Full wwPDB X-ray Structure Validation Report (i)

Jun 14, 2020 – 08:19 pm BST

PDB ID	:	3ABZ
Title	:	Crystal structure of Se-Met labeled Beta-glucosidase from Kluyveromyces marxianus
Authors	:	Yoshida, E.; Hidaka, M.; Fushinobu, S.; Katayama, T.; Kumagai, H.
Deposited on	:	2009-12-25
Resolution	:	2.15 Å(reported)

The following versions of software and data (see references (i)) 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 (i)

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

The reported resolution of this entry is 2.15 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.
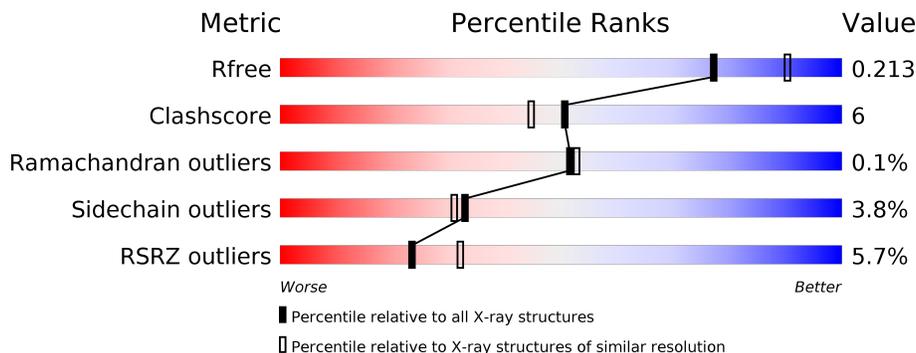
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	845	
1	B	845	
1	C	845	
1	D	845	

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
2	GOL	A	5002	-	-	X	-
2	GOL	B	5006	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 29154 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 Beta-glucosidase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	844	Total 6606	C 4197	N 1110	O 1284	S 5	Se 10	0	0	0
1	B	810	Total 6351	C 4040	N 1065	O 1232	S 4	Se 10	0	0	0
1	C	836	Total 6550	C 4161	N 1102	O 1272	S 5	Se 10	0	0	0
1	D	833	Total 6521	C 4146	N 1096	O 1264	S 5	Se 10	0	0	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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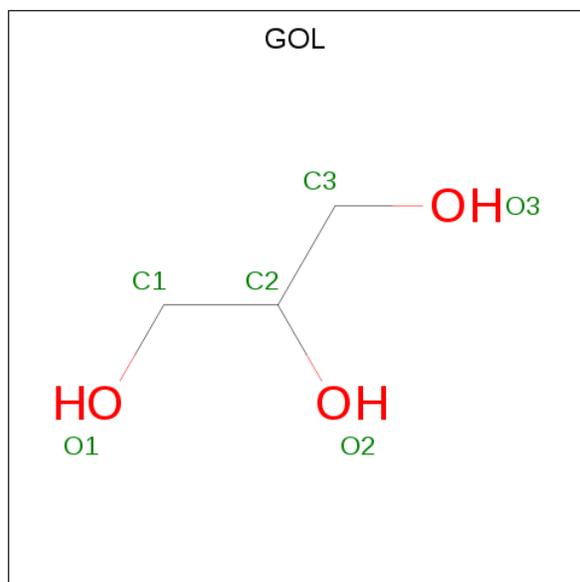
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0

Continued on next page...

Continued from previous page...

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	B	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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	875	Total 875	O 875	0	0
3	B	828	Total 828	O 828	0	0
3	C	701	Total 701	O 701	0	0
3	D	674	Total 674	O 674	0	0

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: Beta-glucosidase I
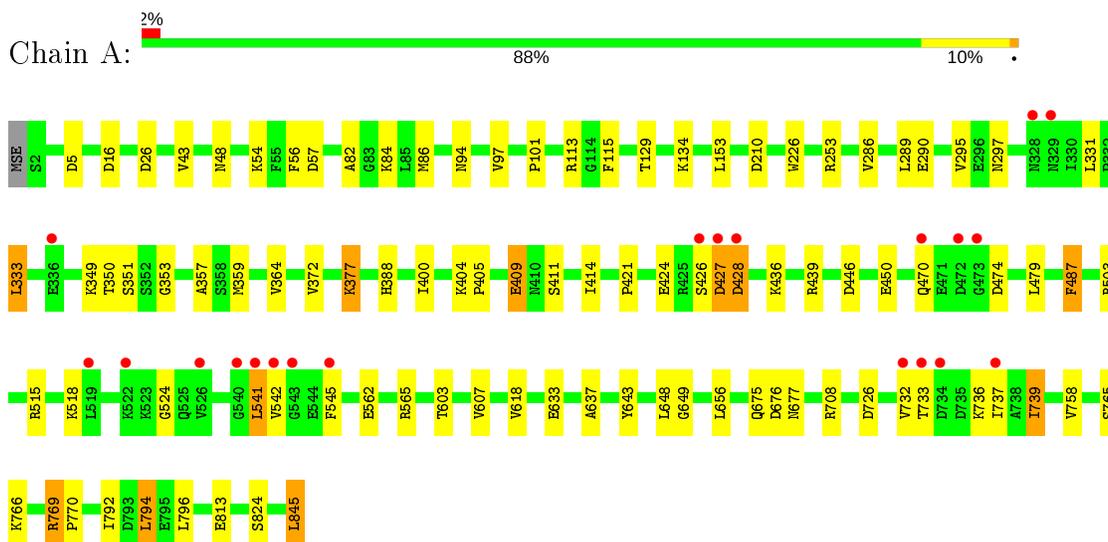
- Molecule 1: Beta-glucosidase I
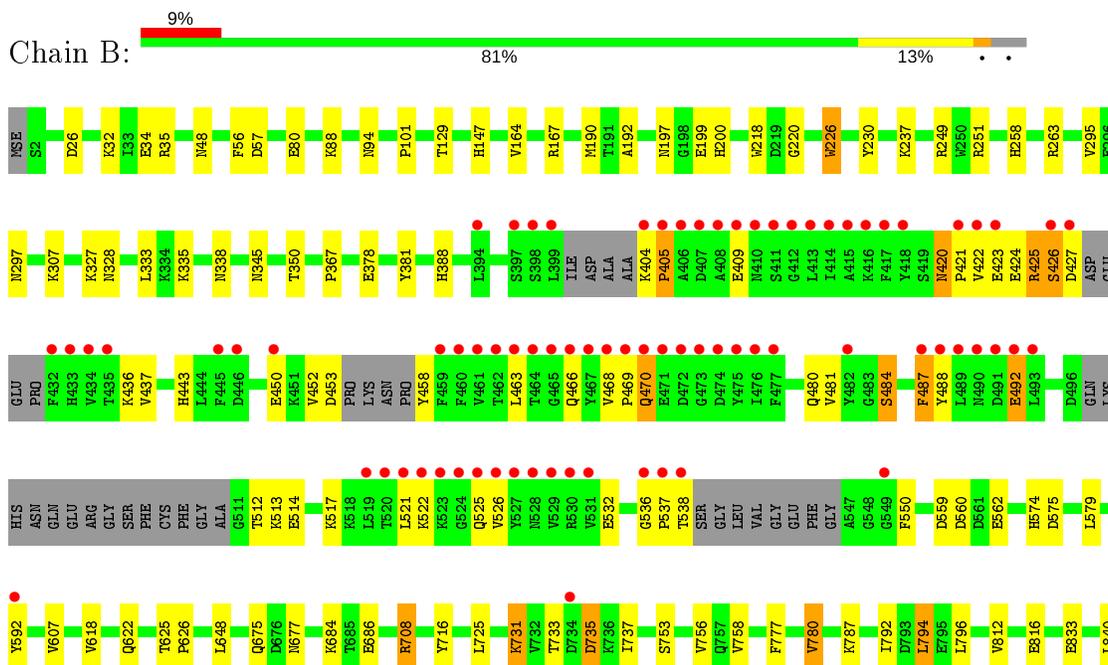
• Molecule 1: Beta-glucosidase I

