



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:02 AM UTC

PDB ID : 6J9X / pdb_00006j9x
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 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

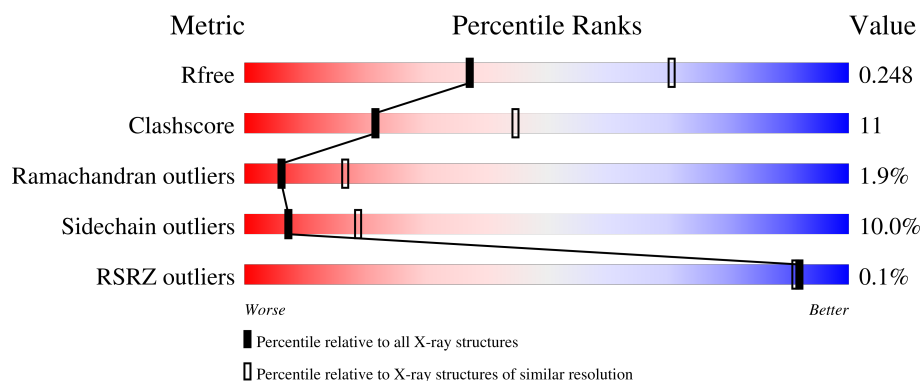
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	518	 64% 28% 6% ..
1	C	518	 69% 27% ..
2	B	518	 75% 20% ..
2	D	518	 70% 26% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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

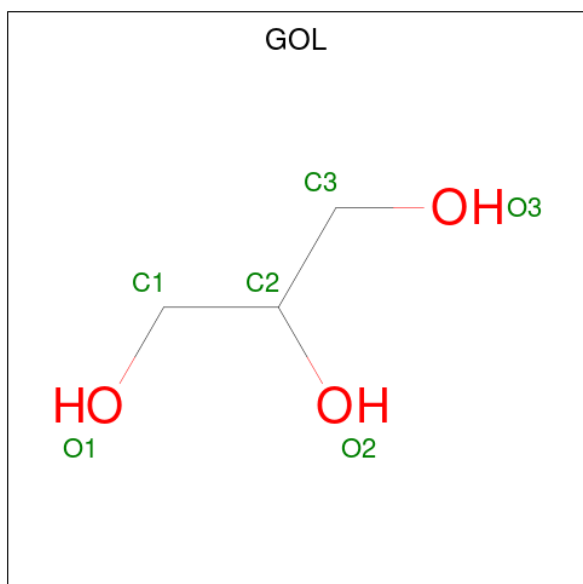
- Molecule 2 is a protein called Glycerol kinase.

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 (CCD ID: 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

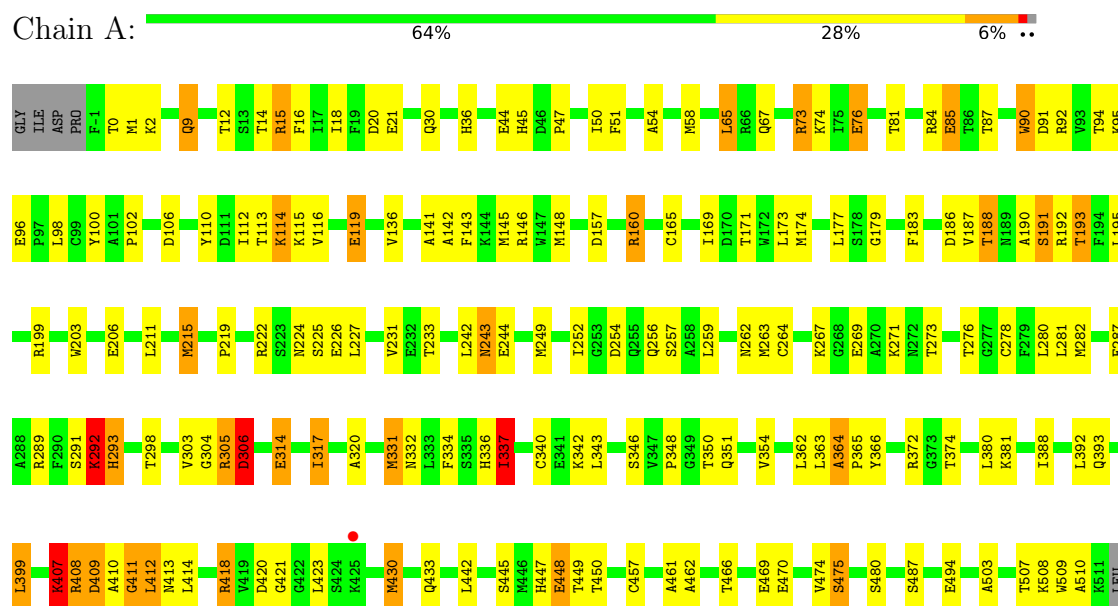
- Molecule 4 is water.

