



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2017 – 12:45 AM EST

PDB ID : 4LQ1  
Title : Crystal Structure of E.Coli Branching Enzyme in complex with maltohexaose  
Authors : Feng, L.; Geiger, J.H.  
Deposited on : unknown  
Resolution : 2.55 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

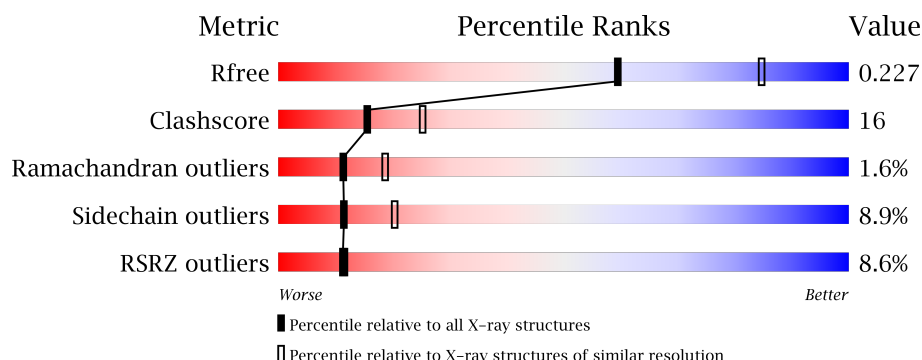
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	612	<div> <div>16%</div> <div>63%</div> <div>28%</div> <div>5%</div> <div>.</div> </div>
1	B	612	<div> <div>11%</div> <div>71%</div> <div>22%</div> <div>.</div> <div>.</div> </div>
1	C	612	<div> <div>5%</div> <div>68%</div> <div>22%</div> <div>5%</div> <div>.</div> </div>
1	D	612	<div> <div>2%</div> <div>73%</div> <div>19%</div> <div>.</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	B	801	-	-	-	X
3	GLC	B	802	-	-	-	X
3	GLC	C	803	-	-	-	X
3	GLC	D	803	-	-	-	X
4	GOL	C	805	-	-	-	X

## 2 Entry composition [i](#)

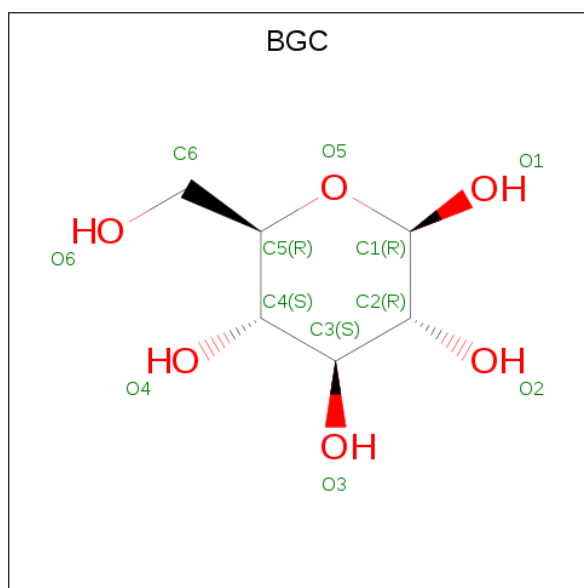
There are 5 unique types of molecules in this entry. The entry contains 20219 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	S	0	1	0
			4817	3080	854	867	16			
1	B	596	Total	C	N	O	S	0	1	0
			4904	3132	871	885	16			
1	C	589	Total	C	N	O	S	0	0	0
			4840	3094	858	872	16			
1	D	593	Total	C	N	O	S	0	8	0
			4954	3163	886	888	17			

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



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

- Molecule 3 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

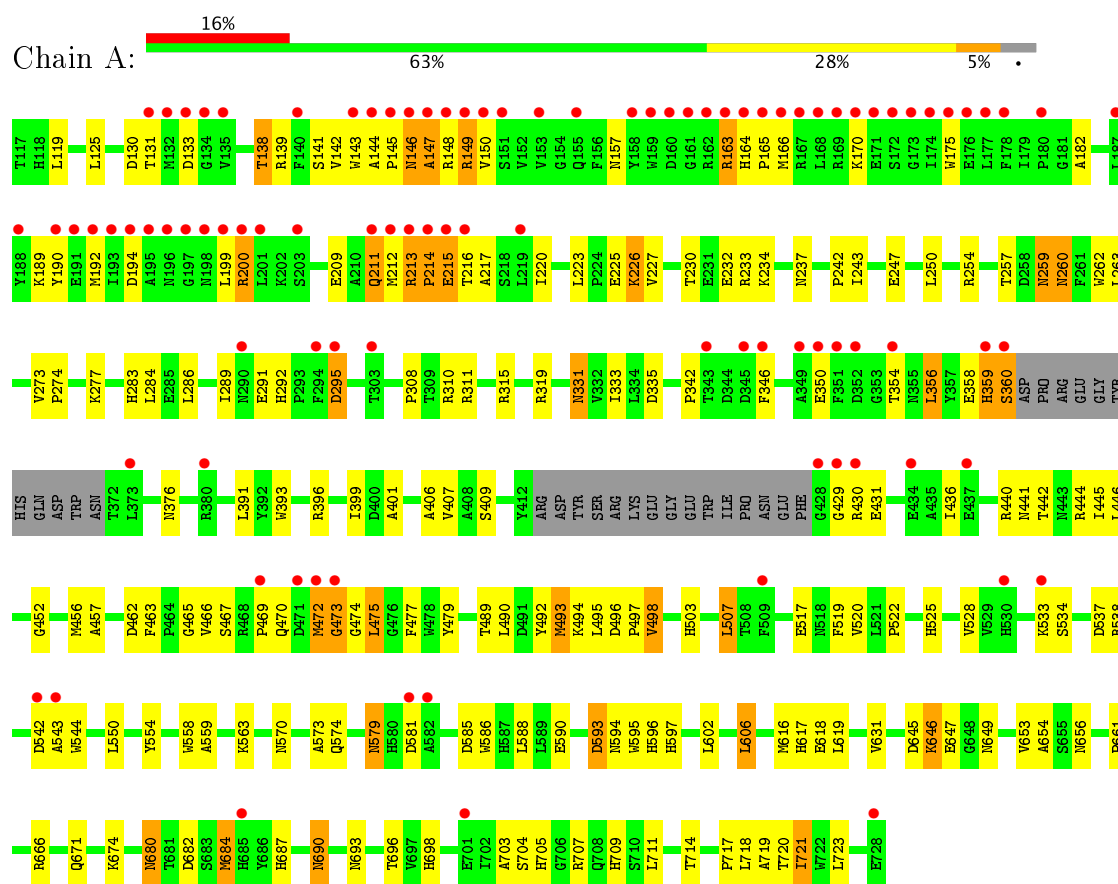
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	101	Total	O	0	0
			101	101		
5	C	159	Total	O	0	0
			159	159		
5	D	232	Total	O	0	0
			232	232		

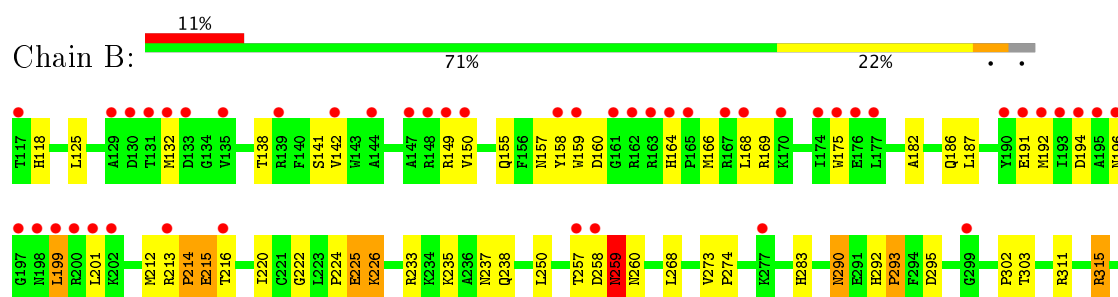
### 3 Residue-property plots [i](#)

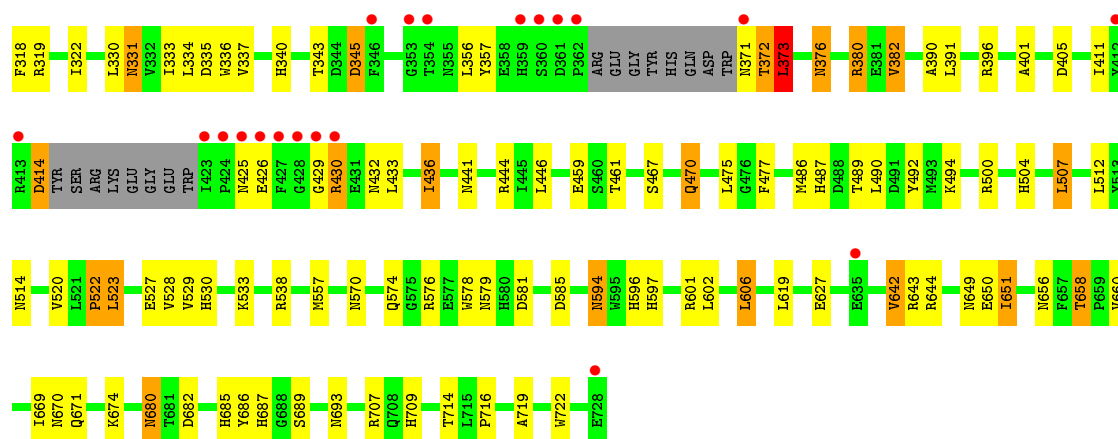
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 1,4-alpha-glucan branching enzyme GlgB

