



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:54 am BST

PDB ID : 6J9X
Title : Crystal structure of Trypanosoma brucei gambiense glycerol kinase phosphorylated at Thr12(pyrophosphatase reaction)
Authors : Balogun, E.O.; Chishima, T.; Ichinose, M.; Inaoka, D.K.; Kido, Y.; Ibrahim, B.; Bringaud, F.; de Koning, H.; McKerrow, J.H.; Watanabe, Y.; Nozaki, T.; Michels, P.A.M.; Harada, S.; Kita, K.; Shiba, T.
Deposited on : 2019-01-24
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

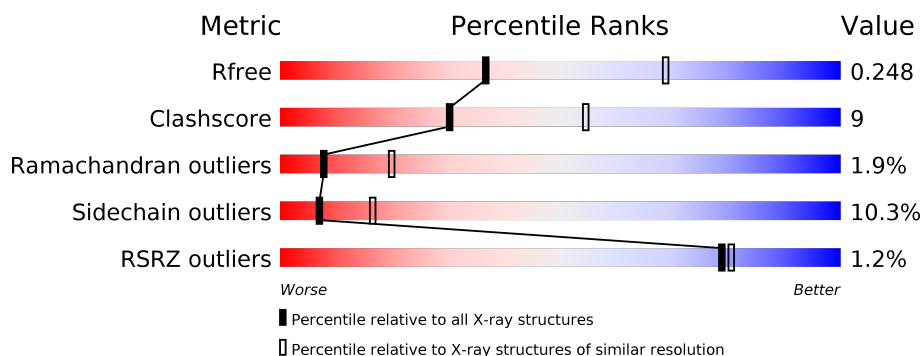
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	518	<div> <div>3%</div> <div>67%</div> <div>27%</div> <div>..</div> </div>
1	C	518	<div> <div>%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>
2	B	518	<div> <div>77%</div> <div>20%</div> <div>..</div> </div>
2	D	518	<div> <div>%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15910 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	P	S	0	0	0
			3961	2499	694	734	1	33			
1	C	513	Total	C	N	O	P	S	0	0	0
			3961	2499	694	734	1	33			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP D3KVM3
A	-4	ILE	-	expression tag	UNP D3KVM3
A	-3	ASP	-	expression tag	UNP D3KVM3
A	-2	PRO	-	expression tag	UNP D3KVM3
A	-1	PHE	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
C	-5	GLY	-	expression tag	UNP D3KVM3
C	-4	ILE	-	expression tag	UNP D3KVM3
C	-3	ASP	-	expression tag	UNP D3KVM3
C	-2	PRO	-	expression tag	UNP D3KVM3
C	-1	PHE	-	expression tag	UNP D3KVM3
C	0	THR	-	expression tag	UNP D3KVM3

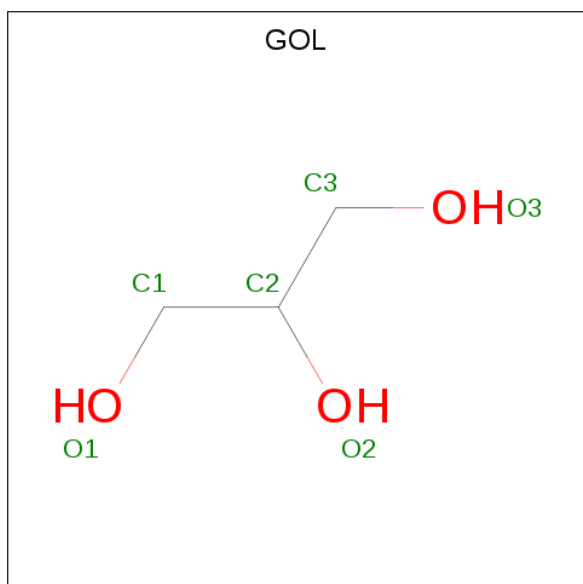
- Molecule 2 is a protein called Glycerol kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	513	Total	C	N	O	S		0	0	0
			3957	2499	694	731	33				
2	D	513	Total	C	N	O	S		0	0	0
			3957	2499	694	731	33				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP D3KVM3
B	-4	ILE	-	expression tag	UNP D3KVM3
B	-3	ASP	-	expression tag	UNP D3KVM3
B	-2	PRO	-	expression tag	UNP D3KVM3
B	-1	PHE	-	expression tag	UNP D3KVM3
B	0	THR	-	expression tag	UNP D3KVM3
D	-5	GLY	-	expression tag	UNP D3KVM3
D	-4	ILE	-	expression tag	UNP D3KVM3
D	-3	ASP	-	expression tag	UNP D3KVM3
D	-2	PRO	-	expression tag	UNP D3KVM3
D	-1	PHE	-	expression tag	UNP D3KVM3
D	0	THR	-	expression tag	UNP D3KVM3

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



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

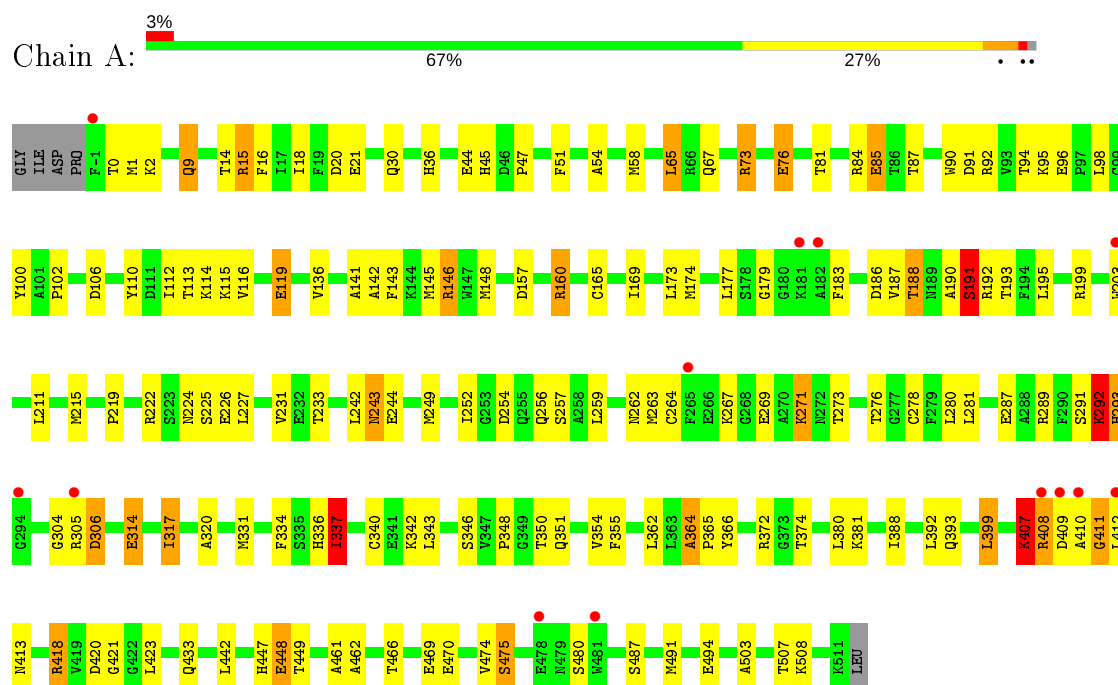
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	11	Total 11	O 11	0	0
4	C	12	Total 12	O 12	0	0
4	D	17	Total 17	O 17	0	0