Chain C:
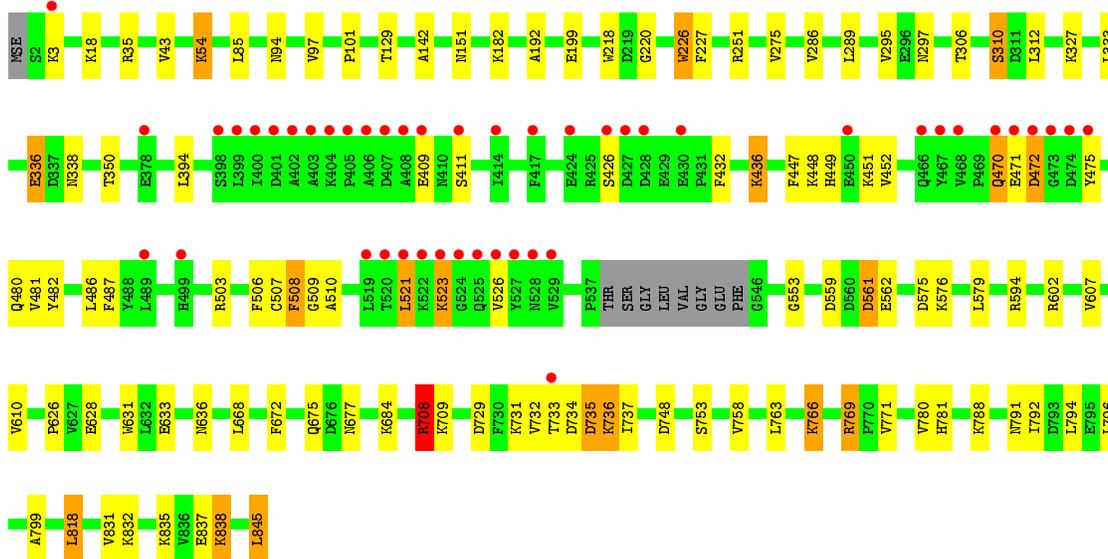
• Molecule 1: Beta-glucosidase I

Chain D:
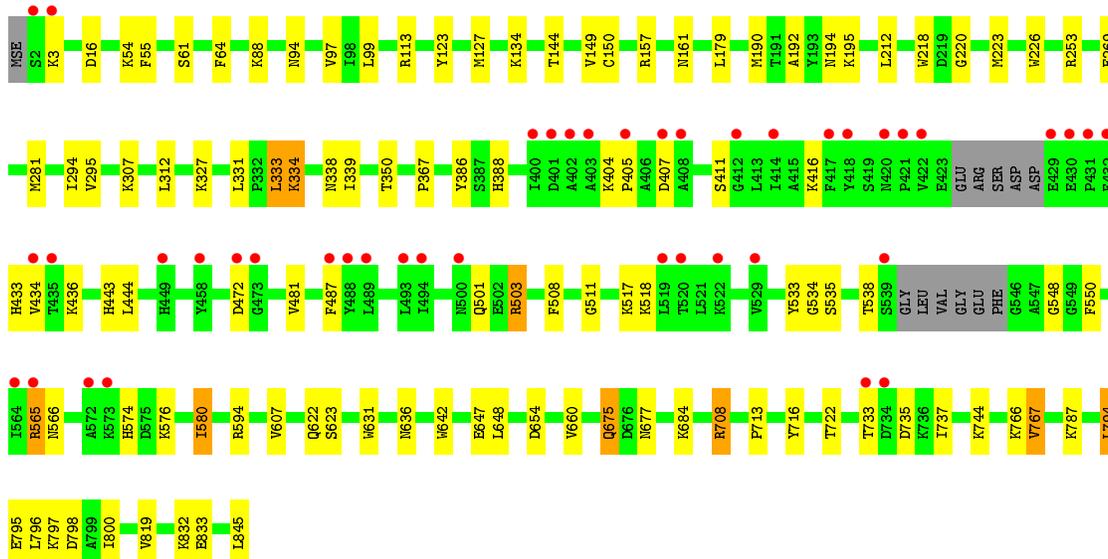
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	245.68Å 148.64Å 119.78Å 90.00° 112.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 48.40 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.15) 99.8 (48.40-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.160 , 0.218 0.156 , 0.213	Depositor DCC
R_{free} test set	10724 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.3	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	29154	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.07	1/6733 (0.0%)	0.88	8/9088 (0.1%)
1	B	1.13	7/6466 (0.1%)	0.90	11/8720 (0.1%)
1	C	1.01	3/6675 (0.0%)	0.85	6/9008 (0.1%)
1	D	0.99	4/6645 (0.1%)	0.84	5/8967 (0.1%)
All	All	1.05	15/26519 (0.1%)	0.87	30/35783 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	795	GLU	CG-CD	5.84	1.60	1.51
1	A	643	TYR	CD1-CE1	-5.67	1.30	1.39
1	B	80	GLU	CB-CG	-5.64	1.41	1.52
1	C	199	GLU	CB-CG	5.53	1.62	1.52
1	C	771	VAL	CB-CG1	5.47	1.64	1.52
1	B	618	VAL	CB-CG1	-5.45	1.41	1.52
1	D	97	VAL	CB-CG1	5.44	1.64	1.52
1	C	199	GLU	CG-CD	5.21	1.59	1.51
1	B	381	TYR	CD1-CE1	-5.20	1.31	1.39
1	D	269	GLU	CG-CD	5.19	1.59	1.51
1	B	716	TYR	CD2-CE2	5.18	1.47	1.39
1	B	226	TRP	CB-CG	5.07	1.59	1.50
1	D	647	GLU	CG-CD	5.05	1.59	1.51
1	B	199	GLU	CB-CG	5.04	1.61	1.52
1	B	592	TYR	CD2-CE2	5.02	1.46	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	113	ARG	NE-CZ-NH1	-8.69	115.95	120.30
1	A	769	ARG	NE-CZ-NH1	-7.39	116.60	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	769	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	C	251	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	B	263	ARG	NE-CZ-NH2	6.89	123.75	120.30
1	B	26	ASP	CB-CG-OD1	6.69	124.33	118.30
1	A	5	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	708	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	C	708	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	708	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	B	263	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	515	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	845	LEU	CB-CG-CD1	5.81	120.88	111.00
1	C	818	LEU	CA-CB-CG	5.74	128.51	115.30
1	B	251	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	B	249	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	D	157	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	594	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	D	113	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	D	594	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	26	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	798	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	560	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	559	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	486	LEU	CA-CB-CG	5.21	127.27	115.30
1	B	559	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	210	ASP	CB-CG-OD1	5.12	122.90	118.30
1	D	767	VAL	CG1-CB-CG2	5.07	119.01	110.90
1	B	167	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	5	ASP	CB-CG-OD2	-5.02	113.78	118.30