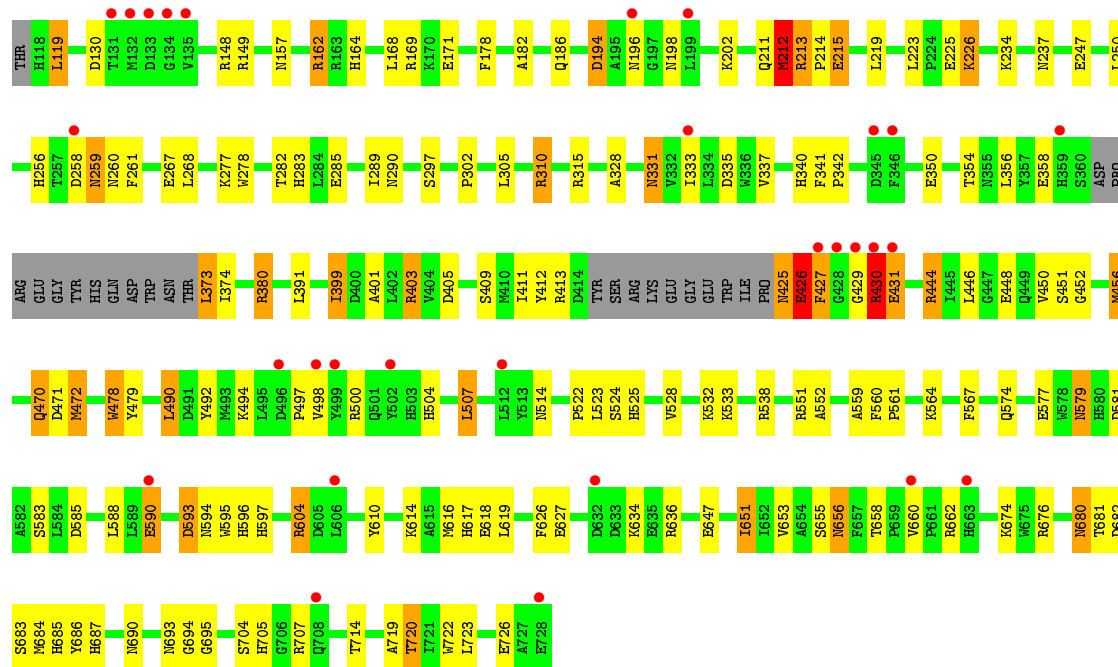


- Molecule 1: 1,4-alpha-glucan branching enzyme GlgB

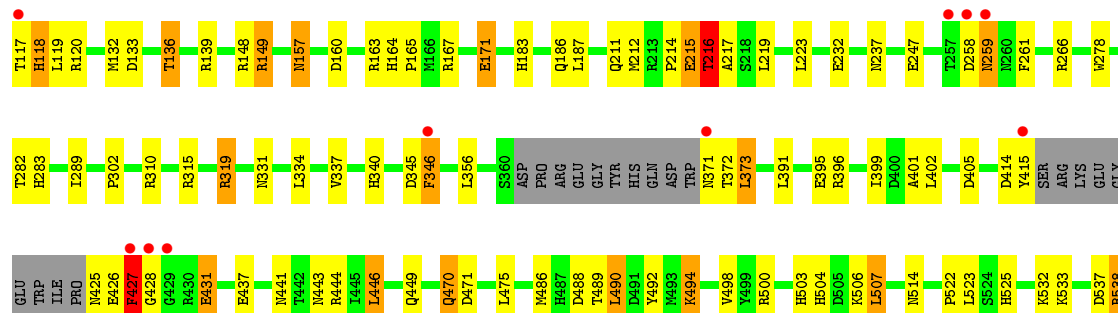
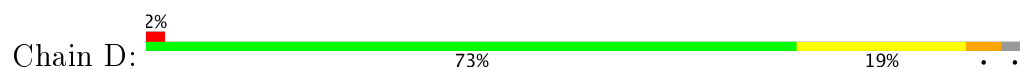




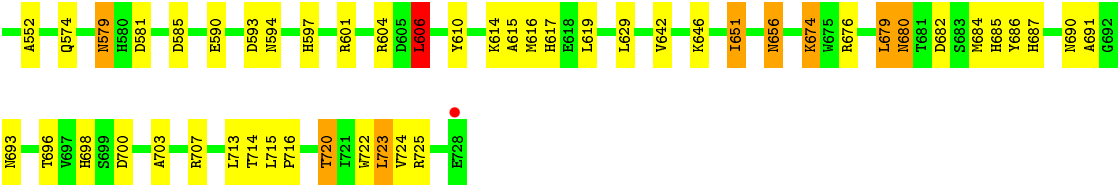
• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB



• Molecule 1: 1,4-alpha-glucan branching enzyme GlgB







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.69Å 104.11Å 186.71Å 90.00° 91.85° 90.00°	Depositor
Resolution (Å)	50.00 – 2.55 42.70 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-2.55) 95.9 (42.70-2.55)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.34 (at 2.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.178 , 0.224 0.181 , 0.227	Depositor DCC
$R_{free}$ test set	11224 reflections (11.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.3	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, GOL, 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	0.37	0/4970	0.52	0/6749
1	B	0.42	0/5061	0.57	1/6874 (0.0%)
1	C	0.53	0/4993	0.62	1/6778 (0.0%)
1	D	0.64	0/5112	0.73	4/6937 (0.1%)
All	All	0.50	0/20136	0.62	6/27338 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	446	LEU	C-N-CA	-6.61	108.42	122.30
1	D	723	LEU	CA-CB-CG	6.07	129.26	115.30
1	D	538	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	403	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	D	606	LEU	CA-CB-CG	5.27	127.43	115.30
1	B	158	TYR	CB-CG-CD1	-5.20	117.88	121.00

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	4817	0	4547	153	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4904	0	4616	149	0
1	C	4840	0	4565	178	0
1	D	4954	0	4664	151	0
2	A	12	0	12	0	0
3	B	23	0	21	0	0
3	C	46	0	42	2	0
3	D	46	0	42	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	12	0	16	0	0
5	A	61	0	0	7	0
5	B	101	0	0	9	0
5	C	159	0	0	10	0
5	D	232	0	0	24	0
All	All	20219	0	18541	630	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 16.

