



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:34 am GMT

PDB ID : 2VR5
Title : Crystal structure of Trex from Sulfolobus Solfataricus in complex with acarbose intermediate and glucose
Authors : Song, H.-N.; Yoon, S.-M.; Lee, S.-J.; Cha, H.-J.; Park, K.-H.; Woo, E.-J.
Deposited on : 2008-03-26
Resolution : 2.80 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 ⓘ symbol.

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 : trunk28620
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) : recalc28949

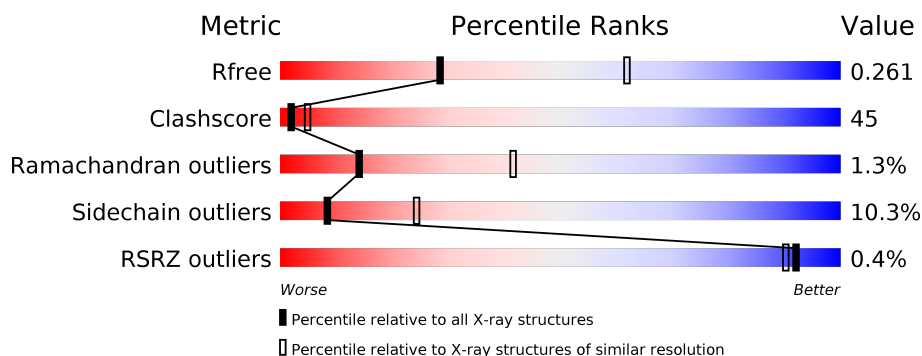
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 $\leq 5\%$. 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	718	
1	B	718	

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	1719	-	-	-	X
2	GLC	A	1720	-	-	-	X
2	GLC	A	1721	-	-	-	X
3	A16	A	1722	X	-	-	X
3	A16	B	1720	X	-	-	X
4	SO4	A	1723	-	-	X	-
5	GOL	A	1724	-	-	-	X

2 Entry composition [i](#)

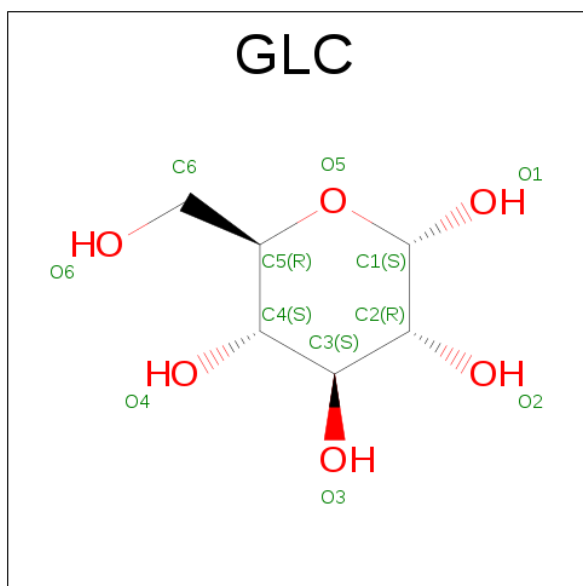
There are 6 unique types of molecules in this entry. The entry contains 12209 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLYCOGEN OPERON PROTEIN GLGX.

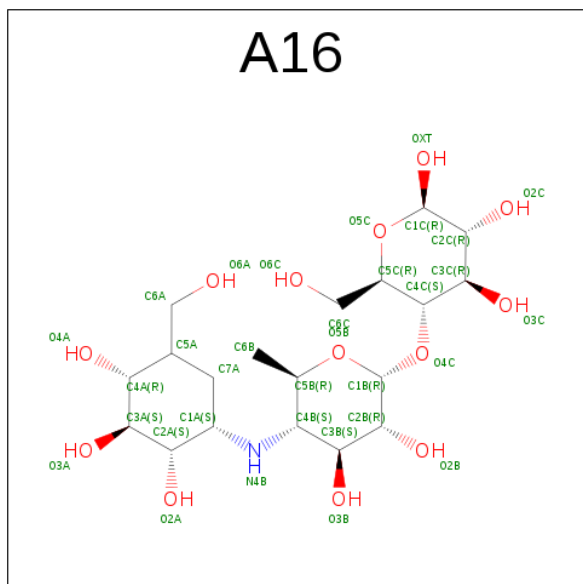
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5848	3753	985	1091	19			
1	B	714	Total	C	N	O	S	0	0	0
			5837	3744	984	1090	19			

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



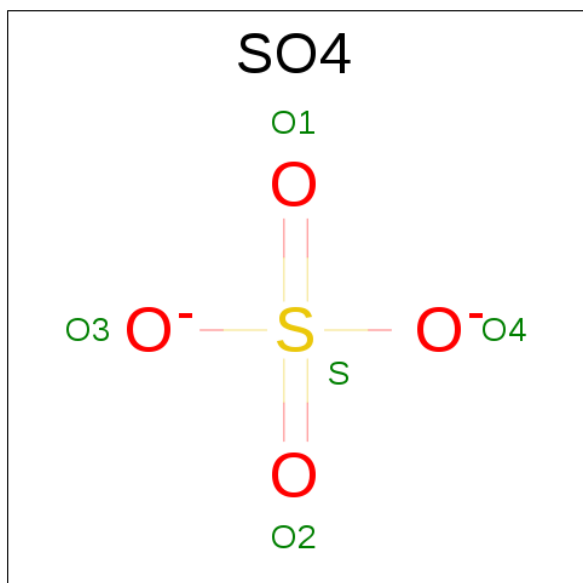
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 4-O-(4,6-DIDEOXY-4-[[[(1S,2S,3S,4R,5S)-2,3,4-TRIHYDROXY-5-(HYDROXYMETHYL)CYCLOHEXYL]AMINO}-ALPHA-D-GLUCOPYRANOSYL)-BETA-D-GLUCOPYRANOSE (three-letter code: A16) (formula: $C_{19}H_{35}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	19	1	12		
3	B	1	Total	C	N	O	0	0
			32	19	1	12		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

