



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:39 am BST

PDB ID : 3WXJ
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 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

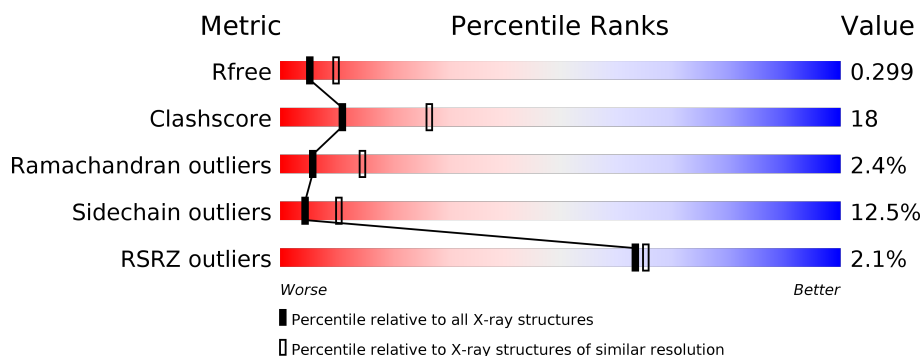
1 Overall quality at a glance

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	
1	B	518	
1	C	518	
1	D	518	

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	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:

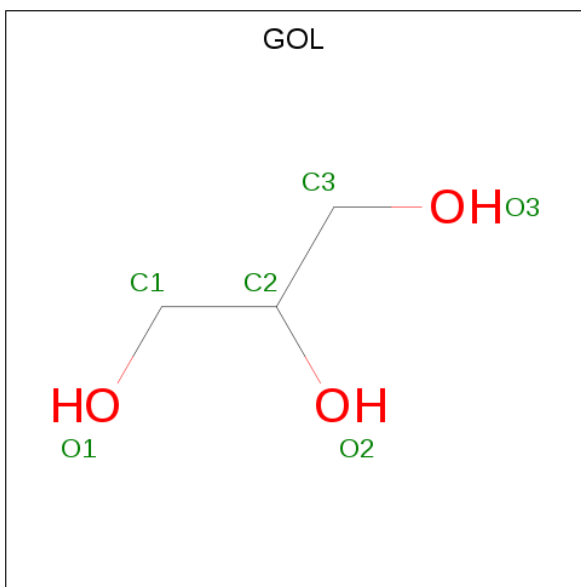
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP D3KVM3
A	-4	ILE	-	EXPRESSION TAG	UNP D3KVM3
A	-3	ASP	-	EXPRESSION TAG	UNP D3KVM3
A	-2	PRO	-	EXPRESSION TAG	UNP D3KVM3
A	-1	PHE	-	EXPRESSION TAG	UNP D3KVM3
A	0	THR	-	EXPRESSION TAG	UNP D3KVM3
B	-5	GLY	-	EXPRESSION TAG	UNP D3KVM3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

Continued on next page...

Continued from previous page...

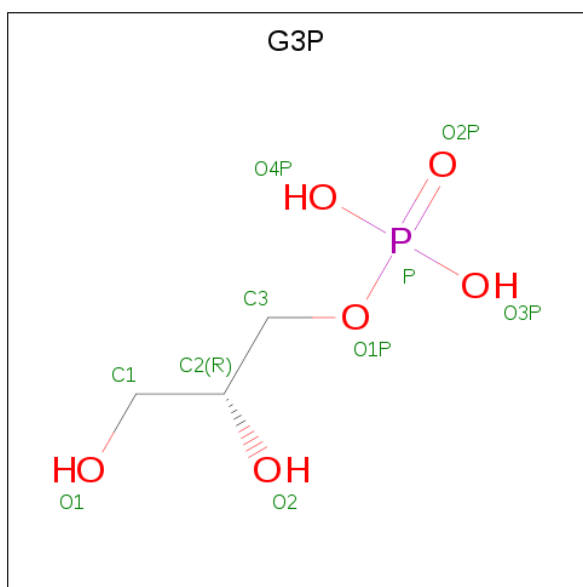
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PRO	-	EXPRESSION TAG	UNP D3KVM3
D	-1	PHE	-	EXPRESSION TAG	UNP D3KVM3
D	0	THR	-	EXPRESSION TAG	UNP D3KVM3

- Molecule 2 is GLYCEROL (three-letter code: 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 (three-letter code: 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		