All (630) 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:527:GLU:O	1:B:538:ARG:NH2	1.75	1.20
1:C:380:ARG:HG2	5:C:972:HOH:O	1.43	1.19
1:B:380:ARG:HH21	1:B:380:ARG:HG2	1.12	1.12
1:C:444:ARG:HG2	1:C:444:ARG:HH21	1.08	1.11
1:A:212:MET:HG2	1:A:213:ARG:H	1.12	1.10
1:D:214:PRO:HA	1:D:215:GLU:O	1.53	1.08
1:A:200:ARG:HG2	1:A:200:ARG:HH11	1.16	1.07
1:C:211:GLN:HA	1:C:212:MET:HB2	1.31	1.06
1:C:162:ARG:HG3	1:C:162:ARG:HH11	1.13	1.06
1:C:426:GLU:HG3	1:C:427:PHE:CD2	1.91	1.05
1:B:430:ARG:H	1:B:430:ARG:HD3	1.19	1.05
1:D:441:ASN:ND2	1:D:444:ARG:HH11	1.54	1.04
1:D:215:GLU:HB2	1:D:217:ALA:H	1.21	1.04
1:A:200:ARG:HH11	1:A:200:ARG:CG	1.70	1.04
1:B:292:HIS:O	1:B:311:ARG:NH1	1.89	1.03
1:D:373:LEU:H	1:D:373:LEU:HD22	1.22	1.03
1:C:470:GLN:N	1:C:470:GLN:HE21	1.60	1.00
1:C:426:GLU:HG3	1:C:427:PHE:HD2	1.26	0.99
1:C:470:GLN:H	1:C:470:GLN:NE2	1.60	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:GLU:HB3	1:D:216:THR:OG1	1.60	0.99
1:C:658:THR:HG22	1:C:660:VAL:H	1.23	0.97
1:D:171:GLU:HG3	5:D:1040:HOH:O	1.64	0.96
1:B:670:ASN:HD21	1:B:707:ARG:HE	1.11	0.95
1:D:441:ASN:HD21	1:D:444:ARG:NH1	1.63	0.95
1:D:693:ASN:HD21	1:D:713:LEU:HB2	1.32	0.94
1:A:232:GLU:HG2	5:A:934:HOH:O	1.68	0.94
1:D:164:HIS:HE1	5:D:1010:HOH:O	1.49	0.94
1:D:470:GLN:HE21	1:D:470:GLN:H	0.95	0.94
1:B:470:GLN:NE2	1:B:470:GLN:H	1.65	0.93
1:B:470:GLN:HE21	1:B:470:GLN:N	1.66	0.93
1:B:380:ARG:HH21	1:B:380:ARG:CG	1.80	0.93
1:C:444:ARG:HG2	1:C:444:ARG:NH2	1.76	0.93
1:D:337:VAL:HG23	1:D:337:VAL:O	1.67	0.92
1:C:225:GLU:O	1:C:226:LYS:CB	2.19	0.90
1:C:157:ASN:HD21	1:C:164:HIS:CD2	1.89	0.90
1:C:574:GLN:NE2	1:C:585:ASP:H	1.69	0.90
1:C:225:GLU:O	1:C:226:LYS:HB3	1.69	0.89
1:A:212:MET:HG2	1:A:213:ARG:N	1.88	0.89
1:A:544:TRP:HE3	5:A:919:HOH:O	1.56	0.89
1:B:670:ASN:ND2	1:B:707:ARG:HE	1.71	0.88
1:B:594:ASN:H	1:B:597:HIS:HD2	1.21	0.88
1:D:215:GLU:HB2	1:D:217:ALA:N	1.89	0.88
1:C:693:ASN:HD21	1:C:714:THR:H	1.21	0.87
1:C:310:ARG:HH11	1:C:310:ARG:HG2	1.38	0.87
1:C:211:GLN:CA	1:C:212:MET:HB2	2.04	0.86
1:C:310:ARG:HH11	1:C:310:ARG:CG	1.88	0.86
1:A:214:PRO:O	1:A:215:GLU:HB2	1.75	0.86
1:A:212:MET:CG	1:A:213:ARG:H	1.85	0.85
1:C:213:ARG:HB3	1:C:214:PRO:HA	1.59	0.85
1:A:225:GLU:O	1:A:226:LYS:HB3	1.75	0.85
1:D:470:GLN:NE2	1:D:470:GLN:H	1.74	0.84
1:B:651:ILE:CD1	1:B:722:TRP:HB3	2.06	0.84
1:B:372:THR:O	1:B:373:LEU:HD23	1.78	0.83
1:C:429:GLY:HA2	1:C:430:ARG:HG3	1.59	0.83
1:C:237:ASN:ND2	1:C:283:HIS:HE1	1.76	0.83
1:C:590:GLU:OE2	1:C:590:GLU:HA	1.76	0.83
1:B:658:THR:CG2	1:B:660:VAL:H	1.92	0.83
1:B:225:GLU:O	1:B:226:LYS:HB2	1.79	0.82
1:B:658:THR:HG22	1:B:660:VAL:H	1.43	0.82
1:A:574:GLN:NE2	1:A:585:ASP:H	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:616:MET:SD	1:D:651:ILE:HG12	2.19	0.81
1:B:237:ASN:ND2	1:B:283:HIS:HE1	1.78	0.81
1:B:470:GLN:HE21	1:B:470:GLN:H	0.84	0.81
1:D:247:GLU:OE1	1:D:525:HIS:HD2	1.62	0.81
1:A:200:ARG:NH1	1:A:200:ARG:HG2	1.87	0.81
1:D:693:ASN:ND2	1:D:713:LEU:HB2	1.94	0.81
1:C:651:ILE:CD1	1:C:722:TRP:HB3	2.11	0.81
1:B:191:GLU:HG2	1:B:201:LEU:HD23	1.63	0.80
1:B:430:ARG:N	1:B:430:ARG:HD3	1.96	0.80
1:D:441:ASN:HD21	1:D:444:ARG:HH11	0.84	0.79
1:C:162:ARG:CG	1:C:162:ARG:HH11	1.94	0.79
1:D:427:PHE:HB3	5:D:1007:HOH:O	1.81	0.79
1:D:282:THR:OG1	1:D:283:HIS:HD2	1.66	0.78
1:D:426:GLU:O	1:D:427:PHE:HB3	1.82	0.78
1:C:412:TYR:CD2	1:C:431:GLU:HB3	2.18	0.78
1:A:474:GLY:O	1:A:475:LEU:HB2	1.84	0.77
1:C:674:LYS:NZ	5:C:1011:HOH:O	2.14	0.77
1:B:169:ARG:HG2	1:B:169:ARG:HH11	1.48	0.77
1:D:302:PRO:HG3	1:D:337:VAL:HG21	1.64	0.76
1:C:340:HIS:HE1	1:C:405:ASP:OD2	1.69	0.76
1:D:713:LEU:HD12	1:D:713:LEU:C	2.06	0.76
1:A:709:HIS:HD2	5:A:924:HOH:O	1.67	0.76
1:B:380:ARG:HG2	1:B:380:ARG:NH2	1.92	0.76
1:D:371:ASN:ND2	1:D:372:THR:H	1.84	0.76
1:C:490:LEU:O	1:C:494:LYS:HG3	1.85	0.76
1:C:213:ARG:HH11	1:C:213:ARG:HB2	1.51	0.75
1:B:651:ILE:HD12	1:B:722:TRP:HB3	1.69	0.75
1:D:492:TYR:CZ	1:D:500:ARG:HG2	2.21	0.75
1:C:157:ASN:HD21	1:C:164:HIS:HD2	1.31	0.74
1:A:211:GLN:OE1	1:A:215:GLU:HB3	1.86	0.74
1:C:444:ARG:CG	1:C:444:ARG:HH21	1.91	0.74
1:D:187:LEU:HD23	1:D:219:LEU:HD12	1.69	0.74
1:C:594:ASN:H	1:C:597:HIS:HD2	1.35	0.74
1:B:376:ASN:O	1:B:382:VAL:HG11	1.88	0.74
1:C:429:GLY:CA	1:C:430:ARG:HG3	2.16	0.74
1:D:346:PHE:N	1:D:346:PHE:HD2	1.85	0.74
1:D:470:GLN:N	1:D:470:GLN:HE21	1.79	0.73
1:D:215:GLU:HB3	1:D:216:THR:HG1	1.53	0.73
1:C:399:ILE:HD11	1:C:401:ALA:O	1.88	0.73
1:A:237:ASN:ND2	1:A:283:HIS:HE1	1.86	0.73
1:D:120:ARG:NH1	1:D:395:GLU:OE1	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ARG:CB	1:C:214:PRO:HA	2.19	0.73
1:B:318:PHE:CZ	1:B:322:ILE:HD11	2.24	0.73
1:C:411:ILE:O	1:C:431:GLU:HB2	1.87	0.73
1:C:532:LYS:C	1:C:533:LYS:HG2	2.08	0.73
1:D:346:PHE:CD2	1:D:346:PHE:N	2.58	0.72
1:A:138:THR:HG22	1:A:182:ALA:O	1.90	0.71
1:C:399:ILE:HD12	1:C:401:ALA:H	1.55	0.71
1:B:257:THR:OG1	5:B:908:HOH:O	2.07	0.71
1:D:149[A]:ARG:HH11	1:D:149[A]:ARG:HB3	1.56	0.71
1:C:341:PHE:CZ	1:C:358:GLU:HB3	2.26	0.71
1:D:340:HIS:HE1	1:D:405:ASP:OD2	1.74	0.70
1:B:372:THR:O	1:B:373:LEU:CD2	2.40	0.69
1:D:214:PRO:CA	1:D:215:GLU:O	2.38	0.69
1:A:472:MET:HG2	1:A:473:GLY:N	2.07	0.69
1:D:247:GLU:OE1	1:D:525:HIS:CD2	2.46	0.69
1:B:212:MET:C	1:B:214:PRO:HA	2.12	0.69
1:B:334:LEU:HD11	5:B:994:HOH:O	1.91	0.69
1:D:149[A]:ARG:HH21	1:D:165:PRO:HB3	1.58	0.68
1:C:636:ARG:HG2	1:C:662:ARG:NH2	2.09	0.68
1:B:693:ASN:HD21	1:B:714:THR:H	1.40	0.68
1:C:213:ARG:HB2	1:C:213:ARG:NH1	2.09	0.68
1:A:292:HIS:O	1:A:311:ARG:NH1	2.27	0.68
1:C:399:ILE:CD1	1:C:401:ALA:O	2.42	0.67
1:D:606:LEU:HD13	1:D:679:LEU:HD11	1.76	0.67
1:C:627:GLU:OE1	1:C:707:ARG:NH2	2.27	0.67
1:D:693:ASN:HD21	1:D:714:THR:H	1.43	0.67
1:D:371:ASN:CG	1:D:372:THR:H	1.96	0.67
1:A:359:HIS:O	1:A:360:SER:HB2	1.95	0.67
1:A:213:ARG:HB2	1:A:214:PRO:CD	2.26	0.66
1:C:157:ASN:ND2	1:C:164:HIS:HD2	1.93	0.66
1:B:430:ARG:CD	1:B:430:ARG:H	2.05	0.66
1:D:373:LEU:N	1:D:373:LEU:HD22	2.01	0.66
1:D:399:ILE:HD11	1:D:402:LEU:CD2	2.25	0.66
1:A:225:GLU:O	1:A:226:LYS:CB	2.44	0.66
1:B:486:MET:CE	1:B:487:HIS:CD2	2.79	0.66
1:A:618:GLU:OE2	1:A:646:LYS:HB2	1.95	0.66
1:B:237:ASN:HD22	1:B:283:HIS:HE1	1.42	0.66
1:C:684:MET:H	1:C:690:ASN:HD22	1.44	0.65
1:D:163:ARG:HD3	5:D:985:HOH:O	1.97	0.65
1:C:616:MET:SD	1:C:651:ILE:HG12	2.36	0.65
1:C:444:ARG:HD3	5:C:982:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:TYR:HD2	1:C:431:GLU:HB3	1.60	0.65
1:B:486:MET:CE	1:B:487:HIS:HD2	2.09	0.65
1:B:224:PRO:HG2	1:B:396:ARG:HB3	1.80	0.64
1:D:149[A]:ARG:NH1	1:D:149[A]:ARG:HB3	2.12	0.64
1:B:651:ILE:HD11	1:B:722:TRP:HB3	1.77	0.64
1:C:532:LYS:O	1:C:533:LYS:HG2	1.96	0.64
1:D:215:GLU:HB3	1:D:216:THR:CB	2.27	0.64
1:B:157:ASN:OD1	1:B:164:HIS:HD2	1.80	0.64
1:B:166:MET:CE	1:B:175:TRP:HB3	2.27	0.64
1:B:380:ARG:NH2	1:B:380:ARG:CG	2.50	0.64
1:C:277:LYS:HD3	1:C:328:ALA:HB1	1.79	0.64
1:C:492:TYR:CE2	1:C:507:LEU:HD21	2.33	0.64
1:C:693:ASN:ND2	1:C:714:THR:H	1.93	0.64
1:C:310:ARG:NH1	1:C:310:ARG:CG	2.57	0.64
1:A:671:GLN:OE1	5:A:930:HOH:O	2.15	0.63
1:A:470:GLN:HA	1:A:474:GLY:HA2	1.80	0.63
1:A:602:LEU:HG	1:A:606:LEU:HD22	1.80	0.63
1:D:258:ASP:O	1:D:259:ASN:ND2	2.31	0.63
1:A:146:ASN:O	1:A:147:ALA:HB3	1.99	0.63
1:A:213:ARG:HB2	1:A:214:PRO:HD3	1.80	0.63
1:D:427:PHE:O	1:D:427:PHE:CG	2.51	0.63
1:B:459:GLU:OE2	1:B:461:THR:OG1	2.16	0.63
1:C:234:LYS:HG2	1:C:452:GLY:HA3	1.79	0.63
1:A:647:GLU:O	1:A:647:GLU:HG3	2.00	0.62
1:C:651:ILE:HD13	1:C:722:TRP:HB3	1.81	0.62
1:D:237:ASN:ND2	1:D:283:HIS:HE1	1.97	0.62
1:B:233:ARG:NH1	5:B:928:HOH:O	2.22	0.62
1:B:166:MET:HE2	1:B:175:TRP:HB3	1.82	0.62
1:D:680:ASN:ND2	1:D:682:ASP:H	1.98	0.62
1:B:594:ASN:H	1:B:597:HIS:CD2	2.11	0.61
1:A:213:ARG:CB	1:A:214:PRO:CD	2.77	0.61
1:D:574:GLN:NE2	1:D:585:ASP:H	1.98	0.61
1:A:469:PRO:HG2	1:A:472:MET:SD	2.40	0.61
1:D:680:ASN:C	1:D:680:ASN:HD22	2.02	0.61
1:C:302:PRO:HG3	1:C:337:VAL:HG21	1.81	0.61
1:C:194:ASP:HB3	1:C:196:ASN:H	1.66	0.61
1:D:117:THR:HB	5:D:1002:HOH:O	2.00	0.61
1:C:574:GLN:HE21	1:C:585:ASP:H	1.46	0.61
1:C:478:TRP:HZ3	5:C:1055:HOH:O	1.84	0.61
1:C:211:GLN:CA	1:C:212:MET:CB	2.77	0.61
1:C:680:ASN:ND2	1:C:682:ASP:H	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:537:ASP:O	5:D:1091:HOH:O	2.17	0.60
1:A:594:ASN:H	1:A:597:HIS:HD2	1.46	0.60
1:A:149:ARG:HA	1:A:175:TRP:CH2	2.36	0.60
1:D:486:MET:O	1:D:490:LEU:HB2	2.02	0.60
1:C:456:MET:HG3	1:C:479:TYR:HB2	1.82	0.60
1:B:680:ASN:HD22	1:B:682:ASP:H	1.48	0.60
1:C:290:ASN:HD21	1:C:337:VAL:CG2	2.14	0.60
1:C:162:ARG:NH1	1:C:162:ARG:HG3	1.95	0.60
1:C:590:GLU:OE2	1:C:590:GLU:CA	2.50	0.60
1:B:166:MET:CE	1:B:175:TRP:CB	2.79	0.59
1:C:213:ARG:CB	1:C:214:PRO:CA	2.80	0.59
1:C:213:ARG:HB3	1:C:214:PRO:CA	2.30	0.59
1:D:504:HIS:HD2	5:D:986:HOH:O	1.84	0.59
1:C:634:LYS:HE2	5:C:945:HOH:O	2.01	0.59
1:C:552:ALA:O	1:C:720:THR:HG21	2.03	0.59
1:A:574:GLN:HE21	1:A:585:ASP:H	1.47	0.59
1:B:214:PRO:O	1:B:215:GLU:O	2.21	0.59
1:A:237:ASN:HD21	1:A:283:HIS:HE1	1.49	0.58
1:C:335:ASP:OD1	1:C:403:ARG:HD3	2.02	0.58
1:D:373:LEU:H	1:D:373:LEU:CD2	2.07	0.58
1:C:290:ASN:HD21	1:C:337:VAL:HG21	1.68	0.58
1:B:138:THR:HG21	1:B:220:ILE:HG21	1.84	0.58
1:C:532:LYS:O	1:C:533:LYS:CG	2.51	0.58
1:B:191:GLU:HG2	1:B:201:LEU:CD2	2.33	0.58
1:C:680:ASN:HD22	1:C:682:ASP:H	1.48	0.58
1:D:258:ASP:O	1:D:259:ASN:CB	2.52	0.58
1:D:319:ARG:NH2	1:D:396:ARG:O	2.37	0.58
1:A:142:VAL:HG21	1:A:190:TYR:CE1	2.38	0.58