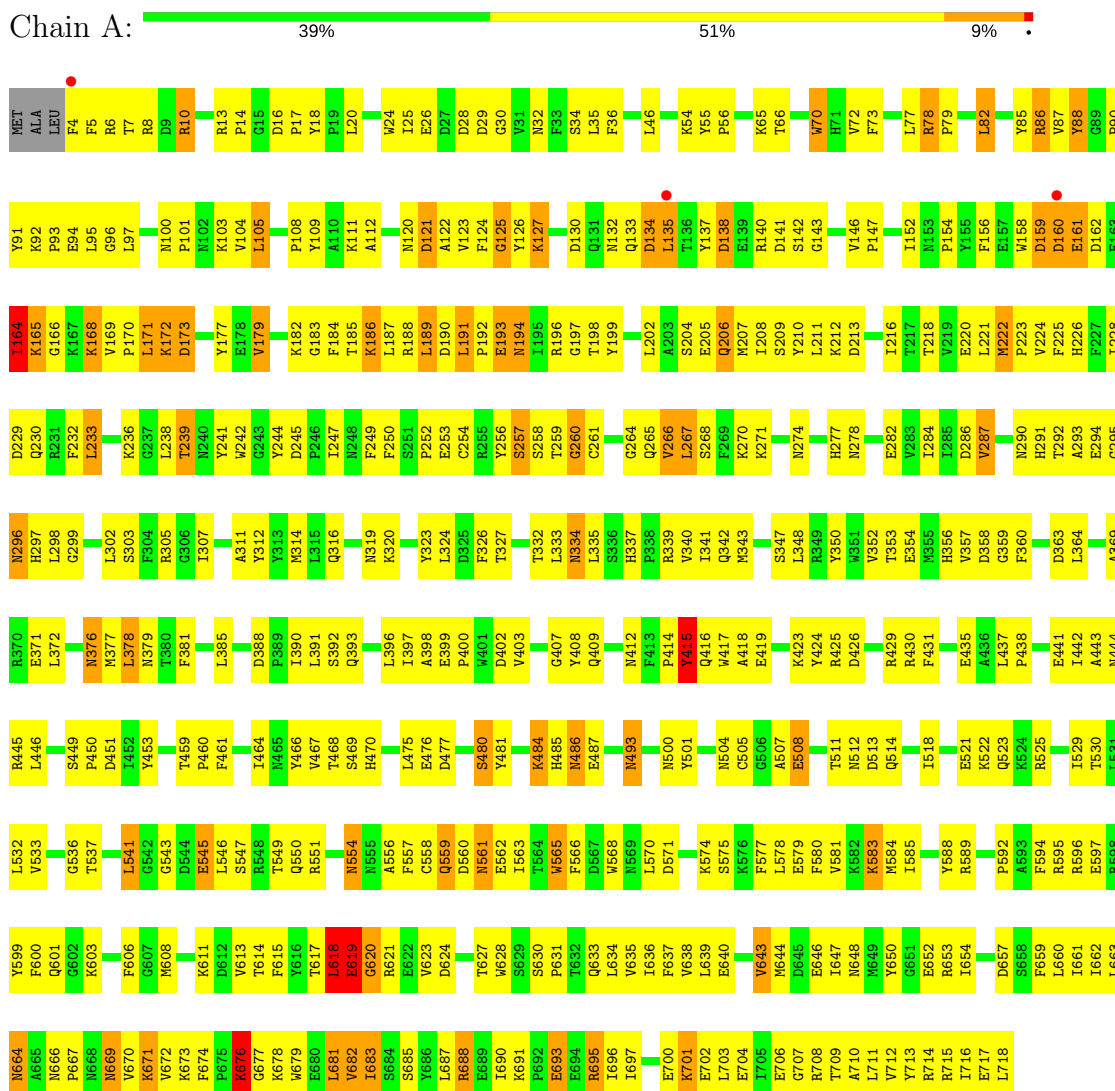
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	213	Total	O	0	0
			213	213		
6	B	188	Total	O	0	0
			188	188		

3 Residue-property plots

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

• Molecule 1: GLYCOGEN OPERON PROTEIN GLGX





4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.81Å 204.81Å 89.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.85 – 2.80 44.45 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (29.85-2.80) 96.6 (44.45-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.214 , 0.266 0.211 , 0.261	Depositor DCC
R_{free} test set	2573 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12209	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GLC, A16, SO4

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	0.21	0/6002	0.32	0/8136
1	B	0.21	0/5990	0.32	0/8120
All	All	0.21	0/11992	0.32	0/16256

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	11
1	B	1	12
All	All	3	23

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	161	GLU	CA
1	A	261	CYS	CA
1	B	372	LEU	CA

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	GLY	Peptide
1	A	161	GLU	Peptide
1	A	165	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	A	259	THR	Peptide
1	A	260	GLY	Peptide
1	A	296	ASN	Peptide
1	A	56	PRO	Peptide
1	A	618	LEU	Peptide
1	A	619	GLU	Peptide
1	A	620	GLY	Peptide
1	A	678	LYS	Peptide
1	B	159	ASP	Peptide
1	B	160	ASP	Peptide
1	B	163	PHE	Peptide
1	B	165	LYS	Peptide
1	B	189	LEU	Peptide
1	B	192	PRO	Peptide
1	B	193	GLU	Peptide
1	B	371	GLU	Peptide
1	B	398	ALA	Peptide
1	B	504	ASN	Peptide
1	B	505	CYS	Peptide
1	B	675	PRO	Peptide

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	5848	0	5662	540	2
1	B	5837	0	5651	503	2
2	A	36	0	36	2	0
2	B	12	0	12	1	0
3	A	32	0	32	1	0
3	B	32	0	32	1	0
4	A	5	0	0	3	0
5	A	6	0	8	3	0
6	A	213	0	0	17	0
6	B	188	0	0	15	0
All	All	12209	0	11433	1043	2

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 45.

