	0.68	0/16154	0.87	15/21859 (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	D	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	501	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	B	92	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	A	329	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	22	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	D	22	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	46	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	108	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	22	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	D	418	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	15	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	65	LEU	CB-CG-CD2	5.18	119.81	111.00
1	D	69	ASP	CB-CG-OD1	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	46	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	66	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	366	TYR	N-CA-C	-5.01	97.48	111.00

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 (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	3951	0	3966	26	0
1	B	3959	0	3976	37	0
1	C	3960	0	3971	25	0
1	D	3960	0	3971	36	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	123	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 (123) 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
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: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: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:B:399[B]:LEU:HD12	1:B:399[B]:LEU:C	2.23	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:A:364:ALA:HB1	1:A:365:PRO:HD3	1.86	0.56
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: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: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: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
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:B:399[B]:LEU:HD23	1:B:433:GLN:CD	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:399[B]:LEU:HD23	1:B:433:GLN:NE2	2.34	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: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: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
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:152:VAL:O	1:B:153:PRO:C	2.59	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

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%)	47	68
1	B	512/514 (100%)	461 (90%)	47 (9%)	4 (1%)	19	35
1	C	512/514 (100%)	483 (94%)	27 (5%)	2 (0%)	34	54
1	D	512/514 (100%)	468 (91%)	41 (8%)	3 (1%)	25	43
All	All	2047/2056 (100%)	1900 (93%)	137 (7%)	10 (0%)	29	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
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 (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	420/421 (100%)	390 (93%)	30 (7%)	14	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	421/421 (100%)	389 (92%)	32 (8%)	13	25
1	C	421/421 (100%)	388 (92%)	33 (8%)	12	24
1	D	421/421 (100%)	390 (93%)	31 (7%)	13	27
All	All	1683/1684 (100%)	1557 (92%)	126 (8%)	13	26

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
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
1	A	199	ARG
1	A	233	THR
1	A	243	ASN
1	A	244	GLU
1	A	271	LYS
1	A	287	GLU
1	A	337	ILE
1	A	342	LYS
1	A	355	PHE
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	483	THR
1	A	491	MET
1	B	9	GLN
1	B	65	LEU
1	B	66	ARG

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Mol	Chain	Res	Type
1	B	73	ARG
1	B	94	THR
1	B	98	LEU
1	B	113	THR
1	B	160	ARG
1	B	163	THR
1	B	166	PHE
1	B	173	LEU
1	B	177	LEU
1	B	187	VAL
1	B	198	LEU
1	B	199	ARG
1	B	243	ASN
1	B	271	LYS
1	B	328	ARG
1	B	329	ARG
1	B	335	SER
1	B	337	ILE
1	B	342	LYS
1	B	362	LEU
1	B	366	TYR
1	B	374	THR
1	B	412	LEU
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	C	9	GLN
1	C	65	LEU
1	C	66	ARG
1	C	73	ARG
1	C	75	ILE
1	C	96	GLU
1	C	113	THR
1	C	146	ARG
1	C	160	ARG
1	C	173	LEU
1	C	177	LEU
1	C	199	ARG
1	C	209	GLU

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Mol	Chain	Res	Type
1	C	233	THR
1	C	244	GLU
1	C	271	LYS
1	C	287	GLU
1	C	329	ARG
1	C	335	SER
1	C	342	LYS
1	C	345	ARG
1	C	351	GLN
1	C	355	PHE
1	C	362	LEU
1	C	366	TYR
1	C	367	TRP
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	D	0	THR
1	D	9	GLN
1	D	65	LEU
1	D	66	ARG
1	D	71	SER
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	199	ARG
1	D	209	GLU
1	D	212	LYS
1	D	271	LYS
1	D	292	LYS
1	D	305	ARG
1	D	337	ILE
1	D	342	LYS
1	D	355	PHE
1	D	362	LEU
1	D	366	TYR

