Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:59 AM GMT

PDB ID	:	2Z1K
Title	:	Crystal Structure of Ttha1563 from Thermus thermophilus HB8
Authors	:	Niwa, H.; Shimada, A.; Matsunaga, E.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-05-08
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

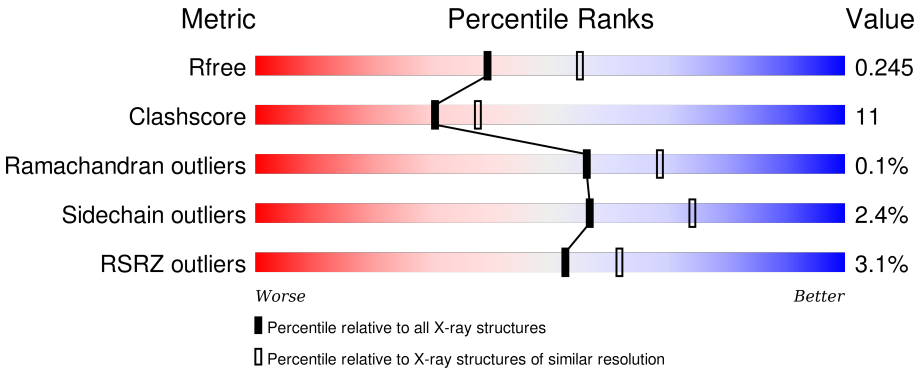
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	475	3% 78% 22%
1	B	475	2% 78% 21%
1	C	475	2% 77% 21%
1	D	475	5% 73% 26%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	A	502	-	-	-	X
2	GLC	A	507	-	-	-	X
2	GLC	D	507	-	-	-	X
3	GLC	A	601	-	-	-	X
3	GLC	A	602	-	-	-	X
3	GLC	A	603	-	-	-	X
3	GLC	B	603	-	-	-	X
3	GLC	C	601	-	-	-	X
3	GLC	C	602	-	-	-	X
3	GLC	C	603	-	-	-	X
3	GLC	D	602	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16422 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 (Neo)pullulanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	Se	0	0	0
			3803	2464	675	655	2	7			
1	B	474	Total	C	N	O	S	Se	0	1	0
			3801	2462	672	658	2	7			
1	C	474	Total	C	N	O	S	Se	0	0	0
			3789	2456	670	654	2	7			
1	D	474	Total	C	N	O	S	Se	0	0	0
			3803	2464	675	655	2	7			

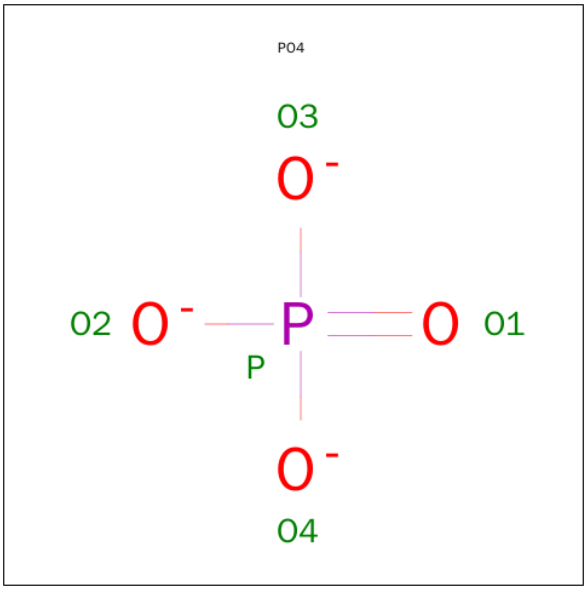
- Molecule 2 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	7	Total	C	O	0	0
			77	42	35		
2	B	7	Total	C	O	0	0
			77	42	35		
2	C	7	Total	C	O	0	0
			77	42	35		
2	D	7	Total	C	O	0	0
			77	42	35		

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	3	Total	C	O	0	0
			33	18	15		
3	B	3	Total	C	O	0	0
			33	18	15		
3	C	3	Total	C	O	0	0
			33	18	15		
3	D	3	Total	C	O	0	0
			33	18	15		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

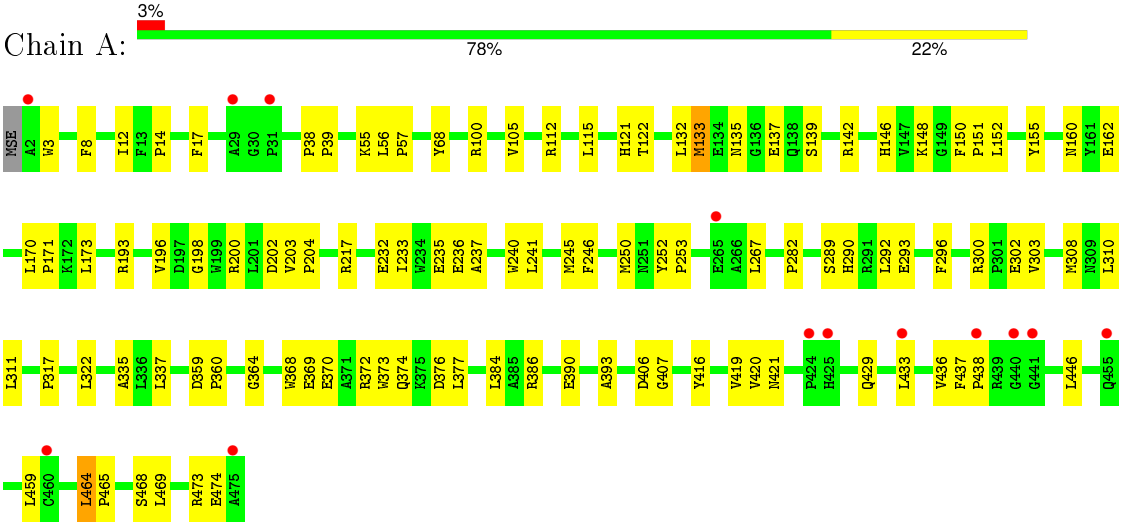
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	166	Total O 166 166	0	0
5	B	227	Total O 227 227	0	0
5	C	197	Total O 197 197	0	0
5	D	191	Total O 191 191	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

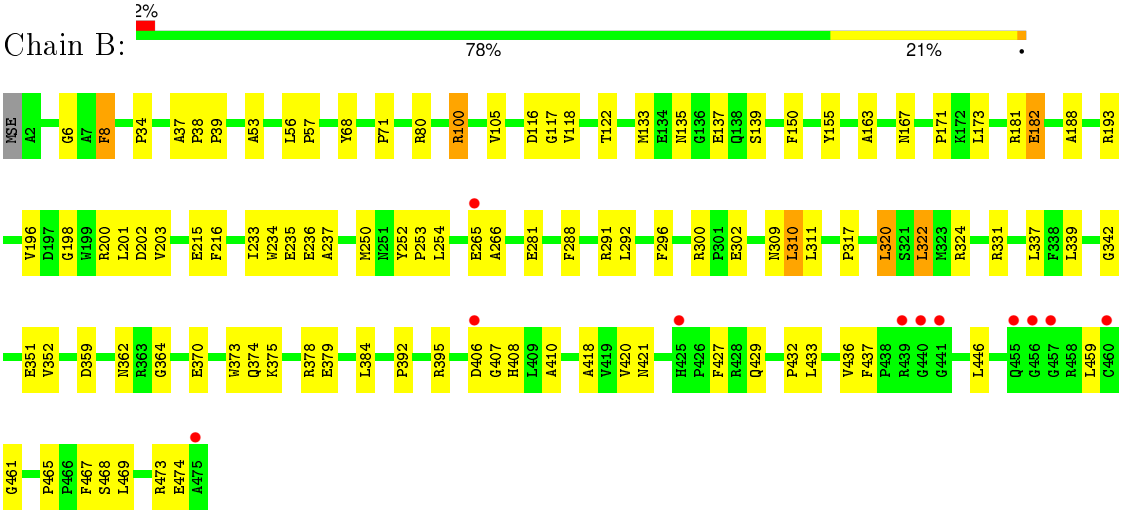
- Molecule 1: (Neo)pullulanase

Chain A:



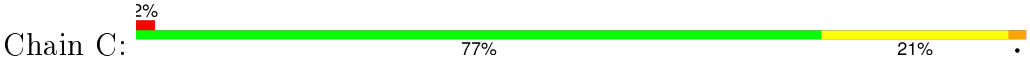
- Molecule 1: (Neo)pullulanase

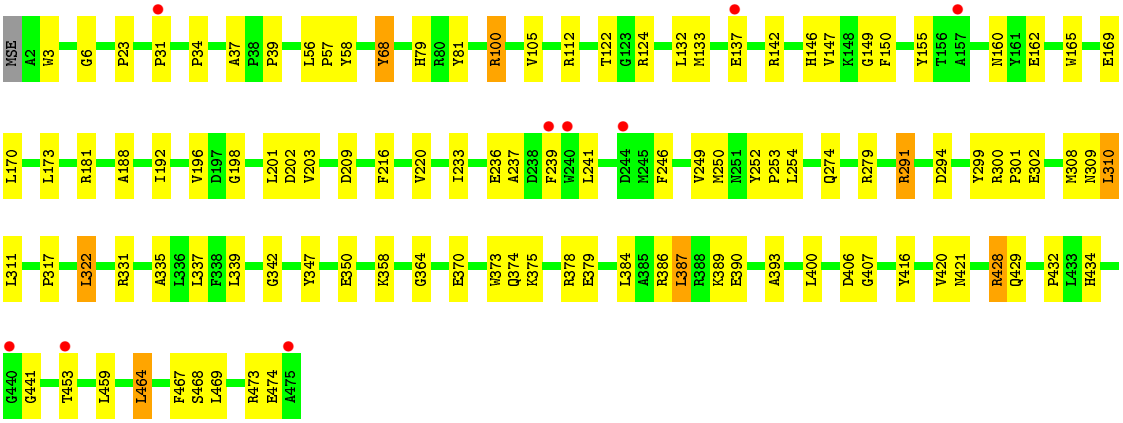
Chain B:



- Molecule 1: (Neo)pullulanase

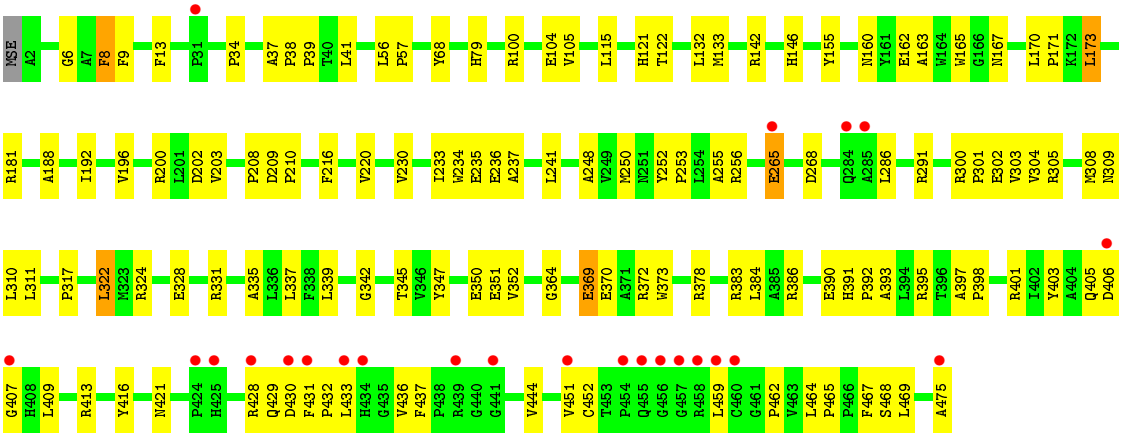
Chain C:





- Molecule 1: (Neo)pullulanase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.14Å 95.90Å 140.60Å 90.00° 94.40° 90.00°	Depositor
Resolution (Å)	46.66 – 2.30 46.66 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.66-2.30) 99.5 (46.66-2.29)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.32 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.236 0.198 , 0.245	Depositor DCC
R_{free} test set	3951 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	26.9	Xtriage
Anisotropy	0.742	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	10 of 79403 reflections (0.013%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16422	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.63 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6636e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4, GLC

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	0.34	0/3926	0.58	0/5339
1	B	0.35	0/3924	0.59	0/5339
1	C	0.34	0/3912	0.59	0/5323
1	D	0.33	0/3926	0.57	0/5339
All	All	0.34	0/15688	0.58	0/21340

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3803	0	3682	82	0
1	B	3801	0	3663	76	0
1	C	3789	0	3654	82	0
1	D	3803	0	3682	96	0
2	A	77	0	63	1	0
2	B	77	0	63	3	0
2	C	77	0	63	1	0
2	D	77	0	63	3	0
3	A	33	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	28	1	0
3	C	33	0	28	2	0
3	D	33	0	28	1	0
4	D	5	0	0	0	0
5	A	166	0	0	3	0
5	B	227	0	0	8	0
5	C	197	0	0	7	0
5	D	191	0	0	5	0
All	All	16422	0	15045	337	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 11.

