Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 03:54 AM EDT

PDB ID	:	3WXK
Title	:	Crystal structure of trypanosoma brucei gambiense glycerol kinase in complex with glycerol
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	:	2.37 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

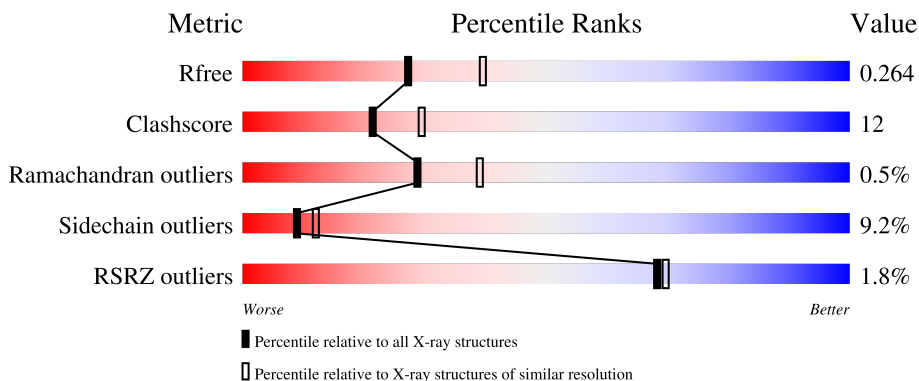|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
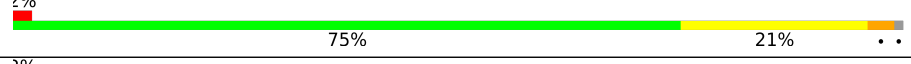*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	Percentile Ranks	Value
Rfree		0.264
Clashscore		12
Ramachandran outliers		0.5%
Sidechain outliers		9.2%
RSRZ outliers		1.8%

Worse   Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	518	74% ... 21% ..
1	B	518	75% ... 21% ..
1	C	518	74% ... 23% ..
1	D	518	75% ... 20% ..

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16111 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	1	0
			3962	2502	695	732	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: $C_3H_8O_3$).
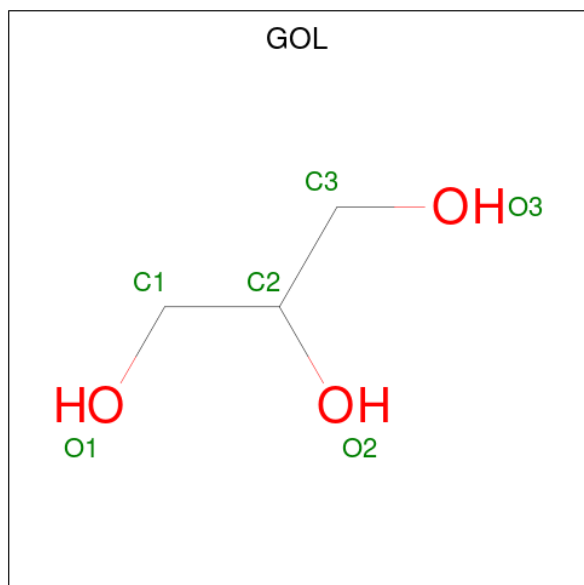
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0	0
2	C	1	Total 6	C 3	O 3	0	0
2	D	1	Total 6	C 3	O 3	0	0
2	D	1	Total 6	C 3	O 3	0	0

- Molecule 3 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).

HEZ
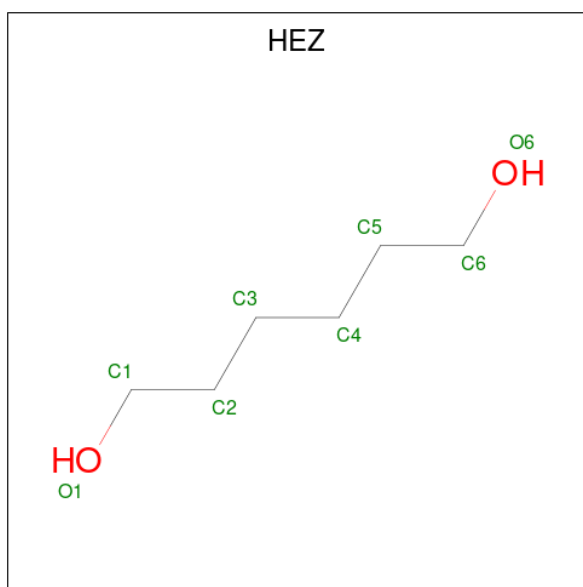
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 8	C 6	O 2	0	0
3	B	1	Total 8	C 6	O 2	0	0
3	C	1	Total 8	C 6	O 2	0	0
3	D	1	Total 8	C 6	O 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total 52	O 52	0	0
4	B	52	Total 52	O 52	0	0
4	C	50	Total 50	O 50	0	0
4	D	50	Total 50	O 50	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glycerol kinase
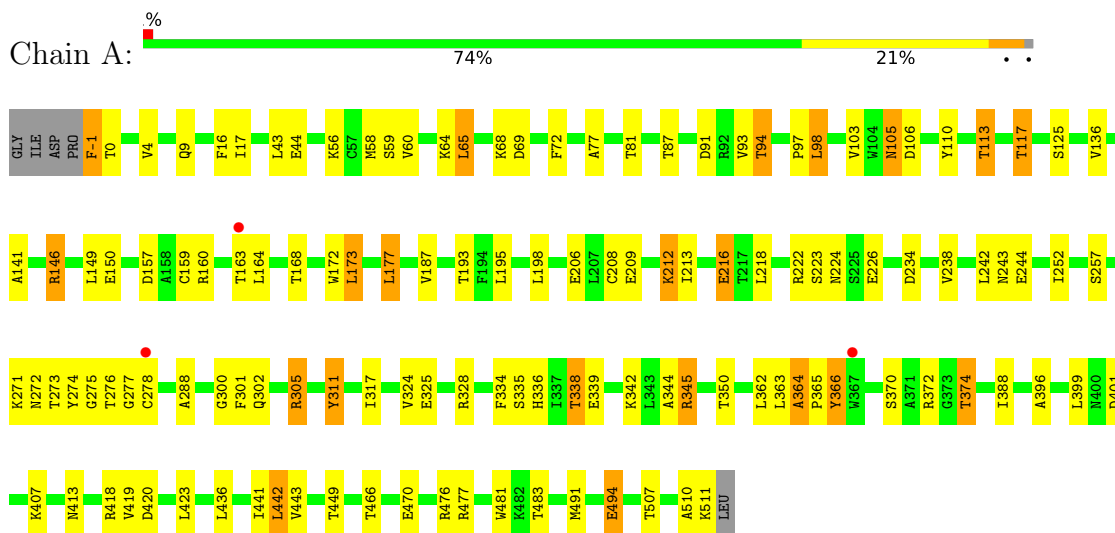
Chain A:

- Molecule 1: Glycerol kinase

Chain B:

- Molecule 1: Glycerol kinase

Chain C:

