Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 05:25 PM EST

PDB ID	:	3AC0
Title	:	Crystal structure of Beta-glucosidase from Kluyveromyces marxianus in complex with glucose
Authors	:	Yoshida, E.; Hidaka, M.; Fushinobu, S.; Katayama, T.; Kumagai, H.
Deposited on	:	2009-12-25
Resolution	:	2.54 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

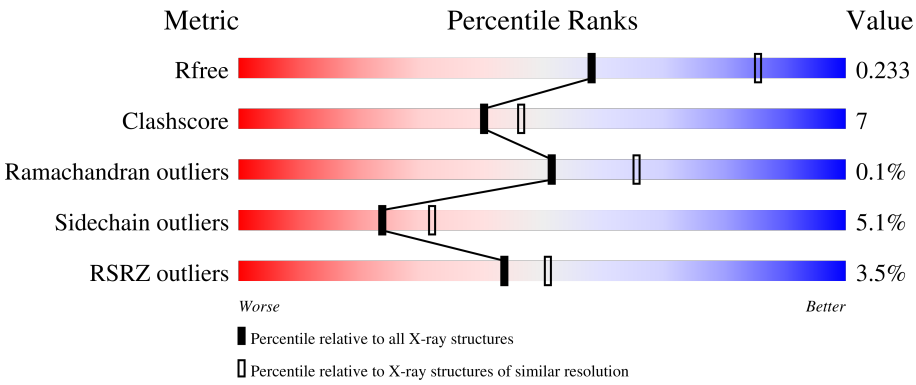
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	845	% 82% 16% •
1	B	845	3% 83% 14% • •
1	C	845	6% 78% 18% • •
1	D	845	3% 78% 18% • •

2 Entry composition (i)

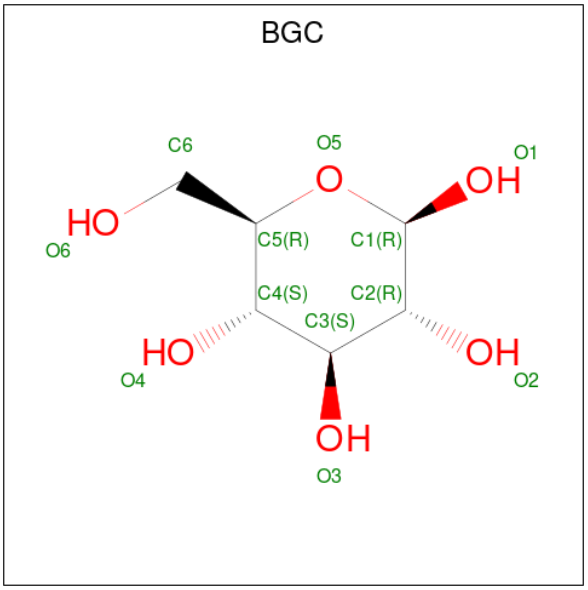
There are 3 unique types of molecules in this entry. The entry contains 27663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	841	6587	4184	1107	1281	15	0	0	0
1	B	825	6462	4104	1091	1253	14	0	0	0
1	C	831	6514	4143	1093	1263	15	0	0	0
1	D	829	6488	4128	1092	1253	15	0	0	0

- Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0
2	B	1	12	6	6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	C	1	12	6	6	0	0
			Total	C	O		
2	D	1	12	6	6	0	0

- Molecule 3 is water.

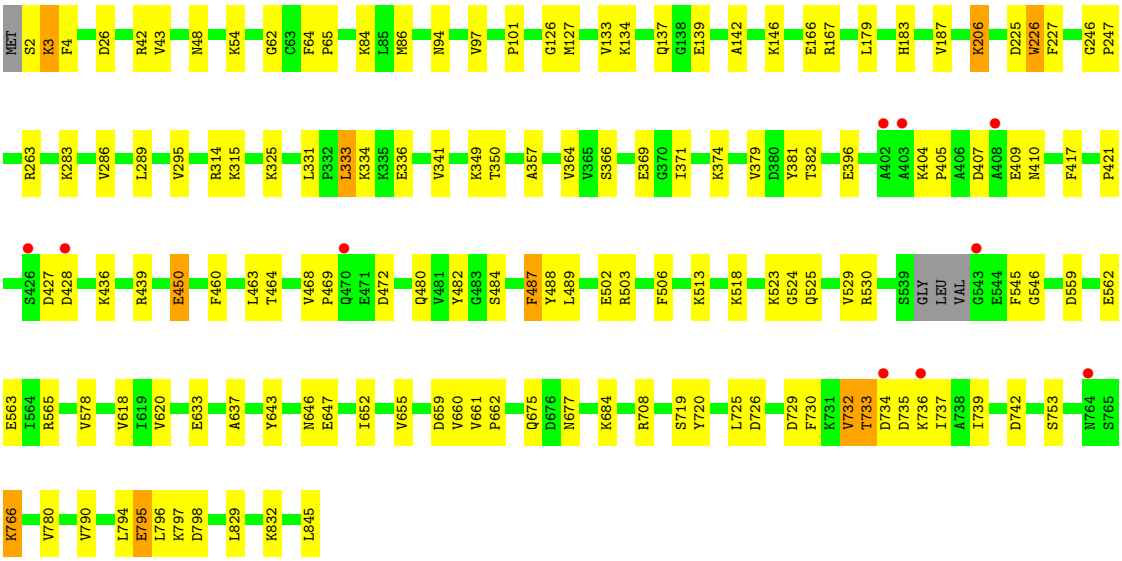
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	448	448	448	0	0
			Total	O		
3	B	446	446	446	0	0
			Total	O		
3	C	345	345	345	0	0
			Total	O		
3	D	325	325	325	0	0

3 Residue-property plots (i)

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

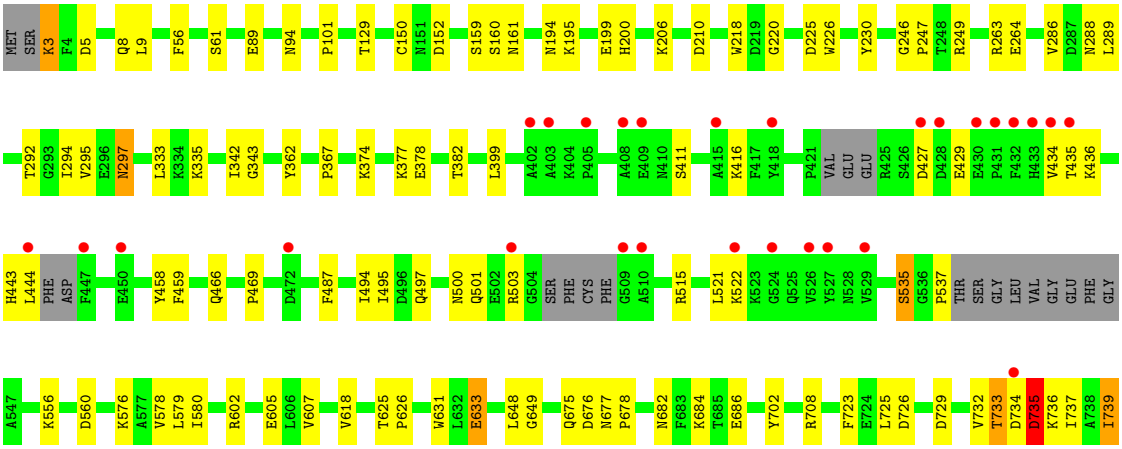
• Molecule 1: Beta-glucosidase I

Chain A:



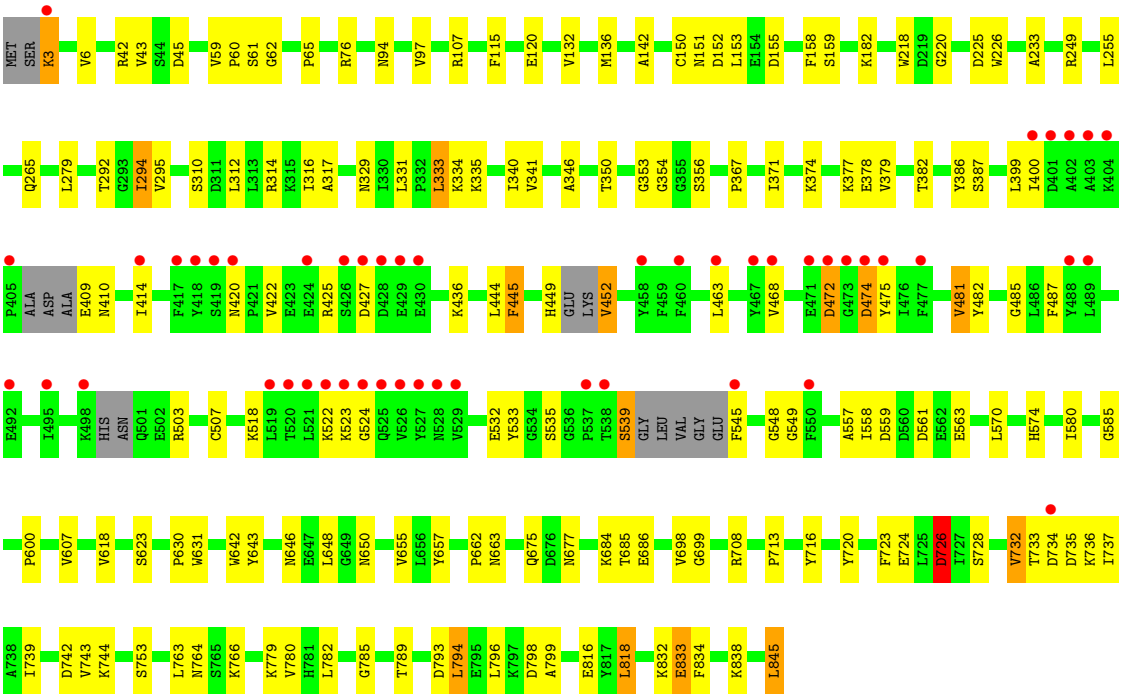
• Molecule 1: Beta-glucosidase I

Chain B:



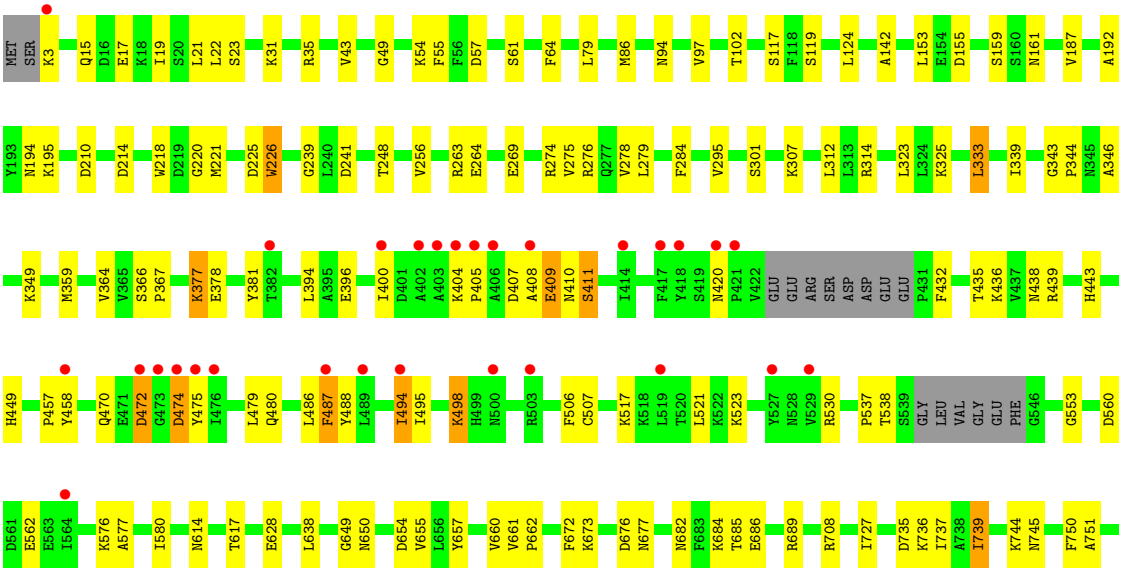
• Molecule 1: Beta-glucosidase I

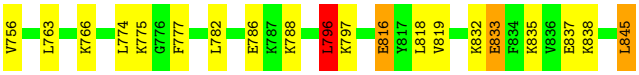
Chain C:



• Molecule 1: Beta-glucosidase I

Chain D:




V756
L763
K766
L774
K775
G776
F777
L782
E786
K787
K788
L796
K797
E816
Y817
L818
V819
K832
E833
F834
K835
V836
E837
K838
L845

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	245.85Å 148.41Å 119.64Å 90.00° 112.84° 90.00°	Depositor
Resolution (Å)	50.00 – 2.54 42.98 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.54) 99.6 (42.98-2.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.169 , 0.242 0.165 , 0.233	Depositor DCC
R_{free} test set	6526 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.7	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	0.95	EDS
Total number of atoms	27663	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: BGC

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	0.89	0/6723	0.82	3/9089 (0.0%)
1	B	0.94	3/6591 (0.0%)	0.86	7/8907 (0.1%)
1	C	0.83	1/6646 (0.0%)	0.81	4/8981 (0.0%)
1	D	0.82	3/6622 (0.0%)	0.80	2/8952 (0.0%)
All	All	0.87	7/26582 (0.0%)	0.82	16/35929 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	816	GLU	CG-CD	6.68	1.61	1.51
1	B	264	GLU	CD-OE2	-5.95	1.19	1.25
1	D	269	GLU	CG-CD	5.79	1.60	1.51
1	D	264	GLU	CD-OE2	-5.70	1.19	1.25
1	B	264	GLU	CD-OE1	-5.21	1.20	1.25
1	C	764	ASN	CB-CG	5.08	1.62	1.51
1	B	723	PHE	CE2-CZ	5.01	1.46	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	579	LEU	CA-CB-CG	8.51	134.86	115.30
1	B	249	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	A	26	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	769	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	42	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	796	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	42	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	560	ASP	CB-CG-OD1	5.53	123.27	118.30
1	B	729	ASP	CB-CG-OD1	5.42	123.17	118.30
1	C	42	ARG	NE-CZ-NH2	-5.41	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	726	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	210	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	249	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	76	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	735	ASP	N-CA-C	5.04	124.62	111.00
1	D	845	LEU	CB-CG-CD1	5.01	119.52	111.00

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	6587	0	6490	96	0
1	B	6462	0	6387	66	0
1	C	6514	0	6427	103	0
1	D	6488	0	6417	113	0
2	A	12	0	12	2	0
2	B	12	0	12	1	0
2	C	12	0	12	1	0
2	D	12	0	12	3	0
3	A	448	0	0	19	0
3	B	446	0	0	11	0
3	C	345	0	0	12	0
3	D	325	0	0	10	0
All	All	27663	0	25769	372	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 7.