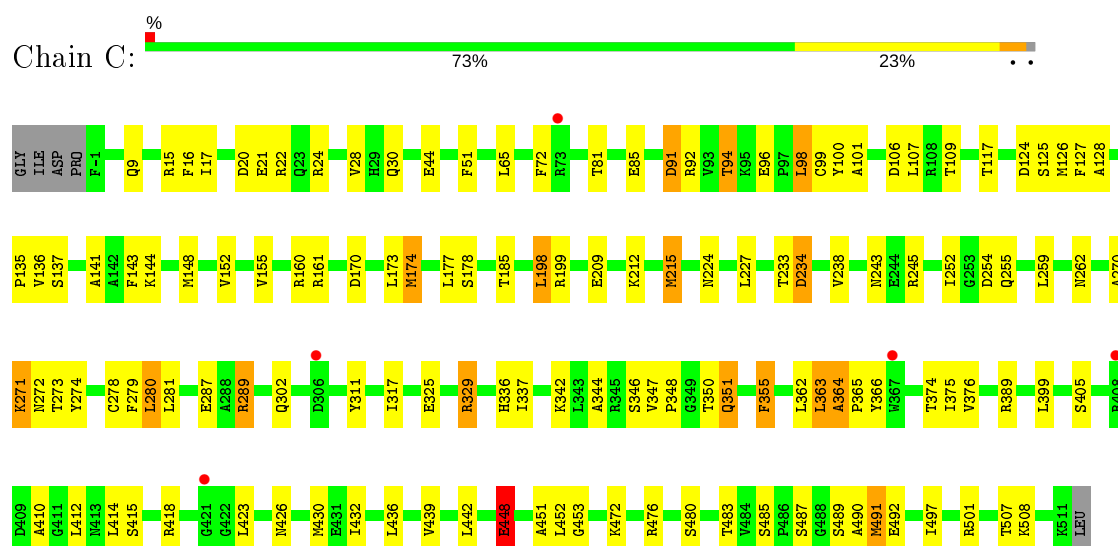
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