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	6606	0	6514	70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6351	0	6279	89	0
1	C	6550	0	6460	74	0
1	D	6521	0	6439	65	0
2	A	24	0	32	10	0
2	B	12	0	16	5	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	875	0	0	13	0
3	B	828	0	0	18	0
3	C	701	0	0	15	0
3	D	674	0	0	10	0
All	All	29154	0	25756	296	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:5001:GOL:H32	3:A:1983:HOH:O	1.54	1.05
1:C:734:ASP:O	1:C:735:ASP:HB3	1.57	1.04
1:A:737:ILE:HD11	1:A:796:LEU:HD23	1.41	1.01
1:C:338:ASN:HB3	1:C:575:ASP:HB2	1.53	0.91
1:D:134:LYS:HE2	3:D:2595:HOH:O	1.70	0.91
1:D:565:ARG:HG2	1:D:565:ARG:HH11	1.35	0.90
1:A:708:ARG:NH2	1:B:708:ARG:NH2	2.27	0.82
1:C:472:ASP:OD2	1:C:523:LYS:HB2	1.80	0.82
1:C:449:HIS:HD2	1:C:451:LYS:H	1.27	0.81
1:D:127:MSE:CE	1:D:179:LEU:HD22	2.12	0.80
1:B:48:ASN:HB3	3:B:2353:HOH:O	1.83	0.79
1:B:517:LYS:HD2	3:B:2238:HOH:O	1.82	0.79
1:B:484:SER:HB3	1:B:538:THR:OG1	1.83	0.78
1:A:84:LYS:HB3	1:A:84:LYS:HZ2	1.47	0.78
1:B:481:VAL:H	1:B:512:THR:HG22	1.48	0.78
1:A:404:LYS:HB3	1:A:405:PRO:HD2	1.66	0.77
1:C:736:LYS:HD2	1:C:737:ILE:N	1.99	0.77
1:A:297:ASN:HB2	3:A:2042:HOH:O	1.86	0.76
3:A:2133:HOH:O	1:B:675:GLN:HG2	1.86	0.75
1:B:350:THR:HG22	3:B:2411:HOH:O	1.88	0.74
1:C:411:SER:O	1:C:436:LYS:HE2	1.87	0.73
1:B:297:ASN:HB3	3:B:2349:HOH:O	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:VAL:HG21	1:A:792:ILE:HD13	1.71	0.72
1:A:439:ARG:H	2:A:5002:GOL:H11	1.54	0.72
1:A:57:ASP:H	2:A:5002:GOL:C3	2.02	0.72
1:B:562:GLU:HG2	3:B:2413:HOH:O	1.90	0.72
1:A:439:ARG:HB2	2:A:5002:GOL:H12	1.70	0.72
1:B:437:VAL:HG13	2:B:5006:GOL:H32	1.70	0.72
1:C:837:GLU:HB3	3:C:863:HOH:O	1.90	0.71
1:C:94:ASN:ND2	1:C:295:VAL:H	1.89	0.71
1:C:471:GLU:HA	1:C:523:LYS:HG2	1.73	0.71
1:B:737:ILE:HD11	1:B:796:LEU:HD23	1.72	0.70
1:D:350:THR:HG22	3:D:2389:HOH:O	1.92	0.70
1:B:164:VAL:H	1:B:197:ASN:HD21	1.39	0.69
1:A:84:LYS:HB3	1:A:84:LYS:NZ	2.06	0.69
1:B:307:LYS:HE2	3:B:2259:HOH:O	1.93	0.69
1:C:794:LEU:HD12	1:C:799:ALA:HB2	1.73	0.69
1:B:426:SER:O	1:B:427:ASP:CB	2.41	0.69
1:D:127:MSE:HE1	1:D:179:LEU:HD22	1.74	0.68
1:D:565:ARG:CG	1:D:565:ARG:HH11	2.06	0.68
1:C:737:ILE:HD11	1:C:796:LEU:HD23	1.76	0.68
1:B:404:LYS:HB2	1:B:405:PRO:HD3	1.75	0.67
1:B:56:PHE:HB2	3:B:2942:HOH:O	1.95	0.67
1:D:327:LYS:HE3	1:D:636:ASN:HD22	1.61	0.66
1:C:733:THR:HB	1:C:736:LYS:HB3	1.75	0.66
1:C:794:LEU:CD1	1:C:799:ALA:HB2	2.26	0.66
1:D:123:TYR:CE1	1:D:127:MSE:HE3	2.30	0.66
1:B:420:ASN:O	1:B:425:ARG:NH1	2.29	0.66
1:C:409:GLU:HB2	3:C:2536:HOH:O	1.96	0.66
1:C:763:LEU:HD21	1:C:818:LEU:HD22	1.76	0.66
1:B:481:VAL:H	1:B:512:THR:CG2	2.08	0.66
1:C:838:LYS:HE2	3:C:1742:HOH:O	1.96	0.66
1:B:218:TRP:CZ2	1:B:220:GLY:HA3	2.32	0.65
1:B:94:ASN:ND2	1:B:295:VAL:H	1.95	0.65
1:B:458:TYR:CZ	1:B:537:PRO:HB2	2.32	0.64
1:B:422:VAL:HG21	1:B:532:GLU:OE1	1.97	0.64
1:A:562:GLU:OE1	1:A:565:ARG:NH1	2.30	0.64
1:C:734:ASP:O	1:C:735:ASP:CB	2.38	0.64
1:B:32:LYS:HE3	1:B:34:GLU:HG2	1.79	0.64
1:D:737:ILE:HB	1:D:794:LEU:HD12	1.80	0.63
1:C:628:GLU:HG3	1:C:672:PHE:O	1.99	0.62
1:D:684:LYS:HD2	3:D:1811:HOH:O	1.97	0.62
1:B:684:LYS:HD3	1:B:686:GLU:HG2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:LEU:HD23	1:D:333:LEU:HD13	1.82	0.61
1:D:535:SER:O	1:D:538:THR:HB	2.00	0.61
1:D:503:ARG:HG2	1:D:511:GLY:O	2.01	0.61
1:A:388:HIS:CD2	3:A:2944:HOH:O	2.53	0.60
1:A:541:LEU:O	1:A:545:PHE:HE1	1.84	0.60