All (372) 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:B:827:ASP:HB3	3:B:1558:HOH:O	1.46	1.12
1:D:562:GLU:HG2	3:D:1448:HOH:O	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:GLU:HG2	3:B:999:HOH:O	1.63	0.97
1:A:737:ILE:HD11	1:A:796:LEU:HD23	1.45	0.96
1:C:763:LEU:HD11	1:C:818:LEU:HD13	1.47	0.94
1:D:346:ALA:O	1:D:367:PRO:HD2	1.69	0.93
1:C:735:ASP:O	1:C:736:LYS:HG2	1.70	0.92
1:B:225:ASP:OD1	2:B:5002:BGC:H1	1.70	0.92
1:D:432:PHE:HB2	1:D:449:HIS:CE1	2.05	0.92
1:B:798:ASP:HA	3:B:956:HOH:O	1.69	0.91
1:A:334:LYS:HD3	3:A:1186:HOH:O	1.70	0.91
1:B:378:GLU:HB3	3:B:1186:HOH:O	1.70	0.91
1:D:3:LYS:HB3	3:D:1064:HOH:O	1.73	0.89
1:C:735:ASP:C	1:C:736:LYS:HG2	1.91	0.88
1:C:449:HIS:O	1:C:452:VAL:HG12	1.74	0.88
1:B:500:ASN:O	1:B:515:ARG:NH2	2.07	0.86
1:D:404:LYS:HD3	1:D:405:PRO:HD2	1.57	0.86
1:C:225:ASP:OD1	2:C:5003:BGC:H1	1.75	0.85
1:B:733:THR:HG21	3:B:1129:HOH:O	1.80	0.82
1:A:334:LYS:HB3	3:A:1186:HOH:O	1.79	0.81
1:B:297:ASN:HB2	3:B:897:HOH:O	1.81	0.79
1:C:472:ASP:OD1	1:C:523:LYS:HB2	1.82	0.79
1:C:728:SER:HB3	1:C:742:ASP:OD2	1.82	0.79
1:D:432:PHE:HB2	1:D:449:HIS:HE1	1.46	0.79
1:C:482:TYR:HD2	1:C:548:GLY:HA3	1.46	0.79
1:B:816:GLU:OE1	1:B:833:GLU:OE2	2.02	0.77
1:A:263:ARG:HB2	1:C:159:SER:HB2	1.67	0.76
1:B:199:GLU:HG2	3:B:862:HOH:O	1.85	0.76
1:D:49:GLY:HA3	1:D:359:MET:HE3	1.64	0.76
1:B:459:PHE:H	1:B:535:SER:HB3	1.50	0.76
1:D:472:ASP:OD2	1:D:523:LYS:HB2	1.86	0.76
1:A:482:TYR:HH	1:A:545:PHE:HD2	1.34	0.75
1:D:737:ILE:HD11	1:D:796:LEU:HD23	1.70	0.74
1:D:409:GLU:CA	1:D:409:GLU:OE2	2.33	0.73
1:A:404:LYS:HB3	1:A:405:PRO:HD2	1.71	0.72
1:A:86:MET:CE	3:A:1538:HOH:O	2.37	0.71
1:C:763:LEU:HD11	1:C:818:LEU:CD1	2.19	0.71
1:C:732:VAL:CG1	1:C:737:ILE:HG12	2.20	0.71
1:A:86:MET:HE3	3:A:1538:HOH:O	1.90	0.71
1:A:766:LYS:HG3	3:A:1512:HOH:O	1.90	0.71
1:A:84:LYS:HE3	1:A:139:GLU:OE2	1.91	0.70
1:A:832:LYS:HE2	3:A:1396:HOH:O	1.91	0.70
1:B:459:PHE:H	1:B:535:SER:CB	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:407:ASP:CG	1:D:408:ALA:H	1.94	0.70
1:D:43:VAL:HG12	1:D:97:VAL:HB	1.74	0.69
1:C:833:GLU:HG3	1:C:834:PHE:N	2.05	0.69
1:D:577:ALA:HB3	1:D:617:THR:HG23	1.75	0.69
1:C:798:ASP:HB3	3:C:900:HOH:O	1.92	0.68
1:D:54:LYS:HE2	3:D:950:HOH:O	1.93	0.68
1:C:452:VAL:HG12	1:C:452:VAL:O	1.91	0.68
1:A:404:LYS:HB3	1:A:405:PRO:CD	2.25	0.67
1:D:480:GLN:NE2	1:D:506:PHE:HB2	2.09	0.66
1:C:452:VAL:O	1:C:452:VAL:CG1	2.44	0.66
1:D:479:LEU:HB3	1:D:495:ILE:CG2	2.26	0.66
1:D:17:GLU:OE2	1:D:35:ARG:NH2	2.27	0.65
1:D:409:GLU:OE2	1:D:409:GLU:N	2.30	0.65
1:A:733:THR:OG1	1:A:734:ASP:N	2.30	0.64
1:B:734:ASP:HB3	1:B:838:LYS:HD3	1.80	0.64
1:C:655:VAL:HG13	1:C:662:PRO:HG3	1.78	0.64
1:D:479:LEU:HB3	1:D:495:ILE:HG21	1.79	0.64
1:D:628:GLU:HG3	1:D:672:PHE:O	1.98	0.64
1:C:733:THR:OG1	1:C:735:ASP:N	2.30	0.64
1:C:444:LEU:HD12	1:C:549:GLY:HA2	1.78	0.63
1:C:474:ASP:HB3	1:C:518:LYS:HE3	1.81	0.63
3:A:1110:HOH:O	1:B:675:GLN:HG2	1.98	0.63
1:B:735:ASP:N	1:B:735:ASP:OD2	2.30	0.63
1:A:502:GLU:CB	1:A:513:LYS:HE3	2.29	0.63
1:B:459:PHE:O	1:B:535:SER:HB3	1.99	0.63
1:D:833:GLU:HG3	3:D:958:HOH:O	1.97	0.63
1:A:633:GLU:HG3	3:A:942:HOH:O	1.98	0.62
1:C:346:ALA:O	1:C:367:PRO:HD2	1.98	0.62
1:D:494:ILE:HD12	1:D:517:LYS:HB3	1.81	0.62
1:D:735:ASP:HB2	1:D:736:LYS:NZ	2.14	0.62
1:A:736:LYS:HD2	3:A:1138:HOH:O	2.01	0.61
1:A:795:GLU:HG3	1:A:798:ASP:OD2	2.00	0.61
1:D:407:ASP:O	1:D:411:SER:HB2	2.00	0.61
1:B:469:PRO:HG3	1:B:521:LEU:HD23	1.82	0.61
1:D:763:LEU:HD11	1:D:818:LEU:HB2	1.81	0.61
1:D:17:GLU:CD	1:D:35:ARG:HH21	2.03	0.61
1:B:737:ILE:HD11	1:B:796:LEU:HD23	1.83	0.60
1:A:97:VAL:HG22	1:A:142:ALA:HB3	1.82	0.60
1:D:686:GLU:O	1:D:689:ARG:HG3	2.02	0.60
1:D:407:ASP:CG	1:D:408:ALA:N	2.55	0.60
1:C:43:VAL:HG12	1:C:97:VAL:HB	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:THR:OG1	1:C:563:GLU:OE2	2.20	0.59
1:D:475:TYR:HB2	1:D:521:LEU:HD13	1.84	0.59
1:C:115:PHE:CE1	1:C:353:GLY:HA3	2.37	0.59
1:C:735:ASP:N	1:C:735:ASP:OD2	2.30	0.59
1:A:349:LYS:HE2	1:A:364:VAL:O	2.03	0.59
1:C:482:TYR:HH	1:C:545:PHE:HD2	1.50	0.59
1:D:727:ILE:HG23	1:D:739:ILE:HD12	1.83	0.59
1:A:225:ASP:OD2	2:A:5001:BGC:H1	2.03	0.59
1:B:416:LYS:HG2	1:B:434:VAL:HG22	1.84	0.59
1:D:479:LEU:CB	1:D:495:ILE:HG21	2.33	0.59
1:D:727:ILE:HG23	1:D:739:ILE:CD1	2.32	0.59
1:C:387:SER:HB2	1:C:600:PRO:HG2	1.85	0.58
1:C:292:THR:HB	1:C:294:ILE:HD12	1.85	0.58
1:C:474:ASP:HB2	1:C:557:ALA:HB3	1.86	0.58
1:C:65:PRO:HA	1:C:643:TYR:O	2.04	0.58
1:A:502:GLU:HB2	1:A:513:LYS:HE3	1.86	0.57
1:C:753:SER:HA	1:C:780:VAL:O	2.05	0.57
1:C:794:LEU:HD13	1:C:799:ALA:HB2	1.85	0.57
1:C:65:PRO:HG2	1:C:316:ILE:HG22	1.85	0.57
1:A:655:VAL:HG13	1:A:662:PRO:HG3	1.85	0.57
1:D:409:GLU:OE2	1:D:409:GLU:C	2.43	0.57
1:D:225:ASP:OD1	2:D:5004:BGC:H1	2.04	0.57
1:D:367:PRO:HG2	1:D:580:ILE:HG21	1.87	0.56
1:A:62:GLY:HA2	1:A:646:ASN:ND2	2.21	0.56
1:B:676:ASP:O	1:B:708:ARG:NH1	2.39	0.56
1:C:292:THR:CB	1:C:294:ILE:HD12	2.35	0.56
1:C:732:VAL:HG12	1:C:737:ILE:HG12	1.88	0.56
1:D:94:ASN:ND2	1:D:295:VAL:H	2.03	0.56
1:A:226:TRP:O	1:A:227:PHE:HB2	2.04	0.56
1:D:487:PHE:HB3	1:D:495:ILE:HB	1.86	0.56
1:C:445:PHE:HB2	3:C:1053:HOH:O	2.05	0.56
1:D:782:LEU:HD21	1:D:788:LYS:HB2	1.88	0.55
1:C:737:ILE:HD11	1:C:796:LEU:HD23	1.86	0.55
1:D:396:GLU:OE2	1:D:439:ARG:HA	2.06	0.55
1:C:482:TYR:HD2	1:C:548:GLY:CA	2.18	0.55
1:A:620:VAL:HG11	1:A:652:ILE:HD13	1.88	0.55
1:D:661:VAL:HG21	1:D:751:ALA:O	2.06	0.55
1:D:49:GLY:HA3	1:D:359:MET:CE	2.36	0.55
1:D:192:ALA:HB1	1:D:194:ASN:OD1	2.07	0.55
1:B:578:VAL:HG22	1:B:618:VAL:CG1	2.37	0.55
1:A:62:GLY:HA2	1:A:646:ASN:HD21	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:TRP:CD2	2:D:5004:BGC:H6C2	2.42	0.54