All (337) 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:406:ASP:CG	1:C:407:GLY:H	1.63	0.99
1:B:100:ARG:HH11	1:B:100:ARG:HG2	1.28	0.98
1:D:406:ASP:CG	1:D:407:GLY:H	1.69	0.95
1:D:311:LEU:HG	1:D:337:LEU:HD11	1.49	0.92
1:D:429:GLN:HB3	1:D:459:LEU:HD23	1.54	0.90
1:A:406:ASP:CG	1:A:407:GLY:H	1.74	0.90
1:B:406:ASP:CG	1:B:407:GLY:H	1.75	0.85
1:C:100:ARG:HH11	1:C:100:ARG:HG2	1.46	0.80
1:C:311:LEU:HG	1:C:337:LEU:HD11	1.65	0.79
1:B:34:PRO:HG2	1:B:37:ALA:HB2	1.64	0.78
1:C:406:ASP:CG	1:C:407:GLY:N	2.35	0.77
1:A:406:ASP:CG	1:A:407:GLY:N	2.39	0.76
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.49	0.76
1:B:465:PRO:HG2	1:B:468:SER:OG	1.86	0.75
1:D:406:ASP:CG	1:D:407:GLY:N	2.39	0.74
1:B:406:ASP:CG	1:B:407:GLY:N	2.41	0.73
1:B:118:VAL:HG22	1:B:202[B]:ASP:OD2	1.88	0.72
1:B:235:GLU:HG2	1:C:301:PRO:HG3	1.73	0.71
1:D:202:ASP:OD1	3:D:603:GLC:C1	2.39	0.70
1:A:429:GLN:HB3	1:A:459:LEU:HD23	1.74	0.70
1:A:56:LEU:HD22	1:A:105:VAL:HG12	1.74	0.70
1:D:132:LEU:HD21	1:D:142:ARG:HA	1.74	0.69
1:D:465:PRO:HG2	1:D:468:SER:OG	1.92	0.69
1:B:200:ARG:NH1	1:B:202[B]:ASP:OD1	2.26	0.68
1:C:233:ILE:HG21	1:C:237:ALA:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ARG:HH11	1:D:100:ARG:HG2	1.59	0.67
1:B:311:LEU:HG	1:B:337:LEU:HD11	1.76	0.67
1:B:433:LEU:O	1:B:436:VAL:HG23	1.96	0.66
1:A:393:ALA:HB3	1:A:416:TYR:HE2	1.61	0.66
1:C:429:GLN:HB3	1:C:459:LEU:HD23	1.77	0.66
1:A:133:MSE:HE1	1:A:155:TYR:HE2	1.61	0.66
1:D:339:LEU:HD11	1:D:469:LEU:HD21	1.77	0.65
1:C:317:PRO:HB2	1:C:322:LEU:HD13	1.76	0.65
1:C:300:ARG:HB3	1:C:302:GLU:OE2	1.97	0.64
1:A:282:PRO:HG3	5:A:658:HOH:O	1.96	0.64
1:A:464:LEU:CD2	1:A:468:SER:HB2	2.28	0.64
1:A:122:THR:O	1:A:171:PRO:HD2	1.98	0.64
1:C:241:LEU:HD21	1:C:249:VAL:HG13	1.79	0.64
1:B:100:ARG:NH1	1:B:100:ARG:HG2	2.07	0.63
1:B:370:GLU:HG2	1:B:373:TRP:CH2	2.34	0.63
1:A:132:LEU:HD21	1:A:142:ARG:HA	1.80	0.63
1:A:289:SER:O	1:A:293:GLU:HG3	1.98	0.62
1:A:386:ARG:O	1:A:390:GLU:HG3	1.99	0.62
1:B:202[A]:ASP:OD1	3:B:603:GLC:C1	2.47	0.62
1:C:132:LEU:HD21	1:C:142:ARG:HA	1.80	0.62
1:A:446:LEU:HD21	1:A:473:ARG:HD3	1.82	0.62
1:B:302:GLU:H	1:B:302:GLU:CD	2.03	0.61
1:C:464:LEU:HD22	1:C:468:SER:HB2	1.83	0.61
1:C:370:GLU:HG2	1:C:373:TRP:CZ3	2.35	0.61
1:C:339:LEU:HD11	1:C:469:LEU:HD21	1.83	0.61
1:C:56:LEU:N	1:C:57:PRO:HD2	2.16	0.61
1:B:56:LEU:HD22	1:B:105:VAL:HG12	1.83	0.60
1:D:433:LEU:O	1:D:436:VAL:HG23	2.02	0.59
1:C:389:LYS:HE3	5:C:617:HOH:O	2.02	0.59
1:A:311:LEU:HG	1:A:337:LEU:HD11	1.84	0.59
1:B:122:THR:O	1:B:171:PRO:HD2	2.02	0.59
1:D:392:PRO:HA	1:D:395:ARG:NH1	2.18	0.58
1:B:317:PRO:HB2	1:B:322:LEU:HD13	1.84	0.58
1:A:56:LEU:N	1:A:57:PRO:HD2	2.18	0.58
1:C:56:LEU:HD23	1:C:105:VAL:HG12	1.84	0.58
1:D:208:PRO:O	1:D:210:PRO:HD3	2.03	0.58
1:D:369:GLU:HG2	1:D:372:ARG:HG3	1.84	0.58
1:C:375:LYS:O	1:C:379:GLU:HG3	2.03	0.58
1:A:317:PRO:HB2	1:A:322:LEU:HD13	1.85	0.57
1:B:100:ARG:CG	1:B:100:ARG:HH11	2.07	0.57
1:C:146:HIS:HB2	1:C:162:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:PRO:HG2	5:B:718:HOH:O	2.03	0.57
1:A:370:GLU:HG2	1:A:373:TRP:CZ3	2.40	0.57
1:C:39:PRO:HG3	1:C:364:GLY:HA2	1.87	0.57
1:A:146:HIS:HB2	1:A:162:GLU:HB2	1.86	0.57
1:D:122:THR:O	1:D:171:PRO:HD2	2.05	0.57
1:A:290:HIS:HA	1:A:293:GLU:OE1	2.04	0.57
1:B:292:LEU:HB3	1:B:296:PHE:CE2	2.39	0.57
1:A:121:HIS:CD2	1:A:170:LEU:HD23	2.40	0.56
1:A:121:HIS:NE2	1:A:170:LEU:HD23	2.20	0.56
1:D:34:PRO:HG2	1:D:37:ALA:HB2	1.86	0.56
1:C:56:LEU:CD2	1:C:105:VAL:HG12	2.36	0.56
5:B:784:HOH:O	1:C:434:HIS:HD2	1.87	0.56
1:A:421:ASN:HB2	1:A:464:LEU:HD13	1.88	0.56
1:D:309:ASN:ND2	1:D:342:GLY:HA3	2.21	0.55
1:B:429:GLN:HB3	1:B:459:LEU:HD23	1.88	0.55
1:A:202:ASP:OD1	3:A:603:GLC:C1	2.54	0.55
1:C:441:GLY:O	1:C:453:THR:HG23	2.07	0.55
1:D:328:GLU:HG2	5:D:920:HOH:O	2.05	0.55
1:B:56:LEU:CD2	1:B:105:VAL:HG12	2.37	0.55
1:D:250:MSE:HE2	1:D:310:LEU:HD13	1.89	0.55
1:C:188:ALA:HB2	1:C:216:PHE:CE1	2.42	0.55
1:D:317:PRO:HB2	1:D:322:LEU:HD13	1.88	0.55
1:D:56:LEU:CD2	1:D:105:VAL:HG12	2.35	0.55
1:A:465:PRO:HG2	1:A:468:SER:OG	2.06	0.55
1:D:236:GLU:CD	1:D:236:GLU:H	2.10	0.54
1:C:370:GLU:HG2	1:C:373:TRP:CH2	2.43	0.54
1:C:170:LEU:HD12	1:C:170:LEU:N	2.22	0.54
1:C:420:VAL:HG22	1:C:469:LEU:CD1	2.36	0.54
1:D:146:HIS:HB2	1:D:162:GLU:HB2	1.88	0.54
1:A:137:GLU:HG2	1:A:150:PHE:CE2	2.43	0.54
1:D:317:PRO:HB2	1:D:322:LEU:CD1	2.38	0.54
1:C:122:THR:HG23	1:C:173:LEU:HD13	1.88	0.54
1:D:310:LEU:H	1:D:310:LEU:HD23	1.72	0.54
1:C:6:GLY:HA2	1:C:342:GLY:O	2.08	0.54
1:C:100:ARG:HH11	1:C:100:ARG:CG	2.19	0.54
1:C:309:ASN:ND2	1:C:342:GLY:HA3	2.23	0.54
1:D:234:TRP:CE2	2:D:501:GLC:H2	2.43	0.53
1:C:241:LEU:HD12	1:C:299:TYR:CE1	2.43	0.53
1:B:56:LEU:N	1:B:57:PRO:HD2	2.23	0.53
1:B:351:GLU:HG2	1:B:352:VAL:HG13	1.91	0.53
1:D:339:LEU:CD1	1:D:469:LEU:HD21	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ARG:NH1	1:B:215:GLU:OE1	2.41	0.53
1:B:421:ASN:O	1:B:467:PHE:HA	2.08	0.53
1:D:133:MSE:HE1	1:D:155:TYR:HE2	1.73	0.53
1:D:39:PRO:HG3	1:D:364:GLY:HA2	1.90	0.53
1:C:34:PRO:HG2	1:C:37:ALA:HB2	1.91	0.53
1:C:147:VAL:HG12	1:C:149:GLY:H	1.72	0.53
1:C:3:TRP:CE3	1:C:112:ARG:HG3	2.43	0.53
1:D:192:ILE:HG13	1:D:220:VAL:HG13	1.91	0.53
1:A:302:GLU:H	1:A:302:GLU:CD	2.12	0.53