1:C:237:ASN:HD22	1:C:283:HIS:HE1	1.48	0.58
1:D:441:ASN:ND2	1:D:444:ARG:NH1	2.37	0.58
1:B:142:VAL:HG12	1:B:166:MET:HE1	1.85	0.58
1:B:670:ASN:HD21	1:B:707:ARG:NE	1.91	0.58
1:C:350:GLU:HA	1:C:354:THR:O	2.04	0.58
1:C:680:ASN:C	1:C:680:ASN:HD22	2.08	0.58
1:D:337:VAL:CG2	1:D:337:VAL:O	2.42	0.58
1:D:601:ARG:HD2	1:D:685[A]:HIS:NE2	2.19	0.58
1:B:157:ASN:OD1	1:B:164:HIS:CD2	2.56	0.57
1:B:514:ASN:ND2	5:B:958:HOH:O	2.37	0.57
1:D:425:ASN:ND2	5:D:925:HOH:O	2.25	0.57
1:A:234:LYS:HD2	1:A:452:GLY:HA3	1.87	0.57
1:B:601:ARG:HD2	1:B:685[A]:HIS:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:VAL:HG23	1:C:337:VAL:O	2.04	0.57
1:C:693:ASN:O	1:C:695:GLY:N	2.37	0.57
1:C:225:GLU:HA	1:C:225:GLU:OE2	2.04	0.57
1:C:427:PHE:O	1:C:427:PHE:CG	2.57	0.57
1:B:258:ASP:O	1:B:260:ASN:N	2.38	0.57
1:B:486:MET:HE3	1:B:487:HIS:CD2	2.40	0.57
1:D:693:ASN:HD21	1:D:713:LEU:CB	2.12	0.57
1:D:494:LYS:HZ3	1:D:494:LYS:HB2	1.70	0.57
1:A:213:ARG:CB	1:A:214:PRO:HD3	2.35	0.57
1:C:282:THR:OG1	1:C:283:HIS:HD2	1.87	0.56
1:D:259:ASN:HB3	1:D:261:PHE:H	1.68	0.56
1:B:290:ASN:C	1:B:290:ASN:HD22	2.03	0.56
1:A:472:MET:CG	1:A:473:GLY:H	2.19	0.56
1:B:260:ASN:O	1:B:260:ASN:ND2	2.38	0.56
1:B:224:PRO:HB2	1:B:319:ARG:NH2	2.20	0.56
1:D:494:LYS:NZ	1:D:494:LYS:HB2	2.20	0.56
1:A:674:LYS:HB3	1:A:696:THR:CG2	2.35	0.56
1:C:579:ASN:ND2	1:C:581:ASP:H	2.03	0.56
1:A:358:GLU:OE2	1:A:358:GLU:N	2.33	0.56
1:C:426:GLU:OE1	1:C:426:GLU:CA	2.53	0.56
1:D:215:GLU:CB	1:D:216:THR:CA	2.83	0.56
1:D:606:LEU:CD1	1:D:679:LEU:HD11	2.36	0.56
1:D:691:ALA:HB3	1:D:716:PRO:HB3	1.87	0.55
1:A:528:VAL:HG12	1:A:534:SER:HA	1.87	0.55
1:C:194:ASP:OD1	1:C:198:ASN:HB2	2.07	0.55
1:C:250:LEU:HD22	1:C:268:LEU:HD13	1.88	0.55
1:B:336:TRP:CZ2	1:B:390:ALA:HB2	2.42	0.55
1:C:504:HIS:HD2	5:C:957:HOH:O	1.90	0.55
1:C:579:ASN:C	1:C:579:ASN:HD22	2.10	0.55
1:B:333:ILE:HG12	1:B:401:ALA:HB3	1.89	0.55
1:B:169:ARG:CG	1:B:169:ARG:HH11	2.19	0.55
1:C:259:ASN:ND2	1:C:261:PHE:H	2.04	0.54
1:A:588:LEU:HD13	1:A:596:HIS:CE1	2.42	0.54
1:B:642:VAL:HG22	1:B:650:GLU:HB2	1.89	0.54
1:D:237:ASN:HD22	1:D:283:HIS:HE1	1.55	0.54
1:A:496:ASP:O	1:A:498:VAL:N	2.40	0.54
1:D:676:ARG:HD2	5:D:1038:HOH:O	2.05	0.54
1:A:472:MET:HG2	1:A:473:GLY:H	1.70	0.54
1:A:680:ASN:HD22	1:A:682:ASP:H	1.54	0.54
1:B:528:VAL:HG11	5:B:945:HOH:O	2.07	0.54
1:C:604:ARG:NH2	5:C:958:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:GLU:HB3	1:D:216:THR:CA	2.37	0.54
1:D:399:ILE:HD11	1:D:402:LEU:HD23	1.90	0.54
1:C:373:LEU:N	1:C:373:LEU:CD2	2.71	0.53
1:C:237:ASN:ND2	1:C:283:HIS:CE1	2.68	0.53
1:D:183:HIS:H	1:D:186:GLN:HE21	1.57	0.53
1:C:426:GLU:HA	1:C:426:GLU:OE1	2.08	0.53
1:A:559:ALA:HB1	1:A:653:VAL:HG21	1.90	0.53
1:C:693:ASN:HD21	1:C:714:THR:N	2.00	0.53
1:D:724:VAL:HG22	1:D:725:ARG:N	2.24	0.53
1:B:125:LEU:HD23	1:B:141:SER:HB3	1.91	0.53
1:B:441:ASN:ND2	1:B:444:ARG:HH22	2.07	0.53
1:A:693:ASN:HD21	1:A:714:THR:H	1.57	0.53
1:C:213:ARG:HA	1:C:215:GLU:N	2.24	0.53
1:C:676:ARG:O	1:C:723:LEU:HA	2.09	0.53
1:A:200:ARG:NH1	1:A:200:ARG:CG	2.42	0.53
1:B:273:VAL:HB	1:B:274:PRO:HD3	1.91	0.53
1:A:150:VAL:HG12	1:A:166:MET:SD	2.49	0.53
1:A:680:ASN:C	1:A:680:ASN:HD22	2.12	0.53
1:D:399:ILE:HD11	1:D:402:LEU:HD21	1.90	0.53
1:A:573:ALA:O	1:A:596:HIS:CE1	2.62	0.53
1:B:504:HIS:HD2	5:B:925:HOH:O	1.91	0.53
1:D:503:HIS:HB3	1:D:506:LYS:HD2	1.90	0.53
1:A:200:ARG:HH11	1:A:200:ARG:HG3	1.67	0.52
1:D:132:MET:SD	1:D:139[B]:ARG:NH1	2.76	0.52
1:D:594:ASN:H	1:D:597:HIS:HD2	1.57	0.52
1:A:406:ALA:HB1	1:A:409:SER:HB3	1.90	0.52
1:A:704:SER:OG	1:A:705:HIS:HD2	1.93	0.52
1:A:150:VAL:HG22	1:A:192:MET:HB2	1.91	0.52
1:A:570:ASN:ND2	5:A:907:HOH:O	2.43	0.52
1:C:148:ARG:HG3	1:C:194:ASP:O	2.09	0.52
1:D:120:ARG:NH2	1:D:449:GLN:OE1	2.42	0.52
1:D:183:HIS:H	1:D:186:GLN:NE2	2.07	0.52
1:D:680:ASN:HD22	1:D:682:ASP:H	1.56	0.52
1:A:125:LEU:HD23	1:A:141:SER:HB3	1.92	0.52
1:A:233:ARG:HG2	1:A:331:ASN:ND2	2.25	0.52
1:A:119:LEU:HD21	1:A:445:ILE:HD13	1.90	0.52
1:B:716:PRO:HB2	1:B:719:ALA:HB3	1.92	0.52
1:D:120:ARG:NH1	1:D:395:GLU:CD	2.62	0.52
1:B:166:MET:HE2	1:B:175:TRP:CB	2.40	0.52
1:A:359:HIS:O	1:A:360:SER:CB	2.57	0.52
1:C:676:ARG:NH1	1:C:726:GLU:OE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:ASN:N	1:B:597:HIS:HD2	2.00	0.52
1:D:289:ILE:HG13	1:D:334:LEU:HD11	1.91	0.52
1:A:674:LYS:HD2	1:A:696:THR:HG21	1.92	0.51
1:B:295:ASP:OD2	1:B:311:ARG:NH2	2.43	0.51
1:D:117:THR:CA	5:D:1002:HOH:O	2.58	0.51
1:D:371:ASN:CG	1:D:372:THR:N	2.62	0.51
1:A:436:ILE:O	1:A:440:ARG:HG3	2.10	0.51
1:A:594:ASN:H	1:A:597:HIS:CD2	2.27	0.51
1:D:489:THR:HG22	1:D:507:LEU:HD12	1.92	0.51
1:A:146:ASN:HD22	1:A:354:THR:CG2	2.23	0.51
1:A:292:HIS:CD2	1:A:311:ARG:NH1	2.79	0.51
1:C:373:LEU:N	5:C:903:HOH:O	2.43	0.51
1:D:157:ASN:C	1:D:157:ASN:HD22	2.14	0.51
1:B:259:ASN:ND2	1:B:259:ASN:H	2.07	0.51
1:D:629:LEU:HD11	1:D:642:VAL:HG23	1.93	0.51
1:D:674:LYS:CB	1:D:674:LYS:NZ	2.73	0.51
1:B:576:ARG:HH21	1:B:585:ASP:CG	2.14	0.51
1:A:289:ILE:HD12	1:A:289:ILE:C	2.31	0.51
1:C:514:ASN:ND2	5:C:1019:HOH:O	2.43	0.51
1:C:614:LYS:HB3	1:C:618:GLU:HG3	1.93	0.51
1:D:117:THR:CB	5:D:1002:HOH:O	2.59	0.51
1:A:593:ASP:OD2	1:A:687:HIS:HE1	1.93	0.50
1:B:492:TYR:CZ	1:B:500:ARG:HG2	2.46	0.50
1:C:285:GLU:OE1	1:C:403:ARG:HD2	2.11	0.50
1:D:614:LYS:NZ	5:D:1024:HOH:O	2.39	0.50
1:D:693:ASN:ND2	1:D:713:LEU:CB	2.72	0.50
1:A:146:ASN:ND2	1:A:354:THR:HG21	2.26	0.50
1:A:262:TRP:CZ3	1:A:311:ARG:HG2	2.47	0.50
1:C:290:ASN:ND2	1:C:337:VAL:HG22	2.26	0.50
1:C:656:ASN:ND2	1:C:658:THR:H	2.08	0.50
1:D:693:ASN:ND2	1:D:714:THR:H	2.09	0.50
1:A:647:GLU:O	1:A:647:GLU:CG	2.60	0.50
1:C:588:LEU:HD13	1:C:596:HIS:CE1	2.47	0.50
1:C:583:SER:HB3	3:C:803:GLC:H62	1.93	0.50
1:B:302:PRO:HG3	1:B:337:VAL:HG21	1.93	0.50
1:A:163:ARG:O	1:A:165:PRO:HD3	2.11	0.50
1:B:149:ARG:O	1:B:192:MET:HA	2.11	0.50
1:B:441:ASN:HD21	1:B:444:ARG:HH22	1.58	0.50
1:C:256:HIS:HB2	1:C:259:ASN:HD21	1.77	0.50
1:B:166:MET:CE	1:B:175:TRP:HB2	2.42	0.50
1:C:194:ASP:HB2	1:C:198:ASN:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:713:LEU:CD1	1:D:713:LEU:C	2.78	0.50
1:B:293:PRO:HD3	1:B:303:THR:HG23	1.93	0.49
1:C:497:PRO:HA	1:C:500:ARG:HD2	1.92	0.49
1:D:674:LYS:HB3	1:D:674:LYS:HZ3	1.77	0.49
1:A:543:ALA:HB1	1:A:595:TRP:HZ3	1.77	0.49
1:B:340:HIS:HE1	1:B:405:ASP:OD2	1.94	0.49
1:B:670:ASN:ND2	1:B:707:ARG:NE	2.52	0.49
1:C:429:GLY:CA	1:C:430:ARG:CG	2.88	0.49
1:C:685:HIS:CE1	1:D:685[A]:HIS:HD2	2.30	0.49
1:D:425:ASN:O	1:D:425:ASN:OD1	2.30	0.49
1:A:474:GLY:O	1:A:475:LEU:CB	2.59	0.49
1:B:235:LYS:HA	1:B:238:GLN:OE1	2.12	0.49
1:C:656:ASN:HD22	1:C:656:ASN:C	2.16	0.49
1:B:643:ARG:O	1:B:650:GLU:HA	2.12	0.49
1:B:150:VAL:O	1:B:166:MET:HG3	2.12	0.49
1:A:295:ASP:N	1:A:295:ASP:OD2	2.45	0.49
1:B:376:ASN:O	1:B:382:VAL:CG1	2.58	0.49
1:C:426:GLU:CG	1:C:427:PHE:CD2	2.80	0.49
1:B:343:THR:HG22	1:B:373:LEU:HD21	1.95	0.49
1:B:224:PRO:HB2	1:B:319:ARG:HH22	1.78	0.49
1:B:470:GLN:NE2	1:B:470:GLN:N	2.42	0.49
1:D:437:GLU:HA	1:D:437:GLU:OE2	2.12	0.49
1:D:278:TRP:O	1:D:604:ARG:HD2	2.13	0.49
1:D:724:VAL:HG22	1:D:725:ARG:H	1.78	0.48
1:B:345:ASP:OD2	1:B:345:ASP:N	2.47	0.48
1:C:157:ASN:ND2	1:C:164:HIS:CD2	2.67	0.48
1:D:214:PRO:HA	1:D:215:GLU:C	2.30	0.48
1:A:645:ASP:OD1	1:A:649:ASN:ND2	2.36	0.48
1:C:256:HIS:CE1	1:C:267:GLU:OE1	2.66	0.48
1:A:215:GLU:HG3	1:A:216:THR:H	1.78	0.48
1:B:237:ASN:ND2	1:B:283:HIS:CE1	2.70	0.48
1:B:259:ASN:ND2	1:B:259:ASN:N	2.61	0.48
1:A:216:THR:O	1:A:217:ALA:HB2	2.13	0.48
1:B:336:TRP:CH2	1:B:390:ALA:HB2	2.49	0.48
1:A:680:ASN:ND2	1:A:682:ASP:H	2.12	0.48
1:A:247:GLU:OE1	1:A:525:HIS:HD2	1.97	0.48
1:B:529:VAL:CG1	1:B:578:TRP:HE3	2.27	0.48
1:B:579:ASN:ND2	1:B:581:ASP:H	2.10	0.48
1:D:215:GLU:CB	1:D:217:ALA:N	2.70	0.48
1:D:258:ASP:O	1:D:259:ASN:HB2	2.14	0.48
1:C:290:ASN:ND2	1:C:337:VAL:CG2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:VAL:O	1:C:450:VAL:HG23	2.14	0.48
1:C:560:PHE:CD2	1:C:561:PRO:HD2	2.48	0.48
1:B:570:ASN:ND2	5:B:945:HOH:O	2.45	0.48
1:C:182:ALA:HA	1:C:186:GLN:HE22	1.79	0.48
1:C:686:TYR:O	1:C:687:HIS:HB2	2.13	0.48
1:B:528:VAL:HA	1:B:533:LYS:O	2.14	0.47
1:C:234:LYS:HE2	1:C:451:SER:O	2.14	0.47
1:D:651:ILE:CD1	1:D:722:TRP:HB3	2.44	0.47
1:D:651:ILE:HD13	1:D:722:TRP:HB3	1.95	0.47
1:A:472:MET:O	1:A:473:GLY:C	2.51	0.47
1:C:684:MET:H	1:C:690:ASN:ND2	2.11	0.47
1:C:552:ALA:O	1:C:720:THR:CG2	2.62	0.47
1:A:542:ASP:OD1	1:A:544:TRP:NE1	2.47	0.47
1:B:411:ILE:HB	1:B:436:ILE:HD11	1.96	0.47
1:A:579:ASN:ND2	1:A:581:ASP:H	2.13	0.47
1:B:492:TYR:CZ	1:B:507:LEU:HD22	2.49	0.47
1:C:237:ASN:HD22	1:C:283:HIS:CE1	2.31	0.47
1:D:117:THR:HA	5:D:1002:HOH:O	2.15	0.47
1:D:646:LYS:NZ	1:D:646:LYS:HB2	2.29	0.47
1:D:167:ARG:NH1	5:D:1122:HOH:O	2.47	0.47
1:D:211:GLN:NE2	1:D:217:ALA:HB3	2.29	0.47
1:A:146:ASN:O	1:A:147:ALA:CB	2.63	0.47
1:B:658:THR:CG2	1:B:660:VAL:HB	2.45	0.47
1:A:142:VAL:CG2	1:A:190:TYR:CE1	2.97	0.47
1:A:654:ALA:HB3	1:A:721:ILE:HD13	1.97	0.47
1:B:644:ARG:HG3	1:B:650:GLU:HB3	1.97	0.47
1:A:243:ILE:HB	1:A:563:LYS:HD2	1.97	0.47
1:A:494:LYS:HB3	1:A:494:LYS:HE2	1.78	0.47
1:B:411:ILE:O	1:B:432:ASN:N	2.47	0.47
1:C:333:ILE:HG12	1:C:401:ALA:HB3	1.97	0.47
1:D:646:LYS:NZ	1:D:646:LYS:CB	2.77	0.47
1:A:259:ASN:HD22	1:A:260:ASN:N	2.13	0.46
1:B:191:GLU:CG	1:B:201:LEU:CD2	2.93	0.46
1:B:213:ARG:HD2	1:B:215:GLU:HB2	1.96	0.46
1:C:259:ASN:H	1:C:259:ASN:ND2	2.13	0.46
1:B:671:GLN:HB3	1:D:498:VAL:HG11	1.97	0.46