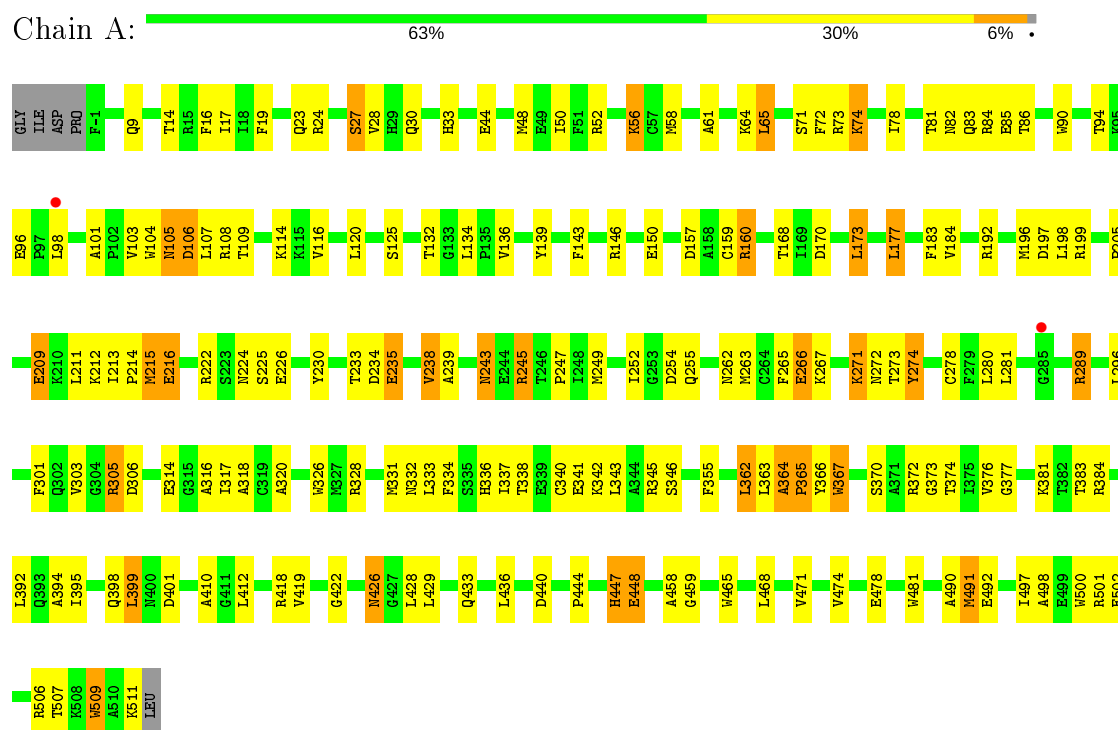
- Molecule 4 is water.

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		

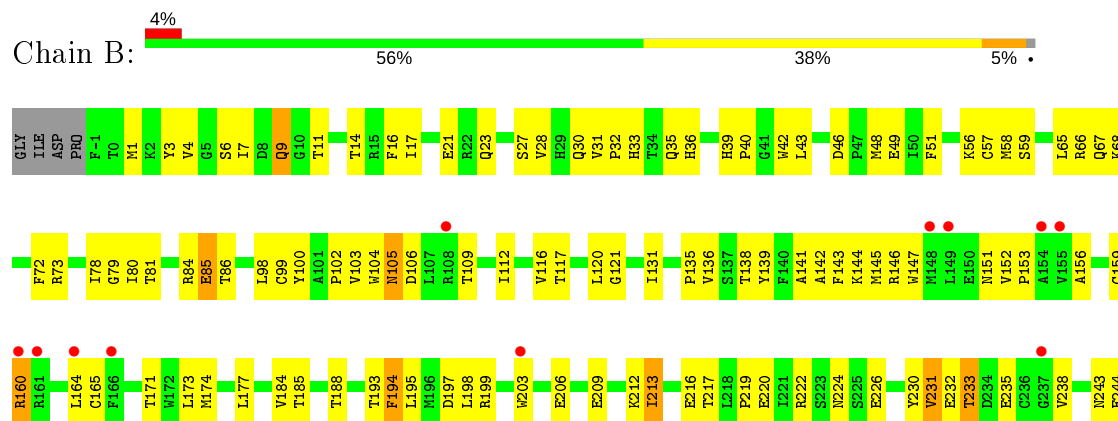
3 Residue-property plots

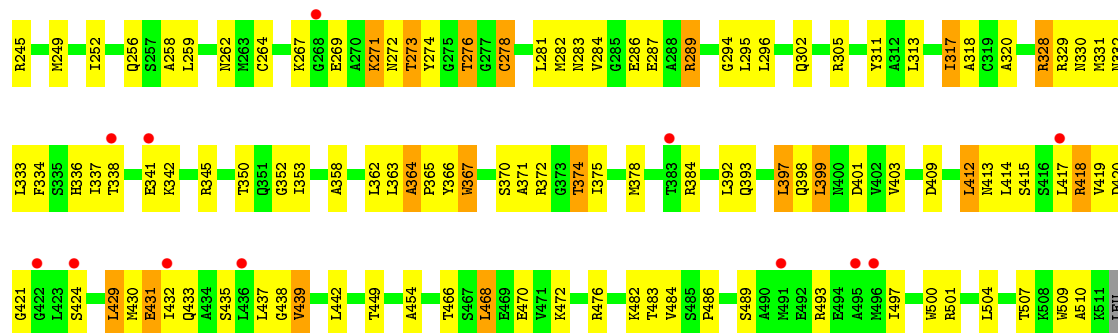
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