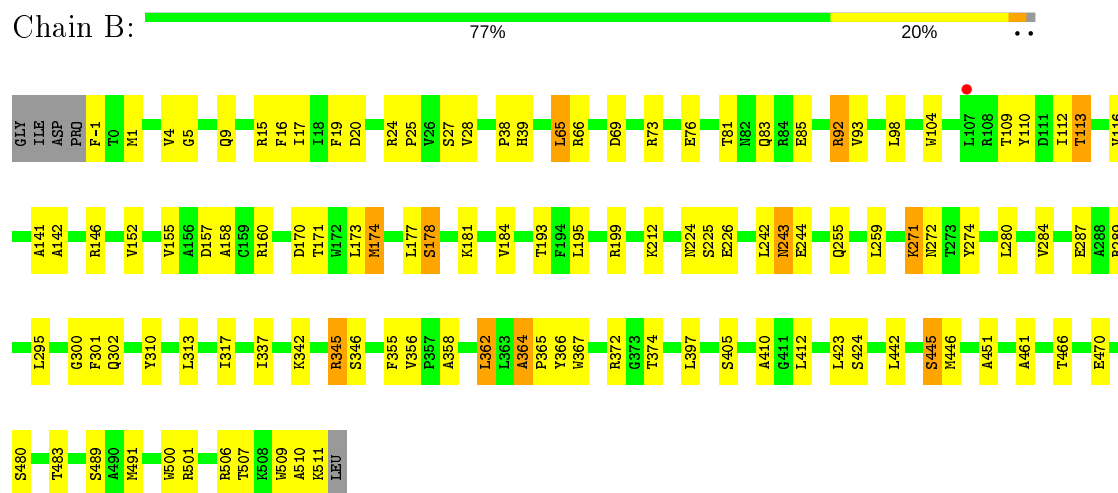
• Molecule 1: Glycerol kinase



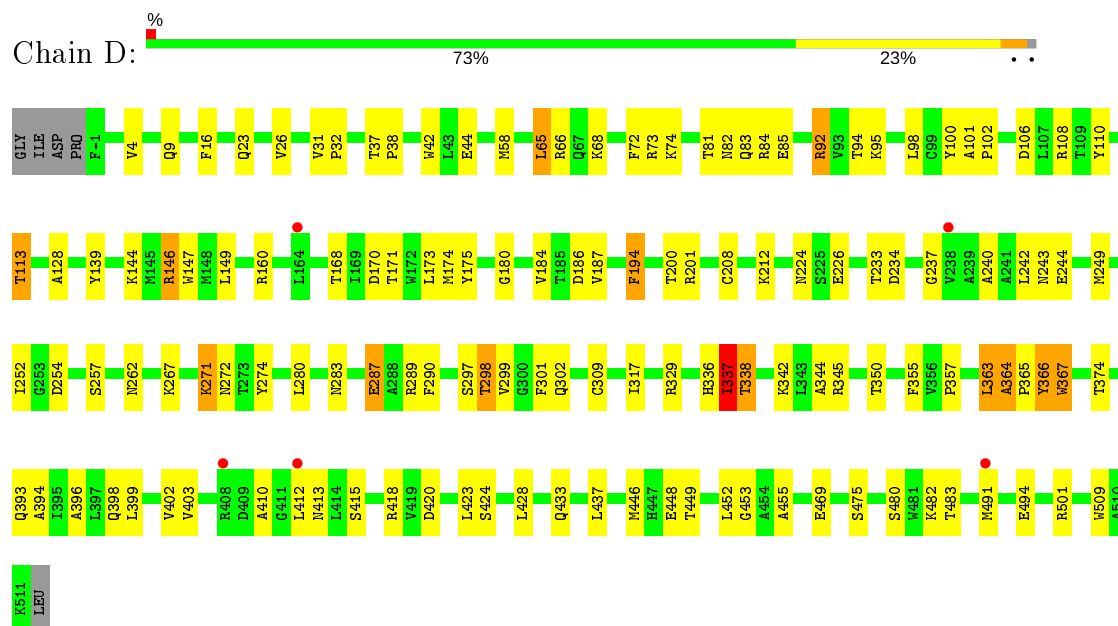
• Molecule 1: Glycerol kinase



- Molecule 2: Glycerol kinase



- Molecule 2: 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	62.38Å 119.34Å 154.73Å 90.00° 90.82° 90.00°	Depositor
Resolution (Å)	19.89 – 2.70 19.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.89-2.70) 99.4 (19.89-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.247 0.185 , 0.248	Depositor DCC
R_{free} test set	3151 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	88.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.129 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15910	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/4031	0.80	1/5452 (0.0%)
1	C	0.55	0/4031	0.79	0/5452
2	B	0.58	0/4039	0.81	0/5465
2	D	0.56	0/4039	0.78	0/5465
All	All	0.56	0/16140	0.79	1/21834 (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	A	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	331	MET	N-CA-C	-5.83	95.25	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	SER	Peptide
1	A	306	ASP	Peptide
1	A	407	LYS	Peptide
1	A	411	GLY	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	3961	0	3968	98	0
1	C	3961	0	3968	74	0
2	B	3957	0	3970	55	0
2	D	3957	0	3970	71	0
3	A	6	0	8	4	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	3	0
4	A	10	0	0	1	0
4	B	11	0	0	2	0
4	C	12	0	0	2	0
4	D	17	0	0	3	0
All	All	15910	0	15908	296	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 9.