1:B:468:VAL:CG2	1:B:526:VAL:HG22	2.31	0.60
1:B:452:VAL:O	1:B:453:ASP:C	2.41	0.59
1:B:816:GLU:HB3	1:B:833:GLU:OE2	2.02	0.59
1:C:791:ASN:HB3	3:C:2502:HOH:O	2.01	0.59
1:D:127:MSE:HE2	1:D:179:LEU:HD22	1.85	0.59
1:B:466:GLN:NE2	3:B:1879:HOH:O	2.35	0.58
1:D:675:GLN:NE2	1:D:675:GLN:H	2.00	0.58
1:A:439:ARG:NH2	2:A:5002:GOL:O3	2.23	0.58
1:A:54:LYS:HE2	3:A:2291:HOH:O	2.04	0.58
1:A:84:LYS:HD2	3:A:2372:HOH:O	2.04	0.58
1:D:94:ASN:ND2	1:D:295:VAL:H	2.02	0.57
1:C:472:ASP:N	1:C:472:ASP:OD2	2.36	0.57
1:B:522:LYS:HE2	1:B:525:GLN:NE2	2.20	0.57
1:D:733:THR:C	1:D:735:ASP:H	2.07	0.57
1:C:508:PHE:N	1:C:508:PHE:HD2	2.02	0.56
1:B:426:SER:O	1:B:427:ASP:HB2	2.04	0.56
1:A:708:ARG:HH22	1:B:708:ARG:NH2	2.04	0.56
1:A:331:LEU:HD21	1:A:618:VAL:HG21	1.88	0.56
1:C:43:VAL:HG12	1:C:97:VAL:HB	1.88	0.56
1:A:737:ILE:HD11	1:A:796:LEU:CD2	2.24	0.56
1:B:388:HIS:CD2	3:B:2561:HOH:O	2.59	0.56
1:C:753:SER:HA	1:C:780:VAL:O	2.06	0.56
1:A:56:PHE:CD1	2:A:5002:GOL:H32	2.41	0.56
1:B:816:GLU:OE1	1:B:833:GLU:OE2	2.22	0.56
1:C:85:LEU:HD22	1:C:312:LEU:HD23	1.88	0.55
1:A:794:LEU:HD12	1:A:794:LEU:O	2.06	0.55
1:A:479:LEU:HD22	1:A:487:PHE:HB2	1.89	0.55
1:B:388:HIS:HD2	3:B:2561:HOH:O	1.87	0.55
1:D:161:ASN:HA	1:D:195:LYS:HB2	1.89	0.55
1:B:469:PRO:HG3	1:B:521:LEU:HD23	1.89	0.55
1:C:781:HIS:O	1:C:788:LYS:HE3	2.07	0.55
1:A:350:THR:HG22	3:A:853:HOH:O	2.07	0.54
1:B:522:LYS:HE2	1:B:525:GLN:HE21	1.72	0.54
1:B:258:HIS:HD2	3:B:2515:HOH:O	1.91	0.54
1:C:576:LYS:HA	3:C:2855:HOH:O	2.08	0.54
1:A:94:ASN:ND2	1:A:295:VAL:H	2.06	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:N	2:A:5002:GOL:O3	2.38	0.53
1:D:565:ARG:NH1	1:D:565:ARG:HG2	2.15	0.53
1:A:101:PRO:HG2	1:A:129:THR:HG23	1.89	0.53
1:A:474:ASP:HB3	1:A:518:LYS:HD2	1.91	0.53
1:C:732:VAL:HG12	3:C:2193:HOH:O	2.08	0.53
1:A:57:ASP:H	2:A:5002:GOL:H32	1.72	0.53
1:C:508:PHE:N	1:C:508:PHE:CD2	2.74	0.53
1:A:758:VAL:CG2	1:A:792:ILE:HD13	2.39	0.52
1:A:388:HIS:HD2	3:A:2944:HOH:O	1.92	0.52
1:B:512:THR:HG23	1:B:513:LYS:O	2.10	0.52
1:C:475:TYR:HB2	1:C:521:LEU:HD22	1.90	0.52
1:C:735:ASP:CG	1:C:735:ASP:O	2.48	0.52
1:D:443:HIS:CE1	1:D:508:PHE:HE2	2.28	0.52
1:A:409:GLU:HB3	3:A:1423:HOH:O	2.09	0.52
1:A:470:GLN:NE2	1:A:470:GLN:HA	2.25	0.52
1:D:404:LYS:HB3	1:D:405:PRO:HD2	1.92	0.52
1:B:675:GLN:NE2	1:B:675:GLN:H	2.08	0.51
1:D:339:ILE:HG22	1:D:576:LYS:HB2	1.91	0.51
1:B:422:VAL:CG2	1:B:532:GLU:OE1	2.58	0.51
1:D:416:LYS:HG2	1:D:434:VAL:HG22	1.93	0.51
1:B:758:VAL:HG21	1:B:792:ILE:HD13	1.93	0.51
1:D:675:GLN:HE21	1:D:675:GLN:H	1.59	0.51
1:B:725:LEU:C	1:B:725:LEU:HD12	2.31	0.51
1:B:453:ASP:O	1:B:453:ASP:OD1	2.30	0.50
1:A:349:LYS:HE2	1:A:364:VAL:O	2.11	0.50
1:D:566:ASN:ND2	3:D:2876:HOH:O	2.43	0.50
1:A:708:ARG:HH22	1:B:708:ARG:HH22	1.58	0.50
1:B:404:LYS:O	1:B:405:PRO:O	2.30	0.50
1:B:536:GLY:N	1:B:537:PRO:CD	2.75	0.50
1:D:443:HIS:HE1	1:D:508:PHE:HE2	1.57	0.50
1:B:57:ASP:H	2:B:5006:GOL:C1	2.24	0.49
1:A:134:LYS:HE2	3:A:3057:HOH:O	2.11	0.49
1:A:765:SER:HB3	1:A:813:GLU:OE1	2.13	0.49
1:B:458:TYR:N	3:B:2207:HOH:O	2.46	0.49
1:B:470:GLN:HE21	1:B:470:GLN:CA	2.25	0.49
1:C:182:LYS:HB2	1:C:845:LEU:HG	1.94	0.49
1:C:97:VAL:HG22	1:C:142:ALA:HB3	1.94	0.49
1:D:501:GLN:HG3	3:D:2137:HOH:O	2.13	0.49
1:A:48:ASN:HD21	1:A:357:ALA:HB1	1.78	0.49
1:B:378:GLU:HG2	3:B:2471:HOH:O	2.13	0.49
1:C:503:ARG:HH21	1:C:510:ALA:HA	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:HIS:CD2	1:C:451:LYS:H	2.18	0.49
1:D:367:PRO:HG2	1:D:580:ILE:HG21	1.95	0.49