All (1043) 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:A:172:LYS:HB2	1:A:461:PHE:CE1	1.61	1.35
1:B:135:LEU:HD21	1:B:321:ARG:NH1	1.42	1.32
1:B:135:LEU:CD2	1:B:321:ARG:HH11	1.49	1.25
1:B:372:LEU:HD12	1:B:373:TYR:N	1.50	1.23
1:B:135:LEU:CD2	1:B:321:ARG:NH1	2.08	1.15
1:A:459:THR:HB	1:A:460:PRO:HD2	1.15	1.14
1:B:482:ASN:HD21	1:B:504:ASN:ND2	1.42	1.14
1:A:161:GLU:OE2	1:A:356:HIS:ND1	1.82	1.13
1:B:372:LEU:C	1:B:372:LEU:HD12	1.66	1.13
1:A:623:VAL:HG13	1:A:627:THR:HG23	1.30	1.11
1:B:164:ILE:HG23	1:B:165:LYS:HD3	1.27	1.11
1:B:192:PRO:O	1:B:195:ILE:HG12	1.48	1.10
1:A:695:ARG:HG2	1:A:696:ILE:HD12	1.12	1.10
1:A:206:GLN:N	1:A:206:GLN:HE21	1.50	1.10
1:B:164:ILE:CG2	1:B:165:LYS:HD3	1.81	1.10
1:A:617:THR:HG22	1:A:618:LEU:H	1.14	1.08
1:A:159:ASP:HB3	6:A:2052:HOH:O	1.53	1.07
1:B:303:SER:O	1:B:307:ILE:HG12	1.56	1.06
1:B:482:ASN:ND2	1:B:504:ASN:ND2	2.02	1.06
1:B:187:LEU:HD22	1:B:565:TRP:HB3	1.38	1.06
1:A:206:GLN:NE2	1:A:206:GLN:H	1.52	1.05
1:A:621:ARG:HB3	6:A:2184:HOH:O	1.53	1.05
1:A:303:SER:O	1:A:307:ILE:HD12	1.57	1.05
1:B:78:ARG:HB3	1:B:79:PRO:HD2	1.37	1.04
1:B:135:LEU:HD11	1:B:321:ARG:HH12	1.24	1.03
1:A:164:ILE:HG13	1:A:164:ILE:O	1.57	1.01
1:B:504:ASN:HB2	1:B:507:ALA:O	1.59	1.00
1:A:695:ARG:HG2	1:A:696:ILE:CD1	1.91	1.00
1:B:372:LEU:C	1:B:372:LEU:CD1	2.30	1.00
1:B:135:LEU:CD1	1:B:321:ARG:HH12	1.76	0.99
1:A:459:THR:HB	1:A:460:PRO:CD	1.93	0.99
1:B:372:LEU:HD12	1:B:373:TYR:CA	1.92	0.99
1:B:135:LEU:CG	1:B:321:ARG:NH1	2.24	0.98
1:A:164:ILE:O	1:A:168:LYS:HD3	1.61	0.98
1:B:89:GLY:HA3	1:B:99:PHE:HD1	1.27	0.98
1:B:164:ILE:HG23	1:B:165:LYS:CD	1.94	0.98
1:A:504:ASN:OD1	1:A:508:GLU:HA	1.64	0.97
1:A:54:LYS:C	1:A:55:TYR:HD2	1.67	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ARG:CG	1:A:696:ILE:HD12	1.94	0.97
1:A:504:ASN:HD21	1:A:507:ALA:HB3	1.24	0.97
1:B:459:THR:HB	1:B:460:PRO:HD2	1.47	0.96
1:A:10:ARG:HH11	1:A:10:ARG:HG2	1.25	0.96
1:A:292:THR:HG22	1:A:293:ALA:N	1.80	0.96
1:B:690:ILE:HD13	1:B:690:ILE:H	1.26	0.95
1:A:634:LEU:HD21	1:A:636:ILE:HD12	1.44	0.95
1:A:292:THR:HG22	1:A:294:GLU:H	1.31	0.95
1:A:339:ARG:HH11	1:A:342:GLN:HE22	1.06	0.94
1:B:331:ASN:HD22	1:B:331:ASN:C	1.69	0.94
1:B:314:MET:HG3	1:B:334:ASN:HB3	1.50	0.93
1:A:339:ARG:NH1	1:A:342:GLN:HE22	1.64	0.93
1:A:172:LYS:HB2	1:A:461:PHE:HE1	1.18	0.93
1:A:549:THR:HG22	1:A:551:ARG:H	1.32	0.93
1:B:636:ILE:HG23	1:B:662:ILE:HD13	1.49	0.92
1:A:618:LEU:O	1:A:672:VAL:HA	1.69	0.92
1:B:339:ARG:HH11	1:B:342:GLN:HE22	1.10	0.92
1:B:414:PRO:O	1:B:417:TRP:HB2	1.69	0.92
1:B:596:ARG:HH21	1:B:646:GLU:HG2	1.34	0.91
1:A:104:VAL:HG11	1:A:143:GLY:HA2	1.52	0.91
1:B:159:ASP:O	1:B:161:GLU:HB2	1.71	0.91
1:B:624:ASP:OD2	6:B:2165:HOH:O	1.87	0.91
1:B:135:LEU:CG	1:B:321:ARG:HH12	1.83	0.90
1:A:172:LYS:CB	1:A:461:PHE:CE1	2.53	0.90
1:B:666:ASN:OD1	1:B:667:PRO:HD2	1.71	0.90
1:B:482:ASN:HD21	1:B:504:ASN:HD21	1.18	0.90
1:A:54:LYS:O	1:A:55:TYR:HD2	1.53	0.90
1:A:82:LEU:H	1:A:82:LEU:HD12	1.37	0.90
1:B:596:ARG:NH2	1:B:646:GLU:HG2	1.87	0.89
1:B:103:LYS:NZ	1:B:125:GLY:H	1.68	0.89
1:B:640:GLU:HB3	1:B:643:VAL:HG22	1.54	0.89
1:B:89:GLY:HA3	1:B:99:PHE:CD1	2.07	0.89
1:B:187:LEU:CD2	1:B:565:TRP:HB3	2.03	0.87
1:A:504:ASN:ND2	1:A:507:ALA:HB3	1.90	0.87
1:B:161:GLU:HA	1:B:161:GLU:OE2	1.73	0.86