1:D:774:LEU:O	1:D:775:LYS:HD3	2.08	0.54
1:A:126:GLY:HA3	1:A:179:LEU:HD12	1.89	0.54
1:B:56:PHE:HB2	1:B:443:HIS:O	2.07	0.54
1:B:733:THR:OG1	1:B:735:ASP:N	2.39	0.54
1:D:339:ILE:HA	1:D:576:LYS:O	2.07	0.54
1:B:342:ILE:HA	1:B:382:THR:O	2.07	0.54
1:A:450:GLU:HG3	3:A:1105:HOH:O	2.08	0.54
1:B:497:GLN:O	1:B:501:GLN:NE2	2.41	0.54
1:C:97:VAL:HG22	1:C:142:ALA:HB3	1.89	0.54
1:B:399:LEU:HD23	1:B:411:SER:HA	1.90	0.54
1:B:459:PHE:O	1:B:535:SER:CB	2.56	0.54
1:C:94:ASN:ND2	1:C:295:VAL:H	2.05	0.53
1:D:474:ASP:OD1	1:D:474:ASP:N	2.41	0.53
1:A:331:LEU:HD23	1:A:333:LEU:HD13	1.91	0.53
1:D:654:ASP:HB3	1:D:660:VAL:HG23	1.90	0.53
1:A:65:PRO:HA	1:A:643:TYR:O	2.09	0.53
1:A:482:TYR:OH	1:A:545:PHE:HD2	1.91	0.53
1:B:342:ILE:HG22	1:B:343:GLY:N	2.22	0.53
1:A:487:PHE:HD2	1:A:488:TYR:N	2.07	0.53
1:C:607:VAL:HG11	1:C:631:TRP:CE2	2.43	0.53
1:A:719:SER:OG	1:A:720:TYR:N	2.42	0.52
1:C:686:GLU:HG3	3:C:966:HOH:O	2.09	0.52
1:A:315:LYS:HE3	3:A:1295:HOH:O	2.10	0.52
1:A:336:GLU:CD	1:A:336:GLU:H	2.12	0.52
1:A:341:VAL:O	1:A:381:TYR:HA	2.09	0.52
1:C:182:LYS:HB2	1:C:845:LEU:HG	1.91	0.52
1:C:218:TRP:CZ2	1:C:220:GLY:HA3	2.44	0.52
1:C:684:LYS:HG2	3:C:849:HOH:O	2.08	0.52
1:A:732:VAL:HG12	1:A:737:ILE:HG13	1.92	0.51
1:D:816:GLU:HG3	1:D:835:LYS:HD2	1.91	0.51
1:C:420:ASN:O	1:C:425:ARG:NH2	2.42	0.51
1:A:64:PHE:CZ	1:A:86:MET:HG3	2.46	0.51
1:B:200:HIS:CD2	1:B:230:TYR:CE2	2.98	0.51
1:D:325:LYS:HB2	1:D:638:LEU:HB3	1.92	0.51
1:A:382:THR:OG1	1:A:563:GLU:OE2	2.29	0.51
1:B:733:THR:OG1	1:B:734:ASP:N	2.42	0.51
1:D:682:ASN:HB3	3:D:1436:HOH:O	2.11	0.51
1:C:485:GLY:HA2	1:C:532:GLU:O	2.10	0.51
1:D:15:GLN:HG3	3:D:941:HOH:O	2.10	0.51
1:A:4:PHE:CD2	1:A:283:LYS:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:PRO:HG2	1:C:716:TYR:HB2	1.92	0.51
1:A:421:PRO:HB3	1:A:460:PHE:CE1	2.46	0.50
1:B:458:TYR:CZ	1:B:537:PRO:HB2	2.47	0.50
1:B:678:PRO:HB3	1:B:702:TYR:CG	2.46	0.50
1:C:132:VAL:O	1:C:136:MET:HG3	2.12	0.50
1:D:400:ILE:HD12	1:D:409:GLU:O	2.11	0.50
1:D:432:PHE:HD1	1:D:449:HIS:ND1	2.09	0.50
1:A:94:ASN:ND2	1:A:295:VAL:H	2.10	0.50
1:C:414:ILE:O	1:C:463:LEU:HA	2.11	0.50
1:D:333:LEU:HB3	1:D:657:TYR:CE2	2.47	0.50
1:A:127:MET:HE3	1:A:179:LEU:HD13	1.93	0.50
1:D:432:PHE:HD1	1:D:449:HIS:CE1	2.28	0.50
1:A:133:VAL:O	1:A:137:GLN:HG3	2.11	0.50
1:A:101:PRO:HB3	3:A:1050:HOH:O	2.12	0.49
1:D:407:ASP:OD2	1:D:408:ALA:N	2.37	0.49
1:C:292:THR:OG1	1:C:294:ILE:HD12	2.12	0.49
1:D:22:LEU:HD21	1:D:275:VAL:CG2	2.42	0.49
1:A:518:LYS:HE3	3:A:1288:HOH:O	2.11	0.49
1:C:570:LEU:O	1:C:574:HIS:ND1	2.45	0.49
1:D:458:TYR:CE2	1:D:538:THR:HA	2.47	0.49
1:B:494:ILE:O	1:B:495:ILE:HG13	2.12	0.49
1:A:371:ILE:HG22	1:A:379:VAL:HG21	1.94	0.49
1:D:745:ASN:ND2	1:D:750:PHE:O	2.36	0.49
1:B:758:VAL:HG21	1:B:792:ILE:HD12	1.94	0.49
1:D:218:TRP:CZ2	1:D:220:GLY:HA3	2.48	0.49
1:C:726:ASP:CB	3:C:909:HOH:O	2.60	0.49
1:C:6:VAL:HG22	1:C:279:LEU:HB3	1.95	0.49
1:C:150:CYS:HA	1:C:152:ASP:OD2	2.13	0.49
1:A:331:LEU:HD21	1:A:618:VAL:HG21	1.95	0.48
1:B:734:ASP:O	1:B:796:LEU:HD12	2.14	0.48
1:D:735:ASP:HB2	1:D:736:LYS:HZ1	1.76	0.48
1:A:366:SER:OG	1:A:369:GLU:HG3	2.14	0.48
1:A:502:GLU:HB3	1:A:513:LYS:HE3	1.94	0.48
1:C:472:ASP:HB2	3:C:921:HOH:O	2.13	0.48
1:D:457:PRO:HD2	1:D:537:PRO:HG2	1.95	0.48
1:C:545:PHE:HB2	3:C:934:HOH:O	2.12	0.48
1:C:735:ASP:O	1:C:736:LYS:CG	2.54	0.48
1:D:782:LEU:HD23	1:D:788:LYS:HD2	1.96	0.48
1:B:297:ASN:CB	3:B:897:HOH:O	2.49	0.48
1:B:725:LEU:HA	1:B:742:ASP:O	2.14	0.48
1:C:742:ASP:OD1	1:C:789:THR:OG1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:LEU:HD11	1:D:498:LYS:HE2	1.95	0.48
1:B:3:LYS:HE3	3:B:1007:HOH:O	2.13	0.48
1:B:94:ASN:ND2	1:B:295:VAL:H	2.12	0.47
1:C:354:GLY:HA3	1:C:585:GLY:O	2.14	0.47
1:D:102:THR:O	1:D:117:SER:HA	2.14	0.47
1:C:107:ARG:HA	1:C:698:VAL:HG13	1.97	0.47
1:D:21:LEU:HD23	1:D:31:LYS:HB3	1.97	0.47
1:A:86:MET:HE2	3:A:1538:HOH:O	2.07	0.47
1:C:120:GLU:CD	1:C:699:GLY:HA3	2.34	0.47
1:D:735:ASP:HB2	1:D:736:LYS:HZ3	1.79	0.47
1:D:673:LYS:O	1:D:676:ASP:HB2	2.15	0.47
1:C:62:GLY:HA2	1:C:646:ASN:HD21	1.80	0.47
1:C:561:ASP:N	1:C:561:ASP:OD1	2.46	0.47
1:D:64:PHE:CZ	1:D:86:MET:HG3	2.50	0.47
1:B:161:ASN:HA	1:B:195:LYS:HB2	1.97	0.47
1:C:733:THR:OG1	1:C:734:ASP:N	2.40	0.47
1:C:3:LYS:HD2	1:C:3:LYS:O	2.15	0.46
1:D:23:SER:OG	1:D:248:THR:HB	2.15	0.46
1:D:432:PHE:CD1	1:D:449:HIS:ND1	2.83	0.46
1:C:422:VAL:HA	1:C:425:ARG:CZ	2.45	0.46
1:C:115:PHE:CZ	1:C:353:GLY:HA3	2.51	0.46
1:B:101:PRO:HG2	1:B:129:THR:HG23	1.98	0.46
1:B:159:SER:HB2	1:D:263:ARG:HB2	1.96	0.46
1:A:187:VAL:HG13	3:A:924:HOH:O	2.16	0.46
1:A:407:ASP:HB3	1:A:409:GLU:H	1.81	0.46
1:C:630:PRO:HB2	3:C:1067:HOH:O	2.14	0.46
1:D:94:ASN:HD22	1:D:295:VAL:H	1.64	0.46
1:A:725:LEU:HG	1:A:829:LEU:HD12	1.96	0.46
1:D:142:ALA:HB1	1:D:187:VAL:HB	1.98	0.46
1:A:84:LYS:HE2	1:A:84:LYS:HB3	1.76	0.46
1:B:678:PRO:HB3	1:B:702:TYR:CD1	2.50	0.46
1:D:210:ASP:O	1:D:214:ASP:HB2	2.16	0.46
1:A:3:LYS:HA	1:A:3:LYS:HD3	1.50	0.46
1:A:708:ARG:NH2	1:B:708:ARG:NH2	2.64	0.46
1:C:333:LEU:HB3	1:C:657:TYR:CE2	2.51	0.46
1:B:578:VAL:HG22	1:B:618:VAL:HG13	1.98	0.45
1:C:724:GLU:HB2	3:C:1122:HOH:O	2.16	0.45
1:A:407:ASP:HB3	1:A:410:ASN:H	1.81	0.45
1:A:684:LYS:HG2	3:A:1002:HOH:O	2.16	0.45
1:A:708:ARG:HG3	3:A:880:HOH:O	2.16	0.45
1:A:725:LEU:HA	1:A:742:ASP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ARG:HB2	1:D:159:SER:HB2	1.99	0.45
1:D:57:ASP:HB2	1:D:435:THR:HG21	1.97	0.45
1:D:432:PHE:CD1	1:D:449:HIS:CE1	3.04	0.45
1:A:733:THR:CG2	1:A:736:LYS:HB2	2.45	0.45
1:B:607:VAL:HG11	1:B:631:TRP:CE2	2.52	0.45
1:C:350:THR:HG22	3:C:1030:HOH:O	2.16	0.45