1:A:16:ASP:CG	1:A:253:ARG:HD2	2.33	0.48
1:A:333:LEU:HD22	1:A:656:LEU:HB3	1.95	0.48
1:A:84:LYS:CB	1:A:84:LYS:NZ	2.73	0.48
1:C:675:GLN:H	1:C:675:GLN:NE2	2.11	0.48
1:D:737:ILE:HB	1:D:794:LEU:CD1	2.43	0.48
1:D:796:LEU:HD22	1:D:800:ILE:HD11	1.94	0.48
1:C:336:GLU:H	1:C:336:GLU:CD	2.14	0.48
1:A:421:PRO:HG2	1:A:424:GLU:HB2	1.95	0.48
1:B:335:LYS:HE2	3:B:2440:HOH:O	2.14	0.48
1:D:54:LYS:HE2	3:D:2324:HOH:O	2.14	0.48
1:D:622:GLN:NE2	1:D:648:LEU:HD13	2.28	0.48
1:C:151:ASN:HB2	1:C:192:ALA:HB1	1.95	0.48
1:C:736:LYS:HD2	1:C:737:ILE:H	1.75	0.48
1:D:127:MSE:HE2	1:D:179:LEU:HD13	1.95	0.48
1:B:338:ASN:ND2	1:B:574:HIS:HA	2.28	0.48
1:D:607:VAL:HG11	1:D:631:TRP:CE2	2.49	0.48
1:B:409:GLU:HA	1:B:436:LYS:NZ	2.29	0.48
1:D:733:THR:O	1:D:735:ASP:N	2.47	0.48
1:B:458:TYR:CE1	1:B:537:PRO:HB2	2.49	0.47
1:A:794:LEU:HD12	1:A:794:LEU:C	2.34	0.47
1:D:433:HIS:ND1	3:D:2743:HOH:O	2.35	0.47
1:D:338:ASN:ND2	1:D:574:HIS:HA	2.30	0.47
1:B:735:ASP:OD1	1:B:735:ASP:N	2.47	0.47
1:C:470:GLN:HA	1:C:470:GLN:HE21	1.79	0.47
1:B:463:LEU:HD22	1:B:550:PHE:CE1	2.49	0.47
1:B:480:GLN:HG2	1:B:514:GLU:HA	1.96	0.47
1:B:422:VAL:HG21	1:B:532:GLU:CD	2.34	0.47
1:C:503:ARG:CZ	1:C:503:ARG:HB3	2.44	0.47
1:A:439:ARG:H	2:A:5002:GOL:C1	2.27	0.47
1:B:443:HIS:C	3:B:2942:HOH:O	2.53	0.47
1:D:334:LYS:HE2	3:D:2244:HOH:O	2.15	0.47
1:A:769:ARG:HB3	1:A:770:PRO:HD2	1.96	0.46
1:A:676:ASP:HB3	1:A:708:ARG:HD3	1.96	0.46
1:C:472:ASP:OD2	1:C:523:LYS:CB	2.57	0.46
1:A:427:ASP:O	3:A:1704:HOH:O	2.20	0.46
1:D:713:PRO:HG2	1:D:716:TYR:HB2	1.98	0.46
1:A:400:ILE:HD12	1:A:414:ILE:HG12	1.98	0.46
1:C:338:ASN:O	1:C:575:ASP:HB3	2.16	0.46
1:A:648:LEU:HD12	1:A:649:GLY:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ALA:HB1	1:D:194:ASN:OD1	2.16	0.46
1:D:607:VAL:HG11	1:D:631:TRP:CD2	2.51	0.46
1:B:345:ASN:HB3	1:B:622:GLN:OE1	2.16	0.46
1:C:218:TRP:CZ2	1:C:220:GLY:HA3	2.52	0.45
1:C:327:LYS:HE2	1:C:636:ASN:HD22	1.81	0.45
1:C:432:PHE:O	1:C:449:HIS:CE1	2.69	0.45
1:B:725:LEU:HD12	1:B:725:LEU:O	2.16	0.45
1:C:54:LYS:HE3	3:C:1010:HOH:O	2.16	0.45
1:C:766:LYS:HB3	3:C:2866:HOH:O	2.16	0.45
1:C:286:VAL:HA	1:C:289:LEU:HG	1.99	0.45
1:C:769:ARG:HD3	1:C:769:ARG:HH11	1.51	0.45
1:A:769:ARG:HB3	1:A:770:PRO:CD	2.47	0.45
1:B:404:LYS:O	1:B:405:PRO:C	2.54	0.45
1:A:43:VAL:HG12	1:A:97:VAL:HB	1.99	0.45
1:B:327:LYS:O	1:B:328:ASN:HB2	2.17	0.45
1:D:88:LYS:HB3	1:D:88:LYS:HE3	1.74	0.45
1:C:561:ASP:HB2	3:C:2617:HOH:O	2.17	0.45
1:A:82:ALA:O	1:A:86:MSE:HG3	2.16	0.44
1:B:487:PHE:HD2	1:B:488:TYR:N	2.15	0.44
1:B:338:ASN:HD22	1:B:575:ASP:H	1.65	0.44
1:C:607:VAL:HG11	1:C:631:TRP:CE2	2.51	0.44
1:D:733:THR:C	1:D:735:ASP:N	2.69	0.44
1:A:153:LEU:HD12	1:A:153:LEU:C	2.38	0.44
1:C:626:PRO:HD3	1:C:668:LEU:HD13	1.98	0.44
1:B:57:ASP:H	2:B:5006:GOL:H11	1.82	0.44
1:C:763:LEU:HD11	1:C:818:LEU:HD13	1.99	0.44
1:B:338:ASN:HD21	1:B:574:HIS:HA	1.83	0.44
1:C:471:GLU:CA	1:C:523:LYS:HG2	2.46	0.44
1:D:534:GLY:HA3	1:D:538:THR:HG21	1.98	0.44
1:C:736:LYS:C	1:C:736:LYS:HD2	2.37	0.44
1:C:838:LYS:HB2	1:C:838:LYS:HE3	1.84	0.44
1:C:708:ARG:HD3	3:C:2241:HOH:O	2.17	0.44
1:D:212:LEU:HD23	1:D:212:LEU:HA	1.92	0.44
1:C:503:ARG:NH2	1:C:509:GLY:O	2.51	0.43
1:A:331:LEU:HD23	1:A:333:LEU:HD13	2.01	0.43
1:A:404:LYS:HB3	1:A:405:PRO:CD	2.41	0.43
1:D:123:TYR:HE1	1:D:127:MSE:HE3	1.79	0.43
1:D:833:GLU:HB3	3:D:2378:HOH:O	2.17	0.43
1:A:675:GLN:NE2	1:A:675:GLN:H	2.15	0.43
1:B:625:THR:HB	1:B:626:PRO:CD	2.49	0.43
