



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 AM UTC

PDB ID : 3WXJ / pdb_00003wxj
Title : Crystal structure of trypanosoma brucei gambiense glycerol kinase in complex with glycerol 3-phosphate
Authors : Balogun, E.O.; Inaoka, D.K.; Shiba, T.; Kido, Y.; Tsuge, C.; Nara, T.; Aoki, T.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Michels, P.A.M.; Kita, K.; Harada, S.
Deposited on : 2014-08-01
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

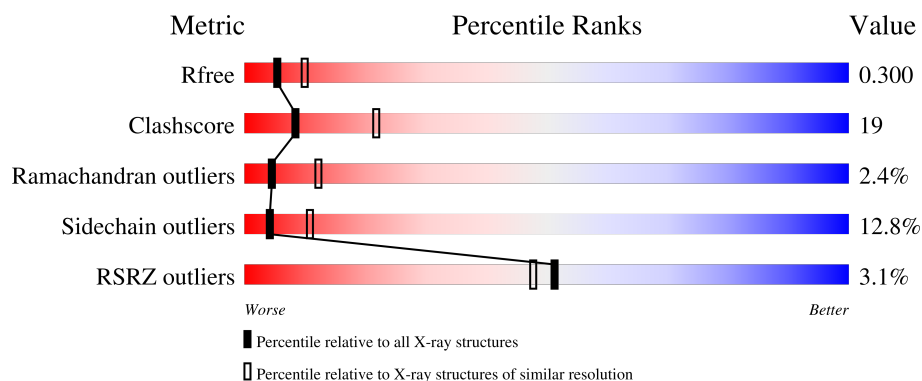
1 Overall quality at a glance

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	61% 31% 7%
1	B	518	4% 55% 38% 6%
1	C	518	2% 61% 32% 5%
1	D	518	5% 57% 32% 10%

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	G3P	C	701	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16015 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glycerol kinase.

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

There are 24 discrepancies between the modelled and reference sequences:

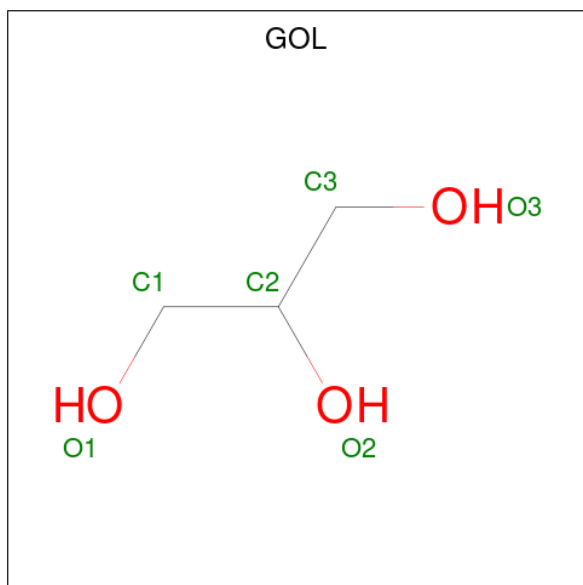
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP D3KVM3
A	-4	ILE	-	expression tag	UNP D3KVM3
A	-3	ASP	-	expression tag	UNP D3KVM3
A	-2	PRO	-	expression tag	UNP D3KVM3
A	-1	PHE	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
B	-5	GLY	-	expression tag	UNP D3KVM3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

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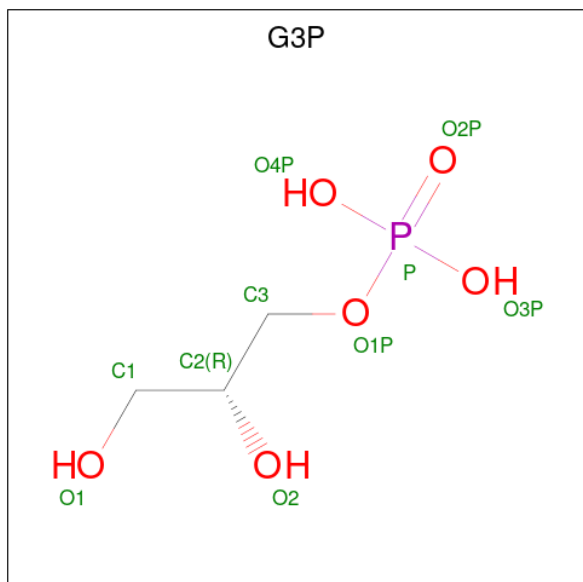
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PRO	-	expression tag	UNP D3KVM3
D	-1	PHE	-	expression tag	UNP D3KVM3
D	0	THR	-	expression tag	UNP D3KVM3

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



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

- Molecule 3 is SN-GLYCEROL-3-PHOSPHATE (CCD ID: G3P) (formula: $C_3H_9O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		

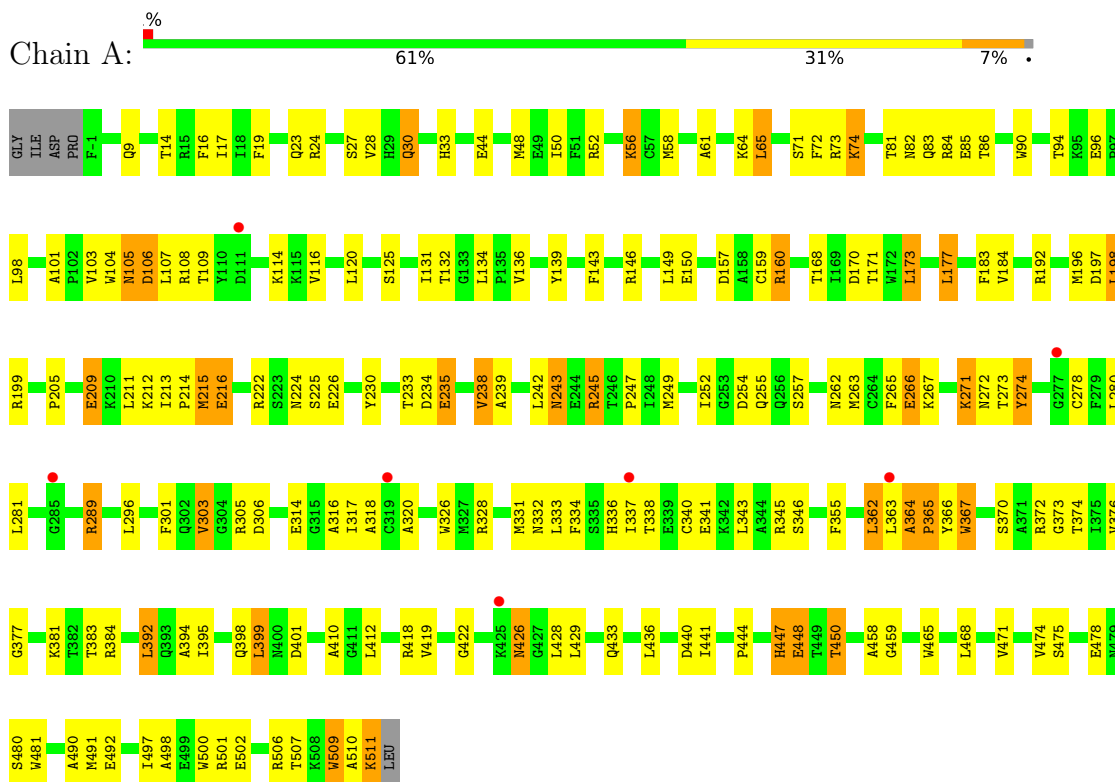
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	30	Total	O	0	0
			30	30		
4	C	38	Total	O	0	0
			38	38		
4	D	41	Total	O	0	0
			41	41		

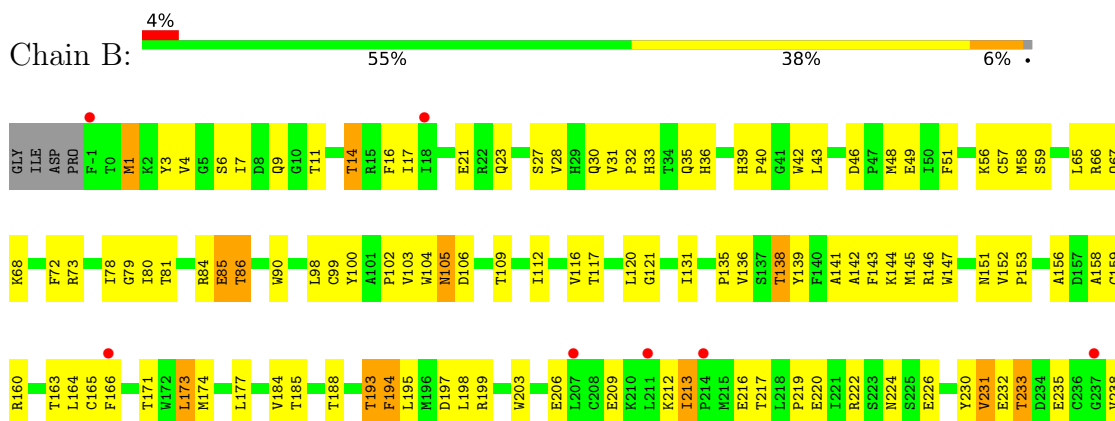
3 Residue-property plots [i](#)

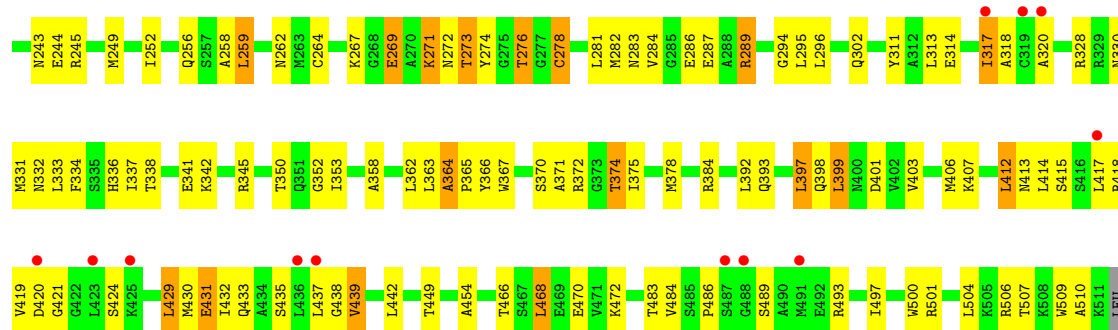
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