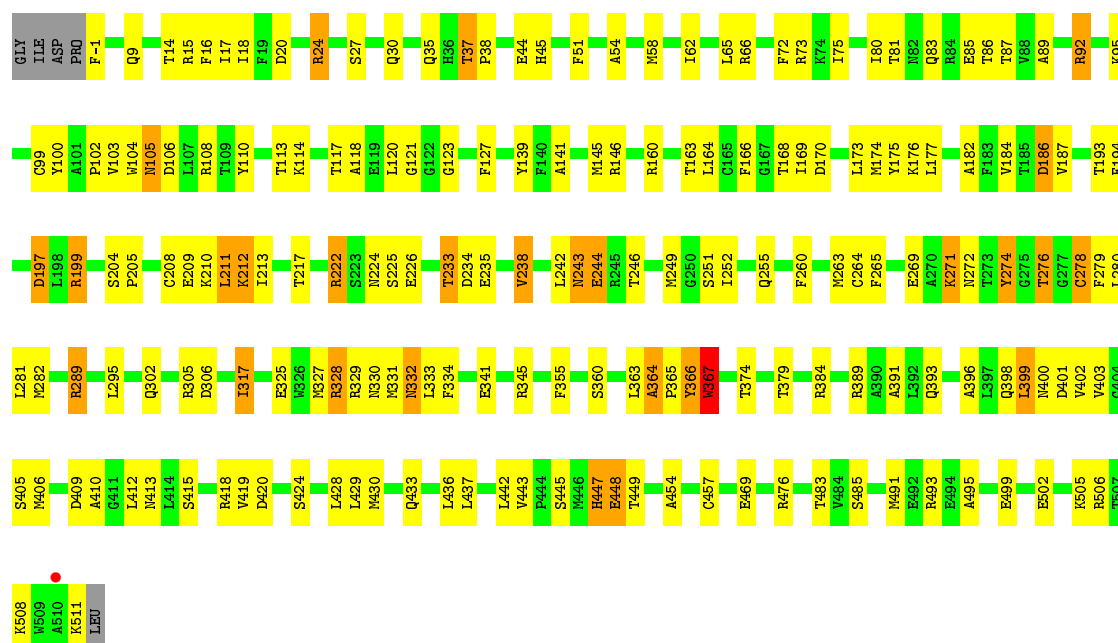
• Molecule 1: Glycerol kinase





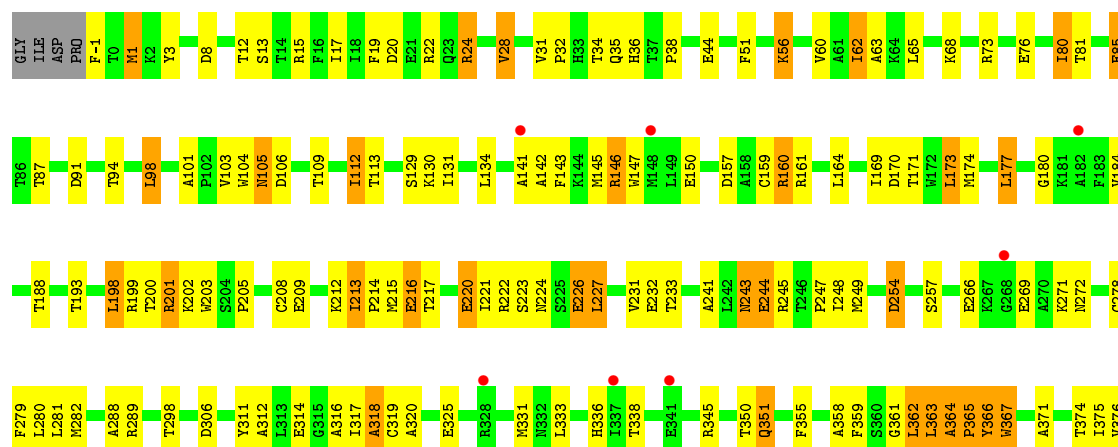
• Molecule 1: Glycerol kinase

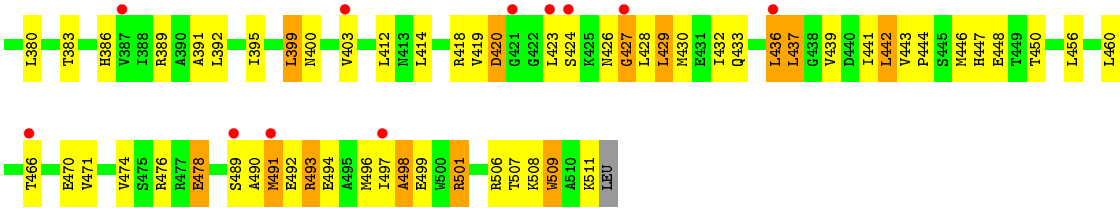
Chain C: 63% 31% 5%



• Molecule 1: Glycerol kinase

Chain D: 59% 31% 9% 3%





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 47.49 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.70) 99.7 (47.49-2.70)	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 , 0.299	Depositor DCC
R_{free} test set	3201 reflections (4.96%)	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 , 52.3	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 [i](#)

5.1 Standard geometry [i](#)

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	0.50	0/4039	0.65	0/5465
1	B	0.53	0/4039	0.63	0/5465
1	C	0.51	0/4039	0.63	0/5465
1	D	0.46	0/4039	0.64	1/5465 (0.0%)
All	All	0.50	0/16156	0.64	1/21860 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	427	GLY	N-CA-C	8.16	133.50	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3957	0	3970	146	0
1	B	3957	0	3970	147	0
1	C	3957	0	3970	134	0
1	D	3957	0	3970	159	0
2	A	6	0	8	1	0
3	B	10	0	7	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	571	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 18.