1:D:532:LYS:O	1:D:533:LYS:HB2	2.15	0.46
1:B:250:LEU:HD22	1:B:268:LEU:HD13	1.96	0.46
1:C:656:ASN:C	1:C:656:ASN:ND2	2.68	0.46
1:C:651:ILE:HD11	1:C:722:TRP:HB3	1.96	0.46
1:D:538:ARG:HD3	5:D:981:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:OD2	1:A:131:THR:N	2.46	0.46
1:A:146:ASN:HD22	1:A:354:THR:HG21	1.81	0.46
1:A:212:MET:CG	1:A:213:ARG:N	2.59	0.46
1:B:520:VAL:O	1:B:522:PRO:HD3	2.14	0.46
1:B:523:LEU:HD22	1:B:557:MET:SD	2.55	0.46
1:C:256:HIS:HE1	1:C:267:GLU:OE1	1.98	0.46
1:D:552:ALA:HA	1:D:720:THR:HG23	1.97	0.46
1:A:273:VAL:HB	1:A:274:PRO:HD3	1.97	0.46
1:C:429:GLY:HA3	1:C:430:ARG:HG3	1.96	0.46
1:D:215:GLU:HA	1:D:216:THR:HG23	1.96	0.46
1:D:431:GLU:H	1:D:431:GLU:HG2	1.39	0.46
1:D:590:GLU:HA	5:D:990:HOH:O	2.14	0.46
1:A:684:MET:H	1:A:690:ASN:ND2	2.14	0.46
1:C:636:ARG:HG2	1:C:662:ARG:CZ	2.45	0.46
1:C:551:ARG:NH1	1:C:681:THR:O	2.45	0.46
1:B:644:ARG:HA	1:B:649:ASN:O	2.16	0.46
1:C:658:THR:HG22	1:C:660:VAL:N	2.08	0.46
1:B:237:ASN:HD22	1:B:283:HIS:CE1	2.28	0.46
1:B:426:GLU:OE2	1:B:433:LEU:HD12	2.16	0.46
1:A:645:ASP:OD2	1:A:649:ASN:N	2.48	0.46
1:A:717:PRO:O	1:A:718:LEU:C	2.54	0.46
1:D:118[A]:HIS:N	5:D:1002:HOH:O	2.49	0.46
1:D:674:LYS:HZ3	1:D:696:THR:HG21	1.81	0.46
1:A:289:ILE:C	1:A:289:ILE:CD1	2.84	0.46
1:A:359:HIS:CD2	1:A:376:ASN:HA	2.51	0.46
1:A:213:ARG:O	1:A:215:GLU:N	2.49	0.45
1:B:169:ARG:HG2	1:B:169:ARG:NH1	2.23	0.45
1:B:486:MET:HE3	1:B:487:HIS:HD2	1.77	0.45
1:D:118[B]:HIS:N	5:D:1002:HOH:O	2.49	0.45
1:D:187:LEU:CD2	1:D:219:LEU:HD12	2.43	0.45
1:A:661:PRO:HB3	1:A:717:PRO:HD3	1.99	0.45
1:B:182:ALA:HA	1:B:186:GLN:OE1	2.15	0.45
1:C:247:GLU:OE1	1:C:525:HIS:HD2	1.99	0.45
1:C:593:ASP:OD2	1:C:687:HIS:HE1	1.99	0.45
1:A:138:THR:HG21	1:A:220:ILE:HD13	1.96	0.45
1:A:209:GLU:OE2	1:A:310:ARG:NH1	2.49	0.45
1:B:425:ASN:OD1	1:B:429:GLY:N	2.50	0.45
1:B:494:LYS:HB3	1:B:494:LYS:HE2	1.74	0.45
1:B:658:THR:HG23	1:B:660:VAL:H	1.74	0.45
1:C:492:TYR:CE2	1:C:507:LEU:CD2	3.00	0.45
1:C:331:ASN:ND2	5:C:928:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:593:ASP:OD2	1:D:687:HIS:HE1	1.99	0.45
1:D:713:LEU:HD11	1:D:715:LEU:HD21	1.97	0.45
1:A:133:ASP:C	1:A:133:ASP:OD1	2.55	0.45
1:A:574:GLN:HG3	1:A:585:ASP:HB2	1.98	0.45
1:B:674:LYS:HE2	1:B:674:LYS:HB2	1.55	0.45
1:C:194:ASP:HB2	1:C:198:ASN:H	1.81	0.45
1:C:278:TRP:O	1:C:604:ARG:HD2	2.17	0.45
1:A:254:ARG:HG2	1:A:586:TRP:NE1	2.32	0.45
1:C:211:GLN:HB3	1:C:212:MET:HB3	1.99	0.45
1:C:552:ALA:HA	1:C:720:THR:CG2	2.47	0.45
1:D:136:THR:HG22	5:D:997:HOH:O	2.16	0.45
1:A:441:ASN:OD1	1:A:444:ARG:NH1	2.46	0.45
1:A:631:VAL:O	1:A:631:VAL:HG22	2.17	0.45
1:D:399:ILE:HD12	1:D:401:ALA:H	1.82	0.45
1:A:550:LEU:HD11	1:A:554:TYR:CZ	2.51	0.45
1:C:528:VAL:O	1:C:577:GLU:HB2	2.17	0.45
1:C:533:LYS:O	1:C:538:ARG:NH2	2.49	0.44
1:A:472:MET:CG	1:A:473:GLY:N	2.71	0.44
1:B:467:SER:HA	1:B:477:PHE:O	2.17	0.44
1:B:574:GLN:NE2	1:B:585:ASP:H	2.14	0.44
1:C:211:GLN:HB3	1:C:212:MET:CB	2.47	0.44
1:C:532:LYS:C	1:C:533:LYS:CG	2.83	0.44
1:D:674:LYS:HD2	1:D:698[B]:HIS:CD2	2.53	0.44
1:A:543:ALA:CB	1:A:595:TRP:HZ3	2.31	0.44
1:A:242:PRO:HD3	1:A:617:HIS:CE1	2.52	0.44
1:C:237:ASN:HD21	1:C:283:HIS:HE1	1.58	0.44
1:D:340:HIS:CE1	1:D:405:ASP:OD2	2.63	0.44
1:A:467:SER:OG	1:A:517:GLU:OE2	2.35	0.44
1:B:669:ILE:O	1:B:707:ARG:HD3	2.17	0.44
1:C:399:ILE:CD1	1:C:401:ALA:H	2.28	0.44
1:A:593:ASP:OD2	1:A:687:HIS:CE1	2.69	0.44
1:B:155:GLN:O	5:B:961:HOH:O	2.21	0.44
1:C:426:GLU:CG	1:C:427:PHE:N	2.78	0.44
1:D:656:ASN:ND2	5:D:1043:HOH:O	2.46	0.44
1:A:143:TRP:CH2	1:A:356:LEU:HD22	2.52	0.44
1:C:225:GLU:O	1:C:226:LYS:HB2	2.11	0.44
1:B:627:GLU:OE1	1:B:707:ARG:NH2	2.49	0.44
1:A:148:ARG:HG2	1:A:148:ARG:H	1.54	0.44
1:D:703:ALA:HA	1:D:707:ARG:O	2.18	0.44
1:A:142:VAL:CG2	1:A:190:TYR:CZ	3.01	0.44
1:C:194:ASP:HB3	1:C:196:ASN:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:525:HIS:HB3	1:C:567:PHE:CE1	2.53	0.44
1:D:258:ASP:O	1:D:259:ASN:CG	2.55	0.44
1:D:414:ASP:O	1:D:415:TYR:CG	2.71	0.44
1:D:615:ALA:HB3	1:D:651:ILE:HG23	1.98	0.44
1:A:496:ASP:C	1:A:498:VAL:N	2.72	0.43
1:B:658:THR:HG22	1:B:660:VAL:N	2.22	0.43
1:C:655:SER:OG	1:C:720:THR:HB	2.18	0.43
1:C:559:ALA:HB1	1:C:653:VAL:HG21	2.00	0.43
1:C:593:ASP:HA	1:C:597:HIS:CD2	2.52	0.43
1:C:610:TYR:O	1:C:617:HIS:HD2	2.01	0.43
1:A:295:ASP:OD2	1:A:311:ARG:NH2	2.52	0.43
1:A:533:LYS:O	1:A:538:ARG:NH2	2.52	0.43
1:C:130:ASP:HB3	1:C:178:PHE:CE2	2.53	0.43
1:A:289:ILE:O	1:A:308:PRO:HA	2.18	0.43
1:A:489:THR:O	1:A:493:MET:HB2	2.18	0.43
1:B:132:MET:HA	1:B:132:MET:CE	2.49	0.43
1:D:399:ILE:CD1	1:D:402:LEU:HD23	2.48	0.43
1:A:237:ASN:ND2	1:A:283:HIS:CE1	2.76	0.43
1:B:191:GLU:CG	1:B:201:LEU:HD23	2.42	0.43
1:C:472:MET:SD	1:C:472:MET:N	2.91	0.43
1:C:579:ASN:C	1:C:579:ASN:ND2	2.72	0.43
1:A:393:TRP:HB3	1:A:399:ILE:HG13	2.00	0.43
1:A:590:GLU:HA	1:A:590:GLU:OE1	2.19	0.43
1:A:463:PHE:O	1:A:466:VAL:HG23	2.19	0.43
1:B:212:MET:O	1:B:214:PRO:HA	2.18	0.43
1:D:118[A]:HIS:H	1:D:118[A]:HIS:CD2	2.31	0.43
1:A:682:ASP:HB2	1:A:719:ALA:HB2	2.01	0.43
1:B:594:ASN:HD21	1:B:596:HIS:HB2	1.83	0.43
1:C:302:PRO:HG3	1:C:337:VAL:CG2	2.49	0.43
1:A:259:ASN:C	1:A:259:ASN:HD22	2.21	0.43
1:A:467:SER:HA	1:A:477:PHE:O	2.18	0.43
1:C:429:GLY:HA3	1:C:430:ARG:CG	2.49	0.43
1:D:427:PHE:N	1:D:428:GLY:HA2	2.33	0.43
1:A:407:VAL:HG21	1:A:457:ALA:HB1	2.01	0.43
1:B:194:ASP:C	1:B:196:ASN:H	2.22	0.43
1:B:213:ARG:N	1:B:214:PRO:CA	2.82	0.43
1:C:492:TYR:CD2	1:C:507:LEU:HD21	2.54	0.43
1:D:610:TYR:O	1:D:617:HIS:HD2	2.01	0.43
1:A:465:GLY:O	1:A:474:GLY:O	2.37	0.42
1:A:495:LEU:HD13	1:A:503:HIS:CD2	2.54	0.42
1:A:517:GLU:HB2	1:A:519:PHE:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ASN:ND2	1:B:290:ASN:C	2.72	0.42
1:C:490:LEU:HA	1:C:490:LEU:HD13	1.86	0.42
3:C:801:GLC:H62	3:C:802:GLC:O5	2.19	0.42
1:A:333:ILE:HG12	1:A:401:ALA:HB3	2.01	0.42
1:A:496:ASP:C	1:A:498:VAL:H	2.21	0.42
1:B:658:THR:HG21	1:B:660:VAL:HB	2.01	0.42
1:C:259:ASN:HD22	1:C:261:PHE:H	1.67	0.42
1:A:223:LEU:HD23	1:A:396:ARG:CZ	2.50	0.42
1:D:579:ASN:ND2	1:D:581:ASP:H	2.18	0.42
1:C:426:GLU:HG3	1:C:427:PHE:N	2.34	0.42
1:C:560:PHE:O	1:C:564:LYS:NZ	2.53	0.42
1:A:284:LEU:HD12	1:A:284:LEU:HA	1.91	0.42
1:B:213:ARG:HD3	1:B:215:GLU:HG3	2.02	0.42
1:D:302:PRO:HG3	1:D:337:VAL:CG2	2.41	0.42
1:A:666:ARG:HA	1:A:711:LEU:O	2.20	0.42
1:B:486:MET:HE1	1:B:487:HIS:CD2	2.53	0.42
1:C:211:GLN:CB	1:C:212:MET:CB	2.97	0.42
1:C:310:ARG:O	1:C:310:ARG:HD2	2.20	0.42
1:C:444:ARG:O	1:C:448:GLU:HG3	2.20	0.42
1:D:171:GLU:CG	5:D:1040:HOH:O	2.43	0.42
1:D:552:ALA:O	1:D:720:THR:CG2	2.68	0.42
1:B:414:ASP:OD2	1:B:414:ASP:N	2.53	0.42
1:C:259:ASN:HD22	1:C:260:ASN:N	2.17	0.41
1:A:250:LEU:HD21	1:A:286:LEU:HD22	2.02	0.41
1:B:213:ARG:CD	1:B:215:GLU:HG3	2.50	0.41
1:B:686:TYR:O	1:B:687:HIS:HB2	2.20	0.41
1:C:682:ASP:HB2	1:C:719:ALA:HB2	2.02	0.41
1:D:514:ASN:ND2	5:D:938:HOH:O	2.52	0.41
1:A:157:ASN:OD1	1:A:164:HIS:CD2	2.74	0.41
1:A:475:LEU:HD12	1:A:475:LEU:HA	1.92	0.41
1:A:492:TYR:CZ	1:A:507:LEU:HD22	2.55	0.41
1:B:199:LEU:HD13	1:B:199:LEU:H	1.84	0.41
1:B:594:ASN:HD22	1:B:596:HIS:H	1.67	0.41
1:A:144:ALA:HA	1:A:145:PRO:HD2	1.92	0.41
1:B:529:VAL:CG1	1:B:578:TRP:CE3	3.03	0.41
1:D:266:ARG:HD3	5:D:1046:HOH:O	2.20	0.41
1:B:222:GLY:O	1:B:315:ARG:NH1	2.41	0.41
1:B:318:PHE:CE2	1:B:322:ILE:HD11	2.53	0.41
1:C:704:SER:OG	1:C:705:HIS:HD2	2.03	0.41
1:A:157:ASN:OD1	1:A:164:HIS:HD2	2.03	0.41
1:B:357:TYR:CD1	1:B:382:VAL:HG23	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:ASN:ND2	1:C:425:ASN:N	2.69	0.41
1:C:431:GLU:C	1:C:431:GLU:OE1	2.59	0.41
1:A:230:THR:O	1:A:234:LYS:HG2	2.20	0.41
1:D:212[A]:MET:HG2	1:D:310:ARG:HG2	2.03	0.41
1:D:443:ASN:O	1:D:446:LEU:O	2.39	0.41
1:D:533:LYS:O	1:D:538:ARG:NH2	2.53	0.41
1:D:684:MET:H	1:D:690:ASN:ND2	2.19	0.41
1:A:442:THR:O	1:A:446:LEU:HG	2.21	0.41
1:D:488:ASP:OD2	5:D:1041:HOH:O	2.22	0.41
1:A:456:MET:HG2	1:A:479:TYR:HB2	2.03	0.41
1:A:709:HIS:CD2	5:A:924:HOH:O	2.54	0.41
1:B:213:ARG:HB2	1:B:215:GLU:HB2	2.03	0.41
1:B:169:ARG:CG	1:B:169:ARG:NH1	2.79	0.41
1:B:489:THR:HG22	1:B:507:LEU:HD12	2.02	0.41
1:D:686:TYR:O	1:D:687:HIS:HB2	2.21	0.41
1:B:213:ARG:N	1:B:214:PRO:HA	2.35	0.41
1:D:232:GLU:H	1:D:232:GLU:CD	2.24	0.41
1:A:703:ALA:HA	1:A:707:ARG:O	2.20	0.40
1:D:646:LYS:HZ1	1:D:646:LYS:HB2	1.86	0.40
1:A:227:VAL:HG22	1:A:319:ARG:NH2	2.36	0.40
1:B:709:HIS:HD2	5:B:910:HOH:O	2.02	0.40
1:B:693:ASN:ND2	1:B:714:THR:H	2.15	0.40
1:C:626:PHE:C	1:C:626:PHE:CD2	2.94	0.40
1:A:520:VAL:HG22	1:A:563:LYS:HB2	2.04	0.40
1:C:130:ASP:HB3	1:C:178:PHE:HE2	1.86	0.40
1:C:426:GLU:C	1:C:426:GLU:OE1	2.60	0.40
1:D:160:ASP:C	1:D:160:ASP:OD1	2.60	0.40
1:D:680:ASN:C	1:D:680:ASN:ND2	2.73	0.40
1:A:189:LYS:HE2	1:A:216:THR:O	2.21	0.40
1:B:602:LEU:HG	1:B:606:LEU:HD22	2.04	0.40
1:C:341:PHE:HA	1:C:342:PRO:HD3	1.92	0.40
1:C:551:ARG:HB3	1:C:681:THR:HB	2.03	0.40
1:A:430:ARG:O	1:A:431:GLU:C	2.59	0.40
1:A:654:ALA:HB3	1:A:721:ILE:CD1	2.51	0.40
1:A:698:HIS:HB3	5:A:902:HOH:O	2.22	0.40
1:B:233:ARG:HG2	1:B:331:ASN:HD21	1.86	0.40
1:C:119:LEU:HA	1:C:119:LEU:HD12	1.83	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	581/612 (95%)	529 (91%)	41 (7%)	11 (2%)	9	14
1	B	591/612 (97%)	544 (92%)	35 (6%)	12 (2%)	9	13
1	C	583/612 (95%)	550 (94%)	25 (4%)	8 (1%)	13	22
1	D	595/612 (97%)	568 (96%)	21 (4%)	6 (1%)	18	31
All	All	2350/2448 (96%)	2191 (93%)	122 (5%)	37 (2%)	11	19