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

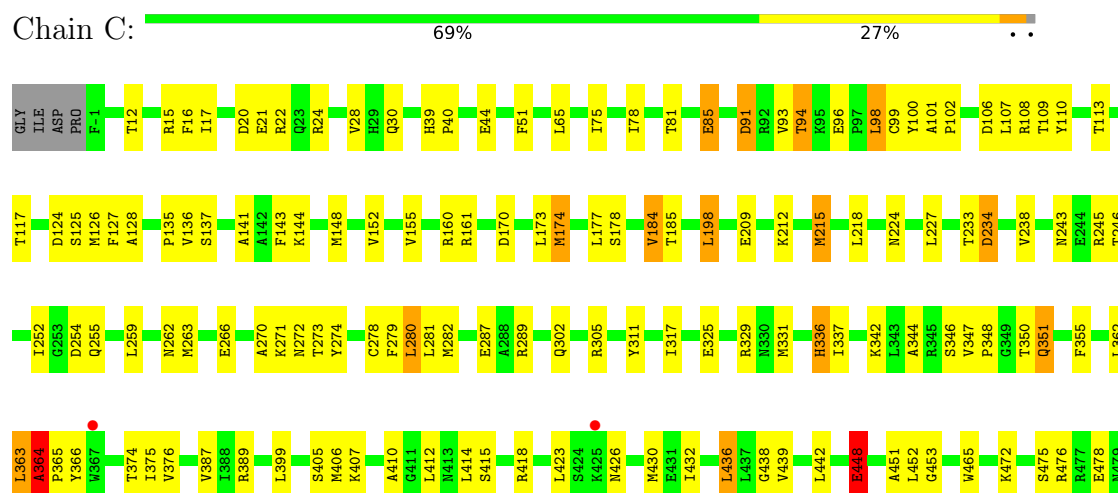
3 Residue-property plots

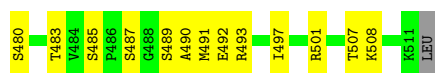
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