1:B:482:ASN:HD21	1:B:504:ASN:CG	1.79	0.86
1:A:218:THR:HG22	1:A:282:GLU:HB2	1.58	0.85
1:B:165:LYS:HD3	1:B:165:LYS:N	1.91	0.85
1:A:339:ARG:HH11	1:A:342:GLN:NE2	1.75	0.85
1:B:187:LEU:HD22	1:B:565:TRP:CB	2.06	0.85
1:B:511:THR:HG22	1:B:512:ASN:H	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:PRO:HG2	1:A:441:GLU:HB2	1.59	0.83
1:A:292:THR:CG2	1:A:293:ALA:N	2.41	0.83
1:A:385:LEU:HD11	1:A:396:LEU:CD1	2.09	0.83
1:B:503:TRP:CZ3	1:B:505:CYS:SG	2.71	0.83
1:B:247:ILE:HD12	1:B:247:ILE:H	1.44	0.83
1:A:385:LEU:HD11	1:A:396:LEU:HD11	1.58	0.83
1:A:624:ASP:H	1:A:627:THR:CG2	1.90	0.82
1:A:561:ASN:HD22	1:A:563:ILE:H	1.25	0.82
1:A:287:VAL:HG21	1:A:360:PHE:HB3	1.61	0.82
1:A:431:PHE:CD1	1:A:442:ILE:HD13	2.15	0.82
1:B:339:ARG:NH1	1:B:342:GLN:HE22	1.77	0.82
1:A:161:GLU:OE1	1:A:277:HIS:HD2	1.61	0.81
1:A:504:ASN:ND2	1:A:507:ALA:CA	2.43	0.81
1:B:682:VAL:HG12	1:B:712:VAL:O	1.80	0.81
1:A:305:ARG:NH1	1:A:323:TYR:OH	2.14	0.81
1:A:560:ASP:OD1	1:A:565:TRP:HH2	1.63	0.81
1:A:158:TRP:HE1	5:A:1724:GOL:H32	1.44	0.80
1:A:617:THR:HG22	1:A:618:LEU:N	1.91	0.80
1:A:103:LYS:HE3	1:A:125:GLY:HA2	1.62	0.80
1:B:261:CYS:HB2	1:B:265:GLN:NE2	1.97	0.80
1:B:303:SER:O	1:B:307:ILE:CG1	2.29	0.80
1:A:126:TYR:OH	1:A:298:LEU:O	1.99	0.80
1:A:715:ARG:HD3	1:A:718:LEU:HB2	1.61	0.80
1:B:42:LYS:HB3	1:B:88:TYR:HB2	1.63	0.80
1:A:637:PHE:CE2	1:A:661:ILE:HB	2.17	0.80
1:B:400:PRO:HA	1:B:413:PHE:CE1	2.17	0.80
1:A:292:THR:CG2	1:A:293:ALA:H	1.94	0.80
1:A:326:PHE:O	1:A:403:VAL:HG22	1.82	0.79
1:B:560:ASP:OD2	1:B:565:TRP:HH2	1.65	0.79
1:A:695:ARG:C	1:A:696:ILE:HD12	2.03	0.79
1:B:504:ASN:CB	1:B:507:ALA:O	2.30	0.79
1:A:54:LYS:O	1:A:55:TYR:CD2	2.36	0.79
1:A:461:PHE:CE2	1:A:597:GLU:HG3	2.17	0.79
1:A:189:LEU:N	1:A:189:LEU:HD13	1.96	0.78
1:A:257:SER:OG	1:A:260:GLY:HA2	1.83	0.78
1:A:437:LEU:HB3	1:A:438:PRO:HD2	1.63	0.78
1:B:103:LYS:HZ2	1:B:125:GLY:H	1.30	0.78
1:A:267:LEU:CD1	1:A:271:LYS:HE2	2.14	0.78
1:B:407:GLY:O	1:B:409:GLN:HG2	1.82	0.78
1:B:135:LEU:HD21	1:B:321:ARG:HH11	0.65	0.78
1:A:161:GLU:OE1	1:A:277:HIS:CD2	2.36	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ASN:ND2	1:A:507:ALA:N	2.31	0.78
1:B:16:ASP:H	1:B:32:ASN:HD21	1.30	0.77
1:B:662:ILE:HG21	1:B:705:ILE:HD13	1.66	0.77
1:A:504:ASN:HD22	1:A:507:ALA:N	1.82	0.77
1:B:93:PRO:O	1:B:321:ARG:HB2	1.84	0.77
1:B:482:ASN:ND2	1:B:504:ASN:CG	2.37	0.77
1:A:277:HIS:HE1	1:A:358:ASP:OD2	1.67	0.77
1:B:623:VAL:HG13	1:B:627:THR:HG23	1.68	0.76
1:A:618:LEU:O	1:A:618:LEU:HD12	1.85	0.76
1:A:161:GLU:O	1:A:164:ILE:HG22	1.84	0.76
1:B:636:ILE:HG12	1:B:662:ILE:HD13	1.66	0.76
1:A:172:LYS:HB2	1:A:461:PHE:CZ	2.18	0.76
1:B:636:ILE:CG2	1:B:662:ILE:HD13	2.15	0.76
1:A:664:ASN:HD21	1:A:666:ASN:HB3	1.52	0.75
1:B:637:PHE:CE2	1:B:661:ILE:HB	2.20	0.75
1:B:157:GLU:OE1	6:B:2062:HOH:O	2.05	0.75
1:B:546:LEU:HD21	1:B:568:TRP:CZ3	2.21	0.75
1:B:189:LEU:HD12	1:B:189:LEU:H	1.51	0.75
1:A:101:PRO:HD2	1:A:137:TYR:OH	1.86	0.75
1:A:172:LYS:O	1:A:595:ARG:HB3	1.87	0.74
1:A:681:LEU:HD22	1:A:682:VAL:H	1.52	0.74
1:B:164:ILE:CG2	1:B:165:LYS:CD	2.59	0.74
1:A:54:LYS:C	1:A:55:TYR:CD2	2.58	0.74
1:B:164:ILE:HG22	1:B:165:LYS:HD3	1.70	0.74
1:B:248:ASN:ND2	1:B:250:PHE:H	1.86	0.74
1:B:314:MET:HG3	1:B:334:ASN:CB	2.18	0.74