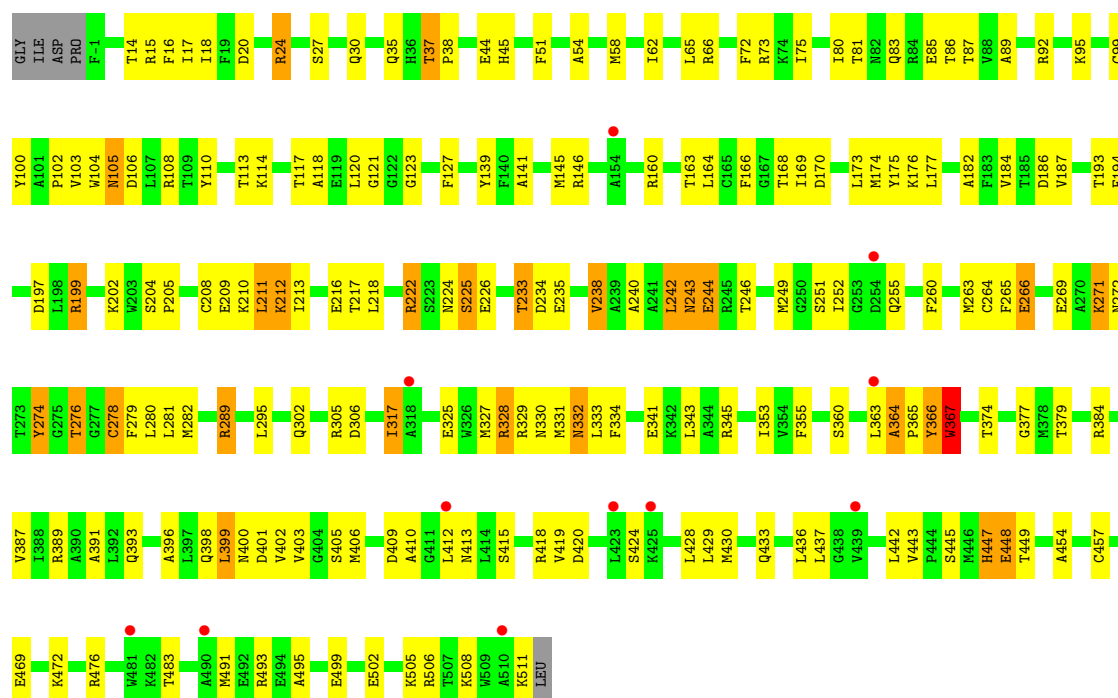


• Molecule 1: Glycerol kinase

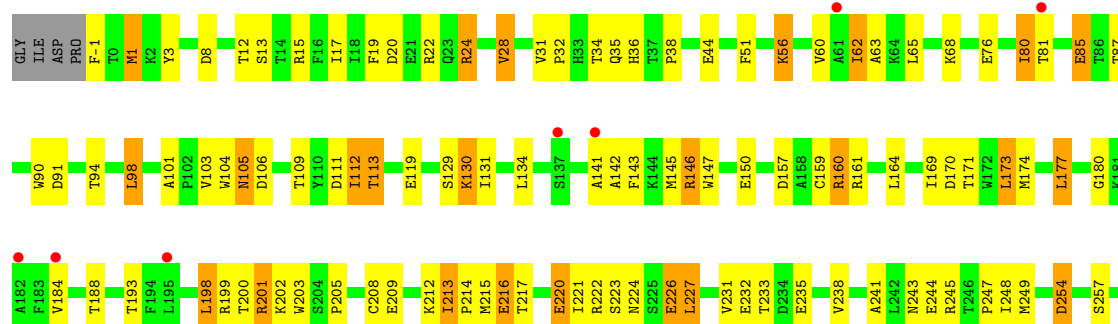


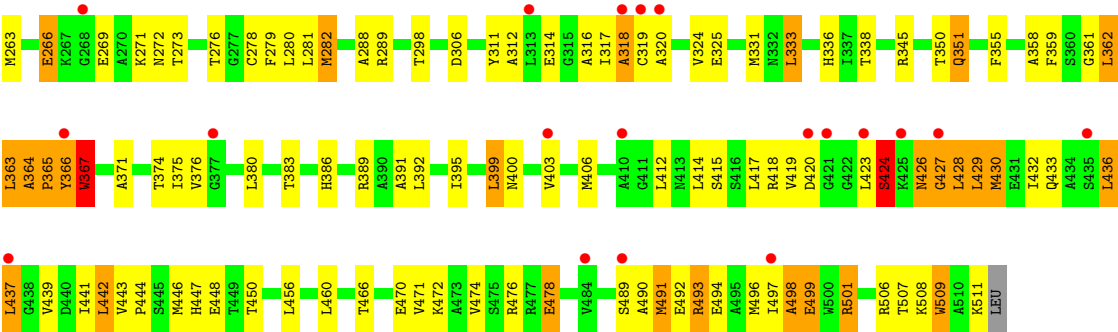


• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.17Å 120.89Å 153.55Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.70) 99.9 (50.00-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.290 0.220 , 0.300	Depositor DCC
R_{free} test set	3201 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
Reported twinning fraction	0.507 for H, K, L 0.493 for h,-k,-l	Depositor
Outliers	0 of 64493 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16015	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, G3P

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	0.66	0/4039	0.92	1/5465 (0.0%)
1	B	0.69	0/4039	0.94	4/5465 (0.1%)
1	C	0.65	0/4039	0.95	4/5465 (0.1%)
1	D	0.59	0/4039	0.97	9/5465 (0.2%)
All	All	0.65	0/16156	0.95	18/21860 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	427	GLY	N-CA-C	16.19	133.50	112.77
1	D	428	LEU	N-CA-C	8.19	122.44	109.50
1	C	243	ASN	N-CA-C	-6.79	100.26	110.24
1	D	430	MET	N-CA-C	-6.78	103.89	111.28
1	D	238	VAL	N-CA-C	6.50	116.53	110.42
1	B	193	THR	N-CA-C	6.23	118.15	111.36
1	D	426	ASN	CA-C-N	5.91	126.50	120.00
1	D	426	ASN	C-N-CA	5.91	126.50	120.00
1	C	240	ALA	N-CA-C	5.85	117.46	111.14
1	C	225	SER	N-CA-C	5.77	116.85	107.32
1	B	90	TRP	N-CA-C	5.28	115.25	108.34
1	D	276	THR	N-CA-C	-5.15	105.74	111.36
1	C	242	LEU	N-CA-C	-5.14	99.39	108.23
1	A	480	SER	N-CA-C	5.12	116.90	110.24
1	D	424	SER	N-CA-C	-5.09	105.91	112.68
1	B	86	THR	N-CA-C	-5.06	102.79	110.28
1	B	259	LEU	N-CA-C	-5.04	105.44	111.03
1	D	90	TRP	N-CA-C	5.03	114.94	108.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3957	0	3970	156	0
1	B	3957	0	3970	158	0
1	C	3957	0	3970	141	0
1	D	3957	0	3970	168	0
2	A	6	0	8	1	0
3	B	10	0	7	1	0
3	C	10	0	7	4	0
3	D	10	0	7	3	0
4	A	42	0	0	3	0
4	B	30	0	0	1	0
4	C	38	0	0	2	0
4	D	41	0	0	1	0
All	All	16015	0	15909	606	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 19.