All (296) 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)
2:D:84:ARG:HD3	3:D:601:GOL:O3	1.56	1.03
2:B:364:ALA:HB1	2:B:365:PRO:HD2	1.53	0.90
1:A:190:ALA:O	1:A:191:SER:HB3	1.77	0.84
1:A:410:ALA:HB3	1:A:411:GLY:HA2	1.62	0.82
1:A:364:ALA:HB1	1:A:365:PRO:HD3	1.62	0.81
1:A:317:ILE:HD11	1:A:320:ALA:HB2	1.62	0.80
1:C:44:GLU:HG2	1:C:100:TYR:HB3	1.64	0.78
1:A:364:ALA:HB1	1:A:365:PRO:CD	2.13	0.77
2:D:84:ARG:CD	3:D:601:GOL:O3	2.34	0.76
1:A:112:ILE:O	1:A:116:VAL:HG23	1.86	0.76
1:A:447:HIS:O	1:A:449:THR:N	2.22	0.73
2:D:364:ALA:HB1	2:D:365:PRO:CD	2.18	0.73
1:C:364:ALA:HB1	1:C:365:PRO:CD	2.19	0.72
2:D:262:ASN:HB3	2:D:418:ARG:HG3	1.70	0.72
1:C:136:VAL:HG13	1:C:143:PHE:CZ	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ARG:HG2	1:A:30:GLN:HG3	1.72	0.71
2:B:364:ALA:HB1	2:B:365:PRO:CD	2.21	0.71
1:A:410:ALA:HB3	1:A:411:GLY:CA	2.22	0.68
1:A:269:GLU:OE1	1:A:418:ARG:NH2	2.27	0.68
1:A:292:LYS:O	1:A:293:HIS:CG	2.47	0.67
1:C:442:LEU:CD1	1:C:483:THR:HG22	2.25	0.66
2:B:356:VAL:HG11	2:B:507:THR:HG21	1.77	0.65
1:A:84:ARG:HE	3:A:601:GOL:C3	2.11	0.64
1:A:136:VAL:HG13	1:A:143:PHE:CE1	2.33	0.63
1:A:408:ARG:HA	1:A:408:ARG:NE	2.14	0.63
1:A:190:ALA:O	1:A:191:SER:CB	2.47	0.62
1:A:44:GLU:HG2	1:A:100:TYR:HB3	1.82	0.62
1:A:292:LYS:O	1:A:293:HIS:CD2	2.54	0.61
1:A:1:MET:SD	1:A:21:GLU:HG2	2.41	0.61
2:D:446:MET:CE	2:D:452:LEU:HD22	2.31	0.61
1:A:372:ARG:O	1:A:374:THR:HG23	2.00	0.60
1:A:110:TYR:O	1:A:113:THR:HG22	2.01	0.60
1:C:374:THR:HG21	1:C:507:THR:HA	1.82	0.60
1:A:364:ALA:CB	1:A:365:PRO:CD	2.80	0.60
2:D:364:ALA:CB	2:D:365:PRO:CD	2.79	0.60
1:A:84:ARG:HE	3:A:601:GOL:H32	1.66	0.60
2:B:271:LYS:O	2:B:280:LEU:HD12	2.02	0.60
1:A:374:THR:HG21	1:A:507:THR:HA	1.83	0.59
1:A:141:ALA:HB3	1:A:193:THR:HA	1.82	0.59
2:B:110:TYR:O	2:B:113:THR:HG22	2.02	0.59
2:B:295:LEU:HD11	2:B:405:SER:HB2	1.83	0.59
1:C:15:ARG:HE	1:C:30:GLN:HE21	1.48	0.59
1:A:85:GLU:HG3	1:A:192:ARG:HB3	1.86	0.58
2:B:17:ILE:HG12	2:B:28:VAL:HG23	1.85	0.58
1:A:273:THR:HA	1:A:420:ASP:O	2.04	0.57
2:B:224:ASN:HD22	2:B:302:GLN:H	1.51	0.57
2:D:65:LEU:HD13	2:D:72:PHE:CG	2.40	0.57
1:A:2:LYS:HD2	1:A:76:GLU:CD	2.24	0.57
2:B:242:LEU:O	2:B:243:ASN:HB3	2.04	0.57
1:A:254:ASP:OD2	3:A:601:GOL:O3	2.23	0.57
2:B:15:ARG:NH2	2:B:17:ILE:HD11	2.20	0.57
2:B:374:THR:HG21	2:B:507:THR:HA	1.87	0.57
2:D:175:TYR:CE1	2:D:180:GLY:HA2	2.39	0.56
1:A:81:THR:HA	1:A:252:ILE:O	2.05	0.56
1:C:262:ASN:HB3	1:C:418:ARG:HG3	1.86	0.56
1:C:273:THR:O	1:C:278:CYS:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASP:C	1:A:20:ASP:OD1	2.43	0.56
2:D:446:MET:HE1	2:D:452:LEU:HD22	1.86	0.56
1:A:263:MET:CE	1:A:475:SER:HB2	2.35	0.56
2:B:274:TYR:HB3	2:B:423:LEU:HB2	1.88	0.56
2:D:224:ASN:HD22	2:D:302:GLN:H	1.54	0.56
1:C:374:THR:CG2	4:D:712:HOH:O	2.54	0.55
2:D:337:ILE:N	2:D:337:ILE:HD13	2.21	0.55
2:D:364:ALA:HB1	2:D:365:PRO:HD3	1.88	0.55
1:A:173:LEU:O	1:A:177:LEU:HB2	2.06	0.55
1:C:364:ALA:CB	1:C:365:PRO:CD	2.84	0.55
2:D:271:LYS:O	2:D:280:LEU:HD12	2.06	0.55
2:B:178:SER:HB2	2:B:181:LYS:H	1.72	0.55
1:C:22:ARG:HD2	1:C:24:ARG:HB2	1.89	0.55
1:C:489:SER:O	1:C:492:GLU:N	2.40	0.55
2:D:102:PRO:HB2	2:D:144:LYS:HD3	1.87	0.55
2:D:74:LYS:HD2	2:D:244:GLU:HG3	1.88	0.55
2:D:23:GLN:HE22	2:D:475:SER:HB2	1.73	0.54
2:D:272:ASN:HB2	2:D:280:LEU:HD13	1.88	0.54
1:C:81:THR:HA	1:C:252:ILE:O	2.07	0.54
1:C:174:MET:O	1:C:178:SER:OG	2.21	0.54
1:A:407:LYS:O	1:A:410:ALA:HA	2.08	0.54
1:A:508:LYS:O	2:B:506:ARG:NH2	2.41	0.54
2:B:372:ARG:O	2:B:374:THR:HG23	2.08	0.54
1:C:364:ALA:HB1	1:C:365:PRO:HD2	1.88	0.54
2:D:364:ALA:HB1	2:D:365:PRO:HD2	1.91	0.53
2:D:398:GLN:O	2:D:402:VAL:HG23	2.08	0.53
1:A:188:THR:HG22	1:A:256:GLN:HG2	1.89	0.53
2:D:171:THR:HG23	2:D:184:VAL:O	2.08	0.53
1:A:113:THR:OG1	1:A:136:VAL:HG12	2.09	0.53
1:A:192:ARG:NH2	1:A:314:GLU:OE1	2.42	0.53
1:C:489:SER:O	1:C:491:MET:N	2.41	0.53
1:A:169:ILE:O	1:A:173:LEU:HB2	2.09	0.53
1:C:272:ASN:HD21	1:C:278:CYS:HB3	1.74	0.53
2:D:234:ASP:OD1	2:D:234:ASP:N	2.39	0.53
2:D:420:ASP:OD1	2:D:449:THR:OG1	2.27	0.53
2:B:272:ASN:HB2	2:B:280:LEU:HD13	1.90	0.53
1:A:271:LYS:HA	1:A:418:ARG:O	2.08	0.52
1:C:501:ARG:CZ	4:C:701:HOH:O	2.56	0.52
1:A:136:VAL:HG13	1:A:143:PHE:CZ	2.45	0.52
1:A:273:THR:O	1:A:278:CYS:HA	2.09	0.52
1:A:399:LEU:HB2	1:A:433:GLN:HE22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LEU:O	2:B:243:ASN:CB	2.57	0.52
1:C:152:VAL:HB	1:C:155:VAL:HB	1.92	0.52
2:D:226:GLU:O	2:D:249:MET:HA	2.09	0.52
2:B:142:ALA:HB2	2:B:195:LEU:HG	1.91	0.51
2:D:396:ALA:HA	2:D:433:GLN:OE1	2.10	0.51
2:D:4:VAL:HG11	2:D:455:ALA:O	2.09	0.51
2:B:17:ILE:HD12	2:B:451:ALA:CB	2.41	0.51
1:A:187:VAL:O	1:A:188:THR:HG23	2.09	0.51
1:A:249:MET:SD	1:A:462:ALA:HB2	2.51	0.51
1:A:227:LEU:HB2	1:A:249:MET:HE3	1.92	0.51
1:C:22:ARG:CD	1:C:24:ARG:HB2	2.41	0.51
1:A:92:ARG:HG3	1:A:165:CYS:SG	2.51	0.51
1:C:497:ILE:O	1:C:501:ARG:HG3	2.11	0.51
2:B:358:ALA:HB2	2:B:362:LEU:HD13	1.92	0.51
1:C:81:THR:OG1	1:C:254:ASP:HA	2.11	0.50
1:A:263:MET:HE3	1:A:475:SER:HB2	1.91	0.50
2:D:290:PHE:HA	2:D:297:SER:OG	2.11	0.50
1:C:350:THR:O	1:C:351:GLN:C	2.48	0.50
2:B:146:ARG:NH1	2:B:212:LYS:O	2.44	0.50
2:D:363:LEU:O	2:D:364:ALA:C	2.48	0.50
1:C:289:ARG:HD3	1:C:410:ALA:HA	1.94	0.50
2:D:224:ASN:ND2	2:D:301:PHE:HA	2.27	0.50
2:D:92:ARG:HH11	2:D:92:ARG:HB3	1.76	0.49
2:B:174:MET:O	2:B:178:SER:OG	2.30	0.49
2:D:336:HIS:CD2	2:D:338:THR:OG1	2.66	0.49
1:C:270:ALA:HB3	1:C:414:LEU:HD11	1.94	0.49
2:D:16:PHE:CD1	2:D:58:MET:HG2	2.48	0.49
2:D:81:THR:OG1	2:D:254:ASP:HA	2.13	0.49
2:B:112:ILE:O	2:B:116:VAL:HG23	2.12	0.49
1:A:278:CYS:HB2	1:A:317:ILE:HG13	1.95	0.49
2:D:81:THR:HA	2:D:252:ILE:O	2.13	0.49
1:A:45:HIS:O	1:A:47:PRO:HD3	2.13	0.48
2:B:20:ASP:OD1	2:B:20:ASP:C	2.51	0.48
2:B:345:ARG:HH21	2:B:345:ARG:HG3	1.77	0.48
2:D:394:ALA:O	2:D:398:GLN:HG3	2.13	0.48
2:B:445:SER:OG	2:B:480:SER:O	2.31	0.48
2:D:350:THR:HG23	2:D:393:GLN:NE2	2.28	0.48
1:A:354:VAL:HG11	1:A:503:ALA:CB	2.44	0.48
1:C:501:ARG:NH1	4:C:701:HOH:O	2.46	0.48
2:D:254:ASP:OD1	3:D:601:GOL:H31	2.13	0.48
1:A:115:LYS:HG3	1:A:119:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ALA:HB3	2:B:193:THR:HA	1.95	0.48
2:B:92:ARG:HB2	4:B:711:HOH:O	2.12	0.48
1:A:410:ALA:CB	1:A:411:GLY:CA	2.88	0.48
1:C:91:ASP:OD1	1:C:94:THR:HG22	2.14	0.48
1:C:91:ASP:CB	1:C:98:LEU:HD11	2.44	0.48
2:B:259:LEU:HA	2:B:271:LYS:HG2	1.96	0.47
1:A:336:HIS:CE1	1:A:337:ILE:HG12	2.48	0.47
1:C:272:ASN:HD22	1:C:280:LEU:HB2	1.78	0.47
1:A:90:TRP:HA	1:A:98:LEU:HD22	1.96	0.47
1:C:347:VAL:HB	1:C:348:PRO:HD2	1.94	0.47
2:D:345:ARG:HH21	2:D:345:ARG:HG3	1.79	0.47
1:A:36:HIS:HB2	1:A:44:GLU:HB3	1.96	0.47