1:B:731:LYS:HE3	1:B:733:THR:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:744:LYS:HB2	1:D:787:LYS:HG3	2.01	0.43
1:A:541:LEU:O	1:A:545:PHE:CE1	2.68	0.43
1:C:758:VAL:HG21	1:C:792:ILE:HD13	2.00	0.43
1:D:339:ILE:HA	1:D:576:LYS:O	2.18	0.43
1:B:420:ASN:HB3	1:B:421:PRO:HD2	2.00	0.43
1:D:190:MSE:HG3	1:D:223:MSE:HG3	2.00	0.43
1:B:404:LYS:C	1:B:405:PRO:O	2.53	0.43
1:C:579:LEU:HD22	1:C:610:VAL:HG11	2.00	0.42
1:D:149:VAL:O	1:D:150:CYS:HB2	2.19	0.42
1:B:480:GLN:HG3	3:B:949:HOH:O	2.18	0.42
1:D:99:LEU:HA	1:D:144:THR:HB	2.01	0.42
1:D:533:TYR:CZ	1:D:535:SER:HA	2.53	0.42
1:D:444:LEU:HB2	1:D:548:GLY:O	2.19	0.42
1:D:218:TRP:CZ2	1:D:220:GLY:HA3	2.54	0.42
1:A:411:SER:O	1:A:436:LYS:HD3	2.18	0.42
1:B:237:LYS:HE3	3:B:2183:HOH:O	2.18	0.42
1:A:115:PHE:CE1	1:A:353:GLY:HA3	2.55	0.42
1:A:737:ILE:HG22	1:A:739:ILE:HG22	2.01	0.42
1:B:56:PHE:CD1	2:B:5006:GOL:H11	2.55	0.42
1:B:812:VAL:HB	1:B:840:LEU:HB3	2.01	0.42
1:C:101:PRO:HG2	1:C:129:THR:HG23	2.00	0.42
1:C:559:ASP:CG	1:C:562:GLU:HB3	2.40	0.42
1:C:708:ARG:NE	3:C:2241:HOH:O	2.52	0.42
1:A:372:VAL:HG13	1:A:377:LYS:O	2.20	0.42
1:A:351:SER:HA	1:A:648:LEU:HD23	2.02	0.42
1:B:101:PRO:HG2	1:B:129:THR:HG23	2.00	0.42
1:D:708:ARG:HD3	3:D:2947:HOH:O	2.19	0.42
1:A:618:VAL:HA	1:A:637:ALA:HB3	2.01	0.42
1:A:824:SER:HB3	2:A:5003:GOL:H32	2.02	0.42
1:C:394:LEU:HB2	1:C:553:GLY:HA2	2.02	0.42
1:D:481:VAL:HG12	1:D:550:PHE:CB	2.50	0.42
1:B:684:LYS:HD3	1:B:686:GLU:CG	2.49	0.42
1:B:753:SER:HA	1:B:780:VAL:O	2.19	0.42
1:D:623:SER:O	1:D:642:TRP:HA	2.19	0.42
1:A:286:VAL:HA	1:A:289:LEU:HG	2.01	0.42
1:A:54:LYS:HA	1:A:446:ASP:OD2	2.20	0.42
1:B:756:VAL:O	1:B:777:PHE:HA	2.20	0.42
1:B:708:ARG:NE	3:B:2054:HOH:O	2.51	0.41
1:B:794:LEU:N	1:B:794:LEU:HD12	2.34	0.41
1:B:88:LYS:HE3	1:B:88:LYS:HB3	1.73	0.41
1:C:350:THR:HG22	3:C:2559:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:LYS:HE2	3:C:1705:HOH:O	2.19	0.41
1:C:684:LYS:HD3	3:C:1417:HOH:O	2.20	0.41
1:A:428:ASP:HA	3:A:1704:HOH:O	2.20	0.41
1:B:147:HIS:HB3	1:B:192:ALA:HA	2.02	0.41
1:B:190:MSE:SE	2:B:5005:GOL:H31	2.70	0.41
1:C:18:LYS:HB3	1:C:275:VAL:HG21	2.03	0.41
1:B:492:GLU:HG3	1:B:492:GLU:O	2.20	0.41
1:B:579:LEU:HD21	1:B:607:VAL:HA	2.01	0.41
1:C:226:TRP:O	1:C:227:PHE:HB2	2.21	0.41
1:C:306:THR:O	1:C:310:SER:HB2	2.20	0.41
1:D:281:MSE:SE	1:D:281:MSE:C	3.09	0.41
1:D:796:LEU:HD22	1:D:800:ILE:CD1	2.50	0.41
1:A:16:ASP:OD1	1:A:253:ARG:HD2	2.20	0.41
1:D:55:PHE:CG	1:D:443:HIS:HD2	2.38	0.41
1:D:64:PHE:CD2	1:D:64:PHE:N	2.89	0.41
1:A:297:ASN:CB	3:A:2042:HOH:O	2.55	0.41
1:D:16:ASP:OD1	1:D:253:ARG:HD2	2.20	0.41
1:B:731:LYS:HE3	1:B:733:THR:CG2	2.50	0.41
1:D:654:ASP:HB3	1:D:660:VAL:HG23	2.03	0.41
1:B:200:HIS:CD2	1:B:230:TYR:CE2	3.09	0.41
1:C:447:PHE:HE2	1:C:452:VAL:HG21	1.85	0.41
1:C:733:THR:HG22	1:C:734:ASP:O	2.21	0.41
1:A:359:MSE:HB3	1:A:359:MSE:HE2	2.02	0.41
1:D:386:TYR:HB3	1:D:388:HIS:CD2	2.56	0.40
1:C:709:LYS:HD2	3:C:895:HOH:O	2.21	0.40
1:B:367:PRO:HD3	1:B:648:LEU:HD11	2.03	0.40
1:A:603:THR:O	1:A:607:VAL:HG23	2.21	0.40
1:C:480:GLN:NE2	1:C:506:PHE:HB2	2.36	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	842/845 (100%)	808 (96%)	33 (4%)	1 (0%)	51	53
1	B	798/845 (94%)	764 (96%)	33 (4%)	1 (0%)	51	53
1	C	832/845 (98%)	796 (96%)	36 (4%)	0	100	100
1	D	827/845 (98%)	789 (95%)	38 (5%)	0	100	100
All	All	3299/3380 (98%)	3157 (96%)	140 (4%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	GLY
1	B	405	PRO