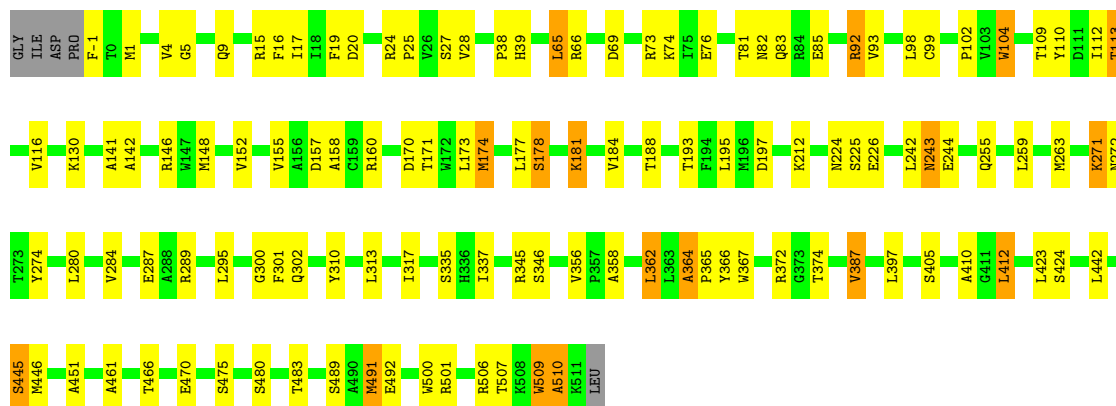
• Molecule 1: Glycerol kinase





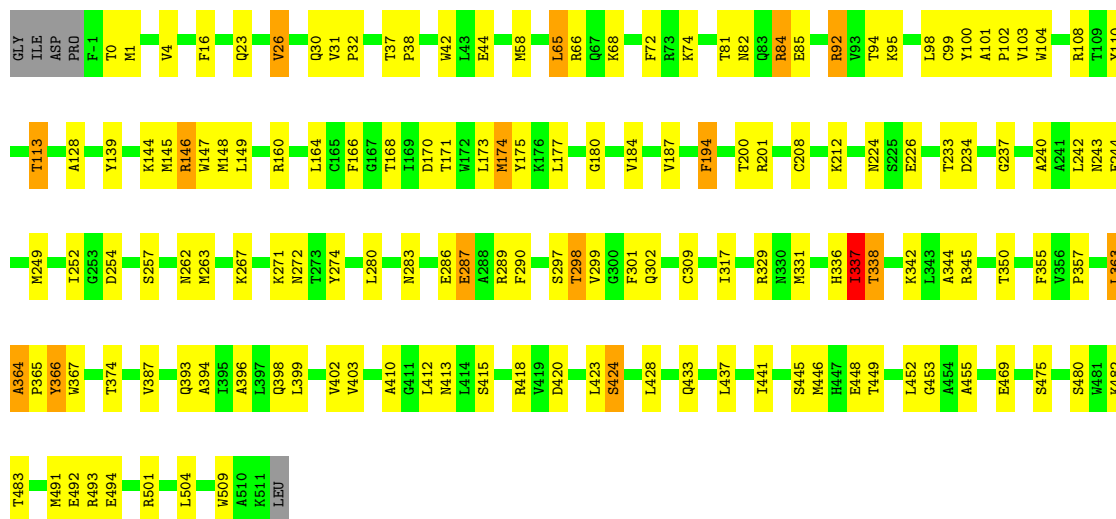
• Molecule 2: Glycerol kinase

Chain B: 75% 20% ..



• Molecule 2: Glycerol kinase

Chain D: 70% 26% ..



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) 99.1 (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 (5.07%)	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 , 58.1	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

5.1 Standard geometry

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

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	0.81	0/4031	1.04	7/5452 (0.1%)
1	C	0.78	0/4031	1.02	8/5452 (0.1%)
2	B	0.83	0/4039	1.07	7/5465 (0.1%)
2	D	0.79	1/4039 (0.0%)	1.02	3/5465 (0.1%)
All	All	0.80	1/16140 (0.0%)	1.04	25/21834 (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	A	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	26	VAL	C-O	-5.41	1.19	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	MET	N-CA-C	-9.88	95.25	110.17
1	A	409	ASP	N-CA-C	7.21	122.10	112.30
2	D	337	ILE	N-CA-C	6.28	122.41	109.34
1	A	332	ASN	N-CA-C	-6.27	102.91	110.44
2	B	387	VAL	N-CA-C	-6.24	104.67	110.53
2	D	164	LEU	N-CA-C	6.09	119.06	110.23
1	A	412	LEU	N-CA-C	6.04	117.07	108.74
2	D	445	SER	N-CA-C	-5.90	104.83	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	188	THR	N-CA-C	-5.84	104.99	111.36
1	C	364	ALA	CA-C-N	-5.80	114.27	121.00
1	C	364	ALA	C-N-CA	-5.80	114.27	121.00
1	C	246	THR	N-CA-C	5.72	117.20	109.24
2	B	412	LEU	N-CA-C	5.58	117.10	109.18
1	C	465	TRP	N-CA-C	-5.57	100.81	109.72
2	B	181	LYS	N-CA-C	5.50	119.16	112.23
1	C	218	LEU	N-CA-C	5.38	116.84	110.07
2	B	82	ASN	N-CA-C	5.22	117.32	109.23
1	C	93	VAL	N-CA-C	5.22	116.13	111.90
1	A	90	TRP	N-CA-C	5.21	115.93	108.74
1	C	184	VAL	N-CA-C	5.20	116.19	108.65
1	C	336	HIS	CB-CA-C	5.14	118.64	109.38
1	A	74	LYS	N-CA-C	5.13	116.88	109.07
2	B	104	TRP	N-CA-C	5.06	117.18	111.11
1	A	303	VAL	N-CA-C	5.03	114.85	107.15
2	B	74	LYS	N-CA-C	5.03	114.97	107.88