• Molecule 1: Glycerol kinase

Chain D:
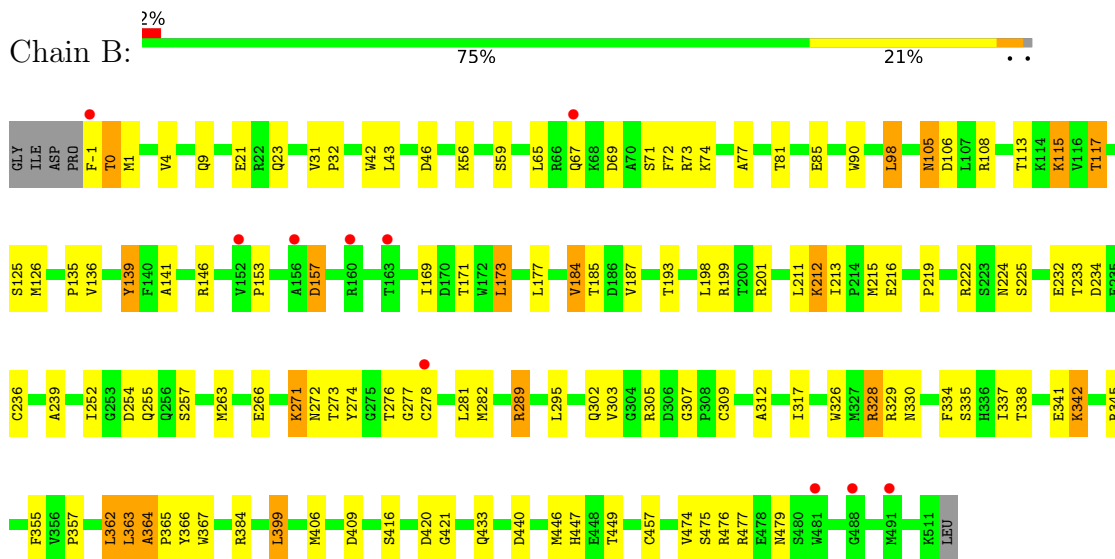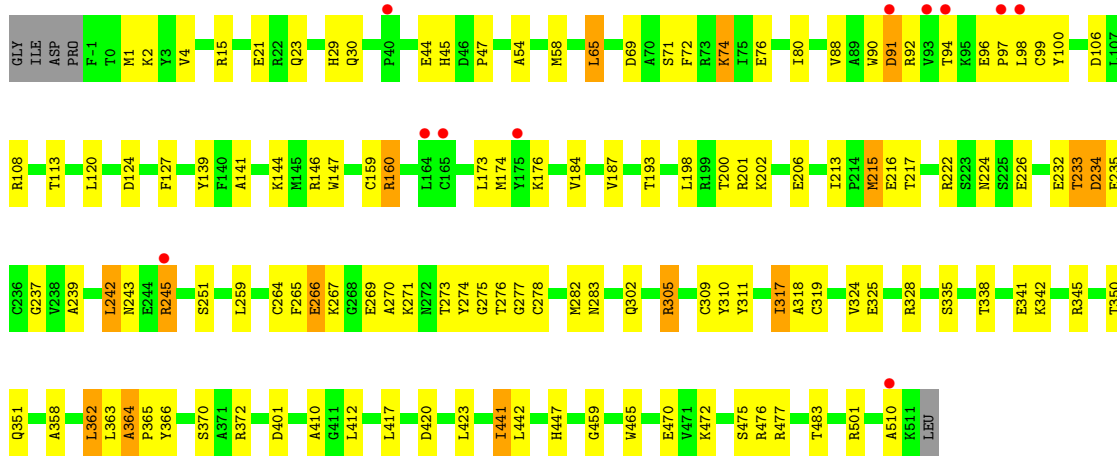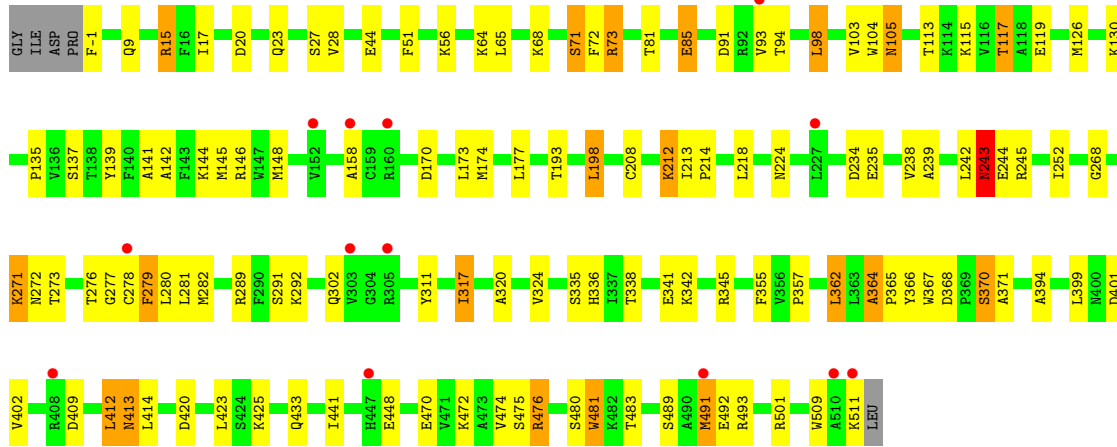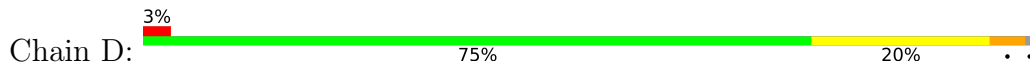
4 Data and refinement statistics ⓘ

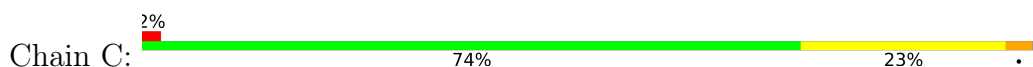| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.48Å 122.14Å 154.51Å 90.00° 90.76° 90.00°	Depositor
Resolution (Å)	30.00 – 2.37 47.91 – 2.37	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.00-2.37) 93.5 (47.91-2.37)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190 , 0.251 0.207 , 0.264	Depositor DCC
R_{free} test set	4415 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.5	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-l	Xtriage
Reported twinning fraction	0.914 for H, K, L 0.086 for -h,-k,l	Depositor
Outliers	0 of 88201 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16111	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.93	2/4039 (0.0%)	0.82	2/5465 (0.0%)
1	B	0.94	0/4039	0.83	2/5465 (0.0%)
1	C	1.04	3/4039 (0.1%)	0.80	1/5465 (0.0%)
1	D	0.88	2/4047 (0.0%)	0.79	0/5476
All	All	0.95	7/16164 (0.0%)	0.81	5/21871 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	309	CYS	CB-SG	-5.86	1.72	1.81
1	A	311	TYR	CD1-CE1	-5.50	1.31	1.39
1	C	310	TYR	CD2-CE2	-5.41	1.31	1.39
1	D	279	PHE	CD1-CE1	-5.25	1.28	1.39
1	A	311	TYR	CD2-CE2	-5.23	1.31	1.39
1	C	310	TYR	CD1-CE1	-5.06	1.31	1.39
1	D	85	GLU	CD-OE1	-5.02	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	345	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	98	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	242	LEU	N-CA-C	-5.24	96.86	111.00
1	B	384	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	99	0
1	B	3957	0	3970	81	0
1	C	3957	0	3970	95	0
1	D	3962	0	3976	107	0
2	A	12	0	16	1	0
2	B	6	0	8	0	0
2	C	12	0	16	2	0
2	D	12	0	16	1	0
3	B	16	0	28	4	0
3	C	8	0	14	0	0
3	D	8	0	14	0	0
4	A	52	0	0	7	0
4	B	52	0	0	3	0
4	C	50	0	0	6	0
4	D	50	0	0	2	0
All	All	16111	0	15998	383	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 12.