1:B:739:ILE:HG13	1:B:740:SER:N	2.29	0.45
1:D:55:PHE:CG	1:D:443:HIS:CD2	3.05	0.45
1:C:533:TYR:OH	1:C:535:SER:HA	2.17	0.44
1:A:43:VAL:HG12	1:A:97:VAL:HB	1.99	0.44
1:B:206:LYS:HE2	3:B:884:HOH:O	2.18	0.44
1:B:625:THR:HB	1:B:626:PRO:CD	2.48	0.44
1:D:349:LYS:HG2	1:D:364:VAL:HB	2.00	0.44
1:C:155:ASP:O	1:C:685:THR:OG1	2.17	0.44
1:C:449:HIS:O	1:C:452:VAL:CG1	2.54	0.44
1:C:158:PHE:HB2	3:C:896:HOH:O	2.17	0.44
1:A:314:ARG:HB2	1:A:647:GLU:HG3	1.99	0.44
1:D:153:LEU:HD13	1:D:155:ASP:HB3	1.99	0.44
1:D:655:VAL:HG13	1:D:662:PRO:HG3	2.00	0.44
1:C:45:ASP:OD2	1:C:356:SER:HB2	2.17	0.44
1:A:396:GLU:OE2	1:A:439:ARG:HA	2.18	0.44
1:B:150:CYS:HA	1:B:152:ASP:OD2	2.17	0.44
1:C:400:ILE:HG12	1:C:410:ASN:O	2.18	0.44
1:B:5:ASP:O	1:B:9:LEU:HD12	2.18	0.43
1:D:276:ARG:NH2	3:D:1130:HOH:O	2.35	0.43
1:A:523:LYS:C	1:A:525:GLN:H	2.21	0.43
1:A:655:VAL:HA	1:A:660:VAL:O	2.19	0.43
1:C:474:ASP:O	1:C:475:TYR:CD1	2.72	0.43
1:D:400:ILE:HD11	1:D:436:LYS:HG3	2.00	0.43
1:B:286:VAL:HA	1:B:289:LEU:HG	1.99	0.43
1:C:708:ARG:NH2	1:D:708:ARG:NH2	2.66	0.43
1:A:464:THR:HG22	1:A:530:ARG:HG3	2.01	0.43
1:D:314:ARG:NE	1:D:650:ASN:HB3	2.32	0.43
1:A:263:ARG:HD2	1:C:159:SER:HB2	2.01	0.43
1:A:546:GLY:HA3	3:A:871:HOH:O	2.17	0.43
1:B:160:SER:O	1:B:194:ASN:HB2	2.18	0.43
1:B:732:VAL:O	1:B:732:VAL:CG2	2.64	0.43
1:B:602:ARG:NH1	1:B:605:GLU:OE1	2.52	0.43
1:D:301:SER:HA	3:D:898:HOH:O	2.19	0.43
1:C:648:LEU:C	1:C:648:LEU:HD12	2.39	0.43
1:D:284:PHE:HD1	3:D:1486:HOH:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:PRO:HD3	1:B:648:LEU:HD11	2.00	0.42
1:C:151:ASN:ND2	3:C:851:HOH:O	2.52	0.42
1:C:374:LYS:HA	1:C:374:LYS:HD3	1.94	0.42
1:A:489:LEU:HD12	1:A:489:LEU:HA	1.81	0.42
1:B:374:LYS:HA	1:B:374:LYS:HD3	1.79	0.42
1:B:578:VAL:HG12	1:B:580:ILE:HD11	2.02	0.42
1:A:134:LYS:HE3	1:A:183:HIS:O	2.19	0.42
1:A:374:LYS:NZ	1:A:659:ASP:OD2	2.46	0.42
1:B:648:LEU:HD12	1:B:649:GLY:N	2.34	0.42
1:A:166:GLU:OE1	1:A:206:LYS:NZ	2.48	0.42
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.91	0.42
1:A:523:LYS:O	1:A:525:GLN:N	2.51	0.42
1:C:314:ARG:CZ	1:C:650:ASN:HB3	2.50	0.42
1:C:386:TYR:CE2	1:C:558:ILE:HG12	2.55	0.42
1:C:539:SER:O	1:C:539:SER:OG	2.38	0.42
1:C:563:GLU:OE1	1:C:563:GLU:HA	2.19	0.42
1:C:723:PHE:HA	1:C:744:LYS:O	2.19	0.42
1:D:79:LEU:HD23	1:D:79:LEU:HA	1.76	0.42
1:B:218:TRP:CZ2	1:B:220:GLY:HA3	2.55	0.42
1:C:371:ILE:HG22	1:C:379:VAL:HG21	2.00	0.42
1:C:744:LYS:HE3	1:C:785:GLY:O	2.19	0.42
1:A:489:LEU:CD1	1:A:529:VAL:HG12	2.49	0.42
1:B:288:ASN:O	1:B:292:THR:HG23	2.19	0.42
1:D:161:ASN:HA	1:D:195:LYS:HB2	2.01	0.42
1:C:233:ALA:HB1	1:C:265:GLN:HB2	2.02	0.42
1:D:323:LEU:HD22	1:D:662:PRO:HG2	2.02	0.42
1:D:744:LYS:HA	1:D:786:GLU:O	2.20	0.42
1:A:661:VAL:HG13	1:A:720:TYR:HB2	2.02	0.41
1:A:146:LYS:HE3	2:A:5001:BGC:O3	2.20	0.41
1:A:336:GLU:CD	1:A:336:GLU:N	2.74	0.41
1:B:736:LYS:HB2	1:B:736:LYS:HE2	1.58	0.41
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.88	0.41
1:A:286:VAL:HA	1:A:289:LEU:HG	2.02	0.41
1:A:350:THR:O	1:A:350:THR:OG1	2.33	0.41
1:A:417:PHE:HA	1:A:460:PHE:O	2.21	0.41
1:A:84:LYS:HE3	1:A:139:GLU:CD	2.41	0.41
1:B:297:ASN:CG	3:B:897:HOH:O	2.59	0.41
1:C:331:LEU:HB3	1:C:720:TYR:OH	2.20	0.41
1:D:226:TRP:CE2	2:D:5004:BGC:H6C2	2.55	0.41
1:A:167:ARG:NH2	3:A:887:HOH:O	2.51	0.41
1:A:730:PHE:CD2	1:A:832:LYS:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:THR:HG23	1:A:736:LYS:H	1.85	0.41
1:D:19:ILE:HG12	1:D:256:VAL:HG11	2.02	0.41
1:D:22:LEU:HD21	1:D:275:VAL:HG22	2.03	0.41
1:A:559:ASP:HB3	1:A:562:GLU:HB3	2.02	0.41
1:D:394:LEU:HB2	1:D:553:GLY:HA2	2.02	0.41
1:D:614:ASN:O	1:D:617:THR:OG1	2.38	0.41
1:A:468:VAL:HA	1:A:469:PRO:HD2	1.88	0.41
1:C:65:PRO:HG3	1:C:317:ALA:HA	2.02	0.41
1:C:340:ILE:HG13	1:C:341:VAL:N	2.34	0.41
1:C:386:TYR:HE2	1:C:558:ILE:HG12	1.86	0.41
1:D:241:ASP:HA	1:D:274:ARG:HD3	2.02	0.41
1:C:62:GLY:HA2	1:C:646:ASN:ND2	2.36	0.41
1:C:481:VAL:HG23	1:C:482:TYR:N	2.34	0.41
1:C:623:SER:O	1:C:642:TRP:HA	2.21	0.41
1:C:684:LYS:HE3	1:C:684:LYS:HB2	2.00	0.41
1:C:743:VAL:HG12	1:C:782:LEU:HD11	2.03	0.41
1:D:119:SER:CB	1:D:124:LEU:HD23	2.50	0.41
1:D:221:MET:SD	1:D:278:VAL:HA	2.60	0.41
1:D:343:GLY:HA2	1:D:344:PRO:HD3	1.84	0.41
1:D:394:LEU:CB	1:D:553:GLY:HA2	2.51	0.41
1:A:48:ASN:HD21	1:A:357:ALA:HB1	1.86	0.41
1:B:89:GLU:OE2	1:B:362:TYR:OH	2.28	0.41
1:B:246:GLY:HA2	1:B:247:PRO:C	2.41	0.41
1:D:349:LYS:HE2	1:D:364:VAL:O	2.21	0.41
1:A:463:LEU:O	1:A:530:ARG:HA	2.21	0.40
1:A:720:TYR:HD1	1:A:720:TYR:HA	1.76	0.40
1:D:685:THR:HG22	3:D:927:HOH:O	2.21	0.40
1:C:59:VAL:HA	1:C:60:PRO:HD3	1.92	0.40
1:A:246:GLY:HA2	1:A:247:PRO:C	2.42	0.40
1:A:480:GLN:NE2	1:A:506:PHE:HB2	2.36	0.40
1:A:753:SER:HA	1:A:780:VAL:O	2.21	0.40
1:C:474:ASP:C	1:C:475:TYR:CD1	2.94	0.40
1:C:663:ASN:OD1	1:C:779:LYS:NZ	2.53	0.40
1:D:314:ARG:CZ	1:D:650:ASN:HB3	2.50	0.40
1:D:367:PRO:HA	1:D:649:GLY:HA2	2.02	0.40
1:D:409:GLU:OE2	1:D:410:ASN:N	2.54	0.40
1:D:377:LYS:O	1:D:378:GLU:C	2.57	0.40
1:D:737:ILE:CD1	1:D:796:LEU:HD23	2.47	0.40
1:A:325:LYS:O	1:A:637:ALA:HA	2.22	0.40
1:A:578:VAL:HG22	1:A:618:VAL:CG1	2.52	0.40
1:D:239:GLY:HA2	1:D:274:ARG:CZ	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:756:VAL:O	1:D:777:PHE:HA	2.22	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	837/845 (99%)	792 (95%)	44 (5%)	1 (0%)	51	65
1	B	815/845 (96%)	776 (95%)	38 (5%)	1 (0%)	51	65
1	C	821/845 (97%)	773 (94%)	46 (6%)	2 (0%)	47	60
1	D	823/845 (97%)	773 (94%)	50 (6%)	0	100	100
All	All	3296/3380 (98%)	3114 (94%)	178 (5%)	4 (0%)	51	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	GLY
1	B	297	ASN
1	C	329	ASN
1	C	524	GLY