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ARG
1	A	215	GLU
1	A	226	LYS
1	A	475	LEU
1	B	215	GLU
1	B	225	GLU
1	B	226	LYS
1	B	530	HIS
1	C	194	ASP
1	C	226	LYS
1	C	426	GLU
1	C	430	ARG
1	D	215	GLU
1	D	345	ASP
1	D	427	PHE
1	B	259	ASN
1	C	212	MET
1	C	694	GLY
1	D	259	ASN
1	A	522	PRO
1	B	159	TRP
1	B	160	ASP

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Mol	Chain	Res	Type
1	B	373	LEU
1	B	522	PRO
1	C	215	GLU
1	D	216	THR
1	D	522	PRO
1	B	372	THR
1	C	522	PRO
1	A	147	ALA
1	A	342	PRO
1	A	214	PRO
1	A	497	PRO
1	A	429	GLY
1	B	293	PRO
1	A	473	GLY
1	B	214	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	497/521 (95%)	450 (90%)	47 (10%)	10	17
1	B	507/521 (97%)	469 (92%)	38 (8%)	16	28
1	C	499/521 (96%)	443 (89%)	56 (11%)	7	12
1	D	511/521 (98%)	472 (92%)	39 (8%)	15	27
All	All	2014/2084 (97%)	1834 (91%)	180 (9%)	11	20