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	3969	112	0
1	C	3961	0	3968	87	0
2	B	3957	0	3970	64	0
2	D	3957	0	3970	86	0
3	A	6	0	8	4	0
3	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	15909	344	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 11.

All (344) 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
1:C:99:CYS:SG	1:C:148:MET:HE2	2.11	0.91
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
2:B:99:CYS:SG	2:B:148:MET:HE2	2.27	0.74
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
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:174:MET:HE3	1:C:184:VAL:HG23	1.77	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:C:102:PRO:HD3	1:C:148:MET:HE3	1.77	0.65
1:A:84:ARG:HE	3:A:601:GOL:C3	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2:LYS:HD2	1:A:76:GLU:CD	2.24	0.61
2:D:145:MET:HE2	2:D:166:PHE:HB3	1.80	0.61
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
2:D:99:CYS:SG	2:D:148:MET:HE2	2.41	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:20:ASP:OD1	1:A:20:ASP:C	2.43	0.59
2:D:102:PRO:HD3	2:D:148:MET:HE3	1.84	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
1:A:263:MET:HE3	1:A:475:SER:HB2	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
1:C:174:MET:O	1:C:178:SER:OG	2.21	0.57
2:D:65:LEU:HD13	2:D:72:PHE:CG	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	2:D:337:ILE:N	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
1:C:350:THR:O	1:C:351:GLN:C	2.48	0.55
2:D:271:LYS:O	2:D:280:LEU:HD12	2.06	0.55
2:D:363:LEU:O	2:D:364:ALA:C	2.48	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:74:LYS:HD2	2:D:244:GLU:HG3	1.88	0.55
2:D:102:PRO:HB2	2:D:144:LYS:HD3	1.87	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: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:B:20:ASP:C	2:B:20:ASP:OD1	2.51	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:102:PRO:HD3	2:B:148:MET:HE3	1.91	0.53
2:B:272:ASN:HB2	2:B:280:LEU:HD13	1.90	0.53
1:C:331:MET:HE1	2:D:387:VAL:HG21	1.89	0.52
1:A:271:LYS:HA	1:A:418:ARG:O	2.08	0.52
2:D:263:MET:HE3	2:D:475:SER:HB2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PRO:CD	1:A:148:MET:HE3	2.40	0.52
1:A:399:LEU:HB2	1:A:433:GLN:HE22	1.75	0.52
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:B:263:MET:HE3	2:B:475:SER:HB2	1.91	0.51
2:D:4:VAL:HG11	2:D:455:ALA:O	2.09	0.51
2:D:396:ALA:HA	2:D:433:GLN:OE1	2.10	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
2:D:290:PHE:HA	2:D:297:SER:OG	2.11	0.50
2:B:146:ARG:NH1	2:B:212:LYS:O	2.44	0.50
2:D:99:CYS:HG	2:D:148:MET:HE2	1.76	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
2:D:446:MET:HE1	2:D:452:LEU:HD22	1.94	0.49
1:A:263:MET:HE3	1:A:475:SER:CB	2.41	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:345:ARG:HH21	2:B:345:ARG:HG3	1.77	0.48
1:A:282:MET:HE2	1:A:414:LEU:HD13	1.95	0.48