1:A:203:VAL:HG23	1:A:203:VAL:O	2.10	0.52
1:D:265:GLU:CD	1:D:265:GLU:H	2.13	0.52
1:A:236:GLU:CD	1:A:236:GLU:H	2.10	0.52
1:A:100:ARG:CG	1:A:100:ARG:HH11	2.22	0.52
1:A:3:TRP:CE3	1:A:112:ARG:HG3	2.44	0.52
1:C:302:GLU:CD	1:C:302:GLU:H	2.12	0.52
1:A:39:PRO:HG3	1:A:364:GLY:HA2	1.91	0.52
1:B:196:VAL:HG12	1:B:198:GLY:H	1.75	0.52
1:D:6:GLY:HA3	1:D:395:ARG:HD2	1.92	0.52
1:B:39:PRO:HG3	1:B:364:GLY:HA2	1.91	0.52
1:D:309:ASN:HD21	1:D:342:GLY:HA3	1.73	0.51
1:D:56:LEU:HD22	1:D:105:VAL:HG12	1.91	0.51
1:C:331:ARG:NH1	5:C:659:HOH:O	2.42	0.51
1:D:421:ASN:O	1:D:467:PHE:HA	2.10	0.51
1:A:437:PHE:CD1	1:A:474:GLU:HG3	2.44	0.51
1:C:31:PRO:HA	5:C:763:HOH:O	2.09	0.51
1:C:100:ARG:HG2	1:C:100:ARG:NH1	2.22	0.51
1:C:254:LEU:HD23	1:C:309:ASN:OD1	2.11	0.51
1:A:133:MSE:HE1	1:A:155:TYR:CE2	2.44	0.51
1:D:444:VAL:HG12	1:D:475:ALA:HB2	1.91	0.51
1:B:100:ARG:CG	1:B:100:ARG:NH1	2.71	0.51
1:A:56:LEU:CD2	1:A:105:VAL:HG12	2.39	0.51
1:C:335:ALA:HB1	1:C:384:LEU:HD22	1.92	0.51
1:D:370:GLU:HG2	1:D:373:TRP:CZ3	2.45	0.51
1:D:252:TYR:N	1:D:253:PRO:CD	2.74	0.51
1:D:429:GLN:HB3	1:D:459:LEU:CD2	2.35	0.50
1:C:181:ARG:NH2	1:C:209:ASP:OD1	2.44	0.50
1:B:233:ILE:HG21	1:B:237:ALA:HB2	1.93	0.50
2:A:505:GLC:O5	2:A:506:GLC:H61	2.11	0.50
1:B:116:ASP:OD2	1:B:202[B]:ASP:OD1	2.29	0.50
1:D:203:VAL:HG23	1:D:203:VAL:O	2.11	0.50
1:B:6:GLY:HA2	1:B:342:GLY:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:GLN:HE21	1:C:358:LYS:HD3	1.77	0.50
1:A:100:ARG:NH1	1:A:100:ARG:HG2	2.24	0.49
1:A:39:PRO:CG	1:A:364:GLY:HA2	2.43	0.49
1:B:375:LYS:O	1:B:379:GLU:HG3	2.12	0.49
1:B:310:LEU:HD23	1:B:310:LEU:H	1.78	0.49
1:C:192:ILE:HG13	1:C:220:VAL:HG13	1.95	0.49
1:C:23:PRO:HB3	5:C:777:HOH:O	2.12	0.49
1:C:58:TYR:CE1	1:C:378:ARG:NH2	2.81	0.49
1:B:410:ALA:HA	1:B:418:ALA:O	2.13	0.49
1:D:268:ASP:HA	1:D:324:ARG:NH2	2.28	0.49
1:A:335:ALA:HA	1:A:384:LEU:HD22	1.95	0.49
1:B:234:TRP:CE2	2:B:501:GLC:H2	2.48	0.49
5:C:723:HOH:O	1:D:301:PRO:HG2	2.12	0.49
1:C:165:TRP:HZ3	2:C:506:GLC:H5	1.77	0.48
1:C:201:LEU:HD12	1:C:246:PHE:CE1	2.48	0.48
1:C:473:ARG:HG2	1:C:473:ARG:HH11	1.78	0.48
1:A:235:GLU:HB3	1:A:236:GLU:OE2	2.14	0.48
1:B:266:ALA:O	1:B:324:ARG:HD2	2.13	0.48
1:C:252:TYR:N	1:C:253:PRO:CD	2.77	0.48
1:D:405:GLN:O	1:D:406:ASP:HB3	2.12	0.48
1:D:122:THR:HG23	1:D:173:LEU:HD13	1.95	0.48
1:B:34:PRO:HG2	1:B:37:ALA:CB	2.41	0.48
1:D:369:GLU:HB3	1:D:372:ARG:HD3	1.94	0.48
1:A:233:ILE:HG21	1:A:237:ALA:HB2	1.96	0.48
1:D:378:ARG:HG2	1:D:378:ARG:HH11	1.79	0.48
1:D:393:ALA:HB3	1:D:416:TYR:HE2	1.79	0.48
1:A:300:ARG:HB3	1:A:302:GLU:OE2	2.14	0.47
1:B:331:ARG:HG2	1:B:331:ARG:HH11	1.79	0.47
1:A:250:MSE:HE2	1:A:310:LEU:HD13	1.96	0.47
1:A:12:ILE:O	1:A:14:PRO:HD3	2.14	0.47
1:D:100:ARG:O	1:D:104:GLU:HG3	2.15	0.47
1:D:121:HIS:CD2	1:D:170:LEU:HD23	2.49	0.47
1:D:56:LEU:N	1:D:57:PRO:HD2	2.30	0.47
1:D:235:GLU:HB3	1:D:236:GLU:OE2	2.13	0.47
1:C:279:ARG:HH11	1:C:279:ARG:HG2	1.79	0.47
1:D:403:TYR:O	1:D:409:LEU:HD12	2.15	0.47
1:B:71:PRO:HB2	1:B:80:ARG:HB3	1.96	0.47
1:A:193:ARG:HD3	5:A:737:HOH:O	2.14	0.47
1:D:451:VAL:O	1:D:452:CYS:HB3	2.15	0.47
1:D:115:LEU:HD11	1:D:196:VAL:HG21	1.96	0.47
1:D:335:ALA:HA	1:D:384:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:O	1:A:436:VAL:HG23	2.15	0.47
1:C:202:ASP:OD1	3:C:603:GLC:C1	2.63	0.47
1:A:252:TYR:N	1:A:253:PRO:CD	2.78	0.47
1:C:137:GLU:HG2	1:C:150:PHE:CE2	2.50	0.46
1:B:420:VAL:HG22	1:B:469:LEU:CD1	2.46	0.46
1:D:13:PHE:CZ	1:D:79:HIS:HA	2.50	0.46
1:B:408:HIS:HB3	1:B:427:PHE:CZ	2.51	0.46
1:B:252:TYR:N	1:B:253:PRO:CD	2.78	0.46
1:B:39:PRO:HD2	5:B:740:HOH:O	2.15	0.46
1:A:420:VAL:HG22	1:A:469:LEU:CD1	2.45	0.46
1:B:201:LEU:HD21	1:B:216:PHE:CZ	2.51	0.46
1:B:300:ARG:HB3	1:B:302:GLU:OE2	2.16	0.46
2:B:504:GLC:O5	2:B:505:GLC:H61	2.16	0.46
1:B:437:PHE:HB3	1:B:474:GLU:OE2	2.16	0.45
1:B:281:GLU:HG2	5:B:798:HOH:O	2.15	0.45
1:D:331:ARG:HG2	1:D:331:ARG:HH11	1.80	0.45
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.79	0.45
1:A:135:ASN:HB2	1:A:139:SER:HB2	1.97	0.45
1:B:163:ALA:HB1	1:B:167:ASN:O	2.16	0.45
1:A:55:LYS:HE3	1:A:368:TRP:CE2	2.52	0.45
1:C:68:TYR:C	1:C:68:TYR:CD1	2.89	0.45
1:D:300:ARG:O	1:D:304:VAL:HG23	2.16	0.45
1:B:310:LEU:H	1:B:310:LEU:CD2	2.29	0.45
1:A:369:GLU:HB3	1:A:372:ARG:HD3	1.98	0.45
1:A:115:LEU:HD11	1:A:196:VAL:HG21	1.99	0.45
1:D:431:PHE:HB2	1:D:432:PRO:HD2	1.99	0.45
1:A:310:LEU:HD23	1:A:310:LEU:H	1.80	0.45
1:C:386:ARG:O	1:C:390:GLU:HG3	2.16	0.45
5:C:723:HOH:O	1:D:302:GLU:HG3	2.16	0.45
1:A:374:GLN:HG3	1:A:377:LEU:H	1.82	0.45
1:B:182:GLU:HG2	5:B:796:HOH:O	2.17	0.45
1:D:230:VAL:HA	1:D:248:ALA:O	2.17	0.45
1:D:241:LEU:HD13	1:D:303:VAL:HG11	1.99	0.45
1:C:233:ILE:CG2	1:C:237:ALA:HB2	2.45	0.44
1:D:286:LEU:HD11	1:D:401:ARG:NH1	2.31	0.44
1:C:347:TYR:O	1:C:350:GLU:HG2	2.17	0.44
1:D:163:ALA:HB1	1:D:167:ASN:O	2.17	0.44
1:C:202:ASP:O	1:C:203:VAL:C	2.55	0.44
1:A:335:ALA:CA	1:A:384:LEU:HD22	2.48	0.44
1:B:320:LEU:HD12	1:B:320:LEU:HA	1.80	0.44
1:A:200:ARG:C	1:A:200:ARG:HD3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:GLU:HG2	1:D:373:TRP:CH2	2.53	0.44
1:D:428:ARG:HD2	1:D:430:ASP:OD2	2.18	0.44
1:C:79:HIS:CE1	1:C:81:TYR:HB2	2.53	0.44
1:C:100:ARG:NH1	1:C:100:ARG:CG	2.79	0.44