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	THR
1	A	139	ARG
1	A	146	ASN
1	A	149	ARG
1	A	163	ARG
1	A	170	LYS

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Mol	Chain	Res	Type
1	A	194	ASP
1	A	199	LEU
1	A	200	ARG
1	A	211	GLN
1	A	257	THR
1	A	259	ASN
1	A	260	ASN
1	A	263	LEU
1	A	277	LYS
1	A	291	GLU
1	A	295	ASP
1	A	315	ARG
1	A	331	ASN
1	A	335	ASP
1	A	346	PHE
1	A	350	GLU
1	A	356	LEU
1	A	359	HIS
1	A	360	SER
1	A	391	LEU
1	A	462	ASP
1	A	472	MET
1	A	490	LEU
1	A	493	MET
1	A	498	VAL
1	A	507	LEU
1	A	537	ASP
1	A	558	TRP
1	A	579	ASN
1	A	593	ASP
1	A	606	LEU
1	A	616	MET
1	A	619	LEU
1	A	646	LYS
1	A	656	ASN
1	A	680	ASN
1	A	684	MET
1	A	690	ASN
1	A	720	THR
1	A	721	ILE
1	A	723	LEU
1	B	118	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	168	LEU
1	B	187	LEU
1	B	199	LEU
1	B	216	THR
1	B	259	ASN
1	B	290	ASN
1	B	315	ARG
1	B	330	LEU
1	B	331	ASN
1	B	335	ASP
1	B	345	ASP
1	B	356	LEU
1	B	371	ASN
1	B	373	LEU
1	B	376	ASN
1	B	380	ARG
1	B	382	VAL
1	B	391	LEU
1	B	414	ASP
1	B	430	ARG
1	B	436	ILE
1	B	446	LEU
1	B	470	GLN
1	B	475	LEU
1	B	490	LEU
1	B	507	LEU
1	B	512	LEU
1	B	523	LEU
1	B	594	ASN
1	B	606	LEU
1	B	619	LEU
1	B	642	VAL
1	B	651	ILE
1	B	656	ASN
1	B	658	THR
1	B	680	ASN
1	B	689	SER
1	C	119	LEU
1	C	149	ARG
1	C	162	ARG
1	C	168	LEU
1	C	169	ARG

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Mol	Chain	Res	Type
1	C	171	GLU
1	C	202	LYS
1	C	212	MET
1	C	213	ARG
1	C	219	LEU
1	C	223	LEU
1	C	258	ASP
1	C	259	ASN
1	C	289	ILE
1	C	297	SER
1	C	305	LEU
1	C	310	ARG
1	C	315	ARG
1	C	331	ASN
1	C	356	LEU
1	C	373	LEU
1	C	374	ILE
1	C	380	ARG
1	C	391	LEU
1	C	399	ILE
1	C	409	SER
1	C	413	ARG
1	C	425	ASN
1	C	426	GLU
1	C	427	PHE
1	C	430	ARG
1	C	431	GLU
1	C	444	ARG
1	C	446	LEU
1	C	456	MET
1	C	470	GLN
1	C	471	ASP
1	C	472	MET
1	C	478	TRP
1	C	490	LEU
1	C	498	VAL
1	C	507	LEU
1	C	523	LEU
1	C	524	SER
1	C	579	ASN
1	C	590	GLU
1	C	593	ASP

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Mol	Chain	Res	Type
1	C	595	TRP
1	C	604	ARG
1	C	619	LEU
1	C	647	GLU
1	C	651	ILE
1	C	656	ASN
1	C	680	ASN
1	C	683	SER
1	C	720	THR
1	D	118[A]	HIS
1	D	118[B]	HIS
1	D	119	LEU
1	D	133	ASP
1	D	136	THR
1	D	148	ARG
1	D	149[A]	ARG
1	D	149[B]	ARG
1	D	157	ASN
1	D	171	GLU
1	D	216	THR
1	D	223	LEU
1	D	315	ARG
1	D	319	ARG
1	D	331	ASN
1	D	346	PHE
1	D	356	LEU
1	D	373	LEU
1	D	391	LEU
1	D	427	PHE
1	D	431	GLU
1	D	470	GLN
1	D	471	ASP
1	D	475	LEU
1	D	490	LEU
1	D	494	LYS
1	D	507	LEU
1	D	523	LEU
1	D	579	ASN
1	D	606	LEU
1	D	619	LEU
1	D	651	ILE
1	D	656	ASN

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Mol	Chain	Res	Type
1	D	674	LYS
1	D	679	LEU
1	D	680	ASN
1	D	700	ASP
1	D	720	THR
1	D	723	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	164	HIS
1	A	196	ASN
1	A	237	ASN
1	A	256	HIS
1	A	259	ASN
1	A	260	ASN
1	A	283	HIS
1	A	326	HIS
1	A	331	ASN
1	A	359	HIS
1	A	376	ASN
1	A	384	ASN
1	A	501	GLN
1	A	503	HIS
1	A	525	HIS
1	A	570	ASN
1	A	574	GLN
1	A	579	ASN
1	A	597	HIS
1	A	617	HIS
1	A	656	ASN
1	A	680	ASN
1	A	687	HIS
1	A	690	ASN
1	A	693	ASN
1	A	705	HIS
1	B	157	ASN
1	B	164	HIS
1	B	198	ASN
1	B	237	ASN
1	B	259	ASN

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Mol	Chain	Res	Type
1	B	260	ASN
1	B	283	HIS
1	B	331	ASN
1	B	340	HIS
1	B	376	ASN
1	B	441	ASN
1	B	470	GLN
1	B	487	HIS
1	B	525	HIS
1	B	545	GLN
1	B	570	ASN
1	B	574	GLN
1	B	579	ASN
1	B	580	HIS
1	B	594	ASN
1	B	597	HIS
1	B	617	HIS
1	B	656	ASN
1	B	670	ASN
1	B	680	ASN
1	B	690	ASN
1	B	693	ASN
1	B	705	HIS
1	C	157	ASN
1	C	164	HIS
1	C	183	HIS
1	C	186	GLN
1	C	237	ASN
1	C	256	HIS
1	C	259	ASN
1	C	283	HIS
1	C	290	ASN
1	C	301	GLN
1	C	331	ASN
1	C	340	HIS
1	C	425	ASN
1	C	470	GLN
1	C	504	HIS
1	C	525	HIS
1	C	570	ASN
1	C	574	GLN
1	C	579	ASN

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Mol	Chain	Res	Type
1	C	597	HIS
1	C	600	GLN
1	C	617	HIS
1	C	656	ASN
1	C	680	ASN
1	C	687	HIS
1	C	690	ASN
1	C	693	ASN
1	C	705	HIS
1	D	157	ASN
1	D	164	HIS
1	D	186	GLN
1	D	237	ASN
1	D	256	HIS
1	D	259	ASN
1	D	283	HIS
1	D	331	ASN
1	D	340	HIS
1	D	371	ASN
1	D	425	ASN
1	D	441	ASN
1	D	443	ASN
1	D	470	GLN
1	D	504	HIS
1	D	525	HIS
1	D	545	GLN
1	D	570	ASN
1	D	574	GLN
1	D	579	ASN
1	D	597	HIS
1	D	617	HIS
1	D	649	ASN
1	D	656	ASN
1	D	680	ASN
1	D	687	HIS
1	D	690	ASN
1	D	693	ASN
1	D	705	HIS
1	D	708	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