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	714/717 (100%)	685 (96%)	29 (4%)	30	41
1	B	700/717 (98%)	664 (95%)	36 (5%)	24	32
1	C	707/717 (99%)	662 (94%)	45 (6%)	17	23
1	D	703/717 (98%)	669 (95%)	34 (5%)	25	34
All	All	2824/2868 (98%)	2680 (95%)	144 (5%)	24	32

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	LYS
1	A	54	LYS
1	A	206	LYS
1	A	226	TRP
1	A	333	LEU
1	A	427	ASP
1	A	428	ASP
1	A	436	LYS
1	A	450	GLU
1	A	472	ASP
1	A	484	SER
1	A	487	PHE
1	A	503	ARG
1	A	565	ARG
1	A	675	GLN
1	A	677	ASN
1	A	726	ASP
1	A	729	ASP
1	A	732	VAL
1	A	733	THR
1	A	735	ASP
1	A	739	ILE
1	A	766	LYS
1	A	790	VAL
1	A	794	LEU
1	A	795	GLU
1	A	797	LYS
1	A	845	LEU
1	B	3	LYS
1	B	8	GLN
1	B	61	SER
1	B	226	TRP

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Mol	Chain	Res	Type
1	B	294	ILE
1	B	333	LEU
1	B	335	LYS
1	B	377	LYS
1	B	427	ASP
1	B	429	GLU
1	B	435	THR
1	B	436	LYS
1	B	444	LEU
1	B	466	GLN
1	B	487	PHE
1	B	503	ARG
1	B	522	LYS
1	B	535	SER
1	B	556	LYS
1	B	576	LYS
1	B	633	GLU
1	B	677	ASN
1	B	682	ASN
1	B	684	LYS
1	B	686	GLU
1	B	726	ASP
1	B	733	THR
1	B	735	ASP
1	B	739	ILE
1	B	766	LYS
1	B	794	LEU
1	B	797	LYS
1	B	833	GLU
1	B	837	GLU
1	B	839	GLU
1	B	845	LEU
1	C	3	LYS
1	C	61	SER
1	C	153	LEU
1	C	226	TRP
1	C	255	LEU
1	C	294	ILE
1	C	310	SER
1	C	312	LEU
1	C	333	LEU
1	C	334	LYS