1:A:461:PHE:HE2	1:A:597:GLU:HG3	1.52	0.73
1:A:164:ILE:O	1:A:168:LYS:CD	2.35	0.73
1:B:400:PRO:HA	1:B:413:PHE:HE1	1.52	0.73
1:A:86:ARG:HH11	1:A:86:ARG:CG	2.01	0.73
1:A:91:TYR:O	1:A:92:LYS:HG2	1.88	0.73
1:B:505:CYS:SG	1:B:519:CYS:CB	2.76	0.73
1:A:319:ASN:HB3	6:A:2103:HOH:O	1.88	0.73
1:A:634:LEU:HD21	1:A:636:ILE:CD1	2.19	0.73
1:B:153:ASN:C	1:B:153:ASN:HD22	1.91	0.73
1:A:398:ALA:HB2	1:A:417:TRP:CE3	2.24	0.73
1:B:161:GLU:CA	1:B:161:GLU:OE2	2.35	0.72
1:B:292:THR:HG22	1:B:294:GLU:H	1.54	0.72
1:A:461:PHE:CZ	1:A:597:GLU:HA	2.24	0.72
1:B:135:LEU:HG	1:B:321:ARG:NH1	2.04	0.72
1:B:248:ASN:ND2	1:B:251:SER:H	1.85	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:HA	1:A:284:ILE:O	1.89	0.72
1:A:504:ASN:ND2	1:A:507:ALA:CB	2.53	0.72
1:A:559:GLN:HG3	1:A:563:ILE:HD12	1.70	0.72
1:B:135:LEU:HD11	1:B:321:ARG:NH1	2.00	0.72
1:A:623:VAL:CG1	1:A:627:THR:HG23	2.14	0.72
1:B:627:THR:HG22	6:B:2165:HOH:O	1.87	0.72
1:B:81:GLN:HE21	1:B:82:LEU:H	1.37	0.72
1:A:6:ARG:HG3	1:A:7:THR:H	1.54	0.72
1:A:669:ASN:N	1:A:669:ASN:HD22	1.87	0.71
1:A:504:ASN:HD21	1:A:507:ALA:CB	2.02	0.71
1:B:186:LYS:O	1:B:196:ARG:HG2	1.90	0.71
1:B:439:TYR:HD1	1:B:632:THR:HG21	1.55	0.71
1:A:523:GLN:HE22	1:A:708:ARG:HB3	1.55	0.71
1:B:165:LYS:CD	1:B:165:LYS:N	2.49	0.71
1:B:560:ASP:OD2	1:B:565:TRP:CH2	2.43	0.71
1:A:192:PRO:HD3	6:A:2069:HOH:O	1.89	0.71
1:A:673:LYS:HE2	1:A:700:GLU:O	1.91	0.71
1:B:339:ARG:HH11	1:B:342:GLN:NE2	1.87	0.71
1:B:484:LYS:HE3	1:B:495:ASP:O	1.88	0.71
1:B:636:ILE:HG23	1:B:662:ILE:CD1	2.19	0.71
1:A:82:LEU:N	1:A:82:LEU:HD12	2.06	0.71
1:A:617:THR:CG2	1:A:618:LEU:H	2.00	0.71
1:B:648:ASN:C	1:B:648:ASN:HD22	1.94	0.71
1:B:674:PHE:CG	1:B:697:ILE:HG21	2.26	0.71
1:A:90:PRO:HB2	1:A:97:LEU:HD13	1.71	0.71
1:B:20:LEU:HB2	1:B:109:TYR:CE2	2.25	0.71
1:B:130:ASP:HB3	6:B:2046:HOH:O	1.91	0.71
1:B:636:ILE:HG12	1:B:662:ILE:CD1	2.21	0.71
1:A:504:ASN:ND2	1:A:507:ALA:C	2.44	0.70
1:A:681:LEU:HD22	1:A:682:VAL:N	2.05	0.70
1:B:120:ASN:O	1:B:123:VAL:HG22	1.90	0.70
1:B:189:LEU:HD12	1:B:189:LEU:N	2.04	0.70
1:B:202:LEU:HD23	1:B:202:LEU:O	1.91	0.70
1:A:257:SER:HB2	1:A:265:GLN:HA	1.72	0.70
1:A:126:TYR:CZ	1:A:298:LEU:HA	2.26	0.70
1:B:715:ARG:HD3	1:B:718:LEU:HB2	1.73	0.70
1:A:13:ARG:HB3	1:A:14:PRO:HD2	1.73	0.70
1:A:546:LEU:HD21	1:A:568:TRP:CZ3	2.27	0.70
1:B:193:GLU:O	1:B:194:ASN:CG	2.30	0.70
1:B:187:LEU:HD22	1:B:565:TRP:CG	2.27	0.70
1:B:505:CYS:SG	1:B:519:CYS:HB3	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:LEU:O	1:A:634:LEU:HD23	1.92	0.70
1:B:372:LEU:HD11	1:B:373:TYR:CD1	2.27	0.70
1:B:709:THR:HG22	1:B:711:LEU:HD11	1.73	0.69
1:B:192:PRO:O	1:B:195:ILE:CG1	2.33	0.69
1:A:164:ILE:CG1	1:A:164:ILE:O	2.36	0.69
1:A:292:THR:HG22	1:A:294:GLU:N	2.07	0.69
1:A:198:THR:HB	1:A:256:TYR:O	1.92	0.69
1:A:337:HIS:O	1:A:341:ILE:HG13	1.93	0.69
1:B:456:ASN:O	1:B:457:ASN:HB2	1.91	0.69
1:A:504:ASN:CG	1:A:507:ALA:O	2.30	0.69
1:A:10:ARG:NH1	1:A:10:ARG:HG2	2.03	0.69
1:B:48:TYR:CD1	1:B:148:LYS:HD3	2.26	0.69
1:A:10:ARG:HH11	1:A:10:ARG:CG	2.01	0.69
1:A:637:PHE:CZ	1:A:661:ILE:HB	2.27	0.69
1:B:111:LYS:HB2	1:B:152:ILE:HD12	1.74	0.69
1:B:312:TYR:O	1:B:333:LEU:HD12	1.93	0.69
1:B:516:VAL:O	1:B:520:ARG:HD3	1.93	0.69
1:A:617:THR:C	1:A:619:GLU:O	2.31	0.68
1:A:379:ASN:HD21	1:A:381:PHE:HB3	1.57	0.68