All (606) 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:D:428:LEU:HD12	1:D:429:LEU:N	1.48	1.26
1:A:364:ALA:HB1	1:A:365:PRO:CD	1.71	1.20
1:B:364:ALA:HB1	1:B:365:PRO:HD3	1.23	1.19
1:A:364:ALA:CB	1:A:365:PRO:HD3	1.75	1.15
1:D:429:LEU:HD12	1:D:429:LEU:O	1.44	1.15
1:D:364:ALA:HB1	1:D:365:PRO:HD3	1.28	1.10
1:D:420:ASP:HB2	1:D:424:SER:HB3	1.26	1.09
1:B:198:LEU:HD23	1:B:198:LEU:O	1.50	1.09
1:A:274:TYR:HB2	1:A:422:GLY:HA3	1.26	1.07
1:C:276:THR:HG23	3:C:701:G3P:O3P	1.51	1.07
1:A:48:MET:O	1:A:52:ARG:HG3	1.52	1.07
1:D:428:LEU:HD12	1:D:429:LEU:H	0.89	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ALA:CB	1:A:365:PRO:CD	2.26	1.03
1:B:341:GLU:O	1:B:345:ARG:HG3	1.60	1.01
1:C:276:THR:CG2	3:C:701:G3P:O3P	2.10	0.99
1:D:428:LEU:CD1	1:D:429:LEU:H	1.74	0.99
1:B:364:ALA:HB1	1:B:365:PRO:CD	1.93	0.99
1:D:423:LEU:HG	1:D:426:ASN:OD1	1.63	0.97
1:A:105:ASN:HD22	1:A:105:ASN:H	1.02	0.97
1:B:226:GLU:O	1:B:249:MET:HA	1.66	0.96
1:D:428:LEU:O	1:D:429:LEU:HB3	1.61	0.95
1:D:428:LEU:CD1	1:D:429:LEU:N	2.30	0.95
1:A:306:ASP:OD1	1:C:212:LYS:HE3	1.67	0.93
1:C:367:TRP:HB2	4:C:817:HOH:O	1.68	0.92
1:D:364:ALA:HB1	1:D:365:PRO:CD	1.98	0.92
1:A:364:ALA:HB1	1:A:365:PRO:HD3	0.91	0.89
1:A:196:MET:HG2	1:A:197:ASP:H	1.36	0.89
1:A:105:ASN:HD22	1:A:105:ASN:N	1.70	0.88
1:B:105:ASN:HD22	1:B:105:ASN:H	1.21	0.88
1:C:199:ARG:H	1:C:199:ARG:HE	1.21	0.87
1:D:1:MET:HE1	1:D:20:ASP:HB2	1.54	0.87
1:C:364:ALA:HB1	1:C:365:PRO:HD3	1.53	0.87
1:B:284:VAL:HG11	1:B:313:LEU:HG	1.57	0.86
1:D:173:LEU:O	1:D:177:LEU:HB2	1.77	0.84
1:D:364:ALA:CB	1:D:365:PRO:CD	2.55	0.83
1:D:403:VAL:HG21	1:D:437:LEU:HD21	1.58	0.83
1:D:420:ASP:CB	1:D:424:SER:HB3	2.09	0.82
1:D:184:VAL:HG11	1:D:222:ARG:NH1	1.95	0.81
1:D:269:GLU:HB3	1:D:418:ARG:HH12	1.45	0.81
1:B:80:ILE:HD12	1:B:174:MET:HG3	1.60	0.81
1:A:222:ARG:HB3	1:A:226:GLU:OE1	1.82	0.80
1:A:341:GLU:O	1:A:345:ARG:HG3	1.82	0.79
1:B:198:LEU:O	1:B:198:LEU:CD2	2.29	0.79
1:B:336:HIS:HB3	1:B:338:THR:HG22	1.64	0.79
1:D:420:ASP:HB2	1:D:424:SER:CB	2.11	0.79
1:C:235:GLU:O	1:C:238:VAL:HG22	1.82	0.78
1:C:447:HIS:H	1:C:447:HIS:CD2	2.02	0.78
1:A:160:ARG:HG2	1:A:160:ARG:HH11	1.49	0.78
1:A:262:ASN:HD22	1:A:271:LYS:HB2	1.47	0.78
1:C:226:GLU:O	1:C:249:MET:HA	1.85	0.77
1:A:86:THR:HG23	1:A:103:VAL:HA	1.68	0.76
1:B:399:LEU:HG	1:B:433:GLN:HE22	1.51	0.76
1:D:491:MET:HG3	1:D:492:GLU:H	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASN:H	1:A:105:ASN:ND2	1.78	0.76
1:A:274:TYR:CB	1:A:422:GLY:HA3	2.14	0.76
1:D:497:ILE:O	1:D:501:ARG:HD3	1.84	0.76
1:C:168:THR:HG22	1:C:169:ILE:H	1.51	0.76
1:D:364:ALA:CB	1:D:365:PRO:HD3	2.11	0.76
1:D:429:LEU:O	1:D:429:LEU:CD1	2.30	0.76
1:C:364:ALA:CB	1:C:365:PRO:CD	2.64	0.76
1:B:271:LYS:HE2	1:B:281:LEU:HD13	1.68	0.75
1:B:318:ALA:H	1:B:363:LEU:HD13	1.52	0.75
1:A:345:ARG:HG2	1:A:428:LEU:HD22	1.67	0.75
1:D:199:ARG:HG2	1:D:288:ALA:HB3	1.67	0.74
1:D:490:ALA:O	1:D:494:GLU:HG2	1.87	0.74
1:C:366:TYR:HE1	1:C:401:ASP:OD1	1.69	0.74
1:B:364:ALA:CB	1:B:365:PRO:CD	2.65	0.74
1:C:222:ARG:HH21	1:C:305:ARG:HE	1.36	0.74
1:C:242:LEU:O	1:C:243:ASN:C	2.29	0.74
1:A:364:ALA:HB3	1:A:365:PRO:CD	2.17	0.74
1:A:274:TYR:HB2	1:A:422:GLY:CA	2.11	0.74
1:A:317:ILE:HD11	1:A:320:ALA:HB2	1.68	0.74
1:D:509:TRP:O	1:D:509:TRP:CG	2.33	0.74
1:D:15:ARG:NH1	1:D:448:GLU:OE1	2.20	0.74
1:D:160:ARG:HG2	1:D:160:ARG:HH11	1.51	0.73
1:D:429:LEU:HA	1:D:432:ILE:HD12	1.67	0.73
1:D:184:VAL:HG11	1:D:222:ARG:HH11	1.51	0.73
1:C:447:HIS:H	1:C:447:HIS:HD2	1.36	0.73
1:A:235:GLU:O	1:A:238:VAL:HG12	1.88	0.73
1:B:282:MET:HE2	1:B:414:LEU:HD13	1.69	0.72
1:B:42:TRP:HA	1:B:106:ASP:OD2	1.89	0.72
1:C:364:ALA:CB	1:C:365:PRO:HD3	2.17	0.72
1:A:17:ILE:HG12	1:A:28:VAL:HG23	1.70	0.71
1:C:72:PHE:CE2	1:C:75:ILE:HG13	2.25	0.71
1:D:1:MET:HE1	1:D:20:ASP:CB	2.19	0.71
1:D:200:THR:C	1:D:201:ARG:HE	1.97	0.71
1:C:419:VAL:HG21	1:C:430:MET:SD	2.30	0.71
1:B:147:TRP:O	1:B:151:ASN:HB2	1.90	0.71
1:C:105:ASN:H	1:C:105:ASN:HD22	1.39	0.70
1:A:233:THR:O	1:A:239:ALA:HB2	1.92	0.70
1:A:103:VAL:O	1:A:106:ASP:HB3	1.92	0.69
1:A:224:ASN:ND2	1:A:301:PHE:HA	2.07	0.69
1:A:83:GLN:O	1:A:83:GLN:HG3	1.92	0.69
1:A:255:GLN:NE2	2:A:601:GOL:H32	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:SER:O	1:D:443:VAL:HG11	1.93	0.69
1:B:282:MET:CE	1:B:414:LEU:HD13	2.23	0.69
1:C:72:PHE:HE2	1:C:75:ILE:HG13	1.56	0.68
1:B:105:ASN:H	1:B:105:ASN:ND2	1.92	0.68
1:D:51:PHE:HZ	1:D:233:THR:HG21	1.59	0.68
1:A:56:LYS:HE3	1:A:56:LYS:HA	1.76	0.68
1:B:198:LEU:HD23	1:B:198:LEU:C	2.17	0.67
1:D:423:LEU:HA	1:D:426:ASN:HB3	1.75	0.67
1:C:364:ALA:HB1	1:C:365:PRO:CD	2.23	0.67
1:D:423:LEU:CG	1:D:426:ASN:OD1	2.41	0.67
1:C:224:ASN:HD22	1:C:302:GLN:H	1.40	0.67
1:B:399:LEU:HG	1:B:433:GLN:NE2	2.09	0.67
1:C:289:ARG:HG2	1:C:410:ALA:HA	1.76	0.67
1:B:401:ASP:CG	1:B:501:ARG:HH22	2.03	0.67
1:A:271:LYS:HE2	1:A:281:LEU:HD13	1.76	0.66
1:C:243:ASN:O	1:C:244:GLU:HB2	1.95	0.66
1:A:509:TRP:NE1	1:B:352:GLY:O	2.29	0.66
1:D:374:THR:HG21	1:D:507:THR:HG22	1.78	0.66
1:B:320:ALA:HB3	4:B:728:HOH:O	1.96	0.66
1:A:362:LEU:O	1:A:367:TRP:HA	1.95	0.66
1:B:188:THR:HG21	1:B:252:ILE:HG13	1.77	0.65
1:C:364:ALA:O	1:C:367:TRP:HE3	1.79	0.65
1:D:426:ASN:HB2	4:D:712:HOH:O	1.96	0.65
1:D:429:LEU:HD12	1:D:429:LEU:C	2.18	0.65
1:D:281:LEU:HG	1:D:314:GLU:HB2	1.79	0.65
1:A:58:MET:HE2	1:A:238:VAL:CG2	2.27	0.65
1:B:197:ASP:OD2	1:B:199:ARG:N	2.30	0.65
1:B:331:MET:HB3	1:B:333:LEU:HG	1.79	0.65
1:A:280:LEU:HD13	1:A:399:LEU:HD11	1.78	0.64
1:C:92:ARG:HB2	1:C:163:THR:O	1.98	0.64
1:D:85:GLU:HB2	1:D:104:TRP:HB3	1.78	0.64
1:D:200:THR:HA	1:D:201:ARG:HH21	1.62	0.64
1:B:105:ASN:HD22	1:B:105:ASN:N	1.90	0.64
1:C:429:LEU:HG	1:C:430:MET:HE2	1.79	0.64
1:B:197:ASP:OD2	1:B:197:ASP:C	2.41	0.63
1:C:197:ASP:OD1	1:C:199:ARG:NH2	2.31	0.63
1:C:168:THR:HB	1:C:170:ASP:OD1	1.99	0.63
1:A:274:TYR:CD1	1:A:274:TYR:N	2.67	0.62
1:A:84:ARG:NH1	1:A:255:GLN:HB2	2.14	0.62
1:A:196:MET:HG2	1:A:197:ASP:N	2.12	0.62
1:A:146:ARG:NH1	1:A:212:LYS:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ARG:O	1:B:313:LEU:HD21	1.99	0.62
1:B:84:ARG:O	1:B:85:GLU:HB2	1.98	0.62
1:B:112:ILE:O	1:B:116:VAL:HG23	1.99	0.62
1:B:397:LEU:HG	1:B:500:TRP:CG	2.35	0.62
1:D:278:CYS:SG	1:D:320:ALA:HB3	2.40	0.62
1:D:266:GLU:HB2	1:D:269:GLU:HG3	1.81	0.61
1:C:95:LYS:O	1:C:176:LYS:NZ	2.32	0.61
1:B:276:THR:HB	3:B:601:G3P:O2P	2.00	0.61
1:B:224:ASN:HD22	1:B:302:GLN:H	1.49	0.61
1:B:203:TRP:HZ2	1:B:219:PRO:O	1.83	0.61
1:C:51:PHE:HE2	1:C:235:GLU:HG3	1.65	0.61
1:D:423:LEU:HG	1:D:426:ASN:CG	2.26	0.61
1:A:272:ASN:HB2	1:A:280:LEU:HD12	1.83	0.60
1:C:429:LEU:HG	1:C:430:MET:CE	2.31	0.60
1:D:419:VAL:HG23	1:D:443:VAL:HG22	1.83	0.60
1:D:272:ASN:HB2	1:D:280:LEU:HG	1.84	0.60
1:B:397:LEU:HD11	1:B:497:ILE:HG12	1.83	0.60
1:C:66:ARG:NH2	1:C:73:ARG:O	2.33	0.60
1:D:226:GLU:O	1:D:227:LEU:HB2	2.01	0.60
1:A:303:VAL:HG21	1:A:468:LEU:HD11	1.82	0.59
1:C:366:TYR:CE1	1:C:401:ASP:OD1	2.53	0.59
1:A:105:ASN:N	1:A:105:ASN:ND2	2.44	0.59
1:A:280:LEU:CD1	1:A:399:LEU:HD11	2.32	0.59
1:B:194:PHE:CD2	1:B:194:PHE:O	2.55	0.59
1:D:143:PHE:HA	1:D:146:ARG:HB3	1.85	0.59
1:D:509:TRP:O	1:D:509:TRP:CD1	2.55	0.59
1:D:177:LEU:HD12	1:D:231:VAL:HG13	1.83	0.59
1:A:384:ARG:HB3	1:B:331:MET:HA	1.85	0.59
1:A:332:ASN:ND2	1:B:332:ASN:O	2.34	0.59
1:B:267:LYS:HB2	1:B:412:LEU:HD21	1.84	0.59
1:C:243:ASN:O	1:C:244:GLU:CB	2.50	0.59
1:C:387:VAL:HG21	1:D:331:MET:HE1	1.85	0.59
1:C:54:ALA:O	1:C:58:MET:HG3	2.02	0.58
1:A:398:GLN:HG2	1:A:500:TRP:CZ2	2.38	0.58
1:C:193:THR:O	1:C:194:PHE:CB	2.52	0.58
1:B:16:PHE:HB2	1:B:57:CYS:HB3	1.85	0.58
1:C:271:LYS:HE2	1:C:281:LEU:HD13	1.84	0.58
1:D:318:ALA:HA	1:D:363:LEU:HD22	1.85	0.58
1:B:198:LEU:CD2	1:B:198:LEU:C	2.73	0.58
1:C:211:LEU:C	1:C:212:LYS:HD2	2.28	0.58
1:B:317:ILE:HD13	1:B:398:GLN:OE1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:VAL:O	1:A:478:GLU:HG2	2.02	0.58
1:B:399:LEU:O	1:B:403:VAL:HG23	2.03	0.58
1:A:73:ARG:O	1:A:74:LYS:HB3	2.04	0.57
1:C:224:ASN:ND2	1:C:302:GLN:H	2.01	0.57
1:D:169:ILE:O	1:D:173:LEU:HB2	2.03	0.57
1:A:490:ALA:C	1:A:492:GLU:H	2.11	0.57
1:A:365:PRO:HG3	1:A:401:ASP:HB3	1.86	0.57
1:D:429:LEU:HA	1:D:432:ILE:CD1	2.34	0.57
1:D:493:ARG:H	1:D:493:ARG:HD2	1.68	0.57
1:C:396:ALA:HA	1:C:433:GLN:OE1	2.05	0.57
1:C:212:LYS:HD2	1:C:212:LYS:N	2.20	0.57
1:B:233:THR:HG23	1:B:238:VAL:CG2	2.34	0.57
1:A:44:GLU:HA	1:A:103:VAL:HG23	1.87	0.56
1:D:316:ALA:O	1:D:364:ALA:N	2.38	0.56
1:A:274:TYR:HD1	1:A:274:TYR:H	1.53	0.56
1:A:364:ALA:HB3	1:A:365:PRO:HD2	1.87	0.56
1:B:195:LEU:HD11	1:B:213:ILE:HG13	1.86	0.56
1:A:214:PRO:C	1:A:216:GLU:H	2.14	0.56
1:A:274:TYR:N	1:A:274:TYR:HD1	2.03	0.56
1:B:51:PHE:HE2	1:B:235:GLU:HG3	1.69	0.56
1:C:87:THR:HG21	1:C:145:MET:HG3	1.87	0.56
1:D:429:LEU:HD11	1:D:433:GLN:HG3	1.87	0.56
1:A:336:HIS:C	1:A:338:THR:H	2.13	0.56
1:B:274:TYR:HB2	1:B:421:GLY:HA3	1.87	0.56
1:B:370:SER:HA	1:B:510:ALA:HB3	1.88	0.56
1:B:17:ILE:HG12	1:B:28:VAL:HG23	1.87	0.56