1:A:430:MET:HE2	1:A:430:MET:HA	1.94	0.48
2:B:445:SER:OG	2:B:480:SER:O	2.31	0.48
2:D:394:ALA:O	2:D:398:GLN:HG3	2.13	0.48
1:C:452:LEU:O	1:C:453:GLY:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:92:ARG:HB2	4:B:711:HOH:O	2.12	0.48
2:B:141:ALA:HB3	2:B:193:THR:HA	1.95	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:69:ASP:OD1	2:B:69:ASP:C	2.56	0.47
2:B:259:LEU:HA	2:B:271:LYS:HG2	1.96	0.47
2:B:491:MET:HE3	2:B:492:GLU:HG3	1.95	0.47
1:C:282:MET:HE2	1:C:414:LEU:HD12	1.94	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:A:91:ASP:OD1	1:A:94:THR:N	2.27	0.47
1:C:198:LEU:HD22	1:C:311:TYR:CE1	2.50	0.47
1:C:376:VAL:HA	2:D:374:THR:HG22	1.96	0.47
2:D:366:TYR:O	2:D:367:TRP:C	2.57	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:C:282:MET:HE2	1:C:414:LEU:CD1	2.44	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:O	1:A:243:ASN:ND2	2.48	0.46
1:A:408:ARG:C	1:A:410:ALA:HB2	2.40	0.46
2:B:170:ASP:CG	2:B:171:THR:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:GLN:HA	2:B:255:GLN:OE1	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:20:ASP:OD1	1:C:20:ASP:C	2.59	0.46
1:C:209:GLU:O	1:C:212:LYS:N	2.47	0.46
1:A:81:THR:OG1	1:A:254:ASP:HA	2.16	0.46
1:A:186:ASP:OD2	1:A:224:ASN:OD1	2.34	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
1:C:91:ASP:HB2	1:C:98:LEU:HD11	1.96	0.46
1:A:331:MET:HE1	2:B:387:VAL:HG21	1.98	0.46
2:D:289:ARG:HD3	2:D:410:ALA:HA	1.98	0.46
1:C:280:LEU:C	1:C:281:LEU:HD12	2.41	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:B:157:ASP:O	2:B:158:ALA:C	2.59	0.46
1:C:263:MET:HE3	1:C:475:SER:OG	2.16	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: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:387:VAL:HG21	2:D:331:MET:HE1	1.98	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:OE1	1:C:448:GLU:HA	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
2:B:197:ASP:OD1	2:B:197:ASP:C	2.61	0.44
1:C:259:LEU:HA	1:C:271:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:HZ	1:A:233:THR:HG21	1.82	0.44
1:A:225:SER:O	1:A:304:GLY:HA2	2.16	0.44
1:A:509:TRP:O	1:A:510:ALA:C	2.60	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
2:D:263:MET:HE3	2:D:475:SER:CB	2.48	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:HG3	2:D:287:GLU:O	2.17	0.44
2:D:492:GLU:O	2:D:493:ARG:C	2.60	0.44
1:C:22:ARG:HG2	1:C:478:GLU:CD	2.43	0.43
1:A:16:PHE:CD2	1:A:58:MET:HA	2.52	0.43
1:A:142:ALA:CB	1:A:195:LEU:HD21	2.48	0.43
1:C:51:PHE:HE1	1:C:177:LEU:HD12	1.83	0.43
1:A:215:MET:HE2	1:A:215:MET:HB3	1.86	0.43
1:A:305:ARG:O	1:A:306:ASP:C	2.61	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
1:C:280:LEU:HD13	1:C:399:LEU:CD1	2.48	0.43
2:D:274:TYR:HB3	2:D:423:LEU:HB2	2.00	0.43
2:D:363:LEU:N	2:D:363:LEU:HD23	2.32	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:HB2	1:A:160:ARG:CZ	2.47	0.43
1:A:252:ILE:HG23	1:A:257:SER:HB2	2.01	0.43