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Mol	Chain	Res	Type
1	C	335	LYS
1	C	377	LYS
1	C	378	GLU
1	C	399	LEU
1	C	409	GLU
1	C	427	ASP
1	C	436	LYS
1	C	445	PHE
1	C	452	VAL
1	C	468	VAL
1	C	472	ASP
1	C	474	ASP
1	C	481	VAL
1	C	487	PHE
1	C	503	ARG
1	C	507	CYS
1	C	522	LYS
1	C	539	SER
1	C	559	ASP
1	C	580	ILE
1	C	618	VAL
1	C	675	GLN
1	C	677	ASN
1	C	726	ASP
1	C	732	VAL
1	C	739	ILE
1	C	766	LYS
1	C	793	ASP
1	C	794	LEU
1	C	816	GLU
1	C	818	LEU
1	C	832	LYS
1	C	833	GLU
1	C	838	LYS
1	C	845	LEU
1	D	61	SER
1	D	226	TRP
1	D	307	LYS
1	D	312	LEU
1	D	333	LEU
1	D	366	SER
1	D	377	LYS

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Mol	Chain	Res	Type
1	D	381	TYR
1	D	409	GLU
1	D	411	SER
1	D	420	ASN
1	D	438	ASN
1	D	470	GLN
1	D	472	ASP
1	D	474	ASP
1	D	487	PHE
1	D	488	TYR
1	D	494	ILE
1	D	498	LYS
1	D	507	CYS
1	D	530	ARG
1	D	560	ASP
1	D	677	ASN
1	D	684	LYS
1	D	739	ILE
1	D	766	LYS
1	D	796	LEU
1	D	797	LYS
1	D	819	VAL
1	D	832	LYS
1	D	833	GLU
1	D	837	GLU
1	D	838	LYS
1	D	845	LEU