1:A:511:THR:HG22	1:A:513:ASP:H	1.59	0.68
1:A:20:LEU:HB2	1:A:109:TYR:CE2	2.28	0.68
1:B:103:LYS:O	1:B:105:LEU:HD22	1.94	0.68
1:B:159:ASP:OD1	1:B:159:ASP:C	2.31	0.68
1:A:661:ILE:HG13	1:A:712:VAL:HG22	1.76	0.68
1:B:48:TYR:CG	1:B:148:LYS:HD3	2.29	0.68
1:B:153:ASN:HD22	1:B:154:PRO:N	1.91	0.68
1:A:202:LEU:O	1:A:202:LEU:HD23	1.95	0.67
1:A:206:GLN:HE21	1:A:206:GLN:H	0.74	0.67
1:B:703:LEU:HB3	6:B:2175:HOH:O	1.94	0.67
1:B:331:ASN:ND2	1:B:331:ASN:C	2.43	0.67
1:A:226:HIS:HA	1:A:253:GLU:OE2	1.94	0.67
1:A:690:ILE:HD12	1:A:690:ILE:H	1.59	0.67
1:B:415:TYR:C	1:B:415:TYR:CD2	2.68	0.66
1:B:81:GLN:HE21	1:B:82:LEU:N	1.93	0.66
1:B:449:SER:N	1:B:450:PRO:HD3	2.10	0.66
1:B:191:LEU:HB3	1:B:195:ILE:HD11	1.77	0.66
1:A:397:ILE:HA	1:A:418:ALA:O	1.94	0.66
1:A:438:PRO:HA	1:A:631:PRO:HA	1.75	0.66
1:A:559:GLN:CG	1:A:563:ILE:HD12	2.26	0.66
1:A:218:THR:CG2	1:A:282:GLU:HB2	2.25	0.66
1:A:161:GLU:CD	1:A:277:HIS:HD2	1.97	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PHE:CE2	1:B:253:GLU:HG3	2.30	0.66
1:A:695:ARG:O	1:A:696:ILE:HD12	1.95	0.66
1:B:624:ASP:O	1:B:627:THR:HG22	1.95	0.66
1:B:437:LEU:HD23	1:B:441:GLU:HG2	1.76	0.66
1:A:664:ASN:HD21	1:A:666:ASN:CB	2.09	0.66
1:B:135:LEU:CD1	1:B:321:ARG:NH1	2.52	0.66
1:B:158:TRP:HB3	1:B:161:GLU:HG2	1.77	0.65
1:B:271:LYS:O	1:B:275:GLU:HG2	1.96	0.65
1:A:511:THR:HG22	1:A:512:ASN:N	2.11	0.65
1:B:615:PHE:CD2	1:B:637:PHE:HB3	2.32	0.65
1:B:126:TYR:CZ	1:B:298:LEU:HA	2.32	0.65
1:A:701:LYS:CG	1:A:702:GLU:N	2.59	0.65
1:B:187:LEU:HD22	1:B:565:TRP:CD1	2.32	0.65
1:B:505:CYS:HB2	1:B:520:ARG:HD2	1.79	0.65
1:A:393:GLN:HA	1:A:393:GLN:NE2	2.11	0.65
1:A:637:PHE:CE2	1:A:661:ILE:CG2	2.80	0.65
1:B:662:ILE:HG21	1:B:705:ILE:CD1	2.26	0.65
1:B:292:THR:HG22	1:B:293:ALA:N	2.12	0.65
1:A:36:PHE:CE1	1:A:339:ARG:HG3	2.31	0.65
1:A:648:ASN:HD21	1:A:652:GLU:HB2	1.61	0.65
1:B:450:PRO:HG3	1:B:599:TYR:CD2	2.31	0.65
1:B:511:THR:HG22	1:B:512:ASN:N	2.12	0.65
1:A:504:ASN:CG	1:A:507:ALA:C	2.55	0.64
1:A:168:LYS:O	1:A:170:PRO:HD3	1.95	0.64
1:B:504:ASN:ND2	1:B:507:ALA:O	2.30	0.64
1:B:636:ILE:CG2	1:B:662:ILE:CD1	2.76	0.64
1:B:661:ILE:CD1	1:B:712:VAL:HG22	2.27	0.64
1:B:679:TRP:CZ3	1:B:715:ARG:HB2	2.32	0.64
1:B:388:ASP:O	1:B:392:SER:HB2	1.96	0.64
1:B:158:TRP:HB3	1:B:161:GLU:CG	2.27	0.64
1:B:379:ASN:ND2	1:B:382:PHE:H	1.96	0.64
1:A:120:ASN:O	1:A:122:ALA:N	2.30	0.64
1:B:640:GLU:HB3	1:B:643:VAL:CG2	2.27	0.64
1:A:486:ASN:HB2	6:A:2147:HOH:O	1.97	0.64
1:A:377:MET:HE3	1:A:409:GLN:HG3	1.80	0.64
1:A:701:LYS:HG3	1:A:702:GLU:H	1.63	0.64
1:A:348:LEU:O	1:A:352:VAL:HG23	1.97	0.63
1:B:654:ILE:HG22	1:B:655:ALA:O	1.97	0.63
1:A:86:ARG:HH11	1:A:86:ARG:HG3	1.62	0.63
1:A:525:ARG:O	1:A:529:ILE:HG13	1.98	0.63
1:B:624:ASP:C	1:B:627:THR:HG22	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:PRO:HG3	1:A:419:GLU:HB2	1.81	0.63
1:A:718:LEU:O	1:A:718:LEU:HD13	1.99	0.63
1:B:608:MET:HG3	1:B:643:VAL:HG12	1.79	0.63
1:B:437:LEU:HD12	1:B:437:LEU:N	2.13	0.63
1:A:585:ILE:O	1:A:589:ARG:HG3	1.99	0.63
1:B:191:LEU:O	1:B:196:ARG:NH1	2.31	0.63
1:B:350:TYR:CE1	1:B:354:GLU:HG2	2.34	0.63
1:A:156:PHE:H	5:A:1724:GOL:H11	1.63	0.62
1:A:703:LEU:HD12	1:A:704:GLU:H	1.64	0.62
1:B:673:LYS:HE2	1:B:700:GLU:HB3	1.80	0.62
1:A:682:VAL:HG22	1:A:683:ILE:HG13	1.81	0.62