1:C:428:ARG:CD	1:C:428:ARG:H	2.29	0.44
1:A:17:PHE:HB3	5:A:608:HOH:O	2.18	0.44
1:D:100:ARG:HG2	1:D:100:ARG:NH1	2.30	0.44
1:A:38:PRO:HA	1:A:39:PRO:HD3	1.92	0.44
1:A:193:ARG:HH11	1:A:193:ARG:HG2	1.81	0.44
1:B:446:LEU:HD21	1:B:473:ARG:HD2	2.00	0.44
1:C:387:LEU:HD12	1:C:387:LEU:HA	1.86	0.44
1:C:203:VAL:O	1:C:203:VAL:HG23	2.18	0.44
1:A:420:VAL:HG22	1:A:469:LEU:HD11	2.00	0.44
1:B:291:ARG:HD2	5:B:787:HOH:O	2.18	0.44
1:C:124:ARG:NH2	1:C:169:GLU:HG2	2.33	0.44
1:B:133:MSE:HE1	1:B:155:TYR:HE2	1.83	0.43
1:D:8:PHE:C	1:D:8:PHE:CD1	2.90	0.43
1:D:200:ARG:C	1:D:200:ARG:HD3	2.38	0.43
1:A:359:ASP:OD1	1:A:360:PRO:HA	2.17	0.43
1:D:165:TRP:HZ3	2:D:506:GLC:H5	1.84	0.43
1:B:203:VAL:O	1:B:203:VAL:HG23	2.18	0.43
1:D:369:GLU:HG2	1:D:372:ARG:CD	2.49	0.43
1:B:202[B]:ASP:O	1:B:203:VAL:C	2.56	0.43
1:D:209:ASP:HB2	5:D:926:HOH:O	2.17	0.43
1:A:240:TRP:HB3	1:A:246:PHE:CD2	2.54	0.43
1:B:370:GLU:HG2	1:B:373:TRP:CZ3	2.54	0.43
1:A:393:ALA:HB3	1:A:416:TYR:CE2	2.47	0.43
1:A:419:VAL:HG12	1:A:464:LEU:HD12	2.00	0.43
1:A:465:PRO:HG2	1:A:468:SER:CB	2.49	0.43
1:A:250:MSE:HE3	1:A:308:MSE:SE	2.69	0.43
1:C:133:MSE:HE1	1:C:155:TYR:HE2	1.84	0.43
1:A:217:ARG:HD2	1:A:245:MSE:O	2.18	0.43
1:C:56:LEU:N	1:C:57:PRO:CD	2.81	0.43
1:B:236:GLU:CD	1:B:236:GLU:H	2.21	0.43
1:B:200:ARG:HE	1:B:250:MSE:SE	2.52	0.42
1:B:38:PRO:HA	1:B:39:PRO:HD3	1.92	0.42
1:A:370:GLU:HG2	1:A:373:TRP:CH2	2.53	0.42
1:C:331:ARG:HH11	1:C:331:ARG:HG2	1.84	0.42
1:D:433:LEU:HD13	1:D:437:PHE:HD2	1.85	0.42
1:C:335:ALA:CA	1:C:384:LEU:HD22	2.49	0.42
1:C:250:MSE:HA	1:C:308:MSE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:391:HIS:HA	1:D:392:PRO:HD2	1.86	0.42
1:D:301:PRO:O	1:D:305:ARG:HG3	2.20	0.42
1:B:188:ALA:HB2	1:B:216:PHE:CE1	2.54	0.42
1:A:446:LEU:HD21	1:A:473:ARG:CD	2.49	0.42
1:A:267:LEU:HD12	1:A:322:LEU:O	2.19	0.42
1:C:416:TYR:CE1	1:C:473:ARG:HD3	2.54	0.42
1:C:393:ALA:HB3	1:C:416:TYR:HE2	1.84	0.42
1:A:292:LEU:HB3	1:A:296:PHE:CE2	2.55	0.42
1:D:347:TYR:O	1:D:350:GLU:HG2	2.20	0.42
1:A:232:GLU:O	1:A:232:GLU:HG2	2.20	0.42
1:A:137:GLU:HG2	1:A:150:PHE:CD2	2.54	0.42
1:D:188:ALA:HB2	1:D:216:PHE:CE1	2.54	0.42
1:B:288:PHE:CE2	1:B:292:LEU:HD11	2.55	0.42
1:A:150:PHE:HA	1:A:151:PRO:C	2.40	0.42
1:D:252:TYR:O	1:D:256:ARG:HG3	2.20	0.42
1:D:305:ARG:NH2	5:D:917:HOH:O	2.53	0.42
1:B:117:GLY:HA2	5:B:614:HOH:O	2.19	0.42
1:D:383:ARG:HH11	1:D:383:ARG:HG2	1.85	0.42
1:B:137:GLU:HG2	1:B:150:PHE:CD2	2.54	0.42
1:D:250:MSE:HA	1:D:308:MSE:HB3	2.02	0.41
1:D:351:GLU:HG2	1:D:352:VAL:HG13	2.02	0.41
1:D:115:LEU:CD1	1:D:196:VAL:HG21	2.50	0.41
1:B:352:VAL:HG12	1:B:378:ARG:HD2	2.02	0.41
1:D:39:PRO:CG	1:D:364:GLY:HA2	2.49	0.41
1:D:444:VAL:CG1	1:D:475:ALA:HB2	2.50	0.41
1:C:473:ARG:NH1	1:C:474:GLU:O	2.53	0.41
1:A:204:PRO:HG2	1:A:233:ILE:HD11	2.02	0.41
1:A:241:LEU:HD13	1:A:303:VAL:HG11	2.02	0.41
1:C:310:LEU:H	1:C:310:LEU:HD23	1.85	0.41
1:A:133:MSE:HG2	1:A:152:LEU:HD12	2.01	0.41
1:D:57:PRO:HG2	5:D:921:HOH:O	2.19	0.41
1:C:236:GLU:OE1	1:D:301:PRO:HG2	2.20	0.41
1:D:386:ARG:O	1:D:390:GLU:HG3	2.20	0.41
1:D:397:ALA:HA	1:D:398:PRO:HD3	1.90	0.41
1:D:133:MSE:HE2	5:D:823:HOH:O	2.20	0.41
1:A:250:MSE:HA	1:A:308:MSE:HB3	2.03	0.41
1:B:254:LEU:HD23	1:B:309:ASN:OD1	2.21	0.41
1:C:335:ALA:CB	1:C:384:LEU:HD22	2.50	0.41
1:B:234:TRP:CD2	2:B:501:GLC:H2	2.55	0.41
1:C:196:VAL:HG12	1:C:198:GLY:H	1.85	0.41
1:D:233:ILE:HG21	1:D:237:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ALA:HB3	5:B:715:HOH:O	2.20	0.41
1:C:239:PHE:C	1:C:239:PHE:CD1	2.94	0.41
1:A:148:LYS:HB2	1:A:160:ASN:OD1	2.21	0.41
1:D:335:ALA:CA	1:D:384:LEU:HD22	2.51	0.41
1:A:436:VAL:C	1:A:438:PRO:HD3	2.41	0.41
1:A:374:GLN:OE1	1:A:376:ASP:HB3	2.21	0.41
2:D:503:GLC:O5	2:D:504:GLC:H61	2.21	0.41
1:D:255:ALA:HB2	1:D:310:LEU:O	2.21	0.41
1:C:149:GLY:N	1:C:160:ASN:OD1	2.54	0.41
1:B:193:ARG:HG2	1:B:193:ARG:NH1	2.36	0.41
1:C:79:HIS:CD2	3:C:602:GLC:H2	2.56	0.41
1:D:181:ARG:NH2	1:D:209:ASP:OD2	2.54	0.41
1:B:8:PHE:CD1	1:B:8:PHE:C	2.95	0.41
1:D:38:PRO:HA	1:D:39:PRO:HD3	1.92	0.40
1:B:359:ASP:HA	1:B:362:ASN:OD1	2.21	0.40
1:A:196:VAL:HG12	1:A:198:GLY:H	1.85	0.40
1:B:392:PRO:HA	1:B:395:ARG:NH1	2.37	0.40
1:C:291:ARG:NH1	1:C:294:ASP:OD2	2.54	0.40
1:B:339:LEU:HD11	1:B:469:LEU:HD21	2.03	0.40
1:D:9:PHE:HB3	1:D:345:THR:HG23	2.01	0.40
1:D:413:ARG:HH11	1:D:413:ARG:HG3	1.86	0.40
1:A:202:ASP:O	1:A:203:VAL:C	2.59	0.40
1:C:421:ASN:O	1:C:467:PHE:HA	2.22	0.40
1:C:432:PRO:HG2	5:C:653:HOH:O	2.21	0.40
1:B:135:ASN:HB2	1:B:139:SER:HB2	2.03	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	472/475 (99%)	446 (94%)	26 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	473/475 (100%)	451 (95%)	21 (4%)	1 (0%)	52 64
1	C	472/475 (99%)	450 (95%)	22 (5%)	0	100 100
1	D	472/475 (99%)	444 (94%)	27 (6%)	1 (0%)	52 64
All	All	1889/1900 (99%)	1791 (95%)	96 (5%)	2 (0%)	56 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	461	GLY
1	D	462	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	379/373 (102%)	374 (99%)	5 (1%)	76 87
1	B	378/373 (101%)	367 (97%)	11 (3%)	50 66
1	C	376/373 (101%)	366 (97%)	10 (3%)	52 70
1	D	379/373 (102%)	369 (97%)	10 (3%)	54 71
All	All	1512/1492 (101%)	1476 (98%)	36 (2%)	57 74