2:B:263:MET:HE3	2:B:475:SER:CB	2.49	0.43
1:C:364:ALA:HB1	1:C:365:PRO:HD3	1.99	0.43
2:D:174:MET:HE2	2:D:174:MET:HB2	1.91	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:108:ARG:C	1:C:110:TYR:H	2.27	0.42
1:A:206:GLU:H	1:A:206:GLU:CD	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:GLN:O	2:B:83:GLN:HG3	2.20	0.42
2:B:364:ALA:CB	2:B:365:PRO:CD	2.92	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:B:102:PRO:CD	2:B:148:MET:HE3	2.49	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:C:406:MET:O	1:C:407:LYS:C	2.63	0.42
1:A:192:ARG:NH2	1:A:314:GLU:CD	2.77	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
2:D:355:PHE:CD2	2:D:355:PHE:C	2.97	0.42
1:C:344:ALA:O	1:C:389:ARG:NH1	2.53	0.42
1:C:438:GLY:C	1:C:439:VAL:HG13	2.45	0.42
2:D:200:THR:O	2:D:201:ARG:HB2	2.19	0.42
1:A:257:SER:OG	1:A:450:THR:O	2.37	0.41
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:D:0:THR:O	2:D:1:MET:C	2.63	0.41
2:B:300:GLY:N	2:B:310:TYR:O	2.47	0.41
1:A:256:GLN:OE1	1:A:256:GLN:N	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:225:SER:OG	2:B:461:ALA:HB2	2.21	0.41
2:D:367:TRP:C	2:D:367:TRP:CD1	2.98	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
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:39:HIS:O	1:C:40:PRO:C	2.64	0.41
2:D:102:PRO:CD	2:D:148:MET:HE3	2.49	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: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:183:PHE:CD2	1:A:219:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:5:GLY:HA3	2:B:16:PHE:CZ	2.56	0.41
2:B:178:SER:HB2	2:B:181:LYS:N	2.36	0.41
2:B:224:ASN:ND2	2:B:301:PHE:HA	2.36	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:84:ARG:HD2	2:D:254:ASP:OD1	2.21	0.41
2:D:128:ALA:HB3	2:D:194:PHE:CZ	2.56	0.41
2:D:208:CYS:O	2:D:212:LYS:N	2.54	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:84:ARG:H	3:A:601:GOL:C3	2.34	0.40
1:A:388:ILE:O	1:A:392:LEU:HG	2.22	0.40
1:C:17:ILE:HD12	1:C:451:ALA:CB	2.52	0.40
1:A:50:ILE:O	1:A:51:PHE:C	2.63	0.40
1:C:432:ILE:HG22	1:C:436:LEU:HD12	2.02	0.40
1:A:317:ILE:C	1:A:317:ILE:HD12	2.46	0.40
2:B:25:PRO:HD3	2:B:446:MET:SD	2.61	0.40
2:B:509:TRP:O	2:B:510:ALA:C	2.65	0.40
1:C:106:ASP:OD1	1:C:106:ASP:C	2.63	0.40
1:C:117:THR:HG23	1:C:125:SER:HA	2.03	0.40
1:A:54:ALA:O	1:A:58:MET:HG3	2.20	0.40
1:A:114:LYS:HA	1:A:114:LYS:CE	2.51	0.40
1:A:116:VAL:HG21	1:A:143:PHE:CE1	2.56	0.40
1:C:224:ASN:HD22	1:C:302:GLN:H	1.69	0.40
2:D:423:LEU:O	2:D:424:SER:C	2.65	0.40
1:A:225:SER:OG	1:A:457:CYS:O	2.34	0.40
1:C:492:GLU:O	1:C:493:ARG:C	2.65	0.40
2:D:103:VAL:O	2:D:104:TRP:C	2.64	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%)	3	8
1	C	510/518 (98%)	450 (88%)	50 (10%)	10 (2%)	6	16
2	B	511/518 (99%)	476 (93%)	30 (6%)	5 (1%)	12	32
2	D	511/518 (99%)	465 (91%)	38 (7%)	8 (2%)	7	20
All	All	2042/2072 (99%)	1834 (90%)	169 (8%)	39 (2%)	6	17