1:D:247:PRO:HB2	1:D:249:MET:HG3	1.88	0.56
1:A:114:LYS:C	1:A:116:VAL:H	2.14	0.56
1:A:392:LEU:HA	1:A:395:ILE:HD12	1.87	0.56
1:B:193:THR:O	1:B:194:PHE:CB	2.54	0.55
1:C:66:ARG:HH12	1:C:243:ASN:ND2	2.04	0.55
1:B:103:VAL:HG12	1:B:104:TRP:H	1.71	0.55
1:C:80:ILE:HD12	1:C:174:MET:HG3	1.88	0.55
1:C:199:ARG:H	1:C:199:ARG:NE	1.99	0.55
1:A:107:LEU:C	1:A:109:THR:H	2.14	0.55
1:A:157:ASP:OD2	1:A:160:ARG:NH2	2.38	0.55
1:D:19:PHE:HA	1:D:24:ARG:O	2.06	0.55
1:B:51:PHE:CE2	1:B:235:GLU:HG3	2.41	0.55
1:D:497:ILE:O	1:D:501:ARG:CD	2.54	0.55
1:B:264:CYS:SG	1:B:418:ARG:NH1	2.80	0.55
1:C:255:GLN:OE1	1:C:279:PHE:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASP:HA	1:A:239:ALA:HB3	1.89	0.55
1:A:497:ILE:O	1:A:501:ARG:HG2	2.06	0.55
1:C:508:LYS:O	1:D:506:ARG:NH2	2.39	0.55
1:B:509:TRP:O	1:B:510:ALA:C	2.49	0.55
1:A:296:LEU:HB2	1:A:314:GLU:HB3	1.89	0.55
1:A:334:PHE:CE2	1:A:340:CYS:HB2	2.42	0.55
1:B:1:MET:HE1	1:B:21:GLU:HG2	1.89	0.55
1:B:46:ASP:HB2	1:B:100:TYR:HE2	1.72	0.54
1:C:328:ARG:C	1:C:328:ARG:HE	2.15	0.54
1:A:222:ARG:HG2	1:A:305:ARG:HH22	1.71	0.54
1:C:208:CYS:HB3	1:C:213:ILE:O	2.06	0.54
1:C:197:ASP:CG	1:C:199:ARG:HH21	2.15	0.54
1:C:274:TYR:N	1:C:274:TYR:CD1	2.76	0.54
1:B:272:ASN:HB2	1:B:417:LEU:HD11	1.89	0.54
1:C:85:GLU:OE1	3:C:701:G3P:O1	2.21	0.54
1:C:89:ALA:HB2	1:C:166:PHE:CE2	2.42	0.54
1:C:226:GLU:OE2	1:C:305:ARG:HA	2.07	0.54
1:B:99:CYS:HB3	1:B:152:VAL:HG11	1.90	0.54
1:A:318:ALA:HB2	1:A:363:LEU:HD13	1.90	0.54
1:B:194:PHE:O	1:B:194:PHE:HD2	1.91	0.54
1:A:224:ASN:HD21	1:A:301:PHE:HA	1.70	0.54
1:B:403:VAL:HG21	1:B:437:LEU:HD11	1.90	0.54
1:A:58:MET:HE2	1:A:238:VAL:HG23	1.89	0.53
1:B:220:GLU:HB3	1:B:222:ARG:HH12	1.72	0.53
1:D:105:ASN:HD22	1:D:105:ASN:H	1.56	0.53
1:D:298:THR:HG23	1:D:312:ALA:HB3	1.90	0.53
1:D:317:ILE:HD11	1:D:399:LEU:HD22	1.90	0.53
1:B:135:PRO:HD2	1:B:296:LEU:HD23	1.90	0.53
1:B:159:CYS:HB2	1:B:164:LEU:HD22	1.90	0.53
1:B:184:VAL:HG12	1:B:222:ARG:NH1	2.23	0.53
1:D:62:ILE:HG22	1:D:63:ALA:N	2.22	0.53
1:B:141:ALA:HB3	1:B:193:THR:HA	1.91	0.53
1:D:282:MET:O	1:D:312:ALA:HA	2.09	0.53
1:B:224:ASN:ND2	1:B:302:GLN:H	2.06	0.53
1:C:506:ARG:NH2	1:D:508:LYS:O	2.32	0.53
1:D:358:ALA:HB2	1:D:362:LEU:HD13	1.91	0.53
1:D:400:ASN:CG	1:D:436:LEU:HD12	2.34	0.53
1:B:294:GLY:O	1:B:367:TRP:CZ3	2.62	0.53
1:D:429:LEU:CD1	1:D:433:GLN:HG3	2.39	0.52
1:B:331:MET:CB	1:B:333:LEU:HG	2.39	0.52
1:C:15:ARG:HE	1:C:30:GLN:HE21	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLU:OE1	1:C:305:ARG:HD3	2.09	0.52
1:C:424:SER:HB3	1:C:443:VAL:HG13	1.92	0.52
1:D:13:SER:HA	1:D:32:PRO:HA	1.92	0.52
1:D:214:PRO:HB3	1:D:216:GLU:OE1	2.09	0.52
1:A:27:SER:HB2	1:A:65:LEU:HG	1.91	0.52
1:B:318:ALA:H	1:B:363:LEU:CD1	2.23	0.52
1:D:355:PHE:CD2	1:D:375:ILE:HG12	2.44	0.52
1:B:171:THR:OG1	1:B:185:THR:HB	2.09	0.52
1:D:1:MET:CE	1:D:20:ASP:HB2	2.34	0.52
1:A:373:GLY:HA3	1:B:378:MET:HB2	1.92	0.52
1:A:429:LEU:O	1:A:433:GLN:HB2	2.09	0.52
1:B:197:ASP:OD2	1:B:198:LEU:N	2.43	0.52
1:B:362:LEU:HB2	1:B:371:ALA:HB3	1.92	0.52
1:C:199:ARG:HE	1:C:199:ARG:N	2.00	0.52
1:D:17:ILE:HG13	1:D:28:VAL:HB	1.91	0.52
1:B:414:LEU:HG	1:B:439:VAL:HG11	1.92	0.52
1:C:168:THR:HG22	1:C:169:ILE:N	2.22	0.52
1:D:157:ASP:O	1:D:161:ARG:HG3	2.10	0.52
1:A:90:TRP:CZ2	1:A:183:PHE:CE1	2.99	0.51
1:B:36:HIS:O	1:B:43:LEU:HA	2.11	0.51
1:D:221:ILE:HG22	1:D:222:ARG:N	2.24	0.51
1:D:257:SER:OG	1:D:450:THR:O	2.24	0.51
1:C:51:PHE:CE2	1:C:235:GLU:HG3	2.45	0.51
1:C:327:MET:HB3	1:C:333:LEU:HD12	1.93	0.51
1:A:84:ARG:NH2	1:A:314:GLU:OE2	2.43	0.51
1:B:1:MET:HE2	1:B:1:MET:HA	1.90	0.51
1:B:131:ILE:O	1:B:198:LEU:N	2.43	0.51
1:B:358:ALA:HB2	1:B:362:LEU:HD13	1.91	0.51
1:D:423:LEU:CD2	1:D:430:MET:SD	2.98	0.51
1:D:489:SER:H	1:D:493:ARG:NH1	2.07	0.51
1:A:345:ARG:NH2	1:A:428:LEU:HB2	2.25	0.51
1:D:319:CYS:O	1:D:320:ALA:C	2.53	0.51
1:C:272:ASN:OD1	1:C:274:TYR:CZ	2.63	0.51
1:B:431:GLU:HA	1:B:484:VAL:HG11	1.93	0.51
1:C:81:THR:HB	1:C:454:ALA:HB2	1.93	0.51
1:C:108:ARG:C	1:C:110:TYR:H	2.18	0.51
1:D:91:ASP:HB2	1:D:98:LEU:HD11	1.93	0.51
1:A:502:GLU:O	1:A:506:ARG:NH1	2.43	0.51
1:B:203:TRP:CZ2	1:B:219:PRO:O	2.64	0.50
1:B:1:MET:HE1	1:B:21:GLU:CD	2.36	0.50
1:A:24:ARG:HH11	1:A:478:GLU:HB3	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PRO:O	1:A:209:GLU:HB2	2.11	0.50
1:C:360:SER:OG	1:D:380:LEU:HD11	2.12	0.50
1:A:136:VAL:HG13	1:A:143:PHE:CE1	2.46	0.50
1:A:265:PHE:C	1:A:266:GLU:HG2	2.36	0.50
1:B:198:LEU:CD2	1:B:311:TYR:HE1	2.25	0.50
1:B:278:CYS:HB3	1:B:317:ILE:O	2.11	0.50
1:D:318:ALA:HA	1:D:363:LEU:HD13	1.93	0.50
1:D:441:ILE:HG23	1:D:441:ILE:O	2.10	0.50
1:C:331:MET:O	1:C:332:ASN:C	2.54	0.50
1:D:24:ARG:HH11	1:D:478:GLU:HB3	1.76	0.50
1:A:447:HIS:ND1	1:A:447:HIS:N	2.50	0.50
1:B:139:TYR:O	1:B:144:LYS:HE2	2.12	0.50
1:B:103:VAL:HG12	1:B:104:TRP:N	2.26	0.50
1:C:141:ALA:HB3	1:C:193:THR:HG22	1.92	0.50
1:B:102:PRO:HB2	1:B:144:LYS:HD3	1.93	0.50
1:D:56:LYS:HE2	1:D:60:VAL:HG23	1.93	0.50
1:D:418:ARG:HA	1:D:442:LEU:O	2.12	0.50
1:C:328:ARG:HB2	1:C:334:PHE:CE2	2.47	0.49
1:D:266:GLU:HG2	1:D:269:GLU:OE2	2.12	0.49
1:A:341:GLU:OE1	1:A:426:ASN:HA	2.13	0.49
1:C:16:PHE:CZ	1:C:58:MET:HE3	2.48	0.49
1:D:429:LEU:CA	1:D:432:ILE:HD12	2.41	0.49
1:B:116:VAL:HA	1:B:120:LEU:HD12	1.95	0.49
1:C:44:GLU:HA	1:C:103:VAL:HG23	1.95	0.49
1:C:364:ALA:HB3	1:C:365:PRO:CD	2.43	0.49
1:D:203:TRP:NE1	1:D:221:ILE:HG13	2.28	0.49
1:A:81:THR:OG1	1:A:254:ASP:HA	2.13	0.49
1:A:90:TRP:CZ2	1:A:183:PHE:HE1	2.31	0.49
1:A:366:TYR:O	1:A:367:TRP:C	2.55	0.49
1:B:7:ILE:HD12	1:B:80:ILE:HG12	1.95	0.49
1:B:1:MET:HE1	1:B:21:GLU:CG	2.43	0.49
1:B:284:VAL:CG1	1:B:313:LEU:HG	2.36	0.49
1:D:491:MET:HG2	1:D:493:ARG:NH1	2.28	0.49
1:A:9:GLN:NE2	1:A:50:ILE:HG23	2.27	0.49
1:C:364:ALA:O	1:C:367:TRP:CE3	2.64	0.49
1:B:256:GLN:O	1:B:259:LEU:HB3	2.13	0.49
1:C:325:GLU:O	1:C:329:ARG:N	2.44	0.49
1:C:398:GLN:O	1:C:402:VAL:HG23	2.13	0.49
1:D:160:ARG:HH11	1:D:160:ARG:CG	2.22	0.49
1:D:414:LEU:HB2	1:D:439:VAL:HG11	1.94	0.48
1:A:23:GLN:NE2	4:A:737:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLU:C	1:B:23:GLN:H	2.21	0.48
1:B:328:ARG:HB2	1:B:334:PHE:CZ	2.48	0.48
1:D:129:SER:C	1:D:131:ILE:H	2.21	0.48
1:D:437:LEU:HD22	1:D:439:VAL:HG22	1.96	0.48
1:C:81:THR:HA	1:C:252:ILE:O	2.14	0.48
1:C:263:MET:HA	1:C:265:PHE:CE1	2.49	0.48
1:C:271:LYS:O	1:C:280:LEU:HD12	2.14	0.48
1:D:188:THR:CG2	1:D:224:ASN:HD21	2.26	0.48
1:A:318:ALA:CB	1:A:363:LEU:HD13	2.43	0.48
1:D:494:GLU:HA	1:D:497:ILE:HD12	1.95	0.48
1:C:145:MET:HE1	1:C:218:LEU:HD21	1.96	0.48
1:A:125:SER:O	1:A:136:VAL:HG23	2.14	0.48
1:C:186:ASP:HB3	1:C:251:SER:HB3	1.96	0.48
1:D:184:VAL:HG12	1:D:220:GLU:HB3	1.96	0.48
1:D:428:LEU:CG	1:D:429:LEU:N	2.77	0.48
1:B:230:TYR:CD2	1:B:245:ARG:HG2	2.49	0.48
1:A:331:MET:HA	1:B:384:ARG:HB3	1.95	0.47
1:A:383:THR:HA	1:B:330:ASN:HB3	1.96	0.47
1:C:35:GLN:HE22	1:C:45:HIS:HE2	1.62	0.47
1:D:62:ILE:HG21	1:D:241:ALA:HB1	1.96	0.47
1:C:282:MET:HB3	1:C:406:MET:SD	2.54	0.47
1:A:64:LYS:HE3	4:A:715:HOH:O	2.14	0.47
1:A:267:LYS:HD2	1:A:412:LEU:HD22	1.95	0.47
1:A:326:TRP:C	1:A:328:ARG:H	2.21	0.47
1:A:9:GLN:NE2	1:A:14:THR:OG1	2.47	0.47
1:A:198:LEU:HD23	1:A:198:LEU:HA	1.71	0.47
1:B:401:ASP:OD2	1:B:501:ARG:NH2	2.46	0.47
1:B:39:HIS:HB3	1:B:40:PRO:HD2	1.96	0.47
1:A:197:ASP:O	1:A:198:LEU:C	2.56	0.47
1:C:17:ILE:HD13	1:C:448:GLU:HG3	1.96	0.47
1:C:37:THR:O	1:C:38:PRO:C	2.56	0.47
1:C:66:ARG:HD3	4:C:803:HOH:O	2.15	0.47
1:D:392:LEU:HD22	1:D:429:LEU:HD22	1.96	0.47
1:B:81:THR:HA	1:B:252:ILE:O	2.14	0.47
1:C:51:PHE:CE1	1:C:176:LYS:HB3	2.50	0.47
1:A:271:LYS:NZ	1:A:273:THR:OG1	2.48	0.46
1:A:372:ARG:O	1:A:374:THR:HG22	2.16	0.46
1:B:466:THR:N	1:B:470:GLU:OE1	2.40	0.46
1:C:225:SER:OG	1:C:457:CYS:O	2.33	0.46
1:A:44:GLU:HA	1:A:101:ALA:O	2.16	0.46
1:D:104:TRP:CD2	3:D:601:G3P:H12	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:474:VAL:O	1:D:478:GLU:HG2	2.14	0.46
1:A:490:ALA:C	1:A:492:GLU:N	2.74	0.46
1:B:198:LEU:CD2	1:B:311:TYR:CE1	2.98	0.46
1:C:102:PRO:HB3	1:C:108:ARG:CZ	2.46	0.46
1:D:159:CYS:HB2	1:D:164:LEU:HD22	1.96	0.46
1:A:33:HIS:ND1	4:A:739:HOH:O	2.35	0.46
1:B:273:THR:O	1:B:278:CYS:HA	2.16	0.46
1:D:22:ARG:HD2	1:D:478:GLU:CD	2.40	0.46
1:A:65:LEU:HD13	1:A:72:PHE:CG	2.50	0.46
1:D:112:ILE:HD12	1:D:112:ILE:H	1.80	0.46
1:A:374:THR:HG21	1:A:507:THR:HA	1.96	0.46
1:B:317:ILE:O	1:B:317:ILE:HG13	2.16	0.46
1:D:44:GLU:HA	1:D:101:ALA:O	2.16	0.46
1:D:141:ALA:HB3	1:D:193:THR:HA	1.98	0.46
1:C:269:GLU:CD	1:C:418:ARG:HH12	2.24	0.46
1:D:12:THR:HA	1:D:35:GLN:NE2	2.30	0.46
1:D:426:ASN:CG	1:D:427:GLY:N	2.74	0.46
1:B:145:MET:HE2	1:B:166:PHE:HB3	1.97	0.46
1:D:103:VAL:O	1:D:104:TRP:C	2.59	0.46
1:D:203:TRP:O	1:D:205:PRO:HD3	2.16	0.46
1:D:198:LEU:HD22	1:D:311:TYR:CE1	2.51	0.45
1:D:441:ILE:O	1:D:441:ILE:CG2	2.64	0.45
1:B:273:THR:HG22	1:B:420:ASP:OD1	2.16	0.45
1:D:142:ALA:HA	1:D:145:MET:HE3	1.96	0.45
1:A:363:LEU:O	1:A:364:ALA:C	2.58	0.45
1:B:374:THR:HG21	1:B:507:THR:HA	1.98	0.45