All (383) 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:C:364:ALA:CB	1:C:365:PRO:HD2	1.63	1.28
1:B:364:ALA:HB1	1:B:365:PRO:CD	1.64	1.27
1:C:364:ALA:HB1	1:C:365:PRO:CD	1.64	1.27
1:B:420:ASP:OD1	1:B:449:THR:HG21	1.40	1.21
1:B:364:ALA:CB	1:B:365:PRO:HD2	1.70	1.18
1:A:336:HIS:CD2	1:A:338:THR:HB	1.78	1.17
1:C:305:ARG:HH11	1:C:305:ARG:HG2	1.11	1.13
1:D:364:ALA:CB	1:D:365:PRO:CD	2.26	1.12
1:D:364:ALA:CB	1:D:365:PRO:HD3	1.79	1.12
1:D:73:ARG:H	1:D:73:ARG:HD3	0.99	1.09
1:D:364:ALA:HB1	1:D:365:PRO:HD3	1.12	1.09
1:A:364:ALA:CB	1:A:365:PRO:HD3	1.83	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ASN:HD22	1:D:244:GLU:N	1.50	1.07
1:A:364:ALA:HB1	1:A:365:PRO:HD3	1.08	1.07
1:D:280:LEU:HD12	1:D:399:LEU:HD12	1.37	1.06
1:B:139:TYR:CE2	3:B:603:HEZ:H31	1.90	1.05
1:D:73:ARG:HD3	1:D:73:ARG:N	1.69	1.04
1:B:364:ALA:HB1	1:B:365:PRO:HD2	1.05	1.04
1:C:91:ASP:OD1	1:C:94:THR:HG23	1.59	1.02
1:A:336:HIS:HD2	1:A:338:THR:HB	1.15	1.01
1:B:278:CYS:SG	1:B:399:LEU:HD11	2.01	1.00
1:C:305:ARG:HH11	1:C:305:ARG:CG	1.75	1.00
1:B:362:LEU:O	1:B:363:LEU:HB2	1.58	0.99
1:A:224:ASN:HD22	1:A:302:GLN:H	1.02	0.99
1:C:364:ALA:HA	4:C:749:HOH:O	1.63	0.97
1:D:364:ALA:HB1	1:D:365:PRO:CD	1.92	0.96
1:D:282:MET:CE	1:D:414:LEU:CD1	2.44	0.95
1:A:466:THR:HA	4:A:726:HOH:O	1.67	0.95
1:D:278:CYS:HB3	1:D:317:ILE:HG12	1.49	0.94
1:A:206:GLU:HB2	4:A:709:HOH:O	1.67	0.93
1:A:364:ALA:HB1	1:A:365:PRO:CD	1.97	0.93
1:A:157:ASP:O	1:A:160:ARG:HB3	1.69	0.92
1:A:224:ASN:ND2	1:A:302:GLN:H	1.67	0.92
1:C:364:ALA:HB1	1:C:365:PRO:HD2	0.92	0.91
1:A:150:GLU:HG2	1:C:202:LYS:HE3	1.53	0.91
1:A:305:ARG:HG3	1:A:305:ARG:HH11	1.34	0.91
1:D:282:MET:CE	1:D:414:LEU:HD12	2.00	0.91
1:D:476:ARG:HH21	1:D:481:TRP:HH2	1.19	0.90
1:D:278:CYS:CB	1:D:317:ILE:HG12	2.01	0.90
1:D:364:ALA:HB3	1:D:365:PRO:CD	1.97	0.90
1:B:341:GLU:O	1:B:345:ARG:HG3	1.73	0.89
1:A:226:GLU:OE1	1:A:305:ARG:HD2	1.73	0.89
1:A:364:ALA:CB	1:A:365:PRO:CD	2.50	0.89
1:D:364:ALA:HB3	1:D:365:PRO:HD2	1.54	0.89
1:D:282:MET:HE1	1:D:414:LEU:HD12	1.55	0.89
1:D:282:MET:HE2	1:D:414:LEU:CD1	2.02	0.88
1:D:367:TRP:HE3	4:D:747:HOH:O	1.58	0.87
1:B:399:LEU:HD23	1:B:433:GLN:OE1	1.73	0.87
1:A:336:HIS:HD2	1:A:338:THR:CB	1.87	0.86
1:C:224:ASN:HD22	1:C:302:GLN:H	1.25	0.85
1:D:105:ASN:HD22	1:D:105:ASN:H	1.23	0.84
1:A:278:CYS:SG	1:A:399:LEU:HD21	2.18	0.84
1:C:184:VAL:HG11	1:C:222:ARG:NH1	1.94	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:HH11	1:A:305:ARG:CG	1.91	0.82
1:D:282:MET:HE2	1:D:414:LEU:HD11	1.59	0.82
1:A:336:HIS:CD2	1:A:338:THR:H	1.98	0.82
1:D:280:LEU:CD1	1:D:399:LEU:HD12	2.10	0.82
1:B:224:ASN:HD22	1:B:302:GLN:H	1.24	0.81
1:B:362:LEU:O	1:B:363:LEU:CB	2.29	0.79
1:D:113:THR:O	1:D:117:THR:HG22	1.83	0.79
1:D:243:ASN:ND2	1:D:244:GLU:N	2.30	0.79
1:B:420:ASP:OD1	1:B:449:THR:CG2	2.29	0.79
1:A:374:THR:HG21	1:A:507:THR:HG22	1.64	0.78
1:C:184:VAL:CG1	1:C:222:ARG:HH11	1.96	0.78
1:A:336:HIS:CD2	1:A:338:THR:CB	2.62	0.78
1:D:73:ARG:N	1:D:73:ARG:CD	2.47	0.77
1:A:60:VAL:O	1:A:64:LYS:HG3	1.83	0.77
1:D:476:ARG:NH2	1:D:481:TRP:HH2	1.83	0.76
1:C:160:ARG:HH11	1:C:160:ARG:HB2	1.52	0.75
1:B:141:ALA:HB3	1:B:193:THR:HA	1.69	0.74
1:C:184:VAL:CG1	1:C:222:ARG:NH1	2.50	0.74
1:B:146:ARG:NH1	1:B:212:LYS:HG3	2.02	0.74
1:A:336:HIS:HD2	1:A:338:THR:H	1.33	0.74
1:C:184:VAL:HG11	1:C:222:ARG:HH11	1.52	0.74
1:A:43:LEU:HD23	1:A:105:ASN:HD21	1.53	0.74
1:C:160:ARG:HH11	1:C:160:ARG:CB	2.01	0.73
1:D:73:ARG:H	1:D:73:ARG:CD	1.91	0.73
1:A:325:GLU:OE2	1:A:328:ARG:NH1	2.22	0.73
1:A:374:THR:CG2	1:A:507:THR:HG22	2.18	0.73
1:B:364:ALA:CB	1:B:365:PRO:CD	2.30	0.72
1:C:341:GLU:OE2	1:C:345:ARG:NH2	2.22	0.71
1:C:341:GLU:O	1:C:345:ARG:HG3	1.90	0.70
1:A:372:ARG:O	1:A:374:THR:HG22	1.91	0.70
1:D:282:MET:HE1	1:D:414:LEU:CD1	2.17	0.70
1:D:276:THR:N	1:D:277:GLY:HA3	2.07	0.70
1:A:272:ASN:ND2	1:A:278:CYS:SG	2.60	0.70
1:C:160:ARG:HH11	1:C:160:ARG:CG	2.05	0.69
1:B:364:ALA:HB1	1:B:365:PRO:HD3	1.71	0.69
1:D:278:CYS:HB3	1:D:317:ILE:CG1	2.22	0.69
1:D:336:HIS:HD2	1:D:338:THR:OG1	1.75	0.69
1:B:1:MET:SD	1:B:21:GLU:HG2	2.33	0.68
1:A:91:ASP:OD1	1:A:94:THR:HG23	1.92	0.68
1:C:23:GLN:HE22	1:C:475:SER:HB2	1.58	0.68
1:B:224:ASN:ND2	1:B:302:GLN:H	1.91	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ASN:HD22	1:D:244:GLU:H	1.42	0.68
1:D:282:MET:CE	1:D:414:LEU:HD11	2.19	0.68
1:D:224:ASN:HD22	1:D:302:GLN:H	1.42	0.67
1:A:150:GLU:HG3	4:A:750:HOH:O	1.94	0.66
1:C:305:ARG:CG	1:C:305:ARG:NH1	2.44	0.65
1:C:266:GLU:O	1:C:269:GLU:HG3	1.97	0.65
1:D:105:ASN:H	1:D:105:ASN:ND2	1.95	0.65
1:C:305:ARG:HG2	1:C:305:ARG:NH1	1.95	0.65
1:A:244:GLU:OE1	1:A:244:GLU:N	2.30	0.65
1:C:317:ILE:HD12	1:C:318:ALA:N	2.12	0.65
1:C:364:ALA:CB	1:C:365:PRO:CD	2.30	0.65
1:C:29:HIS:HD2	4:C:742:HOH:O	1.80	0.64
1:D:413[A]:ASN:ND2	1:D:414:LEU:H	1.95	0.64
1:A:226:GLU:CD	1:A:305:ARG:HD2	2.18	0.64
1:A:274:TYR:HB3	1:A:423:LEU:HB2	1.79	0.64
1:B:184:VAL:HG11	1:B:222:ARG:HD2	1.79	0.64
1:C:147:TRP:O	1:C:147:TRP:CE3	2.51	0.64
1:A:336:HIS:HD2	1:A:338:THR:N	1.96	0.63
1:D:413[A]:ASN:HD22	1:D:414:LEU:H	1.46	0.63
1:A:242:LEU:O	1:A:243:ASN:HB3	1.99	0.63
1:A:305:ARG:CG	1:A:305:ARG:NH1	2.56	0.63
1:B:4:VAL:HG23	1:B:77:ALA:O	1.99	0.62
1:D:489:SER:OG	1:D:491:MET:HB3	1.99	0.62
3:B:602:HEZ:H32	4:B:702:HOH:O	1.99	0.62
1:D:317:ILE:HD11	1:D:320:ALA:HB2	1.81	0.62
1:B:43:LEU:HD23	1:B:105:ASN:HD21	1.65	0.62
1:C:1:MET:HA	1:C:21:GLU:OE2	1.98	0.62
1:B:364:ALA:HB3	1:B:365:PRO:HD2	1.75	0.62
1:C:317:ILE:CD1	1:C:319:CYS:H	2.13	0.62
1:D:23:GLN:HE22	1:D:475:SER:HB2	1.65	0.61
1:D:278:CYS:SG	1:D:399:LEU:HD11	2.40	0.61
1:B:117:THR:HG21	4:B:723:HOH:O	2.00	0.61
1:B:56:LYS:HG3	1:B:236:CYS:SG	2.41	0.61
1:A:-1:PHE:HD1	1:A:0:THR:H	1.47	0.61
1:D:51:PHE:CE2	1:D:235:GLU:HG3	2.36	0.61
1:B:363:LEU:HA	1:B:367:TRP:HD1	1.66	0.60
1:C:45:HIS:O	1:C:47:PRO:HD3	2.00	0.60
1:C:276:THR:N	1:C:277:GLY:HA3	2.16	0.60
1:C:233:THR:OG1	1:C:234:ASP:N	2.30	0.60
1:C:317:ILE:HD12	1:C:319:CYS:H	1.66	0.60
1:A:105:ASN:HD22	1:A:105:ASN:H	1.50	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:LEU:HB3	1:C:441:ILE:HG13	1.83	0.60
1:A:65:LEU:HD22	1:A:69:ASP:HB3	1.84	0.59
1:D:243:ASN:ND2	1:D:243:ASN:C	2.56	0.59
1:C:364:ALA:HB3	1:C:365:PRO:HD2	1.77	0.59
1:C:206:GLU:HB2	4:C:746:HOH:O	2.03	0.58
1:D:144:LYS:O	1:D:148:MET:HG3	2.03	0.58
1:B:272:ASN:ND2	1:B:278:CYS:SG	2.69	0.58
1:A:173:LEU:O	1:A:177:LEU:HB2	2.04	0.58
1:D:268:GLY:HA2	1:D:412:LEU:HD11	1.86	0.57
1:D:105:ASN:HD22	1:D:105:ASN:N	1.99	0.57
1:A:396:ALA:HB1	1:A:436:LEU:HD12	1.86	0.57
1:C:88:VAL:HG12	1:C:90:TRP:HE3	1.69	0.57
1:C:54:ALA:O	1:C:58:MET:HG3	2.05	0.57
1:C:215:MET:O	1:C:216:GLU:C	2.42	0.57
1:D:243:ASN:HD22	1:D:243:ASN:C	2.07	0.57
1:D:271:LYS:HG2	1:D:272:ASN:N	2.20	0.57
1:D:481:TRP:HE3	1:D:481:TRP:O	1.88	0.57
1:C:275:GLY:HA3	2:C:601:GOL:H12	1.87	0.57
1:D:278:CYS:SG	1:D:399:LEU:HD21	2.45	0.57
1:A:224:ASN:HD22	1:A:302:GLN:N	1.87	0.56
1:B:420:ASP:CG	1:B:449:THR:HG21	2.23	0.56
1:D:242:LEU:O	1:D:243:ASN:HB3	2.05	0.56
1:D:509:TRP:C	1:D:511:LYS:H	2.08	0.56
1:B:105:ASN:HD22	1:B:105:ASN:H	1.53	0.56
1:C:358:ALA:HB2	1:C:362:LEU:HD13	1.88	0.56
1:A:146:ARG:NE	4:A:750:HOH:O	2.32	0.56
1:B:416:SER:HB2	1:B:440:ASP:O	2.06	0.55
1:B:106:ASP:OD1	1:B:108:ARG:HG2	2.06	0.55
1:A:110:TYR:O	1:A:113:THR:HG22	2.07	0.55
1:B:278:CYS:SG	1:B:399:LEU:CD1	2.87	0.55
1:C:401:ASP:CG	1:C:501:ARG:HH21	2.10	0.55
1:C:477:ARG:NH2	4:C:709:HOH:O	2.39	0.55
1:D:278:CYS:HB2	1:D:317:ILE:HG12	1.88	0.54
1:A:234:ASP:HB2	4:A:752:HOH:O	2.06	0.54
1:C:124:ASP:O	1:C:127:PHE:HB3	2.07	0.54
1:B:0:THR:HG22	1:B:1:MET:H	1.73	0.54
1:C:160:ARG:HB2	1:C:160:ARG:NH1	2.23	0.54
1:A:198:LEU:HD22	1:A:311:TYR:HE1	1.71	0.54
1:A:222:ARG:HD3	1:A:226:GLU:OE1	2.07	0.54
1:C:184:VAL:HG12	1:C:222:ARG:HH11	1.71	0.54
1:D:85:GLU:OE1	1:D:139:TYR:CE2	2.61	0.54