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	68	TYR
1	A	133	MSE
1	A	173	LEU
1	A	464	LEU
1	B	8	PHE
1	B	68	TYR
1	B	100	ARG
1	B	173	LEU

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Mol	Chain	Res	Type
1	B	182	GLU
1	B	265	GLU
1	B	310	LEU
1	B	320	LEU
1	B	322	LEU
1	B	374	GLN
1	B	384	LEU
1	C	68	TYR
1	C	100	ARG
1	C	291	ARG
1	C	310	LEU
1	C	322	LEU
1	C	374	GLN
1	C	387	LEU
1	C	400	LEU
1	C	428	ARG
1	C	464	LEU
1	D	8	PHE
1	D	41	LEU
1	D	68	TYR
1	D	160	ASN
1	D	173	LEU
1	D	265	GLU
1	D	291	ARG
1	D	322	LEU
1	D	369	GLU
1	D	464	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	88	GLN
1	A	274	GLN
1	B	11	GLN
1	B	70	ASN
1	B	88	GLN
1	B	274	GLN
1	B	434	HIS
1	C	11	GLN
1	C	70	ASN
1	C	88	GLN

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Mol	Chain	Res	Type
1	C	274	GLN
1	C	434	HIS
1	D	11	GLN
1	D	70	ASN
1	D	88	GLN
1	D	274	GLN
1	D	455	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