2:D:344:ALA:HB1	2:D:428:LEU:HD23	1.97	0.47
1:A:350:THR:HG23	1:A:393:GLN:NE2	2.30	0.47
1:C:91:ASP:OD2	1:C:161:ARG:NH2	2.48	0.47
1:C:274:TYR:HB3	1:C:423:LEU:HB2	1.97	0.47
2:D:37:THR:HG22	2:D:42:TRP:O	2.14	0.47
1:C:198:LEU:HD22	1:C:311:TYR:CE1	2.50	0.47
1:A:91:ASP:OD1	1:A:94:THR:N	2.27	0.47
1:C:376:VAL:HA	2:D:374:THR:HG22	1.96	0.47
2:B:284:VAL:HG11	2:B:313:LEU:HD12	1.97	0.47
2:D:146:ARG:O	2:D:149:LEU:N	2.47	0.47
2:D:337:ILE:N	2:D:337:ILE:CD1	2.78	0.47
2:B:364:ALA:CB	2:B:365:PRO:HD2	2.35	0.47
2:B:397:LEU:HD13	2:B:500:TRP:HB2	1.97	0.47
1:C:170:ASP:O	1:C:174:MET:HB2	2.14	0.47
1:A:231:VAL:HG11	1:A:242:LEU:CD1	2.45	0.46
1:C:271:LYS:HA	1:C:418:ARG:O	2.15	0.46
1:A:243:ASN:ND2	1:A:243:ASN:O	2.48	0.46
2:B:255:GLN:OE1	2:B:255:GLN:HA	2.15	0.46
1:C:355:PHE:CD2	1:C:375:ILE:HG12	2.50	0.46
2:D:237:GLY:O	2:D:240:ALA:HB3	2.15	0.46
1:A:410:ALA:CB	1:A:411:GLY:HA2	2.31	0.46
2:D:44:GLU:HA	2:D:101:ALA:O	2.16	0.46
2:D:403:VAL:HG11	2:D:437:LEU:HD22	1.97	0.46
1:C:209:GLU:O	1:C:212:LYS:N	2.47	0.46
1:A:186:ASP:OD2	1:A:224:ASN:OD1	2.34	0.46
1:A:81:THR:OG1	1:A:254:ASP:HA	2.16	0.46
2:B:146:ARG:NH1	2:B:212:LYS:HG3	2.30	0.46
1:C:363:LEU:HB2	1:C:364:ALA:H	1.67	0.46
2:D:257:SER:O	2:D:453:GLY:HA3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:CYS:SG	1:C:148:MET:HE2	2.56	0.46
1:C:91:ASP:HB2	1:C:98:LEU:HD11	1.96	0.46
2:D:289:ARG:HD3	2:D:410:ALA:HA	1.98	0.46
1:C:364:ALA:CB	1:C:365:PRO:HD2	2.46	0.46
1:C:365:PRO:HB3	1:C:405:SER:OG	2.16	0.46
1:A:292:LYS:O	1:A:293:HIS:CB	2.63	0.46
1:A:350:THR:HG23	1:A:393:GLN:HE22	1.81	0.46
1:A:348:PRO:HG2	1:A:351:GLN:HE21	1.79	0.46
2:B:38:PRO:O	2:B:39:HIS:CG	2.69	0.46
2:D:26:VAL:O	2:D:68:LYS:HE3	2.17	0.45
1:C:126:MET:SD	1:C:135:PRO:HB3	2.56	0.45
1:C:99:CYS:SG	1:C:148:MET:CE	3.05	0.45
1:C:255:GLN:OE1	1:C:279:PHE:HB2	2.17	0.45
1:A:146:ARG:HD2	1:A:211:LEU:O	2.17	0.45
1:C:452:LEU:O	1:C:453:GLY:C	2.55	0.45
1:C:15:ARG:NE	1:C:30:GLN:HE21	2.14	0.45
1:A:115:LYS:CG	4:A:709:HOH:O	2.65	0.45
2:B:27:SER:HB2	2:B:65:LEU:HG	1.99	0.45
1:C:325:GLU:HG3	1:C:329:ARG:HG2	1.99	0.45
1:C:448:GLU:HA	1:C:448:GLU:OE1	2.16	0.45
2:D:399:LEU:HD12	2:D:433:GLN:OE1	2.17	0.45
2:B:85:GLU:HB2	2:B:104:TRP:HB3	1.99	0.44
1:C:414:LEU:HD23	1:C:439:VAL:HG21	1.99	0.44
2:D:267:LYS:HA	2:D:283:ASN:O	2.16	0.44
1:C:259:LEU:HA	1:C:271:LYS:HG2	2.00	0.44
1:A:225:SER:O	1:A:304:GLY:HA2	2.16	0.44
1:A:51:PHE:HZ	1:A:233:THR:HG21	1.82	0.44
1:C:44:GLU:HA	1:C:101:ALA:O	2.17	0.44
2:D:168:THR:OG1	2:D:170:ASP:OD1	2.29	0.44
1:A:142:ALA:O	1:A:145:MET:HB2	2.18	0.44
2:D:187:VAL:HG13	2:D:299:VAL:HG11	2.00	0.44
1:A:157:ASP:O	1:A:160:ARG:HB3	2.18	0.44
2:B:112:ILE:HG13	4:B:703:HOH:O	2.16	0.44
1:C:233:THR:HG23	1:C:238:VAL:CG1	2.47	0.44
1:C:374:THR:HG22	4:D:712:HOH:O	2.15	0.44
2:D:287:GLU:O	2:D:287:GLU:HG3	2.17	0.44
1:A:142:ALA:CB	1:A:195:LEU:HD21	2.48	0.43
1:A:16:PHE:CD2	1:A:58:MET:HA	2.52	0.43
1:C:51:PHE:HE1	1:C:177:LEU:HD12	1.83	0.43
2:D:44:GLU:OE1	2:D:100:TYR:HB2	2.18	0.43
2:B:19:PHE:HA	2:B:24:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LEU:HD13	1:C:399:LEU:CD1	2.48	0.43
2:D:363:LEU:HD23	2:D:363:LEU:N	2.32	0.43
2:D:274:TYR:HB3	2:D:423:LEU:HB2	2.00	0.43
1:A:51:PHE:O	1:A:54:ALA:HB3	2.19	0.43
1:A:9:GLN:HG2	1:A:14:THR:HG23	2.00	0.43
2:D:242:LEU:O	2:D:244:GLU:N	2.50	0.43
1:A:263:MET:CE	1:A:475:SER:CB	2.96	0.43
2:B:109:THR:O	2:B:113:THR:HB	2.19	0.43
2:D:298:THR:OG1	2:D:299:VAL:N	2.51	0.43
1:A:160:ARG:CZ	1:A:160:ARG:HB2	2.47	0.43
1:A:252:ILE:HG23	1:A:257:SER:HB2	2.01	0.43
2:B:69:ASP:C	2:B:69:ASP:OD1	2.56	0.43
1:C:364:ALA:HB1	1:C:365:PRO:HD3	1.99	0.43
2:D:298:THR:HA	4:D:707:HOH:O	2.19	0.43
2:D:364:ALA:CB	2:D:365:PRO:HD2	2.47	0.43
1:C:106:ASP:OD1	1:C:107:LEU:N	2.52	0.43
1:C:91:ASP:HB3	1:C:94:THR:CG2	2.49	0.42
1:A:259:LEU:HD12	1:A:264:CYS:SG	2.60	0.42
2:B:364:ALA:CB	2:B:365:PRO:CD	2.92	0.42
2:B:83:GLN:HG3	2:B:83:GLN:O	2.20	0.42
2:D:85:GLU:HB3	2:D:139:TYR:O	2.20	0.42
2:D:108:ARG:HD3	2:D:147:TRP:CZ2	2.54	0.42
2:D:366:TYR:O	2:D:367:TRP:C	2.57	0.42
2:D:82:ASN:OD1	2:D:170:ASP:HB3	2.19	0.42
1:C:124:ASP:O	1:C:127:PHE:HB3	2.19	0.42
1:A:262:ASN:O	1:A:418:ARG:NH1	2.48	0.42
1:C:274:TYR:CB	1:C:423:LEU:HB2	2.50	0.42
1:C:344:ALA:O	1:C:389:ARG:NH1	2.53	0.42
2:D:200:THR:O	2:D:201:ARG:HB2	2.19	0.42
1:A:343:LEU:O	1:A:346:SER:OG	2.30	0.41
1:C:127:PHE:CE1	1:C:128:ALA:HB2	2.55	0.41
2:B:300:GLY:N	2:B:310:TYR:O	2.47	0.41
1:C:20:ASP:OD1	1:C:20:ASP:C	2.59	0.41
1:A:256:GLN:N	1:A:256:GLN:OE1	2.48	0.41
2:B:289:ARG:HD3	2:B:410:ALA:HA	2.02	0.41
1:A:18:ILE:HD13	1:A:65:LEU:HD12	2.02	0.41
1:A:334:PHE:CZ	1:A:340:CYS:HB2	2.56	0.41
2:B:170:ASP:CG	2:B:171:THR:H	2.23	0.41
2:B:225:SER:OG	2:B:461:ALA:HB2	2.21	0.41
1:A:73:ARG:NH1	1:A:244:GLU:OE1	2.53	0.41
2:B:152:VAL:CG1	2:B:155:VAL:HG23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:VAL:HA	2:D:32:PRO:HD3	1.90	0.41
2:B:466:THR:HG23	2:B:470:GLU:OE1	2.20	0.41
1:C:280:LEU:C	1:C:281:LEU:HD12	2.41	0.41
1:A:102:PRO:HD3	1:A:148:MET:CE	2.50	0.41
1:A:470:GLU:O	1:A:474:VAL:HG23	2.20	0.41
2:B:157:ASP:O	2:B:158:ALA:C	2.59	0.41
2:B:445:SER:OG	2:B:480:SER:HB3	2.21	0.41
1:C:141:ALA:O	1:C:144:LYS:N	2.54	0.41
1:C:426:ASN:O	1:C:430:MET:HG2	2.21	0.41
2:D:110:TYR:O	2:D:113:THR:HG22	2.19	0.41
1:A:408:ARG:C	1:A:410:ALA:HB2	2.40	0.41
2:B:178:SER:HB2	2:B:181:LYS:N	2.36	0.41
2:B:5:GLY:HA3	2:B:16:PHE:CZ	2.56	0.41
1:C:16:PHE:O	1:C:28:VAL:HA	2.21	0.41
1:C:233:THR:OG1	1:C:234:ASP:N	2.54	0.41
2:D:208:CYS:O	2:D:212:LYS:N	2.54	0.41
1:A:183:PHE:CD2	1:A:219:PRO:HA	2.56	0.41
1:A:222:ARG:HD3	1:A:226:GLU:OE1	2.21	0.41
1:A:281:LEU:HG	1:A:314:GLU:HG2	2.02	0.41
2:B:224:ASN:ND2	2:B:301:PHE:HA	2.36	0.41
2:D:128:ALA:HB3	2:D:194:PHE:CZ	2.56	0.41
2:D:84:ARG:HD2	2:D:254:ASP:OD1	2.21	0.41
1:A:281:LEU:HG	1:A:314:GLU:CG	2.51	0.41
1:A:36:HIS:HB2	1:A:44:GLU:O	2.22	0.40
1:A:388:ILE:O	1:A:392:LEU:HG	2.22	0.40
1:A:84:ARG:H	3:A:601:GOL:C3	2.34	0.40
1:C:17:ILE:HD12	1:C:451:ALA:CB	2.52	0.40
1:C:432:ILE:HG22	1:C:436:LEU:HD12	2.02	0.40
2:B:25:PRO:HD3	2:B:446:MET:SD	2.61	0.40
1:C:117:THR:HG23	1:C:125:SER:HA	2.03	0.40
1:A:114:LYS:CE	1:A:114:LYS:HA	2.51	0.40
1:A:116:VAL:HG21	1:A:143:PHE:CE1	2.56	0.40
1:A:54:ALA:O	1:A:58:MET:HG3	2.20	0.40
1:C:224:ASN:HD22	1:C:302:GLN:H	1.69	0.40
2:D:83:GLN:O	2:D:83:GLN:HG3	2.21	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	510/518 (98%)	443 (87%)	51 (10%)	16 (3%)	4	9
1	C	510/518 (98%)	450 (88%)	50 (10%)	10 (2%)	7	19
2	B	511/518 (99%)	476 (93%)	30 (6%)	5 (1%)	15	37
2	D	511/518 (99%)	465 (91%)	38 (7%)	8 (2%)	9	24
All	All	2042/2072 (99%)	1834 (90%)	169 (8%)	39 (2%)	8	20