5.3.2 Protein sidechains (i)

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	716/706 (101%)	693 (97%)	23 (3%)	39	38
1	B	690/706 (98%)	670 (97%)	20 (3%)	42	42
1	C	710/706 (101%)	674 (95%)	36 (5%)	24	20
1	D	707/706 (100%)	678 (96%)	29 (4%)	30	29
All	All	2823/2824 (100%)	2715 (96%)	108 (4%)	33	31

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	TRP
1	A	290	GLU
1	A	333	LEU
1	A	377	LYS
1	A	409	GLU
1	A	426	SER
1	A	427	ASP
1	A	428	ASP
1	A	450	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	487	PHE
1	A	503	ARG
1	A	541	LEU
1	A	542	VAL
1	A	633	GLU
1	A	677	ASN
1	A	726	ASP
1	A	732	VAL
1	A	733	THR
1	A	736	LYS
1	A	739	ILE
1	A	766	LYS
1	A	794	LEU
1	A	845	LEU
1	B	35	ARG
1	B	226	TRP
1	B	333	LEU
1	B	420	ASN
1	B	423	GLU
1	B	424	GLU
1	B	425	ARG
1	B	426	SER
1	B	450	GLU
1	B	470	GLN
1	B	484	SER
1	B	487	PHE
1	B	492	GLU
1	B	677	ASN
1	B	731	LYS
1	B	735	ASP
1	B	780	VAL
1	B	787	LYS
1	B	794	LEU
1	B	845	LEU
1	C	3	LYS
1	C	35	ARG
1	C	54	LYS
1	C	226	TRP
1	C	297	ASN
1	C	310	SER
1	C	333	LEU
1	C	336	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	426	SER
1	C	436	LYS
1	C	470	GLN
1	C	472	ASP
1	C	481	VAL
1	C	482	TYR
1	C	487	PHE
1	C	507	CYS
1	C	508	PHE
1	C	521	LEU
1	C	523	LYS
1	C	526	VAL
1	C	561	ASP
1	C	602	ARG
1	C	633	GLU
1	C	677	ASN
1	C	708	ARG
1	C	729	ASP
1	C	731	LYS
1	C	735	ASP
1	C	736	LYS
1	C	748	ASP
1	C	766	LYS
1	C	831	VAL
1	C	832	LYS
1	C	835	LYS
1	C	838	LYS
1	C	845	LEU
1	D	3	LYS
1	D	61	SER
1	D	226	TRP
1	D	294	ILE
1	D	307	LYS
1	D	312	LEU
1	D	333	LEU
1	D	334	LYS
1	D	407	ASP
1	D	411	SER
1	D	436	LYS
1	D	472	ASP
1	D	487	PHE
1	D	503	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	517	LYS
1	D	518	LYS
1	D	565	ARG
1	D	580	ILE
1	D	675	GLN
1	D	677	ASN
1	D	708	ARG
1	D	722	THR
1	D	766	LYS
1	D	767	VAL
1	D	794	LEU
1	D	797	LYS
1	D	819	VAL
1	D	832	LYS
1	D	845	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	94	ASN
1	A	388	HIS
1	A	470	GLN
1	A	480	GLN
1	A	636	ASN
1	A	675	GLN
1	B	48	ASN
1	B	94	ASN
1	B	197	ASN
1	B	258	HIS
1	B	338	ASN
1	B	388	HIS
1	B	470	GLN
1	B	525	GLN
1	B	636	ASN
1	B	675	GLN
1	C	48	ASN
1	C	94	ASN
1	C	449	HIS
1	C	470	GLN
1	C	480	GLN
1	C	525	GLN

Continued from previous page...

Mol	Chain	Res	Type
1	C	636	ASN
1	C	675	GLN
1	D	48	ASN
1	D	94	ASN
1	D	338	ASN
1	D	388	HIS
1	D	443	HIS
1	D	525	GLN
1	D	636	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	5003	-	5,5,5	0.34	0	5,5,5	0.60	0
2	GOL	C	5007	-	5,5,5	0.57	0	5,5,5	0.72	0
2	GOL	D	5008	-	5,5,5	0.49	0	5,5,5	0.94	0
2	GOL	A	5004	-	5,5,5	0.42	0	5,5,5	0.82	0
2	GOL	B	5006	-	5,5,5	0.30	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	GOL	B	5005	-	5,5,5	0.55	0	5,5,5	1.01	0
2	GOL	A	5001	-	5,5,5	0.46	0	5,5,5	0.70	0
2	GOL	A	5002	-	5,5,5	0.78	0	5,5,5	1.66	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	5003	-	-	0/4/4/4	-
2	GOL	C	5007	-	-	2/4/4/4	-
2	GOL	D	5008	-	-	2/4/4/4	-
2	GOL	A	5004	-	-	4/4/4/4	-
2	GOL	B	5006	-	-	4/4/4/4	-
2	GOL	B	5005	-	-	2/4/4/4	-
2	GOL	A	5001	-	-	2/4/4/4	-
2	GOL	A	5002	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5002	GOL	C3-C2-C1	-3.03	99.91	111.70

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5004	GOL	O1-C1-C2-C3
2	B	5006	GOL	O1-C1-C2-C3
2	B	5006	GOL	C1-C2-C3-O3
2	A	5001	GOL	O2-C2-C3-O3
2	A	5002	GOL	C1-C2-C3-O3
2	A	5002	GOL	O2-C2-C3-O3
2	C	5007	GOL	O1-C1-C2-C3
2	D	5008	GOL	C1-C2-C3-O3
2	A	5004	GOL	C1-C2-C3-O3
2	B	5005	GOL	O1-C1-C2-C3

Continued on next page...