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
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

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Mol	Chain	Res	Type
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%)	368 (88%)	52 (12%)	4	11
1	C	420/424 (99%)	380 (90%)	40 (10%)	8	20
2	B	421/425 (99%)	383 (91%)	38 (9%)	9	23
2	D	421/425 (99%)	382 (91%)	39 (9%)	8	21
All	All	1682/1698 (99%)	1513 (90%)	169 (10%)	7	19

All (169) 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
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	114	LYS

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Mol	Chain	Res	Type
1	A	119	GLU
1	A	160	ARG
1	A	171	THR
1	A	174	MET
1	A	193	THR
1	A	199	ARG
1	A	215	MET
1	A	243	ASN
1	A	267	LYS
1	A	276	THR
1	A	280	LEU
1	A	287	GLU
1	A	292	LYS
1	A	298	THR
1	A	305	ARG
1	A	314	GLU
1	A	317	ILE
1	A	337	ILE
1	A	342	LYS
1	A	362	LEU
1	A	363	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	430	MET
1	A	442	LEU
1	A	445	SER
1	A	448	GLU
1	A	466	THR
1	A	469	GLU
1	A	475	SER
1	A	480	SER
1	A	494	GLU
2	B	-1	PHE
2	B	1	MET

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Mol	Chain	Res	Type
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	130	LYS
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	244	GLU
2	B	271	LYS
2	B	287	GLU
2	B	317	ILE
2	B	335	SER
2	B	337	ILE
2	B	346	SER
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
2	B	491	MET
2	B	501	ARG
1	C	21	GLU
1	C	65	LEU
1	C	75	ILE
1	C	78	ILE
1	C	85	GLU
1	C	91	ASP

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Mol	Chain	Res	Type
1	C	94	THR
1	C	96	GLU
1	C	98	LEU
1	C	113	THR
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	215	MET
1	C	227	LEU
1	C	234	ASP
1	C	245	ARG
1	C	266	GLU
1	C	280	LEU
1	C	287	GLU
1	C	305	ARG
1	C	317	ILE
1	C	336	HIS
1	C	337	ILE
1	C	342	LYS
1	C	362	LEU
1	C	363	LEU
1	C	366	TYR
1	C	412	LEU
1	C	415	SER
1	C	436	LEU
1	C	448	GLU
1	C	472	LYS
1	C	476	ARG
1	C	480	SER
1	C	485	SER
1	C	508	LYS
2	D	30	GLN
2	D	65	LEU
2	D	66	ARG
2	D	84	ARG
2	D	92	ARG
2	D	94	THR
2	D	95	LYS
2	D	98	LEU

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Mol	Chain	Res	Type
2	D	113	THR
2	D	146	ARG
2	D	160	ARG
2	D	173	LEU
2	D	174	MET
2	D	177	LEU
2	D	233	THR
2	D	286	GLU
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	363	LEU
2	D	366	TYR
2	D	412	LEU
2	D	413	ASN
2	D	415	SER
2	D	424	SER
2	D	441	ILE
2	D	448	GLU
2	D	469	GLU
2	D	480	SER
2	D	483	THR
2	D	491	MET
2	D	494	GLU
2	D	501	ARG
2	D	504	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	29	HIS
1	A	82	ASN
1	A	83	GLN
1	A	189	ASN
1	A	224	ASN
1	A	262	ASN