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	THR
1	A	203	TRP
1	A	293	HIS
1	A	337	ILE
1	A	364	ALA
1	A	408	ARG
1	A	448	GLU
1	C	364	ALA
1	C	487	SER
2	D	337	ILE
2	D	364	ALA
1	A	191	SER
1	A	487	SER
2	B	243	ASN
2	B	364	ALA
2	B	510	ALA
1	C	215	MET
1	C	448	GLU
1	C	490	ALA
1	A	0	THR
1	A	289	ARG
1	A	292	LYS

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Mol	Chain	Res	Type
1	A	421	GLY
1	A	461	ALA
2	B	226	GLU
2	B	509	TRP
1	C	346	SER
1	C	351	GLN
2	D	38	PRO
2	D	482	LYS
1	A	306	ASP
1	C	243	ASN
2	D	243	ASN
1	A	179	GLY
1	C	85	GLU
1	C	109	THR
2	D	509	TRP
2	D	194	PHE
2	D	357	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	420/424 (99%)	370 (88%)	50 (12%)	5	12
1	C	420/424 (99%)	378 (90%)	42 (10%)	7	18
2	B	421/425 (99%)	380 (90%)	41 (10%)	8	19
2	D	421/425 (99%)	381 (90%)	40 (10%)	8	20
All	All	1682/1698 (99%)	1509 (90%)	173 (10%)	7	16