1:C:14:THR:C	1:C:15:ARG:HG3	2.40	0.45
1:A:343:LEU:HD21	1:A:384:ARG:HH21	1.81	0.45
1:C:20:ASP:OD1	1:C:24:ARG:N	2.30	0.45
1:C:264:CYS:HB3	1:C:269:GLU:O	2.17	0.45
1:D:80:ILE:HD12	1:D:174:MET:HG3	1.97	0.45
1:D:174:MET:HG2	1:D:248:ILE:HG21	1.98	0.45
1:B:392:LEU:HB3	1:B:429:LEU:HD13	1.98	0.45
1:C:175:TYR:HA	1:C:182:ALA:O	2.16	0.45
1:C:396:ALA:HB1	1:C:436:LEU:HD12	1.97	0.45
1:B:66:ARG:O	1:B:67:GLN:C	2.60	0.45
1:B:419:VAL:HG11	1:B:430:MET:SD	2.57	0.45
1:B:3:TYR:CD2	1:B:72:PHE:HD2	2.35	0.45
1:B:46:ASP:HB3	1:B:49:GLU:HB2	1.99	0.45
1:B:86:THR:HG23	1:B:103:VAL:HA	1.98	0.45
1:B:156:ALA:HB1	1:B:160:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:GLU:O	1:B:406:MET:HE3	2.16	0.45
1:B:500:TRP:NE1	1:B:504:LEU:HD11	2.32	0.45
1:C:295:LEU:HD13	1:C:406:MET:HG2	1.99	0.45
1:A:230:TYR:HA	1:A:247:PRO:HA	1.99	0.45
1:D:498:ALA:O	1:D:501:ARG:NE	2.47	0.45
1:B:350:THR:HB	1:B:353:ILE:HG12	1.99	0.45
1:C:233:THR:OG1	1:C:234:ASP:N	2.50	0.45
1:D:263:MET:HE1	1:D:456:LEU:HD11	1.99	0.45
1:D:351:GLN:HG2	1:D:386:HIS:CD2	2.52	0.45
1:B:46:ASP:OD2	1:B:48:MET:HB2	2.17	0.44
1:C:85:GLU:HB3	1:C:139:TYR:O	2.16	0.44
1:A:146:ARG:NH2	1:A:150:GLU:OE2	2.50	0.44
1:B:222:ARG:HD3	1:B:226:GLU:CD	2.43	0.44
1:B:258:ALA:O	1:B:262:ASN:ND2	2.50	0.44
1:B:497:ILE:O	1:B:500:TRP:HB3	2.17	0.44
1:D:109:THR:HG22	1:D:147:TRP:HB2	1.99	0.44
1:A:90:TRP:HB2	1:A:96:GLU:O	2.17	0.44
1:B:142:ALA:O	1:B:145:MET:HB2	2.18	0.44
1:C:278:CYS:HB3	1:C:317:ILE:O	2.17	0.44
1:A:498:ALA:O	1:A:502:GLU:HG2	2.18	0.44
1:D:221:ILE:CG2	1:D:222:ARG:N	2.80	0.44
1:D:429:LEU:HA	1:D:432:ILE:CG1	2.47	0.44
1:C:110:TYR:O	1:C:113:THR:HB	2.16	0.44
1:C:121:GLY:HA3	1:C:127:PHE:CG	2.53	0.44
1:C:341:GLU:HG3	1:C:428:LEU:CB	2.47	0.44
1:A:249:MET:O	1:A:458:ALA:HA	2.17	0.44
1:C:242:LEU:HD13	1:C:246:THR:OG1	2.17	0.44
1:D:24:ARG:HH11	1:D:478:GLU:CB	2.31	0.44
1:D:279:PHE:CZ	3:D:601:G3P:H11	2.52	0.44
1:A:447:HIS:CD2	1:A:448:GLU:OE2	2.71	0.44
1:B:158:ALA:O	1:B:163:THR:OG1	2.33	0.44
1:B:16:PHE:CB	1:B:57:CYS:HB3	2.47	0.44
1:C:389:ARG:HG2	1:C:393:GLN:HE21	1.83	0.44
1:B:9:GLN:HG2	1:B:14:THR:HG23	2.00	0.43
1:C:16:PHE:CD2	1:C:58:MET:HA	2.53	0.43
1:A:107:LEU:O	1:A:109:THR:N	2.51	0.43
1:D:361:GLY:HA2	1:D:371:ALA:O	2.18	0.43
1:D:491:MET:HG3	1:D:492:GLU:N	2.25	0.43
1:A:459:GLY:HA3	1:A:465:TRP:CZ3	2.53	0.43
1:B:116:VAL:O	1:B:121:GLY:N	2.48	0.43
1:D:146:ARG:NH2	1:D:150:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:ILE:HG23	1:C:72:PHE:HE1	1.82	0.43
1:D:208:CYS:HB3	1:D:213:ILE:O	2.18	0.43
1:A:30:GLN:HE21	1:A:30:GLN:HB2	1.63	0.43
1:A:184:VAL:HG11	1:A:222:ARG:NH1	2.33	0.43
1:A:211:LEU:O	1:A:213:ILE:HD12	2.17	0.43
1:B:374:THR:CG2	1:B:507:THR:HG22	2.48	0.43
1:C:355:PHE:C	1:C:355:PHE:CD2	2.95	0.43
1:D:498:ALA:O	1:D:499:GLU:C	2.61	0.43
1:A:159:CYS:SG	1:A:214:PRO:HG2	2.59	0.43
1:B:11:THR:O	1:B:33:HIS:CE1	2.72	0.43
1:B:136:VAL:HG13	1:B:143:PHE:CE1	2.53	0.43
1:C:243:ASN:N	1:C:243:ASN:HD22	2.14	0.43
1:C:447:HIS:O	1:C:448:GLU:CB	2.65	0.43
1:D:85:GLU:HB2	1:D:104:TRP:CB	2.48	0.43
1:A:160:ARG:HG2	1:A:160:ARG:NH1	2.25	0.43
1:A:192:ARG:NH2	1:A:314:GLU:OE2	2.52	0.43
1:B:78:ILE:HD12	1:B:231:VAL:HG21	2.01	0.43
1:B:393:GLN:HG2	1:B:432:ILE:HD13	1.99	0.43
1:C:18:ILE:HD12	1:C:27:SER:HB3	1.99	0.43
1:C:330:ASN:HB3	1:D:383:THR:HA	2.01	0.43
1:D:254:ASP:OD2	3:D:601:G3P:O2	2.30	0.43
1:B:116:VAL:HG11	1:B:143:PHE:HE1	1.83	0.43
1:B:489:SER:O	1:B:493:ARG:HB2	2.19	0.43
1:C:276:THR:HG21	3:C:701:G3P:O3P	2.12	0.43
1:C:495:ALA:O	1:C:499:GLU:HB2	2.17	0.43
1:D:3:TYR:O	1:D:76:GLU:N	2.51	0.43
1:A:19:PHE:HA	1:A:24:ARG:O	2.19	0.43
1:A:370:SER:O	1:A:509:TRP:N	2.49	0.43
1:B:406:MET:O	1:B:407:LYS:C	2.61	0.43
1:B:413:ASN:HB3	1:B:414:LEU:H	1.66	0.43
1:A:257:SER:OG	1:A:450:THR:O	2.37	0.43
1:B:6:SER:HA	1:B:79:GLY:O	2.19	0.43
1:C:168:THR:CG2	1:C:169:ILE:H	2.27	0.43
1:C:400:ASN:HA	1:C:437:LEU:HD21	2.00	0.43
1:C:493:ARG:HE	1:C:493:ARG:HB2	1.64	0.43
1:B:43:LEU:HD23	1:B:105:ASN:HD21	1.83	0.42
1:B:258:ALA:HB3	1:B:271:LYS:NZ	2.34	0.42
1:C:89:ALA:HB1	1:C:164:LEU:HD11	2.01	0.42
1:D:34:THR:HB	1:D:36:HIS:CE1	2.54	0.42
1:A:86:THR:O	1:A:168:THR:HA	2.19	0.42
1:A:160:ARG:HH11	1:A:160:ARG:CG	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LEU:HD12	1:B:173:LEU:HA	1.91	0.42
1:D:22:ARG:O	1:D:478:GLU:HG3	2.18	0.42
1:D:31:VAL:HG21	1:D:56:LYS:HG2	2.02	0.42
1:D:111:ASP:C	1:D:113:THR:H	2.27	0.42
1:D:414:LEU:O	1:D:415:SER:C	2.62	0.42
1:D:428:LEU:O	1:D:429:LEU:CB	2.43	0.42
1:A:132:THR:HB	1:A:134:LEU:HD12	2.01	0.42
1:C:341:GLU:HG3	1:C:428:LEU:HB3	2.01	0.42
1:C:379:THR:HA	1:D:359:PHE:HB3	2.01	0.42
1:C:193:THR:O	1:C:194:PHE:HB3	2.18	0.42
1:C:355:PHE:CD1	1:C:391:ALA:HB2	2.55	0.42
1:C:399:LEU:O	1:C:403:VAL:HG23	2.18	0.42
1:A:199:ARG:HE	1:A:199:ARG:HB2	1.74	0.42
1:B:35:GLN:HB3	1:B:43:LEU:HD11	2.01	0.42
1:D:351:GLN:HG2	1:D:386:HIS:HD2	1.83	0.42
1:A:377:GLY:HA2	1:B:372:ARG:CB	2.48	0.42
1:B:336:HIS:C	1:B:338:THR:N	2.77	0.42
1:D:366:TYR:O	1:D:367:TRP:C	2.62	0.42
1:D:497:ILE:O	1:D:501:ARG:NE	2.53	0.42
1:B:152:VAL:HA	1:B:153:PRO:HD3	1.92	0.42
1:C:118:ALA:HA	1:C:123:GLY:H	1.84	0.42
1:C:353:ILE:HG22	1:C:377:GLY:C	2.45	0.42
1:D:164:LEU:HD23	1:D:217:THR:HG21	2.02	0.42
1:D:419:VAL:O	1:D:444:PRO:HD2	2.20	0.42
1:C:66:ARG:NH1	1:C:243:ASN:ND2	2.68	0.42
1:C:260:PHE:CE1	1:C:265:PHE:HE2	2.38	0.42
1:D:142:ALA:HB2	1:D:193:THR:O	2.20	0.42
1:A:331:MET:HB3	1:A:333:LEU:HG	2.02	0.42
1:C:44:GLU:HG3	1:C:100:TYR:HD1	1.85	0.42
1:C:86:THR:O	1:C:168:THR:HG23	2.20	0.42
1:C:110:TYR:CZ	1:C:114:LYS:HE2	2.55	0.42
1:D:188:THR:HG23	1:D:224:ASN:HD21	1.84	0.42
1:D:423:LEU:HA	1:D:426:ASN:CB	2.46	0.42
1:B:31:VAL:HA	1:B:32:PRO:HD2	1.89	0.41
1:A:16:PHE:HD2	1:A:61:ALA:HB3	1.85	0.41
1:B:267:LYS:HA	1:B:283:ASN:HB3	2.02	0.41
1:C:266:GLU:HG2	1:C:269:GLU:CD	2.45	0.41
1:D:331:MET:HB2	1:D:333:LEU:HD12	2.02	0.41
1:D:493:ARG:HA	1:D:496:MET:HE3	2.01	0.41
1:A:263:MET:HE3	1:A:475:SER:HB2	2.01	0.41
1:B:438:GLY:O	1:B:439:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:VAL:N	1:B:486:PRO:HG3	2.35	0.41
1:D:112:ILE:HG21	1:D:146:ARG:HG2	2.03	0.41
1:A:173:LEU:O	1:A:177:LEU:HB2	2.20	0.41
1:A:226:GLU:O	1:A:249:MET:HA	2.21	0.41
1:A:336:HIS:HB3	1:A:338:THR:HG22	2.02	0.41
1:A:394:ALA:O	1:A:398:GLN:HG3	2.19	0.41
1:C:66:ARG:HH12	1:C:243:ASN:HD21	1.67	0.41
1:D:460:LEU:HD21	1:D:471:VAL:CG2	2.51	0.41
1:A:377:GLY:HA2	1:B:372:ARG:HB2	2.01	0.41
1:B:16:PHE:CD2	1:B:58:MET:HA	2.56	0.41
1:B:105:ASN:ND2	1:B:105:ASN:N	2.58	0.41
1:C:120:LEU:HD13	1:C:210:LYS:HB3	2.01	0.41
1:D:87:THR:HG21	1:D:145:MET:HG2	2.03	0.41
1:D:243:ASN:O	1:D:243:ASN:ND2	2.52	0.41
1:A:263:MET:SD	1:A:471:VAL:HG12	2.60	0.41
1:A:289:ARG:HG2	1:A:410:ALA:HA	2.03	0.41
1:B:269:GLU:HG3	1:B:415:SER:HB2	2.02	0.41
1:D:159:CYS:SG	1:D:214:PRO:HG2	2.61	0.41
1:D:345:ARG:NH1	1:D:428:LEU:HD13	2.35	0.41
1:A:214:PRO:O	1:A:216:GLU:N	2.52	0.41
1:A:398:GLN:HG2	1:A:500:TRP:CH2	2.55	0.41
1:C:447:HIS:CD2	1:C:447:HIS:N	2.76	0.41
1:A:243:ASN:HD22	1:A:243:ASN:HA	1.57	0.41
1:A:355:PHE:CD2	1:A:355:PHE:C	2.97	0.41
1:B:109:THR:OG1	1:B:138:THR:HG22	2.19	0.41
1:D:362:LEU:HD12	1:D:362:LEU:HA	1.95	0.41
1:D:466:THR:N	1:D:470:GLU:OE1	2.53	0.41
1:A:82:ASN:OD1	1:A:170:ASP:HB3	2.21	0.41
1:A:84:ARG:O	1:A:85:GLU:HB2	2.20	0.41
1:A:225:SER:HB3	1:A:303:VAL:HA	2.03	0.41
1:A:336:HIS:C	1:A:338:THR:N	2.79	0.41
1:B:81:THR:HB	1:B:454:ALA:HB2	2.03	0.41
1:C:62:ILE:HG23	1:C:72:PHE:CE1	2.56	0.41
1:D:198:LEU:HD22	1:D:311:TYR:HE1	1.86	0.41
1:A:419:VAL:O	1:A:444:PRO:HD2	2.21	0.41
1:A:510:ALA:O	1:A:511:LYS:C	2.64	0.41
1:B:468:LEU:HD23	1:B:468:LEU:N	2.35	0.41
1:C:333:LEU:HD21	1:D:331:MET:HE3	2.03	0.41
1:D:8:ASP:HB3	1:D:15:ARG:HG3	2.03	0.41
1:D:456:LEU:O	1:D:460:LEU:HG	2.21	0.41
1:A:85:GLU:HB3	1:A:139:TYR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HD13	1:A:399:LEU:CD1	2.49	0.40
1:A:316:ALA:O	1:A:364:ALA:N	2.47	0.40
1:C:15:ARG:NH1	1:C:448:GLU:OE1	2.54	0.40
1:C:164:LEU:O	1:C:217:THR:HG22	2.21	0.40
1:D:391:ALA:O	1:D:395:ILE:HG13	2.21	0.40
1:A:85:GLU:HB2	1:A:104:TRP:HB3	2.03	0.40
1:A:226:GLU:OE1	1:A:305:ARG:NH1	2.54	0.40
1:A:374:THR:HA	1:B:375:ILE:O	2.21	0.40
1:C:204:SER:HA	1:C:205:PRO:HD3	1.96	0.40
1:A:170:ASP:CG	1:A:171:THR:N	2.79	0.40
1:B:504:LEU:C	1:B:506:ARG:H	2.28	0.40
1:C:502:GLU:HA	1:C:505:LYS:HD2	2.03	0.40
1:A:214:PRO:C	1:A:216:GLU:N	2.75	0.40
1:A:233:THR:C	1:A:239:ALA:HB2	2.44	0.40
1:B:287:GLU:HB3	1:B:289:ARG:NH1	2.37	0.40
1:D:170:ASP:OD1	1:D:171:THR:N	2.54	0.40
1:D:364:ALA:HB3	1:D:366:TYR:CE2	2.56	0.40
1:A:107:LEU:C	1:A:109:THR:N	2.77	0.40
1:C:110:TYR:O	1:C:113:THR:N	2.51	0.40
1:D:24:ARG:NH1	1:D:478:GLU:HB3	2.37	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	511/518 (99%)	440 (86%)	57 (11%)	14 (3%)	4	10
1	B	511/518 (99%)	430 (84%)	73 (14%)	8 (2%)	7	20
1	C	511/518 (99%)	449 (88%)	54 (11%)	8 (2%)	7	20
1	D	511/518 (99%)	436 (85%)	56 (11%)	19 (4%)	2	6
All	All	2044/2072 (99%)	1755 (86%)	240 (12%)	49 (2%)	4	12