1:A:695:ARG:CG	1:A:696:ILE:CD1	2.65	0.62
1:B:292:THR:CG2	1:B:293:ALA:N	2.61	0.62
1:A:120:ASN:O	1:A:123:VAL:HG22	1.99	0.62
1:A:187:LEU:HD12	1:A:565:TRP:HB3	1.82	0.62
1:A:654:ILE:HG22	1:A:654:ILE:O	1.98	0.62
1:B:103:LYS:HZ1	1:B:125:GLY:H	1.45	0.62
1:B:228:ILE:HD11	1:B:247:ILE:HG12	1.81	0.62
1:A:311:ALA:O	1:A:312:TYR:HB2	1.99	0.62
1:B:546:LEU:HD21	1:B:568:TRP:CE3	2.34	0.62
1:A:408:TYR:OH	1:A:423:LYS:HE3	2.00	0.62
1:A:634:LEU:C	1:A:634:LEU:HD23	2.20	0.62
1:A:241:TYR:CE1	1:A:565:TRP:HZ3	2.18	0.62
1:B:232:PHE:CE1	1:B:233:LEU:HD13	2.34	0.62
1:B:348:LEU:O	1:B:352:VAL:HG23	1.98	0.62
1:B:398:ALA:HB2	1:B:417:TRP:CZ3	2.34	0.62
1:B:657:ASP:HB2	1:B:659:PHE:CE1	2.35	0.62
1:A:523:GLN:NE2	1:A:708:ARG:HB3	2.14	0.61
1:A:7:THR:HG22	4:A:1723:SO4:O3	2.01	0.61
1:A:312:TYR:O	1:A:333:LEU:HD12	2.00	0.61
1:A:82:LEU:H	1:A:82:LEU:CD1	2.12	0.61
1:B:372:LEU:HD12	1:B:373:TYR:HA	1.81	0.61
1:B:559:GLN:HG3	1:B:561:ASN:HD21	1.64	0.61
1:A:623:VAL:HG13	1:A:627:THR:CG2	2.19	0.61
1:B:296:ASN:ND2	1:B:297:HIS:O	2.33	0.61
1:A:232:PHE:CE1	1:A:233:LEU:HD13	2.36	0.61
1:A:543:GLY:N	1:A:545:GLU:OE2	2.30	0.61
1:B:195:ILE:O	1:B:195:ILE:HG13	1.98	0.61
1:B:439:TYR:CD1	1:B:632:THR:HG21	2.36	0.61
1:A:277:HIS:CE1	1:A:358:ASP:OD2	2.49	0.61
1:A:172:LYS:CB	1:A:461:PHE:HE1	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:GLN:HG2	1:B:563:ILE:HD12	1.82	0.61
1:A:316:GLN:HB3	6:A:2103:HOH:O	2.00	0.61
1:B:314:MET:CG	1:B:334:ASN:HB3	2.27	0.61
1:B:397:ILE:HG23	1:B:464:ILE:HD12	1.82	0.61
1:A:477:ASP:OD2	1:A:549:THR:HG23	2.00	0.61
1:A:648:ASN:HB3	1:A:654:ILE:HD11	1.82	0.61
1:A:91:TYR:C	1:A:92:LYS:HG2	2.21	0.61
1:B:177:TYR:CD2	1:B:179:VAL:HG22	2.35	0.61
1:A:287:VAL:CG2	1:A:360:PHE:HB3	2.31	0.60
1:A:187:LEU:CD1	1:A:565:TRP:HB3	2.31	0.60
1:B:185:THR:O	1:B:196:ARG:CG	2.48	0.60
1:A:111:LYS:HD2	1:A:350:TYR:CZ	2.36	0.60
1:B:248:ASN:HD22	1:B:251:SER:H	1.48	0.60
1:B:180:HIS:CE1	1:B:182:LYS:HB3	2.37	0.60
1:B:450:PRO:O	1:B:454:LEU:HB3	2.00	0.60
1:A:184:PHE:CD2	1:A:185:THR:HG23	2.36	0.60
1:A:177:TYR:CE2	1:A:179:VAL:HG13	2.36	0.60
1:A:398:ALA:HB2	1:A:417:TRP:CZ3	2.35	0.60
1:A:468:THR:HG21	1:A:475:LEU:N	2.16	0.60
1:A:6:ARG:HG3	1:A:7:THR:N	2.15	0.60
1:B:395:LYS:O	1:B:396:LEU:HD23	2.00	0.60
1:B:591:HIS:HB3	1:B:656:ASP:OD1	2.02	0.60
1:A:624:ASP:H	1:A:627:THR:HG22	1.66	0.60
1:A:644:MET:O	1:A:653:ARG:HD3	2.02	0.60
1:A:292:THR:HG22	1:A:293:ALA:H	1.51	0.60
1:A:611:LYS:O	1:A:640:GLU:CG	2.49	0.60
1:B:517:VAL:O	1:B:520:ARG:HB2	2.02	0.60
1:A:194:ASN:ND2	1:A:194:ASN:O	2.35	0.60
1:A:314:MET:HE2	1:A:332:THR:CG2	2.32	0.59
1:A:239:THR:HG21	1:A:560:ASP:HB3	1.83	0.59
1:B:486:ASN:HB3	1:B:489:ASN:ND2	2.16	0.59
1:B:625:GLU:C	6:B:2165:HOH:O	2.41	0.59
1:B:78:ARG:HB3	1:B:79:PRO:CD	2.25	0.59
1:B:159:ASP:O	1:B:161:GLU:CB	2.48	0.59
1:B:398:ALA:O	1:B:400:PRO:HD3	2.02	0.59
1:B:459:THR:CB	1:B:460:PRO:HD2	2.29	0.59
1:B:503:TRP:HZ3	1:B:505:CYS:SG	2.22	0.59
1:B:504:ASN:OD1	1:B:504:ASN:N	2.32	0.59
1:A:671:LYS:HD2	1:A:671:LYS:N	2.17	0.59
1:B:361:ARG:O	1:B:361:ARG:HD3	2.02	0.59
1:B:105:LEU:HD12	1:B:302:LEU:C	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASP:OD1	1:B:131:GLN:N	2.36	0.59
1:B:459:THR:HB	1:B:460:PRO:CD	2.27	0.59
1:A:618:LEU:C	1:A:618:LEU:HD12	2.23	0.59