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	15	ARG
1	A	65	LEU
1	A	67	GLN

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Mol	Chain	Res	Type
1	A	73	ARG
1	A	76	GLU
1	A	85	GLU
1	A	87	THR
1	A	95	LYS
1	A	96	GLU
1	A	106	ASP
1	A	119	GLU
1	A	146	ARG
1	A	160	ARG
1	A	174	MET
1	A	191	SER
1	A	199	ARG
1	A	215	MET
1	A	243	ASN
1	A	267	LYS
1	A	271	LYS
1	A	276	THR
1	A	280	LEU
1	A	287	GLU
1	A	292	LYS
1	A	305	ARG
1	A	314	GLU
1	A	317	ILE
1	A	337	ILE
1	A	342	LYS
1	A	355	PHE
1	A	362	LEU
1	A	366	TYR
1	A	380	LEU
1	A	381	LYS
1	A	399	LEU
1	A	407	LYS
1	A	409	ASP
1	A	412	LEU
1	A	413	ASN
1	A	418	ARG
1	A	423	LEU
1	A	442	LEU
1	A	448	GLU
1	A	466	THR
1	A	469	GLU

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Mol	Chain	Res	Type
1	A	475	SER
1	A	480	SER
1	A	491	MET
1	A	494	GLU
2	B	-1	PHE
2	B	1	MET
2	B	4	VAL
2	B	9	GLN
2	B	65	LEU
2	B	66	ARG
2	B	73	ARG
2	B	76	GLU
2	B	81	THR
2	B	92	ARG
2	B	93	VAL
2	B	98	LEU
2	B	113	THR
2	B	160	ARG
2	B	173	LEU
2	B	174	MET
2	B	177	LEU
2	B	178	SER
2	B	184	VAL
2	B	199	ARG
2	B	244	GLU
2	B	271	LYS
2	B	287	GLU
2	B	317	ILE
2	B	337	ILE
2	B	342	LYS
2	B	345	ARG
2	B	346	SER
2	B	355	PHE
2	B	362	LEU
2	B	366	TYR
2	B	367	TRP
2	B	412	LEU
2	B	424	SER
2	B	442	LEU
2	B	445	SER
2	B	483	THR
2	B	489	SER

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Mol	Chain	Res	Type
2	B	491	MET
2	B	501	ARG
2	B	511	LYS
1	C	9	GLN
1	C	21	GLU
1	C	65	LEU
1	C	72	PHE
1	C	91	ASP
1	C	92	ARG
1	C	94	THR
1	C	96	GLU
1	C	98	LEU
1	C	137	SER
1	C	160	ARG
1	C	173	LEU
1	C	174	MET
1	C	185	THR
1	C	198	LEU
1	C	199	ARG
1	C	215	MET
1	C	227	LEU
1	C	234	ASP
1	C	245	ARG
1	C	271	LYS
1	C	280	LEU
1	C	287	GLU
1	C	289	ARG
1	C	317	ILE
1	C	329	ARG
1	C	336	HIS
1	C	337	ILE
1	C	342	LYS
1	C	355	PHE
1	C	362	LEU
1	C	363	LEU
1	C	366	TYR
1	C	412	LEU
1	C	415	SER
1	C	448	GLU
1	C	472	LYS
1	C	476	ARG
1	C	480	SER