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Mol	Chain	Res	Type
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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	224	ASN
1	A	243	ASN
1	A	272	ASN
1	B	23	GLN
1	B	29	HIS
1	B	224	ASN
1	B	272	ASN
1	B	302	GLN
1	B	336	HIS
1	C	23	GLN
1	C	29	HIS
1	C	224	ASN
1	C	243	ASN
1	C	272	ASN
1	C	302	GLN
1	C	336	HIS
1	C	351	GLN
1	D	23	GLN
1	D	29	HIS
1	D	224	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 monosaccharides 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	B	602	-	5,5,5	0.57	0	5,5,5	0.43	0
3	GOL	D	602	-	5,5,5	0.44	0	5,5,5	0.75	0
2	6Y0	D	601	-	18,18,18	1.55	3 (16%)	25,25,25	1.92	5 (20%)
2	6Y0	A	601	-	18,18,18	1.60	2 (11%)	25,25,25	1.91	5 (20%)
2	6Y0	C	601	-	18,18,18	1.67	3 (16%)	25,25,25	1.93	7 (28%)
3	GOL	C	602	-	5,5,5	0.56	0	5,5,5	1.08	0
2	6Y0	B	601	-	18,18,18	1.51	4 (22%)	25,25,25	2.09	6 (24%)
3	GOL	A	602	-	5,5,5	0.49	0	5,5,5	0.61	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	B	602	-	-	0/4/4/4	-
3	GOL	D	602	-	-	0/4/4/4	-
2	6Y0	D	601	-	-	2/4/4/4	0/2/2/2
2	6Y0	A	601	-	-	0/4/4/4	0/2/2/2
2	6Y0	C	601	-	-	0/4/4/4	0/2/2/2
3	GOL	C	602	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6Y0	B	601	-	-	2/4/4/4	0/2/2/2
3	GOL	A	602	-	-	1/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	6Y0	CAJ-CAM	-4.62	1.42	1.50
2	D	601	6Y0	CAJ-CAM	-4.43	1.43	1.50
2	A	601	6Y0	CAJ-CAM	-4.29	1.43	1.50
2	B	601	6Y0	CAJ-CAM	-3.99	1.43	1.50
2	A	601	6Y0	CAG-CAM	3.06	1.41	1.35
2	C	601	6Y0	CAG-CAM	2.99	1.41	1.35
2	B	601	6Y0	CAG-CAM	2.63	1.40	1.35
2	D	601	6Y0	CAG-CAM	2.58	1.40	1.35
2	D	601	6Y0	CAP-CAM	-2.25	1.41	1.46
2	B	601	6Y0	CAG-CAO	-2.13	1.40	1.44
2	B	601	6Y0	CAP-CAM	-2.07	1.42	1.46
2	C	601	6Y0	CAP-CAM	-2.00	1.42	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	6Y0	CAJ-CAM-CAP	5.23	124.69	118.62
2	C	601	6Y0	CAJ-CAM-CAP	5.08	124.52	118.62
2	A	601	6Y0	CAJ-CAM-CAP	4.88	124.28	118.62
2	D	601	6Y0	CAJ-CAM-CAP	4.77	124.16	118.62
2	D	601	6Y0	CAL-CAN-CAQ	4.68	123.09	118.43
2	B	601	6Y0	OAK-CAO-OAB	4.52	122.21	116.44
2	B	601	6Y0	CAL-CAN-CAQ	3.89	122.30	118.43
2	A	601	6Y0	OAB-CAO-CAG	-3.77	118.14	125.84
2	A	601	6Y0	CAQ-OAK-CAO	-3.76	118.78	121.99
2	B	601	6Y0	OAB-CAO-CAG	-3.72	118.23	125.84
2	D	601	6Y0	OAK-CAO-OAB	3.48	120.88	116.44
2	A	601	6Y0	OAK-CAO-OAB	3.38	120.75	116.44
2	B	601	6Y0	CAE-CAL-CAN	-3.09	116.89	120.06
2	C	601	6Y0	OAB-CAO-CAG	-3.07	119.58	125.84
2	A	601	6Y0	OAK-CAO-CAG	2.97	120.99	117.17
2	C	601	6Y0	OAK-CAO-CAG	2.65	120.58	117.17
2	C	601	6Y0	OAK-CAO-OAB	2.59	119.74	116.44
2	C	601	6Y0	CAE-CAL-CAN	-2.58	117.41	120.06
2	C	601	6Y0	CAQ-OAK-CAO	-2.53	119.83	121.99
2	D	601	6Y0	OAB-CAO-CAG	-2.49	120.75	125.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	6Y0	CAE-CAL-CAN	-2.49	117.50	120.06
2	C	601	6Y0	CAF-CAE-CAL	2.10	122.67	120.50
2	B	601	6Y0	CAQ-OAK-CAO	-2.06	120.23	121.99

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%)	-0.24	0	100	100	16, 33, 53, 75	1 (0%)
1	B	513/514 (99%)	0.20	24 (4%)	31	33	19, 48, 74, 110	1 (0%)
1	C	513/514 (99%)	-0.23	1 (0%)	95	95	15, 33, 54, 79	1 (0%)
1	D	513/514 (99%)	0.12	15 (2%)	51	55	20, 47, 73, 98	1 (0%)
All	All	2052/2056 (99%)	-0.04	40 (1%)	66	69	15, 39, 69, 110	4 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	367	TRP	4.6
1	B	447	HIS	4.3
1	D	447	HIS	4.0
1	B	488	GLY	3.8
1	B	306	ASP	3.6
1	B	0	THR	3.5
1	B	155	VAL	3.4
1	D	-1	ALA	3.4
1	B	-1	ALA	3.4
1	B	149	LEU	3.3
1	D	491	MET	3.3
1	C	367	TRP	3.0
1	D	0	THR	3.0
1	D	318	ALA	2.8
1	B	178	SER	2.8
1	B	160	ARG	2.7
1	D	488	GLY	2.7
1	B	491	MET	2.6
1	D	421	GLY	2.6
1	B	367	TRP	2.5
1	B	162	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	305	ARG	2.4
1	D	494	GLU	2.4
1	B	212	LYS	2.4
1	B	116	VAL	2.3
1	B	243	ASN	2.3
1	D	305	ARG	2.3
1	D	160	ARG	2.3
1	B	121	GLY	2.3
1	D	155	VAL	2.2
1	B	408	ARG	2.2
1	B	265	PHE	2.2
1	B	266	GLU	2.1
1	B	209	GLU	2.1
1	B	421	GLY	2.1
1	B	308	PRO	2.1
1	D	212	LYS	2.1
1	B	73	ARG	2.0
1	D	408	ARG	2.0
1	D	276	THR	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, 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	B	601	17/17	0.78	0.31	55,81,88,91	0
2	6Y0	D	601	17/17	0.85	0.26	68,80,86,87	0
3	GOL	C	602	6/6	0.85	0.23	40,43,48,57	0
2	6Y0	A	601	17/17	0.90	0.17	38,44,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6Y0	C	601	17/17	0.90	0.17	37,42,47,47	0
3	GOL	A	602	6/6	0.94	0.13	41,47,48,51	0
3	GOL	B	602	6/6	0.96	0.13	22,24,26,28	0
3	GOL	D	602	6/6	0.96	0.13	24,28,33,41	0

6.5 Other polymers (i)

There are no such residues in this entry.