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	B	278	CYS
1	C	364	ALA
1	C	448	GLU
1	D	227	LEU
1	D	364	ALA
1	A	74	LYS
1	A	108	ARG
1	A	215	MET
1	A	245	ARG
1	A	337	ILE
1	A	367	TRP
1	A	426	ASN
1	B	364	ALA
1	C	244	GLU
1	C	278	CYS
1	C	367	TRP
1	D	318	ALA
1	D	367	TRP
1	D	491	MET
1	D	498	ALA
1	D	499	GLU
1	A	209	GLU
1	A	509	TRP
1	C	99	CYS
1	D	130	LYS
1	D	180	GLY
1	D	223	SER
1	D	244	GLU
1	D	336	HIS
1	D	365	PRO
1	D	509	TRP
1	A	491	MET
1	B	435	SER
1	C	332	ASN
1	D	226	GLU
1	D	254	ASP
1	A	365	PRO
1	B	342	LYS
1	C	104	TRP
1	D	38	PRO
1	D	363	LEU

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Mol	Chain	Res	Type
1	A	238	VAL
1	B	194	PHE
1	B	212	LYS
1	B	231	VAL
1	B	337	ILE
1	D	112	ILE
1	A	252	ILE

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	421/425 (99%)	379 (90%)	42 (10%)	7	19
1	B	421/425 (99%)	371 (88%)	50 (12%)	5	13
1	C	421/425 (99%)	367 (87%)	54 (13%)	4	11
1	D	421/425 (99%)	352 (84%)	69 (16%)	2	6
All	All	1684/1700 (99%)	1469 (87%)	215 (13%)	4	11