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:THR:HG23	1:A:470:GLU:OE1	2.08	0.54
1:B:328:ARG:HH11	1:B:328:ARG:CG	2.21	0.53
1:A:117:THR:HG22	1:A:136:VAL:HG11	1.90	0.53
1:A:242:LEU:O	1:A:243:ASN:CB	2.57	0.53
1:D:268:GLY:CA	1:D:412:LEU:HD11	2.38	0.53
1:C:160:ARG:HH11	1:C:160:ARG:HG2	1.71	0.53
1:A:223:SER:HB2	1:A:302:GLN:HG2	1.89	0.53
1:B:146:ARG:NH1	1:B:212:LYS:CG	2.71	0.53
1:B:328:ARG:HH11	1:B:328:ARG:HG2	1.74	0.53
1:D:336:HIS:CD2	1:D:338:THR:OG1	2.60	0.53
1:C:141:ALA:HB3	1:C:193:THR:HA	1.90	0.52
1:B:474:VAL:HG22	1:B:477:ARG:HH12	1.74	0.52
1:B:184:VAL:CG1	1:B:222:ARG:HD2	2.39	0.52
1:C:224:ASN:ND2	1:C:302:GLN:H	2.02	0.52
1:D:324:VAL:HG21	1:D:423:LEU:HD21	1.90	0.52
1:A:141:ALA:HB3	1:A:193:THR:HA	1.91	0.52
1:C:232:GLU:OE1	1:C:245:ARG:NH1	2.43	0.52
1:C:273:THR:HA	1:C:420:ASP:OD2	2.10	0.52
1:B:252:ILE:HG23	1:B:257:SER:HB2	1.91	0.51
1:D:224:ASN:ND2	1:D:302:GLN:H	2.07	0.51
1:D:20:ASP:C	1:D:20:ASP:OD1	2.49	0.51
1:D:98:LEU:HD21	1:D:158:ALA:HB3	1.93	0.51
1:B:126:MET:SD	1:B:135:PRO:HB3	2.51	0.51
1:C:160:ARG:NH1	1:C:160:ARG:HG2	2.26	0.51
1:B:125:SER:O	1:B:136:VAL:HG23	2.11	0.50
1:B:85:GLU:OE1	1:B:139:TYR:CE1	2.64	0.50
1:B:234:ASP:OD2	1:B:234:ASP:N	2.39	0.50
1:D:51:PHE:HE2	1:D:235:GLU:HG3	1.77	0.50
1:A:494:GLU:O	1:A:494:GLU:OE2	2.29	0.50
1:D:72:PHE:HA	1:D:73:ARG:HH11	1.75	0.50
1:C:370:SER:HA	1:C:510:ALA:HB3	1.94	0.50
1:D:238:VAL:HG23	1:D:239:ALA:N	2.26	0.50
1:C:239:ALA:O	1:C:242:LEU:O	2.30	0.50
1:A:277:GLY:HA3	2:A:602:GOL:O2	2.12	0.49
1:D:115:LYS:HG3	1:D:119:GLU:OE1	2.13	0.49
1:D:476:ARG:NH2	1:D:481:TRP:CH2	2.71	0.49
1:C:139:TYR:O	1:C:144:LYS:HE2	2.12	0.49
1:D:279:PHE:CZ	2:D:602:GOL:H32	2.47	0.49
1:D:489:SER:C	1:D:493:ARG:HE	2.16	0.49
1:B:201:ARG:HD3	1:B:309:CYS:SG	2.53	0.49
1:D:198:LEU:HD22	1:D:311:TYR:HE1	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:THR:N	1:A:470:GLU:OE1	2.31	0.49
1:B:81:THR:OG1	1:B:254:ASP:HA	2.13	0.49
1:C:267:LYS:HE3	1:C:412:LEU:HD21	1.95	0.48
1:A:209:GLU:O	1:A:212:LYS:HD2	2.12	0.48
1:B:211:LEU:O	1:B:212:LYS:HG2	2.12	0.48
1:D:280:LEU:HD12	1:D:399:LEU:CD1	2.27	0.48
1:B:274:TYR:O	1:B:421:GLY:HA3	2.13	0.48
1:C:274:TYR:HB3	1:C:423:LEU:HB2	1.96	0.48
1:B:225:SER:OG	1:B:457:CYS:O	2.20	0.48
1:D:44:GLU:HA	1:D:103:VAL:HG23	1.96	0.48
1:A:442:LEU:HB3	1:A:481:TRP:CE3	2.49	0.48
1:B:90:TRP:HA	1:B:98:LEU:HD22	1.96	0.48
1:C:91:ASP:OD1	1:C:94:THR:CG2	2.48	0.48
1:B:303:VAL:O	1:B:307:GLY:HA3	2.13	0.48
1:B:355:PHE:O	1:B:357:PRO:HD3	2.14	0.48
1:D:235:GLU:O	1:D:238:VAL:HG13	2.14	0.47
1:A:336:HIS:N	1:A:339:GLU:OE1	2.30	0.47
1:A:477:ARG:NH2	4:A:713:HOH:O	2.29	0.47
1:B:282:MET:O	1:B:312:ALA:HA	2.14	0.47
1:D:71:SER:O	1:D:73:ARG:HD2	2.14	0.47
1:A:159:CYS:HB2	1:A:164:LEU:HD22	1.95	0.47
1:B:115:LYS:HE2	1:B:115:LYS:HB3	1.64	0.47
1:C:65:LEU:HD22	1:C:69:ASP:HB3	1.97	0.47
1:C:328:ARG:HD2	1:C:335:SER:O	2.14	0.47
1:C:358:ALA:O	1:C:372:ARG:HA	2.14	0.47
1:D:433:GLN:HG2	1:D:441:ILE:HD11	1.97	0.47
1:A:198:LEU:HD22	1:A:311:TYR:CE1	2.49	0.47
1:D:357:PRO:HD3	1:D:394:ALA:HB1	1.96	0.46
1:D:15:ARG:NH2	1:D:448:GLU:OE1	2.49	0.46
1:A:419:VAL:CG2	1:A:443:VAL:HG22	2.46	0.46
1:B:363:LEU:HA	1:B:367:TRP:CD1	2.49	0.46
1:A:407:LYS:HD2	1:A:413:ASN:HA	1.97	0.46
1:B:342:LYS:HA	1:B:342:LYS:HD3	1.74	0.46
1:C:200:THR:O	1:C:201:ARG:HB2	2.15	0.46
1:A:81:THR:HA	1:A:252:ILE:O	2.16	0.46
1:A:224:ASN:ND2	1:A:302:GLN:N	2.50	0.46
1:B:271:LYS:HE3	1:B:281:LEU:HD13	1.96	0.46
1:C:92:ARG:HD3	4:C:733:HOH:O	2.16	0.46
1:D:291:SER:HA	1:D:409:ASP:OD2	2.15	0.46
1:C:184:VAL:HG12	1:C:222:ARG:NH1	2.28	0.45
1:C:283:ASN:C	1:C:283:ASN:OD1	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:THR:N	1:B:277:GLY:HA3	2.32	0.45
1:C:176:LYS:HD2	1:C:176:LYS:HA	1.43	0.45
1:D:362:LEU:HD22	1:D:371:ALA:CB	2.46	0.45
1:A:64:LYS:O	1:A:68:LYS:HG2	2.17	0.45
1:A:366:TYR:CE1	1:A:401:ASP:OD1	2.70	0.45
1:C:324:VAL:HG21	1:C:423:LEU:HD21	1.99	0.45
1:D:271:LYS:HE2	1:D:281:LEU:HD13	1.98	0.45
1:A:328:ARG:HB2	1:A:334:PHE:CE2	2.51	0.45
1:C:198:LEU:O	1:C:311:TYR:OH	2.27	0.45
1:B:69:ASP:C	1:B:71:SER:H	2.18	0.45
1:C:74:LYS:HE3	1:C:76:GLU:OE2	2.16	0.45
1:A:366:TYR:HE1	1:A:401:ASP:OD1	2.00	0.45
1:A:97:PRO:HD3	1:A:172:TRP:CH2	2.52	0.45
1:A:288:ALA:HB2	1:A:311:TYR:CE1	2.52	0.45
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.31	0.44
1:D:17:ILE:HD13	1:D:28:VAL:HG23	1.99	0.44
1:A:157:ASP:O	1:A:160:ARG:CB	2.53	0.44
1:C:96:GLU:HB3	1:C:97:PRO:HD2	2.00	0.44
1:C:350:THR:O	1:C:351:GLN:HB2	2.17	0.44
1:A:275:GLY:N	1:A:277:GLY:O	2.50	0.44
1:C:160:ARG:CG	1:C:160:ARG:NH1	2.70	0.44
1:A:65:LEU:HD13	1:A:72:PHE:CG	2.52	0.44
1:B:171:THR:OG1	1:B:185:THR:HB	2.17	0.44
1:D:413[A]:ASN:ND2	1:D:414:LEU:N	2.63	0.44
1:A:243:ASN:OD1	1:A:244:GLU:OE1	2.36	0.44
1:B:185:THR:HG22	1:B:219:PRO:HG2	2.00	0.44