All (571) 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:O	1:D:429:LEU:HD12	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:O	1:B:198:LEU:HD23	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:105:ASN:H	1:A:105:ASN:ND2	1.78	0.80
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:CD2	1:C:447:HIS:H	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
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:A:364:ALA:HB3	1:A:365:PRO:CD	2.17	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:D:160:ARG:HG2	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:HD2	1:C:447:HIS:H	1.36	0.73
1:A:235:GLU:O	1:A:238:VAL:HG12	1.88	0.73
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: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:HD22	1:C:105:ASN:H	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:C:242:LEU:O	1:C:243:ASN:C	2.29	0.69
1:A:255:GLN:NE2	2:A:601:GOL:H32	2.08	0.69
1:A:83:GLN:HG3	1:A:83:GLN:O	1.92	0.69
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:HA	1:A:56:LYS:HE3	1.76	0.68
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:243:ASN:O	1:C:244:GLU:HB2	1.95	0.67
1:C:289:ARG:HG2	1:C:410:ALA:HA	1.76	0.67
1:D:200:THR:C	1:D:201:ARG:HE	1.97	0.67
1:A:271:LYS:HE2	1:A:281:LEU:HD13	1.76	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:281:LEU:HG	1:D:314:GLU:HB2	1.79	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: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:58:MET:HE3	1:A:78:ILE:HD13	1.80	0.63
1:B:198:LEU:C	1:B:198:LEU:HD23	2.17	0.63
1:A:274:TYR:CD1	1:A:274:TYR:N	2.67	0.62
1:A:196:MET:HG2	1:A:197:ASP:N	2.12	0.62
1:A:84:ARG:NH1	1:A:255:GLN:HB2	2.14	0.62
1:A:146:ARG:NH1	1:A:212:LYS:O	2.33	0.62
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:401:ASP:CG	1:B:501:ARG:HH22	2.03	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: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:C:95:LYS:O	1:C:176:LYS:NZ	2.32	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:429:LEU:C	1:D:429:LEU:HD12	2.18	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:B:282:MET:HE2	1:B:414:LEU:HD13	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:TYR:CE1	1:C:401:ASP:OD1	2.53	0.59
1:A:105:ASN:ND2	1:A:105:ASN:N	2.44	0.59
1:A:280:LEU:CD1	1:A:399:LEU:HD11	2.32	0.59
1:B:194:PHE:O	1:B:194:PHE:CD2	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:B:197:ASP:C	1:B:197:ASP:OD2	2.41	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: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:317:ILE:HD13	1:B:398:GLN:OE1	2.04	0.58
1:A:474:VAL:O	1:A:478:GLU:HG2	2.02	0.58
1:D:1:MET:CE	1:D:20:ASP:HB2	2.34	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: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:HD2	1:D:493:ARG:H	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:274:TYR:HD1	1:A:274:TYR:N	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:B:274:TYR:HB2	1:B:421:GLY:HA3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:199:ARG:NE	1:C:199:ARG:H	1.99	0.55
1:C:80:ILE:HD12	1:C:174:MET:HG3	1.88	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
1:D:62:ILE:HG22	1:D:63:ALA:N	2.22	0.55
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: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:46:ASP:HB2	1:B:100:TYR:HE2	1.72	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:A:490:ALA:C	1:A:492:GLU:H	2.11	0.54
1:C:274:TYR:CD1	1:C:274:TYR:N	2.76	0.54
1:B:198:LEU:C	1:B:198:LEU:CD2	2.73	0.54
1:B:272:ASN:HB2	1:B:417:LEU:HD11	1.89	0.54
1:C:226:GLU:OE2	1:C:305:ARG:HA	2.07	0.54
1:C:89:ALA:HB2	1:C:166:PHE:CE2	2.42	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: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:C:211:LEU:C	1:C:212:LYS:HD2	2.28	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:358:ALA:HB2	1:D:362:LEU:HD13	1.91	0.53
1:C:506:ARG:NH2	1:D:508:LYS:O	2.32	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
1:C:226:GLU:OE1	1:C:305:ARG:HD3	2.09	0.52
1:D:221:ILE:HG22	1:D:222:ARG:N	2.24	0.52
1:C:424:SER:HB3	1:C:443:VAL:HG13	1.92	0.52
1:D:214:PRO:HB3	1:D:216:GLU:OE1	2.09	0.52