15 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	A	801	-	12,12,12	0.48	0	17,17,17	0.96	1 (5%)
3	GLC	B	801	3	12,12,12	0.56	0	17,17,17	0.92	0
3	GLC	B	802	3	11,11,12	0.66	0	13,15,17	1.31	2 (15%)
4	GOL	B	803	-	5,5,5	0.38	0	5,5,5	0.42	0
3	GLC	C	801	3	12,12,12	0.57	0	17,17,17	0.89	0
3	GLC	C	802	3	11,11,12	0.59	0	13,15,17	1.11	1 (7%)
3	GLC	C	803	3	12,12,12	0.63	0	17,17,17	0.68	0
3	GLC	C	804	3	11,11,12	0.68	0	13,15,17	1.29	2 (15%)
4	GOL	C	805	-	5,5,5	0.55	0	5,5,5	1.29	0
3	GLC	D	801	3	12,12,12	0.55	0	17,17,17	0.64	0
3	GLC	D	802	3	11,11,12	0.44	0	13,15,17	2.74	2 (15%)
3	GLC	D	803	3	12,12,12	0.66	0	17,17,17	0.86	1 (5%)
3	GLC	D	804	3	11,11,12	0.72	0	13,15,17	1.60	2 (15%)
4	GOL	D	805	-	5,5,5	0.40	0	5,5,5	0.59	0
4	GOL	D	806	-	5,5,5	0.29	0	5,5,5	0.39	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	BGC	A	801	-	-	0/2/22/22	0/1/1/1
3	GLC	B	801	3	-	0/2/22/22	0/1/1/1
3	GLC	B	802	3	-	0/2/19/22	0/1/1/1
4	GOL	B	803	-	-	0/4/4/4	0/0/0/0
3	GLC	C	801	3	-	0/2/22/22	0/1/1/1
3	GLC	C	802	3	-	0/2/19/22	0/1/1/1
3	GLC	C	803	3	-	0/2/22/22	0/1/1/1
3	GLC	C	804	3	-	0/2/19/22	0/1/1/1
4	GOL	C	805	-	-	0/4/4/4	0/0/0/0
3	GLC	D	801	3	-	0/2/22/22	0/1/1/1
3	GLC	D	802	3	-	0/2/19/22	0/1/1/1
3	GLC	D	803	3	-	0/2/22/22	0/1/1/1
3	GLC	D	804	3	-	0/2/19/22	0/1/1/1
4	GOL	D	805	-	-	0/4/4/4	0/0/0/0
4	GOL	D	806	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802	GLC	C2-C3-C4	-4.19	103.58	110.88
3	D	803	GLC	O2-C2-C3	-2.26	105.43	110.36
3	C	804	GLC	C2-C3-C4	-2.23	106.99	110.88
3	C	804	GLC	C3-C4-C5	-2.13	106.47	110.22
2	A	801	BGC	C4-C3-C2	-2.11	107.11	110.84
3	B	802	GLC	C1-O5-C5	2.19	115.18	112.17
3	B	802	GLC	C3-C4-C5	2.72	115.01	110.22
3	D	804	GLC	C1-C2-C3	2.99	113.44	109.65
3	C	802	GLC	C1-O5-C5	3.01	116.32	112.17
3	D	804	GLC	C1-O5-C5	3.43	116.89	112.17
3	D	802	GLC	C1-O5-C5	8.24	123.53	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	GLC	1	0
3	C	802	GLC	1	0
3	C	803	GLC	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	586/612 (95%)	0.81	96 (16%) <b>2</b> <b>2</b>	59, 87, 129, 153	4 (0%)
1	B	596/612 (97%)	0.56	67 (11%) <b>6</b> <b>6</b>	58, 82, 123, 153	8 (1%)
1	C	589/612 (96%)	0.35	29 (4%) 30 33	48, 69, 89, 109	6 (1%)
1	D	593/612 (96%)	0.14	11 (1%) 67 70	40, 53, 75, 100	9 (1%)
All	All	2364/2448 (96%)	0.47	203 (8%) <b>11</b> <b>11</b>	40, 73, 119, 153	27 (1%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	PRO	7.4
1	A	428	GLY	7.0
1	A	175	TRP	6.7
1	A	290	ASN	6.5
1	A	201	LEU	6.3
1	B	353	GLY	6.2
1	A	199	LEU	6.2
1	A	149	ARG	6.1
1	B	199	LEU	5.9
1	C	431	GLU	5.6
1	B	132	MET	5.6
1	C	132	MET	5.5
1	A	360	SER	5.5
1	A	145	PRO	5.5
1	A	214	PRO	5.3
1	A	144	ALA	5.3
1	A	148	ARG	5.1
1	A	213	ARG	5.1
1	A	166	MET	5.1
1	D	371	ASN	5.0
1	A	159	TRP	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	728	GLU	4.9
1	A	194	ASP	4.9
1	A	212	MET	4.9
1	A	195	ALA	4.9
1	D	429	GLY	4.8
1	B	277	LYS	4.8
1	B	197	GLY	4.8
1	A	170	LYS	4.8
1	B	371	ASN	4.7
1	A	177	LEU	4.7
1	A	197	GLY	4.7
1	A	429	GLY	4.7
1	A	146	ASN	4.7
1	A	191	GLU	4.7
1	A	133	ASP	4.6
1	B	430	ARG	4.6
1	A	151	SER	4.6
1	A	158	TYR	4.4
1	A	196	ASN	4.4
1	B	167	ARG	4.4
1	A	171	GLU	4.4
1	B	427	PHE	4.3
1	B	196	ASN	4.3
1	B	142	VAL	4.3
1	A	472	MET	4.3
1	A	473	GLY	4.3
1	A	343	THR	4.2
1	A	193	ILE	4.2
1	A	150	VAL	4.2
1	B	216	THR	4.2
1	C	430	ARG	4.2
1	B	429	GLY	4.1
1	B	193	ILE	4.1
1	A	294	PHE	4.1
1	D	728	GLU	4.0
1	B	131	THR	4.0
1	A	135	VAL	4.0
1	B	177	LEU	4.0
1	C	427	PHE	3.9
1	C	258	ASP	3.9
1	B	148	ARG	3.9
1	B	133	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	134	GLY	3.9
1	B	361	ASP	3.9
1	A	162	ARG	3.8
1	B	425	ASN	3.8
1	D	258	ASP	3.8
1	C	346	PHE	3.7
1	C	135	VAL	3.7
1	B	149	ARG	3.7
1	B	201	LEU	3.7
1	B	200	ARG	3.7
1	A	211	GLN	3.7
1	A	200	ARG	3.6
1	A	530	HIS	3.6
1	B	158	TYR	3.6
1	B	175	TRP	3.6
1	B	150	VAL	3.6
1	A	168	LEU	3.6
1	A	167	ARG	3.6
1	B	144	ALA	3.6
1	D	428	GLY	3.5
1	B	159	TRP	3.5
1	A	164	HIS	3.5
1	A	190	TYR	3.4
1	A	192	MET	3.4
1	D	117	THR	3.3
1	A	354	THR	3.3
1	B	213	ARG	3.3
1	A	132	MET	3.3
1	B	413	ARG	3.3
1	A	153	VAL	3.3
1	B	257	THR	3.2
1	A	131	THR	3.2
1	C	499	TYR	3.2
1	B	135	VAL	3.2
1	B	162	ARG	3.2
1	B	191	GLU	3.2
1	C	359	HIS	3.2
1	A	728	GLU	3.1
1	C	428	GLY	3.1
1	C	133	ASP	3.1
1	C	429	GLY	3.1
1	B	258	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	423	ILE	3.1
1	C	498	VAL	3.1
1	A	581	ASP	3.1
1	A	147	ALA	3.1
1	A	430	ARG	3.1
1	B	129	ALA	3.1
1	B	194	ASP	3.1
1	A	216	THR	3.1
1	A	143	TRP	3.0
1	A	351	PHE	3.0
1	B	170	LYS	3.0
1	A	134	GLY	3.0
1	D	427	PHE	3.0
1	C	660	VAL	3.0
1	A	188	TYR	2.9
1	A	178	PHE	2.9
1	A	346	PHE	2.9
1	B	161	GLY	2.9
1	B	176	GLU	2.9
1	B	202	LYS	2.9
1	B	424	PRO	2.9
1	A	543	ALA	2.9
1	A	180	PRO	2.8
1	C	502	TYR	2.8
1	B	174	ILE	2.8
1	B	168	LEU	2.8
1	B	360	SER	2.8
1	A	163	ARG	2.8
1	A	469	PRO	2.8
1	B	412	TYR	2.8
1	A	172	SER	2.8
1	A	173	GLY	2.7
1	C	131	THR	2.7
1	B	139	ARG	2.7
1	C	606	LEU	2.7
1	B	147	ALA	2.7
1	D	415	TYR	2.7
1	B	635	GLU	2.7
1	A	215	GLU	2.7
1	A	198	ASN	2.7
1	A	165	PRO	2.7
1	B	428	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	346	PHE	2.6
1	A	169	ARG	2.6
1	A	140	PHE	2.6
1	A	352	ASP	2.6
1	B	117	THR	2.6
1	A	160	ASP	2.6
1	C	512	LEU	2.6
1	A	533	LYS	2.5
1	B	164	HIS	2.5
1	C	590	GLU	2.5
1	B	165	PRO	2.5
1	A	471	ASP	2.5
1	B	346	PHE	2.5
1	C	496	ASP	2.5
1	A	685[A]	HIS	2.5
1	C	199	LEU	2.5
1	C	345	ASP	2.5
1	B	354	THR	2.5
1	A	380	ARG	2.4
1	B	192	MET	2.4
1	A	542	ASP	2.4
1	A	349	ALA	2.4
1	A	174	ILE	2.4
1	A	295	ASP	2.4
1	C	632	ASP	2.3
1	D	259	ASN	2.3
1	C	708	GLN	2.3
1	A	373	LEU	2.3
1	A	303	THR	2.2
1	A	187	LEU	2.2
1	B	728	GLU	2.2
1	A	176	GLU	2.2
1	A	434	GLU	2.2
1	A	701	GLU	2.2
1	D	257	THR	2.2
1	B	195	ALA	2.2
1	B	299	GLY	2.2
1	B	163	ARG	2.2
1	A	161	GLY	2.2
1	A	203	SER	2.2
1	A	345	ASP	2.1
1	B	190	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	196	ASN	2.1
1	A	437	GLU	2.1
1	A	509	PHE	2.1
1	A	219	LEU	2.1
1	A	582	ALA	2.1
1	B	130	ASP	2.1
1	B	426	GLU	2.1
1	A	359	HIS	2.1
1	B	359	HIS	2.1
1	C	663	HIS	2.1
1	B	198	ASN	2.1
1	A	350	GLU	2.0
1	A	155	GLN	2.0
1	C	333	ILE	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. 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	C	805	6/6	0.75	0.29	3.54	70,71,71,71	0
3	GLC	C	803	12/12	0.92	0.35	3.17	88,89,90,90	0
3	GLC	B	801	12/12	0.78	0.27	2.64	114,114,115,115	0
3	GLC	D	803	12/12	0.91	0.31	2.53	73,74,75,75	0
3	GLC	B	802	11/12	0.90	0.33	2.07	115,115,115,115	0
2	BGC	A	801	12/12	0.72	0.32	1.92	99,99,99,100	0
3	GLC	D	804	11/12	0.89	0.28	1.84	72,75,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLC	D	802	11/12	0.69	0.29	1.63	96,97,98,98	0
3	GLC	D	801	12/12	0.89	0.31	1.59	97,98,98,98	0
3	GLC	C	802	11/12	0.91	0.28	1.53	93,93,94,94	0
3	GLC	C	804	11/12	0.86	0.30	1.28	85,87,88,88	0
4	GOL	B	803	6/6	0.94	0.17	-0.04	66,68,69,70	0
4	GOL	D	805	6/6	0.93	0.14	-1.20	56,60,61,62	0
4	GOL	D	806	6/6	0.97	0.10	-1.75	60,61,62,63	0
3	GLC	C	801	12/12	0.92	0.26	-	93,93,94,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.