1:C:15:ARG:HG3	1:C:30:GLN:HG3	1.99	0.44
1:C:80:ILE:O	1:C:251:SER:HA	2.18	0.44
1:A:91:ASP:OD2	1:A:163:THR:HG23	2.18	0.44
1:A:113:THR:O	1:A:117:THR:HG22	2.17	0.44
1:B:187:VAL:HG13	1:B:222:ARG:O	2.17	0.44
1:D:64:LYS:O	1:D:68:LYS:HG3	2.17	0.44
1:D:91:ASP:HB3	1:D:94:THR:OG1	2.17	0.44
1:D:489:SER:HA	1:D:493:ARG:HH21	1.83	0.44
1:B:153:PRO:O	1:B:157:ASP:OD1	2.36	0.44
1:C:276:THR:HB	2:C:601:GOL:H2	1.99	0.44
1:C:270:ALA:HB2	1:C:282:MET:HG3	2.00	0.44
1:D:126:MET:SD	1:D:135:PRO:HB3	2.58	0.44
1:A:374:THR:HG23	1:A:507:THR:HG22	1.97	0.43
1:C:90:TRP:HA	1:C:98:LEU:HD22	2.01	0.43
1:C:267:LYS:HA	1:C:283:ASN:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:HB2	1:B:334:PHE:CZ	2.52	0.43
1:C:44:GLU:HG3	1:C:100:TYR:CB	2.49	0.43
1:D:341:GLU:O	1:D:345:ARG:HG3	2.18	0.43
1:D:357:PRO:HD3	1:D:394:ALA:CB	2.49	0.43
1:B:105:ASN:HB2	3:B:602:HEZ:H11	1.99	0.43
1:B:446:MET:HB2	1:B:479:ASN:OD1	2.18	0.43
1:A:374:THR:HG21	1:A:507:THR:CG2	2.43	0.43
1:D:81:THR:HA	1:D:252:ILE:O	2.19	0.43
1:B:42:TRP:HA	1:B:106:ASP:OD2	2.18	0.43
1:A:216:GLU:H	1:A:216:GLU:HG3	1.65	0.43
1:C:265:PHE:HD1	1:C:472:LYS:HE3	1.83	0.43
1:A:44:GLU:HA	1:A:103:VAL:HG23	2.01	0.42
1:A:477:ARG:NH1	4:A:713:HOH:O	2.48	0.42
1:B:254:ASP:OD2	1:B:255:GLN:HG2	2.19	0.42
1:B:363:LEU:HB3	1:B:364:ALA:H	1.52	0.42
1:B:73:ARG:HG3	1:B:74:LYS:HG2	2.01	0.42
1:A:300:GLY:O	1:A:301:PHE:HB3	2.19	0.42
1:A:324:VAL:HG21	1:A:423:LEU:HD21	2.01	0.42
1:A:336:HIS:HD2	1:A:338:THR:CA	2.30	0.42
1:D:425:LYS:HB2	1:D:425:LYS:HE2	1.72	0.42
1:D:509:TRP:C	1:D:511:LYS:N	2.72	0.42
1:A:113:THR:O	1:A:117:THR:CG2	2.68	0.42
1:B:289:ARG:HG2	1:B:409:ASP:O	2.19	0.42
1:B:326:TRP:O	1:B:330:ASN:HB2	2.20	0.42
1:D:170:ASP:O	1:D:174:MET:HG3	2.20	0.42
1:D:368:ASP:OD1	1:D:370:SER:HB2	2.19	0.42
1:B:31:VAL:HG13	1:B:32:PRO:HD2	2.00	0.42
1:D:401:ASP:OD2	1:D:501:ARG:NH2	2.46	0.42
1:C:410:ALA:HB1	1:C:412:LEU:HD12	2.02	0.42
1:C:472:LYS:HD3	4:C:743:HOH:O	2.19	0.42
1:A:252:ILE:HG23	1:A:257:SER:HB2	2.02	0.41
1:D:208:CYS:HB3	1:D:213:ILE:O	2.20	0.41
1:D:212:LYS:O	1:D:214:PRO:HD3	2.19	0.41
1:A:372:ARG:HA	1:A:372:ARG:HD3	1.85	0.41
1:D:85:GLU:HB2	1:D:104:TRP:HB3	2.02	0.41
1:D:282:MET:HE2	1:D:414:LEU:HD12	1.75	0.41
1:A:344:ALA:HB2	1:A:388:ILE:HG22	2.03	0.41
1:A:418:ARG:HD2	1:A:418:ARG:N	2.35	0.41
1:B:23:GLN:HE22	1:B:475:SER:HB2	1.85	0.41
1:C:147:TRP:O	1:C:147:TRP:CD2	2.74	0.41
1:B:233:THR:O	1:B:239:ALA:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLU:OE1	1:C:100:TYR:HB2	2.21	0.41
1:C:47:PRO:HB2	1:C:97:PRO:HG3	2.03	0.41
1:D:213:ILE:HG21	1:D:218:LEU:HD21	2.03	0.41
1:A:117:THR:HB	1:A:125:SER:HA	2.02	0.41
1:A:420:ASP:OD1	1:A:449:THR:OG1	2.38	0.41
1:A:273:THR:HA	1:A:420:ASP:OD2	2.21	0.41
1:C:80:ILE:HD12	1:C:174:MET:HG3	2.02	0.41
1:A:208:CYS:HB3	1:A:213:ILE:O	2.20	0.41
1:B:295:LEU:HD13	1:B:406:MET:HG3	2.01	0.41
3:B:602:HEZ:O1	3:B:603:HEZ:H62	2.20	0.41
1:D:142:ALA:O	1:D:145:MET:HB2	2.21	0.41
1:B:106:ASP:OD1	4:B:725:HOH:O	2.22	0.41
1:C:325:GLU:OE2	1:C:328:ARG:NH1	2.53	0.41
1:C:459:GLY:HA3	1:C:465:TRP:CZ3	2.55	0.41
1:C:108:ARG:HD3	1:C:147:TRP:CE2	2.55	0.41
1:C:215:MET:O	1:C:217:THR:N	2.52	0.41
1:D:137:SER:C	1:D:139:TYR:H	2.24	0.41
1:D:170:ASP:OD1	1:D:170:ASP:N	2.51	0.41
1:D:364:ALA:HB1	1:D:402:VAL:HG22	2.03	0.41
1:A:370:SER:HA	1:A:510:ALA:HB3	2.03	0.41
1:B:90:TRP:CA	1:B:98:LEU:HD22	2.51	0.41
1:B:273:THR:HG23	1:B:420:ASP:OD2	2.21	0.41
1:C:363:LEU:HB3	1:C:364:ALA:H	1.16	0.41
1:D:130:LYS:HA	1:D:130:LYS:HD3	1.84	0.41
1:A:-1:PHE:HD1	1:A:0:THR:N	2.16	0.40
1:B:69:ASP:C	1:B:71:SER:N	2.74	0.40
1:C:65:LEU:HD13	1:C:72:PHE:CG	2.56	0.40
1:A:146:ARG:HH12	1:A:149:LEU:HD12	1.86	0.40
1:A:195:LEU:HD13	1:A:218:LEU:HD11	2.04	0.40
1:B:447:HIS:O	1:B:449:THR:N	2.46	0.40
1:C:215:MET:HE2	1:C:215:MET:HB3	1.62	0.40
1:D:271:LYS:NZ	1:D:273:THR:OG1	2.41	0.40
1:A:4:VAL:HG23	1:A:77:ALA:O	2.20	0.40
1:A:16:PHE:CD2	1:A:58:MET:HA	2.57	0.40
1:C:259:LEU:CD1	1:C:264:CYS:HB2	2.51	0.40
1:B:169:ILE:O	1:B:173:LEU:HB2	2.21	0.40
1:C:108:ARG:HD3	1:C:147:TRP:CZ2	2.56	0.40
1:D:130:LYS:HD2	4:D:720:HOH:O	2.21	0.40
1:D:141:ALA:HB3	1:D:193:THR:HA	2.04	0.40
1:D:470:GLU:O	1:D:474:VAL:HG23	2.21	0.40
1:C:235:GLU:C	1:C:237:GLY:N	2.72	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ILE:O	1:D:317:ILE:HG13	2.16	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%)	485 (95%)	25 (5%)	1 (0%)	47	61
1	B	511/518 (99%)	480 (94%)	27 (5%)	4 (1%)	19	27
1	C	511/518 (99%)	492 (96%)	17 (3%)	2 (0%)	34	46
1	D	512/518 (99%)	476 (93%)	33 (6%)	3 (1%)	25	34
All	All	2045/2072 (99%)	1933 (94%)	102 (5%)	10 (0%)	29	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	B	364	ALA
1	C	364	ALA
1	D	364	ALA
1	B	215	MET
1	B	337	ILE
1	D	243	ASN
1	C	226	GLU
1	B	363	LEU
1	D	480	SER