1:D:13:SER:HA	1:D:32:PRO:HA	1.92	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: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:423:LEU:HG	1:D:426:ASN:CG	2.26	0.51
1:A:214:PRO:C	1:A:216:GLU:H	2.14	0.51
1:A:336:HIS:C	1:A:338:THR:H	2.13	0.51
1:C:327:MET:HB3	1:C:333:LEU:HD12	1.93	0.51
1:C:51:PHE:CE2	1:C:235:GLU:HG3	2.45	0.51
1:A:84:ARG:NH2	1:A:314:GLU:OE2	2.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LYS:C	1:A:116:VAL:H	2.14	0.51
1:A:345:ARG:NH2	1:A:428:LEU:HB2	2.25	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: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:A:107:LEU:C	1:A:109:THR:H	2.14	0.50
1:B:203:TRP:CZ2	1:B:219:PRO:O	2.64	0.50
1:A:205:PRO:O	1:A:209:GLU:HB2	2.11	0.50
1:A:24:ARG:HH11	1:A:478:GLU:HB3	1.75	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:B:278:CYS:HB3	1:B:317:ILE:O	2.11	0.50
1:B:198:LEU:CD2	1:B:311:TYR:HE1	2.25	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:D:24:ARG:HH11	1:D:478:GLU:HB3	1.76	0.50
1:B:509:TRP:O	1:B:510:ALA:C	2.49	0.50
1:D:1:MET:HE1	1:D:20:ASP:HB2	1.94	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:D:257:SER:OG	1:D:450:THR:O	2.24	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:C:328:ARG:C	1:C:328:ARG:HE	2.15	0.50
1:B:102:PRO:HB2	1:B:144:LYS:HD3	1.93	0.50
1:D:418:ARG:HA	1:D:442:LEU:O	2.12	0.50
1:D:56:LYS:HE2	1:D:60:VAL:HG23	1.93	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: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:90:TRP:CZ2	1:A:183:PHE:HE1	2.31	0.49
1:A:81:THR:OG1	1:A:254:ASP:HA	2.13	0.49
1:B:7:ILE:HD12	1:B:80:ILE:HG12	1.95	0.49
1:B:284:VAL:CG1	1:B:313:LEU:HG	2.36	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:436:LEU:HD23	1:D:496:MET:HE3	1.95	0.48
1:B:328:ARG:HB2	1:B:334:PHE:CZ	2.48	0.48
1:C:197:ASP:CG	1:C:199:ARG:HH21	2.15	0.48
1:D:437:LEU:HD22	1:D:439:VAL:HG22	1.96	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:C:81:THR:HA	1:C:252:ILE:O	2.14	0.48
1:D:188:THR:CG2	1:D:224:ASN:HD21	2.26	0.48
1:D:400:ASN:CG	1:D:436:LEU:HD12	2.34	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: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:383:THR:HA	1:B:330:ASN:HB3	1.96	0.47
1:A:331:MET:HA	1:B:384:ARG:HB3	1.95	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:267:LYS:HD2	1:A:412:LEU:HD22	1.95	0.47
1:A:64:LYS:HE3	4:A:715:HOH:O	2.14	0.47
1:A:9:GLN:NE2	1:A:14:THR:OG1	2.47	0.47
1:A:198:LEU:HA	1:A:198:LEU:HD23	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:C:17:ILE:HD13	1:C:448:GLU:HG3	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:474:VAL:O	1:D:478:GLU:HG2	2.14	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:C:108:ARG:C	1:C:110:TYR:H	2.18	0.46
1:D:159:CYS:HB2	1:D:164:LEU:HD22	1.96	0.46
1:D:319:CYS:O	1:D:320:ALA:C	2.53	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:A:65:LEU:HD13	1:A:72:PHE:CG	2.50	0.46
1:D:112:ILE:H	1:D:112:ILE:HD12	1.80	0.46
1:A:374:THR:HG21	1:A:507:THR:HA	1.96	0.46
1:B:317:ILE:HG13	1:B:317:ILE:O	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:D:12:THR:HA	1:D:35:GLN:NE2	2.30	0.46
1:D:203:TRP:O	1:D:205:PRO:HD3	2.16	0.46
1:A:265:PHE:C	1:A:266:GLU:HG2	2.36	0.45
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:C:331:MET:O	1:C:332:ASN:C	2.54	0.45
1:B:374:THR:HG21	1:B:507:THR:HA	1.98	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:429:LEU:HG	1:C:430:MET:HE3	1.98	0.45
1:C:264:CYS:HB3	1:C:269:GLU:O	2.17	0.45
1:D:174:MET:HG2	1:D:248:ILE:HG21	1.98	0.45
1:D:80:ILE:HD12	1:D:174:MET:HG3	1.97	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:419:VAL:HG11	1:B:430:MET:SD	2.57	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
1:B:46:ASP:HB3	1:B:49:GLU:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:500:TRP:NE1	1:B:504:LEU:HD11	2.32	0.45
1:B:3:TYR:CD2	1:B:72:PHE:HD2	2.35	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: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:A:366:TYR:O	1:A:367:TRP:C	2.55	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:D:129:SER:C	1:D:131:ILE:H	2.21	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:C:37:THR:O	1:C:38:PRO:C	2.56	0.44