Full wwPDB X-ray Structure Validation Report 3ABZ

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	5001	GOL	C1-C2-C3-O3
2	A	5004	GOL	O1-C1-C2-O2
2	A	5004	GOL	O2-C2-C3-O3
2	B	5006	GOL	O2-C2-C3-O3
2	B	5006	GOL	O1-C1-C2-O2
2	B	5005	GOL	O1-C1-C2-O2
2	C	5007	GOL	O1-C1-C2-O2
2	D	5008	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5003	GOL	1	0
2	B	5006	GOL	4	0
2	B	5005	GOL	1	0
2	A	5001	GOL	1	0
2	A	5002	GOL	8	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	834/845 (98%)	-0.15	21 (2%)	57	65	12, 25, 51, 69	0
1	B	800/845 (94%)	0.12	77 (9%)	8	11	12, 22, 67, 98	0
1	C	826/845 (97%)	0.11	46 (5%)	24	33	14, 32, 65, 94	0
1	D	823/845 (97%)	0.11	43 (5%)	27	35	14, 34, 58, 73	0
All	All	3283/3380 (97%)	0.04	187 (5%)	23	32	12, 28, 61, 98	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	403	ALA	7.7
1	C	408	ALA	6.5
1	B	526	VAL	6.4
1	B	472	ASP	6.2
1	B	434	VAL	6.1
1	B	408	ALA	5.9
1	B	538	THR	5.9
1	D	403	ALA	5.9
1	B	422	VAL	5.7
1	B	415	ALA	5.6
1	B	445	PHE	5.4
1	B	404	LYS	5.4
1	B	527	TYR	5.4
1	C	406	ALA	5.3
1	B	407	ASP	5.2
1	B	468	VAL	5.1
1	C	521	LEU	4.9
1	C	402	ALA	4.9
1	C	405	PRO	4.9
1	B	522	LYS	4.9
1	B	467	TYR	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	463	LEU	4.7
1	C	475	TYR	4.7
1	B	435	THR	4.5
1	A	541	LEU	4.5
1	A	428	ASP	4.4
1	B	488	TYR	4.4
1	D	2	SER	4.4
1	D	422	VAL	4.4
1	B	519	LEU	4.4
1	B	414	ILE	4.4
1	B	524	GLY	4.4
1	C	526	VAL	4.3
1	B	475	TYR	4.2
1	B	529	VAL	4.2
1	B	411	SER	4.1
1	B	525	GLN	4.1
1	C	401	ASP	4.1
1	A	540	GLY	4.0
1	D	408	ALA	4.0
1	B	528	ASN	4.0
1	A	426	SER	3.9
1	C	472	ASP	3.9
1	B	399	LEU	3.9
1	A	732	VAL	3.9
1	D	418	TYR	3.9
1	D	431	PRO	3.9
1	B	413	LEU	3.9
1	A	737	ILE	3.9
1	A	733	THR	3.8
1	C	426	SER	3.8
1	B	461	VAL	3.8
1	B	409	GLU	3.8
1	C	428	ASP	3.8
1	B	471	GLU	3.8
1	D	430	GLU	3.7
1	C	409	GLU	3.7
1	B	462	THR	3.7
1	A	542	VAL	3.7
1	A	543	GLY	3.6
1	C	471	GLU	3.6
1	B	536	GLY	3.6
1	C	522	LYS	3.5

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	418	TYR	3.5
1	B	417	PHE	3.5
1	B	464	THR	3.5
1	D	402	ALA	3.5
1	B	433	HIS	3.5
1	A	734	ASP	3.5
1	B	523	LYS	3.5
1	B	521	LEU	3.4
1	B	476	ILE	3.4
1	B	465	GLY	3.4
1	C	527	TYR	3.4
1	B	426	SER	3.4
1	B	531	VAL	3.4
1	B	406	ALA	3.3
1	D	494	ILE	3.3
1	B	489	LEU	3.3
1	B	487	PHE	3.3
1	A	522	LYS	3.3
1	C	525	GLN	3.3
1	B	410	ASN	3.2
1	C	528	ASN	3.2
1	C	400	ILE	3.2
1	B	490	ASN	3.2
1	D	420	ASN	3.2
1	C	529	VAL	3.2
1	A	329	ASN	3.2
1	A	472	ASP	3.1
1	C	524	GLY	3.1
1	D	429	GLU	3.1
1	D	539	SER	3.1
1	B	412	GLY	3.0
1	C	523	LYS	3.0
1	B	432	PHE	3.0
1	B	477	PHE	3.0
1	C	424	GLU	3.0
1	D	472	ASP	3.0
1	C	399	LEU	3.0
1	D	529	VAL	3.0
1	D	488	TYR	2.9
1	C	474	ASP	2.9
1	C	520	THR	2.9
1	D	3	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	398	SER	2.9
1	C	450	GLU	2.9
1	B	460	PHE	2.8
1	B	520	THR	2.8
1	C	411	SER	2.8
1	B	492	GLU	2.8
1	B	427	ASP	2.8
1	C	519	LEU	2.8
1	D	401	ASP	2.8
1	B	405	PRO	2.8
1	B	734	ASP	2.7
1	C	473	GLY	2.7
1	D	519	LEU	2.7
1	D	487	PHE	2.7
1	C	430	GLU	2.7
1	C	407	ASP	2.7
1	C	427	ASP	2.6
1	C	733	THR	2.6
1	C	468	VAL	2.6
1	A	545	PHE	2.6
1	C	378	GLU	2.6
1	D	458	TYR	2.6
1	D	432	PHE	2.6
1	C	499	HIS	2.6
1	C	398	SER	2.5
1	A	328	ASN	2.5
1	B	482	TYR	2.5
1	C	470	GLN	2.5
1	C	466	GLN	2.5
1	D	473	GLY	2.5
1	A	526	VAL	2.5
1	B	416	LYS	2.5
1	D	500	ASN	2.5
1	B	450	GLU	2.5
1	B	397	SER	2.4
1	B	549	GLY	2.4
1	B	421	PRO	2.4
1	B	530	ARG	2.4
1	D	421	PRO	2.4
1	D	733	THR	2.4
1	C	404	LYS	2.4
1	D	434	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	417	PHE	2.4
1	D	489	LEU	2.4
1	D	400	ILE	2.4
1	D	564	ILE	2.4
1	B	466	GLN	2.4
1	C	489	LEU	2.4
1	B	493	LEU	2.3
1	B	537	PRO	2.3
1	D	522	LYS	2.3
1	C	467	TYR	2.3
1	B	394	LEU	2.3
1	B	470	GLN	2.3
1	D	520	THR	2.3
1	C	3	LYS	2.3
1	B	491	ASP	2.3
1	C	414	ILE	2.3
1	B	459	PHE	2.2
1	D	414	ILE	2.2
1	D	734	ASP	2.2
1	D	572	ALA	2.2
1	A	427	ASP	2.2
1	C	417	PHE	2.2
1	D	405	PRO	2.2
1	D	407	ASP	2.2
1	B	446	ASP	2.2
1	A	336	GLU	2.1
1	D	573	LYS	2.1
1	D	435	THR	2.1
1	B	423	GLU	2.1
1	D	412	GLY	2.1
1	B	474	ASP	2.1
1	A	470	GLN	2.1
1	D	449	HIS	2.1
1	A	473	GLY	2.1
1	B	469	PRO	2.0
1	B	592	TYR	2.0
1	D	565	ARG	2.0
1	D	493	LEU	2.0
1	A	519	LEU	2.0
1	B	473	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	5004	6/6	0.86	0.12	37,39,40,44	0
2	GOL	C	5007	6/6	0.88	0.25	33,38,40,46	0
2	GOL	D	5008	6/6	0.92	0.19	35,37,38,39	0
2	GOL	B	5006	6/6	0.93	0.21	50,51,54,58	0
2	GOL	A	5001	6/6	0.93	0.17	29,37,38,41	0
2	GOL	B	5005	6/6	0.94	0.16	34,40,41,45	0
2	GOL	A	5002	6/6	0.95	0.21	27,31,39,41	0
2	GOL	A	5003	6/6	0.96	0.14	30,37,44,48	0

6.5 Other polymers (i)

There are no such residues in this entry.