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	56	LYS
1	A	65	LEU
1	A	71	SER
1	A	94	THR
1	A	98	LEU
1	A	105	ASN
1	A	106	ASP
1	A	120	LEU
1	A	131	ILE
1	A	149	LEU
1	A	160	ARG
1	A	173	LEU
1	A	177	LEU

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Mol	Chain	Res	Type
1	A	198	LEU
1	A	215	MET
1	A	216	GLU
1	A	235	GLU
1	A	242	LEU
1	A	243	ASN
1	A	245	ARG
1	A	266	GLU
1	A	271	LYS
1	A	274	TYR
1	A	278	CYS
1	A	289	ARG
1	A	303	VAL
1	A	346	SER
1	A	362	LEU
1	A	376	VAL
1	A	381	LYS
1	A	392	LEU
1	A	399	LEU
1	A	418	ARG
1	A	436	LEU
1	A	440	ASP
1	A	441	ILE
1	A	447	HIS
1	A	448	GLU
1	A	450	THR
1	A	481	TRP
1	A	511	LYS
1	B	1	MET
1	B	4	VAL
1	B	14	THR
1	B	27	SER
1	B	30	GLN
1	B	56	LYS
1	B	59	SER
1	B	65	LEU
1	B	68	LYS
1	B	73	ARG
1	B	85	GLU
1	B	98	LEU
1	B	105	ASN
1	B	117	THR