1:D:279:PHE:CZ	3:D:601:G3P:H11	2.52	0.44
1:D:24:ARG:HH11	1:D:478:GLU:CB	2.31	0.44
1:A:447:HIS:CD2	1:A:448:GLU:OE2	2.71	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:B:21:GLU:C	1:B:23:GLN:H	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ARG:NH2	1:D:150:GLU:OE2	2.51	0.43
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:211:LEU:O	1:A:213:ILE:HD12	2.17	0.43
1:A:184:VAL:HG11	1:A:222:ARG:NH1	2.33	0.43
1:A:30:GLN:HB2	1:A:30:GLN:HE21	1.63	0.43
1:B:374:THR:CG2	1:B:507:THR:HG22	2.48	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:197:ASP:O	1:A:198:LEU:C	2.56	0.43
1:A:192:ARG:NH2	1:A:314:GLU:OE2	2.52	0.43
1:B:393:GLN:HG2	1:B:432:ILE:HD13	1.99	0.43
1:B:78:ILE:HD12	1:B:231:VAL:HG21	2.01	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: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:495:ALA:O	1:C:499:GLU:HB2	2.17	0.43
1:C:276:THR:HG21	3:C:701:G3P:O3P	2.12	0.43
1:C:85:GLU:OE1	3:C:701:G3P:O1	2.21	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:326:TRP:C	1:A:328:ARG:H	2.21	0.43
1:A:370:SER:O	1:A:509:TRP:N	2.49	0.43
1:B:413:ASN:HB3	1:B:414:LEU:H	1.66	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:160:ARG:CG	1:A:160:ARG:HH11	2.25	0.42
1:A:86:THR:O	1:A:168:THR:HA	2.19	0.42
1:B:173:LEU:HA	1:B:173:LEU:HD12	1.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HB2	1:A:199:ARG:HE	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: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: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:110:TYR:CZ	1:C:114:LYS:HE2	2.55	0.42
1:C:86:THR:O	1:C:168:THR:HG23	2.20	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:A:490:ALA:C	1:A:492:GLU:N	2.74	0.41
1:B:267:LYS:HA	1:B:283:ASN:HB3	2.02	0.41
1:D:254:ASP:OD2	3:D:601:G3P:O2	2.30	0.41
1:D:331:MET:HB2	1:D:333:LEU:HD12	2.02	0.41
1:B:438:GLY:O	1:B:439:VAL:HG13	2.20	0.41
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:D:22:ARG:HD2	1:D:478:GLU:CD	2.40	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:THR:C	1:C:15:ARG:HG3	2.40	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:B:105:ASN:ND2	1:B:105:ASN:N	2.58	0.41
1:B:16:PHE:CD2	1:B:58:MET:HA	2.56	0.41
1:A:377:GLY:HA2	1:B:372:ARG:HB2	2.01	0.41
1:C:120:LEU:HD13	1:C:210:LYS:HB3	2.01	0.41
1:D:243:ASN:ND2	1:D:243:ASN:O	2.52	0.41
1:D:87:THR:HG21	1:D:145:MET:HG2	2.03	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:C:269:GLU:CD	1:C:418:ARG:HH12	2.24	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:D:426:ASN:CG	1:D:427:GLY:N	2.74	0.41
1:A:243:ASN:HD22	1:A:243:ASN:HA	1.57	0.41
1:B:109:THR:OG1	1:B:138:THR:HG22	2.19	0.41
1:D:103:VAL:O	1:D:104:TRP:C	2.59	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:225:SER:HB3	1:A:303:VAL:HA	2.03	0.41
1:A:82:ASN:OD1	1:A:170:ASP:HB3	2.21	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:84:ARG:O	1:A:85:GLU:HB2	2.20	0.41
1:B:81:THR:HB	1:B:454:ALA:HB2	2.03	0.41
1:A:363:LEU:O	1:A:364:ALA:C	2.58	0.41
1:A:419:VAL:O	1:A:444:PRO:HD2	2.21	0.41
1:B:468:LEU:HD23	1:B:468:LEU:N	2.35	0.41
1:D:456:LEU:O	1:D:460:LEU:HG	2.21	0.41
1:D:8:ASP:HB3	1:D:15:ARG:HG3	2.03	0.41
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:A:85:GLU:HB3	1:A:139:TYR:O	2.21	0.40
1:C:164:LEU:O	1:C:217:THR:HG22	2.21	0.40
1:C:15:ARG:NH1	1:C:448:GLU:OE1	2.54	0.40
1:D:391:ALA:O	1:D:395:ILE:HG13	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLU:OE1	1:A:305:ARG:NH1	2.54	0.40
1:A:85:GLU:HB2	1:A:104:TRP:HB3	2.03	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:C:502:GLU:HA	1:C:505:LYS:HD2	2.03	0.40
1:B:287:GLU:HB3	1:B:289:ARG:NH1	2.37	0.40
1:B:66:ARG:O	1:B:67:GLN:C	2.60	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: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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	511/518 (99%)	440 (86%)	57 (11%)	14 (3%)	5	12
1	B	511/518 (99%)	430 (84%)	73 (14%)	8 (2%)	9	24
1	C	511/518 (99%)	449 (88%)	54 (11%)	8 (2%)	9	24
1	D	511/518 (99%)	436 (85%)	56 (11%)	19 (4%)	3	7
All	All	2044/2072 (99%)	1755 (86%)	240 (12%)	49 (2%)	6	15