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Mol	Chain	Res	Type
1	C	485	SER
1	C	491	MET
1	C	508	LYS
2	D	9	GLN
2	D	65	LEU
2	D	66	ARG
2	D	73	ARG
2	D	92	ARG
2	D	94	THR
2	D	95	LYS
2	D	98	LEU
2	D	106	ASP
2	D	113	THR
2	D	146	ARG
2	D	160	ARG
2	D	173	LEU
2	D	174	MET
2	D	186	ASP
2	D	233	THR
2	D	271	LYS
2	D	287	GLU
2	D	298	THR
2	D	309	CYS
2	D	317	ILE
2	D	329	ARG
2	D	337	ILE
2	D	338	THR
2	D	342	LYS
2	D	355	PHE
2	D	363	LEU
2	D	366	TYR
2	D	367	TRP
2	D	412	LEU
2	D	413	ASN
2	D	415	SER
2	D	424	SER
2	D	448	GLU
2	D	469	GLU
2	D	480	SER
2	D	483	THR
2	D	491	MET
2	D	494	GLU

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Mol	Chain	Res	Type
2	D	501	ARG

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

Mol	Chain	Res	Type
1	A	82	ASN
1	A	189	ASN
1	A	224	ASN
1	A	272	ASN
1	A	393	GLN
1	A	413	ASN
1	A	433	GLN
2	B	23	GLN
2	B	224	ASN
2	B	243	ASN
2	B	332	ASN
2	B	413	ASN
1	C	23	GLN
1	C	30	GLN
1	C	224	ASN
1	C	272	ASN
1	C	293	HIS
2	D	23	GLN
2	D	224	ASN
2	D	243	ASN
2	D	272	ASN
2	D	413	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	TPO	A	12	1	8,10,11	1.48	1 (12%)	10,14,16	1.86	2 (20%)
1	TPO	C	12	1	8,10,11	1.52	1 (12%)	10,14,16	1.61	2 (20%)

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
1	TPO	A	12	1	-	5/9/11/13	-
1	TPO	C	12	1	-	5/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	TPO	P-OG1	3.92	1.66	1.59
1	C	12	TPO	P-OG1	3.86	1.66	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	TPO	CG2-CB-CA	-4.58	104.12	113.16
1	C	12	TPO	CG2-CB-CA	-3.07	107.11	113.16
1	A	12	TPO	P-OG1-CB	2.66	131.25	123.21
1	C	12	TPO	CB-CA-N	-2.07	100.80	114.41

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	12	TPO	N-CA-CB-CG2
1	A	12	TPO	N-CA-CB-OG1
1	A	12	TPO	C-CA-CB-CG2
1	A	12	TPO	O-C-CA-CB
1	C	12	TPO	N-CA-CB-CG2
1	C	12	TPO	N-CA-CB-OG1
1	C	12	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
1	A	12	TPO	CB-OG1-P-O3P
1	C	12	TPO	CB-OG1-P-O2P
1	C	12	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	GOL	C	601	-	5,5,5	0.41	0	5,5,5	0.49	0
3	GOL	D	601	-	5,5,5	0.39	0	5,5,5	1.73	1 (20%)
3	GOL	A	601	-	5,5,5	0.53	0	5,5,5	1.60	1 (20%)
3	GOL	B	601	-	5,5,5	0.32	0	5,5,5	0.41	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	C	601	-	-	2/4/4/4	-
3	GOL	D	601	-	-	1/4/4/4	-
3	GOL	A	601	-	-	2/4/4/4	-
3	GOL	B	601	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	601	GOL	C3-C2-C1	-2.54	101.81	111.70
3	D	601	GOL	C3-C2-C1	-2.49	102.02	111.70

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	GOL	O1-C1-C2-C3
3	A	601	GOL	O1-C1-C2-C3
3	C	601	GOL	O1-C1-C2-O2
3	B	601	GOL	C1-C2-C3-O3
3	D	601	GOL	O2-C2-C3-O3
3	B	601	GOL	O2-C2-C3-O3
3	A	601	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	601	GOL	3	0
3	A	601	GOL	4	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	512/518 (98%)	0.09	13 (2%) 57 59	65, 99, 136, 174	1 (0%)
1	C	512/518 (98%)	-0.07	5 (0%) 82 83	67, 96, 122, 160	1 (0%)
2	B	513/518 (99%)	-0.14	1 (0%) 95 96	64, 86, 110, 128	1 (0%)
2	D	513/518 (99%)	-0.11	5 (0%) 82 83	66, 93, 117, 144	1 (0%)
All	All	2050/2072 (98%)	-0.06	24 (1%) 79 80	64, 93, 125, 174	4 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	ASP	8.9
1	A	410	ALA	6.5
1	C	367	TRP	5.4
1	A	182	ALA	4.8
1	A	408	ARG	4.3
1	A	481	TRP	3.9
2	D	408	ARG	3.1
2	D	164	LEU	3.0
1	C	73	ARG	3.0
1	C	306	ASP	2.8
1	A	-1	PHE	2.8
1	A	265	PHE	2.7
1	A	203	TRP	2.6
1	C	408	ARG	2.6
2	D	491	MET	2.6
1	C	421	GLY	2.6
1	A	294	GLY	2.5
1	A	412	LEU	2.5
2	D	412	LEU	2.4
1	A	478	GLU	2.4
1	A	305	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	181	LYS	2.1
2	B	107	LEU	2.1
2	D	238	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	A	12	11/12	0.89	0.16	64,83,113,122	0
1	TPO	C	12	11/12	0.91	0.13	74,88,131,136	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
3	GOL	A	601	6/6	0.87	0.19	78,87,102,117	0
3	GOL	B	601	6/6	0.93	0.18	75,89,99,101	0
3	GOL	D	601	6/6	0.94	0.18	77,82,84,88	0
3	GOL	C	601	6/6	0.96	0.18	70,76,82,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.