40 carbohydrates 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	GLC	A	501	2	11,11,12	0.52	0	14,15,17	0.61	0
2	GLC	A	502	2	11,11,12	0.60	0	14,15,17	0.78	0
2	GLC	A	503	2	11,11,12	0.59	0	14,15,17	0.62	0
2	GLC	A	504	2	11,11,12	0.51	0	14,15,17	0.63	1 (7%)
2	GLC	A	505	2	11,11,12	0.57	0	14,15,17	0.65	0
2	GLC	A	506	2	11,11,12	0.61	0	14,15,17	0.68	0
2	GLC	A	507	2	11,11,12	0.60	0	14,15,17	0.67	0
3	GLC	A	601	3	11,11,12	0.46	0	14,15,17	0.55	0
3	GLC	A	602	3	11,11,12	0.54	0	14,15,17	0.58	0
3	GLC	A	603	3	11,11,12	0.44	0	14,15,17	0.63	0
2	GLC	B	501	2	11,11,12	0.52	0	14,15,17	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLC	B	502	2	11,11,12	0.63	0	14,15,17	0.60	0
2	GLC	B	503	2	11,11,12	0.54	0	14,15,17	0.75	0
2	GLC	B	504	2	11,11,12	0.52	0	14,15,17	0.56	0
2	GLC	B	505	2	11,11,12	0.41	0	14,15,17	0.56	0
2	GLC	B	506	2	11,11,12	0.51	0	14,15,17	0.73	0
2	GLC	B	507	2	11,11,12	0.54	0	14,15,17	0.61	0
3	GLC	B	601	3	11,11,12	0.51	0	14,15,17	0.50	0
3	GLC	B	602	3	11,11,12	0.60	0	14,15,17	0.53	0
3	GLC	B	603	3	11,11,12	0.47	0	14,15,17	0.93	1 (7%)
2	GLC	C	501	2	11,11,12	0.56	0	14,15,17	0.58	0
2	GLC	C	502	2	11,11,12	0.66	0	14,15,17	0.84	0
2	GLC	C	503	2	11,11,12	0.54	0	14,15,17	0.65	1 (7%)
2	GLC	C	504	2	11,11,12	0.55	0	14,15,17	0.60	0
2	GLC	C	505	2	11,11,12	0.51	0	14,15,17	0.61	0
2	GLC	C	506	2	11,11,12	0.62	0	14,15,17	0.63	0
2	GLC	C	507	2	11,11,12	0.60	0	14,15,17	0.76	1 (7%)
3	GLC	C	601	3	11,11,12	0.54	0	14,15,17	0.50	0
3	GLC	C	602	3	11,11,12	0.53	0	14,15,17	0.58	0
3	GLC	C	603	3	11,11,12	0.45	0	14,15,17	0.58	0
2	GLC	D	501	2	11,11,12	0.51	0	14,15,17	0.70	0
2	GLC	D	502	2	11,11,12	0.67	0	14,15,17	0.72	0
2	GLC	D	503	2	11,11,12	0.59	0	14,15,17	0.65	1 (7%)
2	GLC	D	504	2	11,11,12	0.51	0	14,15,17	0.66	1 (7%)
2	GLC	D	505	2	11,11,12	0.54	0	14,15,17	0.61	0
2	GLC	D	506	2	11,11,12	0.56	0	14,15,17	0.62	0
2	GLC	D	507	2	11,11,12	0.60	0	14,15,17	0.72	1 (7%)
3	GLC	D	601	3	11,11,12	0.60	0	14,15,17	0.57	0
3	GLC	D	602	3	11,11,12	0.54	0	14,15,17	0.59	0
3	GLC	D	603	3	11,11,12	0.41	0	14,15,17	0.73	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	GLC	A	501	2	-	0/2/19/22	0/1/1/1
2	GLC	A	502	2	-	0/2/19/22	0/1/1/1
2	GLC	A	503	2	-	0/2/19/22	0/1/1/1
2	GLC	A	504	2	-	0/2/19/22	0/1/1/1
2	GLC	A	505	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	506	2	-	0/2/19/22	0/1/1/1
2	GLC	A	507	2	-	0/2/19/22	0/1/1/1
3	GLC	A	601	3	-	0/2/19/22	0/1/1/1
3	GLC	A	602	3	-	0/2/19/22	0/1/1/1
3	GLC	A	603	3	-	0/2/19/22	0/1/1/1
2	GLC	B	501	2	-	0/2/19/22	0/1/1/1
2	GLC	B	502	2	-	0/2/19/22	0/1/1/1
2	GLC	B	503	2	-	0/2/19/22	0/1/1/1
2	GLC	B	504	2	-	0/2/19/22	0/1/1/1
2	GLC	B	505	2	-	0/2/19/22	0/1/1/1
2	GLC	B	506	2	-	0/2/19/22	0/1/1/1
2	GLC	B	507	2	-	0/2/19/22	0/1/1/1
3	GLC	B	601	3	-	0/2/19/22	0/1/1/1
3	GLC	B	602	3	-	0/2/19/22	0/1/1/1
3	GLC	B	603	3	-	0/2/19/22	0/1/1/1
2	GLC	C	501	2	-	0/2/19/22	0/1/1/1
2	GLC	C	502	2	-	0/2/19/22	0/1/1/1
2	GLC	C	503	2	-	0/2/19/22	0/1/1/1
2	GLC	C	504	2	-	0/2/19/22	0/1/1/1
2	GLC	C	505	2	-	0/2/19/22	0/1/1/1
2	GLC	C	506	2	-	0/2/19/22	0/1/1/1
2	GLC	C	507	2	-	0/2/19/22	0/1/1/1
3	GLC	C	601	3	-	0/2/19/22	0/1/1/1
3	GLC	C	602	3	-	0/2/19/22	0/1/1/1
3	GLC	C	603	3	-	0/2/19/22	0/1/1/1
2	GLC	D	501	2	-	0/2/19/22	0/1/1/1
2	GLC	D	502	2	-	0/2/19/22	0/1/1/1
2	GLC	D	503	2	-	0/2/19/22	0/1/1/1
2	GLC	D	504	2	-	0/2/19/22	0/1/1/1
2	GLC	D	505	2	-	0/2/19/22	0/1/1/1
2	GLC	D	506	2	-	0/2/19/22	0/1/1/1
2	GLC	D	507	2	-	0/2/19/22	0/1/1/1
3	GLC	D	601	3	-	0/2/19/22	0/1/1/1
3	GLC	D	602	3	-	0/2/19/22	0/1/1/1
3	GLC	D	603	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	603	GLC	C2-C3-C4	-2.36	107.03	111.04
2	D	503	GLC	C1-O5-C5	2.00	114.79	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	504	GLC	C1-O5-C5	2.10	114.91	112.25
2	C	503	GLC	C1-O5-C5	2.12	114.94	112.25
2	D	507	GLC	C1-O5-C5	2.16	114.98	112.25
2	D	504	GLC	C1-O5-C5	2.19	115.03	112.25
2	C	507	GLC	C1-O5-C5	2.27	115.13	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	505	GLC	1	0
2	A	506	GLC	1	0
3	A	603	GLC	1	0
2	B	501	GLC	2	0
2	B	504	GLC	1	0
2	B	505	GLC	1	0
3	B	603	GLC	1	0
2	C	506	GLC	1	0
3	C	602	GLC	1	0
3	C	603	GLC	1	0
2	D	501	GLC	1	0
2	D	503	GLC	1	0
2	D	504	GLC	1	0
2	D	506	GLC	1	0
3	D	603	GLC	1	0