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

Mol	Chain	Res	Type
1	A	48	ASN
1	A	94	ASN
1	A	388	HIS
1	A	480	GLN
1	A	525	GLN
1	A	636	ASN
1	A	675	GLN
1	B	48	ASN
1	B	94	ASN
1	B	151	ASN
1	B	183	HIS

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Mol	Chain	Res	Type
1	B	338	ASN
1	B	525	GLN
1	B	636	ASN
1	B	675	GLN
1	C	94	ASN
1	C	151	ASN
1	C	443	HIS
1	C	525	GLN
1	C	636	ASN
1	C	675	GLN
1	C	682	ASN
1	D	48	ASN
1	D	94	ASN
1	D	151	ASN
1	D	183	HIS
1	D	373	ASN
1	D	388	HIS
1	D	443	HIS
1	D	480	GLN
1	D	500	ASN
1	D	636	ASN
1	D	764	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BGC	B	5002	-	12,12,12	0.81	0	17,17,17	2.16	4 (23%)
2	BGC	A	5001	-	12,12,12	0.69	0	17,17,17	1.59	3 (17%)
2	BGC	C	5003	-	12,12,12	0.60	0	17,17,17	0.75	0
2	BGC	D	5004	-	12,12,12	0.84	0	17,17,17	1.66	3 (17%)

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	BGC	B	5002	-	-	0/2/22/22	0/1/1/1
2	BGC	A	5001	-	-	0/2/22/22	0/1/1/1
2	BGC	C	5003	-	-	0/2/22/22	0/1/1/1
2	BGC	D	5004	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5002	BGC	C1-O5-C5	5.56	124.15	113.66
2	B	5002	BGC	O1-C1-O5	-4.95	95.51	110.38
2	A	5001	BGC	C1-O5-C5	4.50	122.15	113.66
2	D	5004	BGC	O1-C1-O5	-3.25	100.63	110.38
2	D	5004	BGC	C3-C4-C5	-3.18	104.57	110.24
2	B	5002	BGC	O5-C1-C2	2.92	115.50	110.28
2	D	5004	BGC	O2-C2-C1	2.69	115.39	109.16
2	B	5002	BGC	O4-C4-C5	-2.67	102.67	109.30
2	A	5001	BGC	O1-C1-O5	-2.53	102.78	110.38
2	A	5001	BGC	O5-C1-C2	2.42	114.59	110.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	5002	BGC	1	0
2	A	5001	BGC	2	0
2	C	5003	BGC	1	0
2	D	5004	BGC	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 (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	841/845 (99%)	-0.27	10 (1%)	79	84	15, 31, 60, 77	0
1	B	825/845 (97%)	-0.18	28 (3%)	45	52	15, 26, 76, 97	0
1	C	831/845 (98%)	-0.00	50 (6%)	21	25	18, 38, 87, 105	0
1	D	829/845 (98%)	0.04	29 (3%)	44	51	19, 43, 80, 99	0
All	All	3326/3380 (98%)	-0.10	117 (3%)	44	51	15, 35, 80, 105	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	406	ALA	5.2
1	A	543	GLY	5.0
1	C	403	ALA	4.9
1	D	403	ALA	4.9
1	D	402	ALA	4.7
1	D	408	ALA	4.5
1	C	526	VAL	4.5
1	C	521	LEU	4.3
1	A	403	ALA	4.2
1	C	428	ASP	4.1
1	C	402	ALA	4.1
1	C	400	ILE	4.0
1	D	418	TYR	3.9
1	C	473	GLY	3.9
1	B	403	ALA	3.7
1	A	428	ASP	3.6
1	B	447	PHE	3.6
1	D	473	GLY	3.6
1	C	401	ASP	3.6
1	B	431	PRO	3.5
1	C	527	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	420	ASN	3.5
1	B	434	VAL	3.5
1	D	405	PRO	3.5
1	C	417	PHE	3.4
1	D	494	ILE	3.4
1	B	428	ASP	3.3
1	B	503	ARG	3.3
1	C	426	SER	3.3
1	B	402	ALA	3.2
1	C	472	ASP	3.2
1	B	435	THR	3.2
1	B	526	VAL	3.2
1	C	458	TYR	3.2
1	C	475	TYR	3.2
1	A	426	SER	3.1
1	C	427	ASP	3.1
1	B	509	GLY	3.1
1	D	474	ASP	3.1
1	D	475	TYR	3.1
1	B	433	HIS	3.0
1	C	519	LEU	3.0
1	C	528	ASN	2.9
1	B	405	PRO	2.9
1	B	418	TYR	2.9
1	C	430	GLU	2.9
1	C	405	PRO	2.8
1	D	519	LEU	2.8
1	C	525	GLN	2.8
1	C	495	ILE	2.8
1	D	529	VAL	2.8
1	B	472	ASP	2.8
1	B	734	ASP	2.8
1	B	444	LEU	2.8
1	C	420	ASN	2.8
1	C	522	LYS	2.8
1	C	414	ILE	2.8
1	D	400	ILE	2.8
1	D	564	ILE	2.7
1	D	421	PRO	2.7
1	A	402	ALA	2.7
1	D	500	ASN	2.7
1	C	419	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	427	ASP	2.7
1	B	432	PHE	2.6
1	D	503	ARG	2.6
1	C	524	GLY	2.6
1	C	468	VAL	2.6
1	C	498	LYS	2.6
1	D	472	ASP	2.6
1	D	487	PHE	2.5
1	D	489	LEU	2.5
1	C	545	PHE	2.5
1	A	408	ALA	2.5
1	D	476	ILE	2.5
1	B	408	ALA	2.5
1	C	460	PHE	2.4
1	C	492	GLU	2.4
1	C	474	ASP	2.4
1	C	734	ASP	2.4
1	B	522	LYS	2.4
1	C	488	TYR	2.4
1	C	471	GLU	2.4
1	D	417	PHE	2.4
1	B	510	ALA	2.4
1	B	415	ALA	2.3
1	C	550	PHE	2.3
1	D	458	TYR	2.3
1	C	538	THR	2.3
1	B	529	VAL	2.3
1	B	450	GLU	2.3
1	D	3	LYS	2.3
1	B	527	TYR	2.3
1	C	477	PHE	2.2
1	C	418	TYR	2.2
1	A	764	ASN	2.2
1	C	489	LEU	2.2
1	C	429	GLU	2.2
1	C	467	TYR	2.2
1	A	470	GLN	2.2
1	C	424	GLU	2.2
1	D	382	THR	2.2
1	D	414	ILE	2.2
1	C	404	LYS	2.2
1	C	529	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	736	LYS	2.1
1	C	520	THR	2.1
1	D	527	TYR	2.1
1	D	404	LYS	2.1
1	B	430	GLU	2.1
1	C	537	PRO	2.1
1	C	463	LEU	2.1
1	B	409	GLU	2.1
1	C	523	LYS	2.1
1	C	3	LYS	2.0
1	B	524	GLY	2.0
1	A	734	ASP	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 monosaccharides 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	BGC	A	5001	12/12	0.96	0.19	20,28,32,37	0
2	BGC	D	5004	12/12	0.97	0.19	32,36,38,41	0
2	BGC	C	5003	12/12	0.98	0.16	28,34,38,42	0
2	BGC	B	5002	12/12	0.98	0.12	25,28,30,33	0

6.5 Other polymers (i)

There are no such residues in this entry.