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	10
1	B	421/425 (99%)	383 (91%)	38 (9%)	9	12
1	C	421/425 (99%)	385 (91%)	36 (9%)	10	14
1	D	422/425 (99%)	382 (90%)	40 (10%)	8	11
All	All	1685/1700 (99%)	1529 (91%)	156 (9%)	9	11

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	PHE
1	A	9	GLN
1	A	17	ILE
1	A	56	LYS
1	A	59	SER
1	A	65	LEU
1	A	87	THR
1	A	93	VAL
1	A	94	THR
1	A	98	LEU
1	A	105	ASN
1	A	106	ASP
1	A	113	THR
1	A	117	THR
1	A	146	ARG
1	A	168	THR
1	A	173	LEU
1	A	177	LEU
1	A	187	VAL
1	A	212	LYS
1	A	216	GLU
1	A	238	VAL
1	A	271	LYS
1	A	276	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	305	ARG
1	A	317	ILE
1	A	335	SER
1	A	338	THR
1	A	342	LYS
1	A	345	ARG
1	A	350	THR
1	A	362	LEU
1	A	363	LEU
1	A	366	TYR
1	A	374	THR
1	A	441	ILE
1	A	442	LEU
1	A	476	ARG
1	A	483	THR
1	A	491	MET
1	A	494	GLU
1	A	511	LYS
1	B	-1	PHE
1	B	0	THR
1	B	9	GLN
1	B	59	SER
1	B	65	LEU
1	B	67	GLN
1	B	72	PHE
1	B	98	LEU
1	B	105	ASN
1	B	113	THR
1	B	115	LYS
1	B	117	THR
1	B	139	TYR
1	B	157	ASP
1	B	173	LEU
1	B	177	LEU
1	B	184	VAL
1	B	198	LEU
1	B	199	ARG
1	B	212	LYS
1	B	213	ILE
1	B	216	GLU
1	B	232	GLU
1	B	263	MET