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	A	238	VAL
1	B	194	PHE
1	B	212	LYS
1	B	231	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	383 (91%)	38 (9%)	9	22
1	B	421/425 (99%)	365 (87%)	56 (13%)	4	9
1	C	421/425 (99%)	365 (87%)	56 (13%)	4	9
1	D	421/425 (99%)	360 (86%)	61 (14%)	3	8
All	All	1684/1700 (99%)	1473 (88%)	211 (12%)	4	10

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	SER
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	160	ARG
1	A	173	LEU
1	A	177	LEU
1	A	215	MET
1	A	216	GLU
1	A	235	GLU
1	A	243	ASN
1	A	245	ARG
1	A	266	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	271	LYS
1	A	274	TYR
1	A	278	CYS
1	A	289	ARG
1	A	305	ARG
1	A	342	LYS
1	A	346	SER
1	A	355	PHE
1	A	362	LEU
1	A	376	VAL
1	A	381	LYS
1	A	399	LEU
1	A	418	ARG
1	A	436	LEU
1	A	440	ASP
1	A	447	HIS
1	A	448	GLU
1	A	481	TRP
1	A	491	MET
1	A	511	LYS
1	B	1	MET
1	B	4	VAL
1	B	9	GLN
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
1	B	146	ARG
1	B	160	ARG
1	B	165	CYS
1	B	177	LEU
1	B	206	GLU
1	B	209	GLU
1	B	213	ILE
1	B	216	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	217	THR
1	B	232	GLU
1	B	233	THR
1	B	243	ASN
1	B	244	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	305	ARG
1	B	317	ILE
1	B	328	ARG
1	B	329	ARG
1	B	366	TYR
1	B	367	TRP
1	B	374	THR
1	B	397	LEU
1	B	399	LEU
1	B	409	ASP
1	B	412	LEU
1	B	418	ARG
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	476	ARG
1	B	482	LYS
1	B	483	THR
1	C	-1	PHE
1	C	9	GLN
1	C	24	ARG
1	C	37	THR
1	C	65	LEU
1	C	83	GLN
1	C	92	ARG
1	C	105	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	106	ASP
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	186	ASP
1	C	187	VAL
1	C	197	ASP
1	C	199	ARG
1	C	209	GLU
1	C	211	LEU
1	C	212	LYS
1	C	222	ARG
1	C	233	THR
1	C	238	VAL
1	C	243	ASN
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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	469	GLU
1	C	476	ARG
1	C	483	THR
1	C	485	SER
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	73	ARG
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	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	243	ASN
1	D	244	GLU
1	D	245	ARG
1	D	271	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	289	ARG
1	D	306	ASP
1	D	325	GLU
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	412	LEU
1	D	420	ASP
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	476	ARG
1	D	478	GLU
1	D	493	ARG
1	D	501	ARG
1	D	511	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	23	GLN
1	A	30	GLN
1	A	105	ASN
1	A	224	ASN
1	A	243	ASN
1	A	255	GLN
1	A	262	ASN
1	A	272	ASN
1	A	293	HIS
1	A	302	GLN
1	A	336	HIS
1	A	479	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	30	GLN
1	B	39	HIS