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Mol	Chain	Res	Type
1	A	272	ASN
1	A	336	HIS
1	A	393	GLN
1	A	400	ASN
1	A	413	ASN
2	B	23	GLN
2	B	29	HIS
2	B	36	HIS
2	B	224	ASN
2	B	243	ASN
2	B	332	ASN
2	B	351	GLN
2	B	393	GLN
2	B	413	ASN
1	C	23	GLN
1	C	30	GLN
1	C	83	GLN
1	C	224	ASN
1	C	243	ASN
1	C	272	ASN
1	C	351	GLN
2	D	23	GLN
2	D	224	ASN
2	D	243	ASN
2	D	272	ASN
2	D	386	HIS

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	C	12	1	8,10,11	1.58	1 (12%)	10,14,16	1.67	4 (40%)
1	TPO	A	12	1	8,10,11	1.54	1 (12%)	10,14,16	1.93	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	C	12	1	-	5/9/11/13	-
1	TPO	A	12	1	-	4/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	TPO	P-OG1	4.10	1.66	1.59
1	C	12	TPO	P-OG1	4.04	1.66	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	TPO	CG2-CB-CA	-4.69	104.12	113.26
1	C	12	TPO	CG2-CB-CA	-3.16	107.11	113.26
1	A	12	TPO	P-OG1-CB	2.92	131.25	123.33
1	C	12	TPO	OG1-P-O1P	-2.06	101.97	109.33
1	C	12	TPO	CB-CA-N	-2.05	100.80	114.17
1	C	12	TPO	P-OG1-CB	2.02	128.81	123.33

There are no chirality outliers.

All (9) 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
1	C	12	TPO	CB-OG1-P-O1P

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Mol	Chain	Res	Type	Atoms
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 oligosaccharides 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	0.42	0	5,5,5	0.50	0
3	GOL	D	601	-	5,5,5	0.41	0	5,5,5	1.86	2 (40%)
3	GOL	B	601	-	5,5,5	0.32	0	5,5,5	0.43	0
3	GOL	A	601	-	5,5,5	0.56	0	5,5,5	1.72	1 (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
3	GOL	C	601	-	-	2/4/4/4	-
3	GOL	D	601	-	-	1/4/4/4	-
3	GOL	B	601	-	-	2/4/4/4	-
3	GOL	A	601	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	GOL	C3-C2-C1	-2.72	101.81	111.80
3	D	601	GOL	C3-C2-C1	-2.67	102.02	111.80
3	D	601	GOL	O2-C2-C1	2.11	117.92	109.18

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	GOL	O1-C1-C2-C3
3	C	601	GOL	O1-C1-C2-C3
3	C	601	GOL	O1-C1-C2-O2
3	B	601	GOL	C1-C2-C3-O3
3	B	601	GOL	O2-C2-C3-O3
3	D	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 [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	512/518 (98%)	-0.52	1 (0%) 91 90	61, 99, 136, 174	1 (0%)
1	C	512/518 (98%)	-0.65	2 (0%) 88 87	61, 96, 122, 160	1 (0%)
2	B	513/518 (99%)	-0.70	0 100 100	58, 86, 110, 128	1 (0%)
2	D	513/518 (99%)	-0.65	0 100 100	56, 93, 117, 144	1 (0%)
All	All	2050/2072 (98%)	-0.63	3 (0%) 92 91	56, 93, 125, 174	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	LYS	2.2
1	C	367	TRP	2.2
1	C	425	LYS	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	C	12	11/12	0.85	0.09	74,88,131,136	0
1	TPO	A	12	11/12	0.86	0.08	64,83,113,122	0

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
3	GOL	D	601	6/6	0.87	0.10	77,82,84,88	0
3	GOL	A	601	6/6	0.88	0.11	78,87,102,117	0
3	GOL	B	601	6/6	0.90	0.08	75,89,99,101	0
3	GOL	C	601	6/6	0.94	0.07	70,76,82,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.