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
4	PO4	D	800	-	4,4,4	1.17	0	6,6,6	0.27	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
4	PO4	D	800	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	467/475 (98%)	-0.08	13 (2%) 56 66	16, 31, 46, 59	0
1	B	467/475 (98%)	-0.23	11 (2%) 62 71	12, 25, 44, 64	0
1	C	467/475 (98%)	-0.12	9 (1%) 70 76	15, 27, 52, 65	0
1	D	467/475 (98%)	-0.02	24 (5%) 32 41	12, 29, 63, 80	0
All	All	1868/1900 (98%)	-0.11	57 (3%) 52 62	12, 28, 52, 80	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	475	ALA	7.6
1	A	460	CYS	5.2
1	A	440	GLY	4.7
1	C	475	ALA	4.4
1	D	459	LEU	4.2
1	B	475	ALA	4.1
1	D	455	GLN	4.1
1	D	457	GLY	4.1
1	B	441	GLY	4.0
1	D	433	LEU	3.9
1	A	455	GLN	3.8
1	D	441	GLY	3.6
1	D	456	GLY	3.6
1	B	455	GLN	3.6
1	D	439	ARG	3.5
1	D	454	PRO	3.5
1	B	440	GLY	3.4
1	A	438	PRO	3.4
1	C	239	PHE	3.3
1	B	456	GLY	3.3
1	C	31	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	425	HIS	3.3
1	B	265	GLU	3.1
1	A	475	ALA	3.0
1	D	430	ASP	2.9
1	B	425	HIS	2.8
1	A	441	GLY	2.8
1	A	265	GLU	2.8
1	A	424	PRO	2.7
1	D	31	PRO	2.7
1	B	439	ARG	2.7
1	B	460	CYS	2.7
1	B	406	ASP	2.6
1	D	451	VAL	2.6
1	D	407	GLY	2.6
1	A	425	HIS	2.5
1	C	453	THR	2.5
1	D	424	PRO	2.4
1	D	460	CYS	2.4
1	D	431	PHE	2.4
1	D	458	ARG	2.3
1	A	31	PRO	2.3
1	C	440	GLY	2.3
1	D	434	HIS	2.3
1	D	406	ASP	2.2
1	D	428	ARG	2.2
1	A	2	ALA	2.2
1	D	265	GLU	2.2
1	D	284	GLN	2.1
1	B	457	GLY	2.1
1	D	285	ALA	2.1
1	A	433	LEU	2.1
1	C	137	GLU	2.1
1	C	157	ALA	2.1
1	A	29	ALA	2.0
1	C	240	TRP	2.0
1	C	244	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	GLC	C	601	11/12	0.79	0.30	7.28	55,56,57,57	0
3	GLC	D	602	11/12	0.88	0.18	4.64	30,33,35,37	0
2	GLC	D	507	11/12	0.92	0.20	4.43	40,40,42,43	0
3	GLC	C	602	11/12	0.81	0.23	3.60	43,47,49,52	0
3	GLC	A	601	11/12	0.85	0.24	3.14	52,53,55,55	0
3	GLC	A	602	11/12	0.84	0.20	2.83	40,44,47,50	0
3	GLC	B	603	11/12	0.88	0.17	2.53	23,27,29,31	0
2	GLC	A	502	11/12	0.90	0.18	2.47	41,43,47,48	0
3	GLC	A	603	11/12	0.84	0.17	2.38	36,41,42,42	0
3	GLC	C	603	11/12	0.86	0.19	2.30	43,45,46,46	0
2	GLC	A	507	11/12	0.87	0.17	2.10	43,45,46,51	0
2	GLC	C	502	11/12	0.80	0.26	1.79	59,63,66,67	0
3	GLC	D	603	11/12	0.92	0.16	1.69	28,32,34,35	0
2	GLC	D	502	11/12	0.92	0.18	1.04	38,42,44,44	0
3	GLC	B	602	11/12	0.92	0.12	0.97	20,26,27,31	0
2	GLC	D	501	11/12	0.94	0.15	0.65	37,40,42,44	0
2	GLC	C	507	11/12	0.91	0.14	0.42	56,58,60,62	0
3	GLC	D	601	11/12	0.91	0.12	0.21	39,41,41,43	0
2	GLC	C	501	11/12	0.91	0.13	-0.02	45,53,55,55	0
3	GLC	B	601	11/12	0.91	0.12	-0.18	31,32,35,36	0
2	GLC	A	501	11/12	0.91	0.12	-0.22	37,41,42,43	0
2	GLC	B	501	11/12	0.96	0.10	-0.40	22,23,26,26	0
2	GLC	B	502	11/12	0.95	0.09	-0.57	23,25,28,30	0
2	GLC	B	507	11/12	0.97	0.08	-2.19	22,24,25,29	0
2	GLC	C	506	11/12	0.84	0.17	-	65,67,69,71	0
2	GLC	B	504	11/12	0.86	0.16	-	37,39,40,44	0
2	GLC	B	505	11/12	0.91	0.13	-	31,33,36,37	0
2	GLC	D	504	11/12	0.93	0.11	-	45,46,48,49	0
2	GLC	C	503	11/12	0.81	0.20	-	70,72,73,73	0
2	GLC	A	504	11/12	0.90	0.14	-	54,56,56,57	0
2	GLC	A	503	11/12	0.82	0.20	-	50,56,56,57	0
2	GLC	A	506	11/12	0.88	0.18	-	54,55,58,59	0
2	GLC	D	505	11/12	0.92	0.16	-	44,45,46,47	0
2	GLC	B	503	11/12	0.92	0.12	-	31,33,36,38	0
2	GLC	C	505	11/12	0.82	0.19	-	72,73,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GLC	D	506	11/12	0.93	0.17	-	41,42,44,45	0
2	GLC	B	506	11/12	0.96	0.09	-	31,33,34,34	0
2	GLC	D	503	11/12	0.84	0.21	-	42,45,47,48	0
2	GLC	A	505	11/12	0.86	0.15	-	54,56,57,57	0
2	GLC	C	504	11/12	0.90	0.15	-	74,76,77,78	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	PO4	D	800	5/5	0.96	0.12	-0.22	55,55,56,57	0

6.5 Other polymers (i)

There are no such residues in this entry.