1	B	67	GLN
1	B	105	ASN
1	B	224	ASN
1	B	243	ASN
1	B	302	GLN
1	B	336	HIS
1	B	433	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	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	351	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	G3P	C	701	-	9,9,9	1.29	1 (11%)	11,12,12	1.59	3 (27%)
3	G3P	B	601	-	9,9,9	0.62	0	11,12,12	0.77	0
2	GOL	A	601	-	5,5,5	0.45	0	5,5,5	0.46	0
3	G3P	D	601	-	9,9,9	1.73	3 (33%)	11,12,12	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
3	G3P	C	701	-	-	5/8/8/8	-
3	G3P	B	601	-	-	0/8/8/8	-
2	GOL	A	601	-	-	4/4/4/4	-
3	G3P	D	601	-	-	7/8/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	601	G3P	P-O4P	-2.91	1.43	1.54
3	D	601	G3P	P-O3P	-2.66	1.44	1.54
3	C	701	G3P	P-O4P	-2.51	1.45	1.54
3	D	601	G3P	P-O2P	-2.06	1.43	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	G3P	P-O1P-C3	3.54	128.06	118.30
3	C	701	G3P	O2-C2-C1	-2.58	97.78	109.12
3	C	701	G3P	O3P-P-O4P	2.13	115.76	107.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
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	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	O1-C1-C2-C3
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
3	C	701	G3P	4	0
3	B	601	G3P	1	0
2	A	601	GOL	1	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%)	0.01	2 (0%) 92 93	38, 62, 77, 83	1 (0%)
1	B	513/518 (99%)	0.13	23 (4%) 33 31	42, 70, 90, 96	1 (0%)
1	C	513/518 (99%)	0.04	1 (0%) 95 96	34, 64, 76, 82	1 (0%)
1	D	513/518 (99%)	0.12	18 (3%) 44 44	45, 70, 91, 98	1 (0%)
All	All	2052/2072 (99%)	0.08	44 (2%) 63 65	34, 67, 85, 98	4 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	427	GLY	4.7
1	D	421	GLY	4.4
1	D	423	LEU	4.1
1	B	491	MET	3.6
1	B	436	LEU	3.6
1	B	417	LEU	3.3
1	B	155	VAL	3.2
1	B	422	GLY	3.1
1	D	489	SER	3.1
1	D	491	MET	3.0
1	D	182	ALA	2.9
1	B	166	PHE	2.9
1	A	98	LEU	2.7
1	D	148	MET	2.7
1	B	148	MET	2.7
1	D	436	LEU	2.6
1	B	164	LEU	2.5
1	C	510	ALA	2.5
1	A	285	GLY	2.5
1	B	203	TRP	2.4
1	B	268	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	154	ALA	2.4
1	D	328	ARG	2.4
1	D	387	VAL	2.4
1	B	160	ARG	2.3
1	B	432	ILE	2.3
1	D	341	GLU	2.2
1	B	496	MET	2.2
1	B	424	SER	2.2
1	B	338	THR	2.2
1	B	149	LEU	2.2
1	D	424	SER	2.1
1	B	108	ARG	2.1
1	D	466	THR	2.1
1	B	383	THR	2.1
1	B	161	ARG	2.1
1	B	341	GLU	2.1
1	D	268	GLY	2.1
1	B	495	ALA	2.1
1	D	337	ILE	2.0
1	D	497	ILE	2.0
1	B	237	GLY	2.0
1	D	403	VAL	2.0
1	D	141	ALA	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 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	G3P	C	701	10/10	0.91	0.18	47,52,60,60	0
2	GOL	A	601	6/6	0.91	0.18	51,52,53,54	0
3	G3P	B	601	10/10	0.96	0.16	65,67,69,70	0
3	G3P	D	601	10/10	0.96	0.15	48,50,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.