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Mol	Chain	Res	Type
1	B	138	THR
1	B	146	ARG
1	B	165	CYS
1	B	173	LEU
1	B	177	LEU
1	B	206	GLU
1	B	209	GLU
1	B	213	ILE
1	B	216	GLU
1	B	217	THR
1	B	232	GLU
1	B	233	THR
1	B	243	ASN
1	B	244	GLU
1	B	269	GLU
1	B	271	LYS
1	B	273	THR
1	B	276	THR
1	B	286	GLU
1	B	289	ARG
1	B	295	LEU
1	B	317	ILE
1	B	366	TYR
1	B	374	THR
1	B	397	LEU
1	B	399	LEU
1	B	412	LEU
1	B	424	SER
1	B	429	LEU
1	B	431	GLU
1	B	439	VAL
1	B	442	LEU
1	B	449	THR
1	B	468	LEU
1	B	472	LYS
1	B	483	THR
1	C	24	ARG
1	C	37	THR
1	C	65	LEU
1	C	83	GLN
1	C	105	ASN
1	C	106	ASP

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Mol	Chain	Res	Type
1	C	117	THR
1	C	146	ARG
1	C	160	ARG
1	C	173	LEU
1	C	177	LEU
1	C	184	VAL
1	C	187	VAL
1	C	199	ARG
1	C	202	LYS
1	C	209	GLU
1	C	211	LEU
1	C	212	LYS
1	C	216	GLU
1	C	222	ARG
1	C	233	THR
1	C	238	VAL
1	C	266	GLU
1	C	271	LYS
1	C	274	TYR
1	C	276	THR
1	C	289	ARG
1	C	306	ASP
1	C	317	ILE
1	C	328	ARG
1	C	343	LEU
1	C	345	ARG
1	C	363	LEU
1	C	366	TYR
1	C	367	TRP
1	C	374	THR
1	C	384	ARG
1	C	399	LEU
1	C	405	SER
1	C	409	ASP
1	C	412	LEU
1	C	413	ASN
1	C	415	SER
1	C	420	ASP
1	C	442	LEU
1	C	445	SER
1	C	447	HIS
1	C	449	THR

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Mol	Chain	Res	Type
1	C	469	GLU
1	C	472	LYS
1	C	476	ARG
1	C	483	THR
1	C	491	MET
1	C	511	LYS
1	D	-1	PHE
1	D	1	MET
1	D	24	ARG
1	D	28	VAL
1	D	56	LYS
1	D	62	ILE
1	D	65	LEU
1	D	68	LYS
1	D	80	ILE
1	D	81	THR
1	D	85	GLU
1	D	94	THR
1	D	98	LEU
1	D	105	ASN
1	D	106	ASP
1	D	113	THR
1	D	119	GLU
1	D	130	LYS
1	D	134	LEU
1	D	146	ARG
1	D	160	ARG
1	D	173	LEU
1	D	177	LEU
1	D	198	LEU
1	D	201	ARG
1	D	202	LYS
1	D	209	GLU
1	D	212	LYS
1	D	213	ILE
1	D	215	MET
1	D	216	GLU
1	D	220	GLU
1	D	232	GLU
1	D	235	GLU
1	D	245	ARG
1	D	266	GLU

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Mol	Chain	Res	Type
1	D	271	LYS
1	D	273	THR
1	D	282	MET
1	D	289	ARG
1	D	306	ASP
1	D	324	VAL
1	D	325	GLU
1	D	333	LEU
1	D	338	THR
1	D	350	THR
1	D	351	GLN
1	D	362	LEU
1	D	366	TYR
1	D	367	TRP
1	D	376	VAL
1	D	389	ARG
1	D	399	LEU
1	D	406	MET
1	D	412	LEU
1	D	417	LEU
1	D	424	SER
1	D	429	LEU
1	D	436	LEU
1	D	437	LEU
1	D	442	LEU
1	D	446	MET
1	D	447	HIS
1	D	472	LYS
1	D	476	ARG
1	D	478	GLU
1	D	493	ARG
1	D	501	ARG
1	D	511	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	30	GLN
1	A	105	ASN
1	A	151	ASN
1	A	224	ASN

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Mol	Chain	Res	Type
1	A	243	ASN
1	A	255	GLN
1	A	262	ASN
1	A	272	ASN
1	A	293	HIS
1	A	336	HIS
1	A	398	GLN
1	A	479	ASN
1	B	30	GLN
1	B	67	GLN
1	B	105	ASN
1	B	151	ASN
1	B	302	GLN
1	B	336	HIS
1	B	351	GLN
1	B	433	GLN
1	C	23	GLN
1	C	30	GLN
1	C	35	GLN
1	C	105	ASN
1	C	151	ASN
1	C	224	ASN
1	C	243	ASN
1	C	272	ASN
1	C	351	GLN
1	C	393	GLN
1	C	447	HIS
1	D	23	GLN
1	D	36	HIS
1	D	67	GLN
1	D	105	ASN
1	D	151	ASN
1	D	224	ASN
1	D	302	GLN
1	D	332	ASN
1	D	413	ASN
1	D	447	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	GOL	A	601	-	5,5,5	0.46	0	5,5,5	0.48	0
3	G3P	B	601	-	9,9,9	0.62	0	10,12,12	0.78	0
3	G3P	C	701	-	9,9,9	1.33	1 (11%)	10,12,12	1.27	2 (20%)
3	G3P	D	601	-	9,9,9	1.78	4 (44%)	10,12,12	1.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	601	-	-	4/4/4/4	-
3	G3P	B	601	-	-	0/8/8/8	-
3	G3P	C	701	-	-	5/8/8/8	-
3	G3P	D	601	-	-	6/8/8/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	G3P	P-O4P	-3.01	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	G3P	P-O3P	-2.75	1.44	1.54
3	C	701	G3P	P-O4P	-2.59	1.45	1.54
3	D	601	G3P	P-O2P	-2.12	1.43	1.50
3	D	601	G3P	P-O1P	-2.06	1.53	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	G3P	O2-C2-C1	-2.75	97.78	109.18
3	C	701	G3P	O3P-P-O4P	2.12	115.76	107.80

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GOL	O1-C1-C2-C3
2	A	601	GOL	C1-C2-C3-O3
2	A	601	GOL	O2-C2-C3-O3
3	C	701	G3P	C1-C2-C3-O1P
3	C	701	G3P	C3-O1P-P-O4P
3	C	701	G3P	C3-O1P-P-O2P
3	C	701	G3P	C3-O1P-P-O3P
3	D	601	G3P	C1-C2-C3-O1P
3	D	601	G3P	O2-C2-C3-O1P
3	D	601	G3P	C3-O1P-P-O2P
3	D	601	G3P	C3-O1P-P-O3P
3	C	701	G3P	O2-C2-C3-O1P
2	A	601	GOL	O1-C1-C2-O2
3	D	601	G3P	O1-C1-C2-O2
3	D	601	G3P	C3-O1P-P-O4P

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GOL	1	0
3	B	601	G3P	1	0
3	C	701	G3P	4	0
3	D	601	G3P	3	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	513/518 (99%)	0.27	7 (1%) 73 72	38, 62, 77, 83	1 (0%)
1	B	513/518 (99%)	0.54	19 (3%) 45 41	42, 70, 90, 96	1 (0%)
1	C	513/518 (99%)	0.33	11 (2%) 63 61	34, 64, 76, 82	1 (0%)
1	D	513/518 (99%)	0.60	26 (5%) 33 29	45, 70, 90, 98	1 (0%)
All	All	2052/2072 (99%)	0.44	63 (3%) 51 48	34, 67, 85, 98	4 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	LYS	5.3
1	D	497	ILE	4.5
1	B	425	LYS	4.4
1	D	425	LYS	4.4
1	C	425	LYS	4.0
1	D	182	ALA	3.6
1	D	484	VAL	3.5
1	D	427	GLY	3.4
1	C	154	ALA	3.3
1	B	319	CYS	3.2
1	D	423	LEU	3.2
1	D	318	ALA	3.1
1	A	363	LEU	3.0
1	D	319	CYS	2.9
1	D	195	LEU	2.9
1	D	435	SER	2.9
1	B	320	ALA	2.9
1	B	417	LEU	2.8
1	D	141	ALA	2.8
1	A	285	GLY	2.8
1	D	489	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	421	GLY	2.7
1	B	423	LEU	2.6
1	B	317	ILE	2.6
1	D	61	ALA	2.6
1	A	319	CYS	2.6
1	B	237	GLY	2.5
1	B	488	GLY	2.5
1	C	490	ALA	2.5
1	D	320	ALA	2.5
1	D	313	LEU	2.4
1	B	18	ILE	2.4
1	C	510	ALA	2.3
1	C	481	TRP	2.3
1	B	166	PHE	2.3
1	D	410	ALA	2.3
1	D	377	GLY	2.3
1	B	436	LEU	2.2
1	B	437	LEU	2.2
1	C	412	LEU	2.2
1	B	491	MET	2.2
1	D	366	TYR	2.2
1	B	214	PRO	2.2
1	C	363	LEU	2.2
1	D	403	VAL	2.2
1	A	277	GLY	2.2
1	C	254	ASP	2.2
1	D	420	ASP	2.2
1	C	439	VAL	2.2
1	D	137	SER	2.2
1	B	211	LEU	2.1
1	C	423	LEU	2.1
1	A	111	ASP	2.1
1	D	437	LEU	2.1
1	C	318	ALA	2.1
1	B	207	LEU	2.1
1	A	337	ILE	2.1
1	D	184	VAL	2.1
1	B	-1	PHE	2.1
1	D	81	THR	2.1
1	B	487	SER	2.0
1	B	420	ASP	2.0
1	D	268	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	601	6/6	0.90	0.10	51,52,53,54	0
3	G3P	C	701	10/10	0.90	0.10	47,52,60,60	0
3	G3P	B	601	10/10	0.94	0.09	65,67,69,70	0
3	G3P	D	601	10/10	0.94	0.14	48,50,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.