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type
1	B	266	GLU
1	B	271	LYS
1	B	289	ARG
1	B	305	ARG
1	B	317	ILE
1	B	328	ARG
1	B	329	ARG
1	B	335	SER
1	B	338	THR
1	B	342	LYS
1	B	362	LEU
1	B	366	TYR
1	B	399	LEU
1	B	476	ARG
1	C	2	LYS
1	C	4	VAL
1	C	65	LEU
1	C	71	SER
1	C	74	LYS
1	C	91	ASP
1	C	99	CYS
1	C	106	ASP
1	C	113	THR
1	C	120	LEU
1	C	146	ARG
1	C	159	CYS
1	C	160	ARG
1	C	173	LEU
1	C	187	VAL
1	C	213	ILE
1	C	215	MET
1	C	233	THR
1	C	234	ASP
1	C	243	ASN
1	C	245	ARG
1	C	266	GLU
1	C	271	LYS
1	C	278	CYS
1	C	305	ARG
1	C	317	ILE
1	C	338	THR
1	C	342	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	362	LEU
1	C	366	TYR
1	C	441	ILE
1	C	442	LEU
1	C	447	HIS
1	C	470	GLU
1	C	476	ARG
1	C	483	THR
1	D	-1	PHE
1	D	9	GLN
1	D	15	ARG
1	D	27	SER
1	D	56	LYS
1	D	65	LEU
1	D	71	SER
1	D	73	ARG
1	D	93	VAL
1	D	98	LEU
1	D	105	ASN
1	D	117	THR
1	D	146	ARG
1	D	173	LEU
1	D	177	LEU
1	D	198	LEU
1	D	212	LYS
1	D	234	ASP
1	D	243	ASN
1	D	245	ARG
1	D	271	LYS
1	D	289	ARG
1	D	292	LYS
1	D	317	ILE
1	D	335	SER
1	D	342	LYS
1	D	355	PHE
1	D	362	LEU
1	D	366	TYR
1	D	370	SER
1	D	412	LEU
1	D	413[A]	ASN
1	D	413[B]	ASN
1	D	420	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	472	LYS
1	D	476	ARG
1	D	481	TRP
1	D	483	THR
1	D	491	MET
1	D	492	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	39	HIS
1	A	105	ASN
1	A	224	ASN
1	A	272	ASN
1	A	302	GLN
1	A	336	HIS
1	B	23	GLN
1	B	30	GLN
1	B	105	ASN
1	B	224	ASN
1	B	272	ASN
1	B	293	HIS
1	B	302	GLN
1	C	23	GLN
1	C	35	GLN
1	C	39	HIS
1	C	105	ASN
1	C	224	ASN
1	C	262	ASN
1	C	272	ASN
1	C	302	GLN
1	C	336	HIS
1	C	393	GLN
1	D	23	GLN
1	D	105	ASN
1	D	151	ASN
1	D	224	ASN
1	D	243	ASN
1	D	336	HIS
1	D	433	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

11 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	C	602	-	5,5,5	0.44	0	5,5,5	0.45	0
3	HEZ	D	603	-	7,7,7	0.50	0	6,6,6	0.31	0
2	GOL	A	602	-	5,5,5	0.46	0	5,5,5	0.33	0
3	HEZ	B	603	-	7,7,7	0.51	0	6,6,6	0.29	0
2	GOL	A	601	-	5,5,5	0.50	0	5,5,5	0.43	0
2	GOL	C	601	-	5,5,5	0.33	0	5,5,5	0.31	0
2	GOL	D	601	-	5,5,5	0.34	0	5,5,5	0.58	0
2	GOL	D	602	-	5,5,5	0.28	0	5,5,5	0.63	0
3	HEZ	B	602	-	7,7,7	0.49	0	6,6,6	0.39	0
3	HEZ	C	603	-	7,7,7	0.52	0	6,6,6	0.48	0
2	GOL	B	601	-	5,5,5	0.57	0	5,5,5	0.90	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	C	602	-	-	4/4/4/4	-
3	HEZ	D	603	-	-	5/5/5/5	-
2	GOL	A	602	-	-	4/4/4/4	-
3	HEZ	B	603	-	-	4/5/5/5	-
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	C	601	-	-	0/4/4/4	-
2	GOL	D	601	-	-	0/4/4/4	-
2	GOL	D	602	-	-	0/4/4/4	-
3	HEZ	B	602	-	-	4/5/5/5	-
3	HEZ	C	603	-	-	3/5/5/5	-
2	GOL	B	601	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	GOL	O1-C1-C2-C3
2	A	602	GOL	C1-C2-C3-O3
2	B	601	GOL	C1-C2-C3-O3
2	C	602	GOL	O1-C1-C2-C3
2	C	602	GOL	C1-C2-C3-O3
2	A	602	GOL	O2-C2-C3-O3
2	C	602	GOL	O2-C2-C3-O3
2	A	601	GOL	O1-C1-C2-C3
2	A	602	GOL	O1-C1-C2-O2
3	C	603	HEZ	C2-C3-C4-C5
3	C	603	HEZ	C1-C2-C3-C4
3	D	603	HEZ	C2-C3-C4-C5
3	B	603	HEZ	C2-C3-C4-C5
3	B	603	HEZ	C3-C4-C5-C6
3	B	602	HEZ	C1-C2-C3-C4
3	B	602	HEZ	C4-C5-C6-O6
3	D	603	HEZ	C4-C5-C6-O6
3	B	602	HEZ	O1-C1-C2-C3
2	C	602	GOL	O1-C1-C2-O2
3	D	603	HEZ	O1-C1-C2-C3
3	B	602	HEZ	C2-C3-C4-C5
3	D	603	HEZ	C3-C4-C5-C6

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	601	GOL	O1-C1-C2-O2
3	C	603	HEZ	O1-C1-C2-C3
3	D	603	HEZ	C1-C2-C3-C4
2	A	601	GOL	O1-C1-C2-O2
2	B	601	GOL	O2-C2-C3-O3
2	B	601	GOL	O1-C1-C2-C3
3	B	603	HEZ	O1-C1-C2-C3
3	B	603	HEZ	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	GOL	1	0
3	B	603	HEZ	2	0
2	C	601	GOL	2	0
2	D	602	GOL	1	0
3	B	602	HEZ	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(Å²)	Q<0.9
1	A	513/518 (99%)	0.17	3 (0%)	89	89	34, 49, 63, 72	1 (0%)
1	B	513/518 (99%)	0.17	10 (1%)	66	68	30, 53, 69, 87	1 (0%)
1	C	513/518 (99%)	0.19	11 (2%)	63	65	32, 51, 68, 75	1 (0%)
1	D	513/518 (99%)	0.13	13 (2%)	57	59	31, 51, 69, 84	1 (0%)
All	All	2052/2072 (99%)	0.17	37 (1%)	68	70	30, 51, 67, 87	4 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	491	MET	6.4
1	B	491	MET	5.3
1	A	278	CYS	4.4
1	B	152	VAL	4.2
1	D	511	LYS	3.8
1	B	160	ARG	3.3
1	C	175	TYR	3.3
1	B	-1	PHE	3.1
1	B	278	CYS	3.1
1	D	510	ALA	3.0
1	D	278	CYS	2.9
1	D	160	ARG	2.9
1	D	158	ALA	2.8
1	B	163	THR	2.8
1	D	447	HIS	2.8
1	B	488	GLY	2.7
1	B	481	TRP	2.6
1	C	91	ASP	2.6
1	D	152	VAL	2.6
1	D	227	LEU	2.5
1	C	93	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	97	PRO	2.4
1	B	156	ALA	2.4
1	C	94	THR	2.4
1	C	98	LEU	2.3
1	D	408	ARG	2.2
1	C	40	PRO	2.2
1	C	245	ARG	2.2
1	D	305	ARG	2.2
1	B	67	GLN	2.2
1	C	164	LEU	2.2
1	D	303	VAL	2.2
1	A	367	TRP	2.1
1	C	165	CYS	2.1
1	D	93	VAL	2.1
1	C	510	ALA	2.0
1	A	163	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEZ	B	602	8/8	0.73	0.29	63,66,67,67	0
3	HEZ	B	603	8/8	0.75	0.28	58,62,63,64	0
3	HEZ	D	603	8/8	0.78	0.26	52,56,57,58	0
3	HEZ	C	603	8/8	0.85	0.18	49,51,52,53	0
2	GOL	A	602	6/6	0.86	0.21	58,60,63,65	0
2	GOL	D	602	6/6	0.87	0.19	60,61,61,62	0
2	GOL	C	602	6/6	0.88	0.27	50,58,61,65	0

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	C	601	6/6	0.89	0.25	72,73,74,75	0
2	GOL	A	601	6/6	0.94	0.14	58,59,60,63	0
2	GOL	D	601	6/6	0.96	0.13	38,40,43,45	0
2	GOL	B	601	6/6	0.96	0.14	31,34,36,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.