1:A:78:ARG:HB3	1:A:79:PRO:HD2	1.84	0.59
1:B:164:ILE:CG2	1:B:165:LYS:CE	2.81	0.59
1:A:172:LYS:HG2	1:A:173:ASP:OD1	2.02	0.59
1:B:626:LYS:N	6:B:2165:HOH:O	2.35	0.59
1:B:648:ASN:ND2	1:B:650:TYR:H	2.01	0.59
1:A:703:LEU:HD12	1:A:704:GLU:N	2.17	0.59
1:B:87:VAL:HG21	1:B:307:ILE:HA	1.85	0.59
1:A:425:ARG:NH1	1:A:426:ASP:OD2	2.36	0.58
1:A:581:VAL:O	1:A:585:ILE:HG13	2.03	0.58
1:B:411:GLY:N	1:B:419:GLU:OE1	2.36	0.58
1:A:385:LEU:HD23	1:A:391:LEU:HD13	1.85	0.58
1:B:304:PHE:HE2	1:B:343:MET:HE1	1.69	0.58
1:A:670:VAL:C	1:A:671:LYS:HD2	2.24	0.58
1:B:679:TRP:CH2	1:B:715:ARG:HB2	2.39	0.58
1:A:637:PHE:CE2	1:A:661:ILE:CB	2.87	0.58
1:A:88:TYR:CD2	1:A:88:TYR:N	2.70	0.58
1:B:429:ARG:HE	1:B:478:LEU:HD13	1.68	0.58
1:A:477:ASP:HA	1:A:480:SER:HB2	1.86	0.58
1:A:297:HIS:CD2	1:A:298:LEU:HG	2.39	0.58
1:A:561:ASN:ND2	1:A:563:ILE:H	1.99	0.58
1:A:674:PHE:O	1:A:700:GLU:HA	2.02	0.58
1:A:397:ILE:HG12	1:A:418:ALA:HB3	1.86	0.58
1:B:690:ILE:HD13	1:B:690:ILE:N	2.10	0.58
1:A:425:ARG:O	1:A:429:ARG:HB2	2.03	0.57
1:A:595:ARG:NH1	1:A:595:ARG:HB2	2.19	0.57
1:B:640:GLU:OE2	1:B:715:ARG:NH2	2.37	0.57
1:A:189:LEU:H	1:A:189:LEU:HD13	1.70	0.57
1:A:449:SER:N	1:A:450:PRO:HD3	2.20	0.57
1:B:78:ARG:CB	1:B:79:PRO:HD2	2.19	0.57
1:A:316:GLN:HA	1:A:324:LEU:HD21	1.86	0.57
1:B:188:ARG:HG2	1:B:568:TRP:NE1	2.19	0.57
1:A:459:THR:CB	1:A:460:PRO:HD2	2.08	0.57
1:B:648:ASN:HD21	1:B:652:GLU:H	1.51	0.57
1:A:189:LEU:HA	1:A:196:ARG:NH2	2.19	0.57
1:A:661:ILE:HD12	1:A:661:ILE:N	2.19	0.57
1:A:88:TYR:N	1:A:88:TYR:HD2	2.02	0.57
1:B:326:PHE:CD2	1:B:370:ARG:HD2	2.40	0.57
1:A:182:LYS:HA	1:A:197:GLY:HA2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:THR:H	1:B:331:ASN:HD21	1.52	0.57
1:A:159:ASP:C	1:A:161:GLU:H	2.06	0.57
1:B:554:ASN:ND2	1:B:554:ASN:C	2.57	0.56
1:B:672:VAL:HB	6:B:2175:HOH:O	2.05	0.56
1:B:437:LEU:HD22	1:B:442:ILE:HD11	1.87	0.56
1:B:450:PRO:HG3	1:B:599:TYR:CE2	2.40	0.56
1:B:486:ASN:HB3	1:B:489:ASN:HD22	1.69	0.56
1:B:432:TRP:CH2	1:B:710:ALA:HB2	2.41	0.56
1:A:290:ASN:OD1	1:A:291:HIS:HD2	1.88	0.56
1:A:546:LEU:HD21	1:A:568:TRP:CE3	2.39	0.56
1:A:647:ILE:HG22	1:A:648:ASN:O	2.06	0.56
1:A:222:MET:HB3	1:A:223:PRO:HD2	1.87	0.56
1:A:560:ASP:OD1	1:A:565:TRP:CH2	2.51	0.56
1:A:160:ASP:CB	1:A:278:ASN:HD21	2.19	0.56
1:A:701:LYS:CG	1:A:702:GLU:H	2.18	0.56
1:B:297:HIS:O	1:B:298:LEU:HB2	2.05	0.56
1:B:559:GLN:CG	1:B:563:ILE:HD12	2.35	0.56
1:A:511:THR:HG22	1:A:513:ASP:N	2.20	0.56
1:A:565:TRP:HE3	1:A:565:TRP:N	2.03	0.56
1:A:695:ARG:O	1:A:696:ILE:CD1	2.53	0.56
1:B:222:MET:HB3	1:B:223:PRO:HD2	1.88	0.56
1:A:385:LEU:CD2	1:A:391:LEU:HD13	2.36	0.56
1:B:94:GLU:HA	1:B:321:ARG:CB	2.36	0.56
1:A:398:ALA:O	1:A:400:PRO:HD3	2.06	0.55
1:B:596:ARG:CZ	1:B:646:GLU:HG2	2.35	0.55
1:B:664:ASN:ND2	1:B:707:GLY:HA2	2.21	0.55
1:B:7:THR:HG23	1:B:7:THR:O	2.06	0.55
1:B:554:ASN:HD22	1:B:554:ASN:C	2.10	0.55
1:A:86:ARG:CG	1:A:86:ARG:NH1	2.63	0.55
1:B:13:ARG:HB3	1:B:14:PRO:HD2	1.87	0.55
1:B:305:ARG:HG3	1:B:309:ASN:OD1	2.06	0.55
1:B:633:GLN:OE1	1:B:666:ASN:HA	2.07	0.55
1:A:296:ASN:ND2	1:A:297:HIS:O	2.40	0.55
1:A:16:ASP:N	1:A:32:ASN:HD21	2.04	0.55
1:A:402:ASP:OD1	1:A:407:GLY:HA3	2.06	0.55
1:A:521:GLU:HB3	1:A:687:LEU:HD21	1.87	0.55
1:A:353:THR:HG21	1:A:390:ILE:HD13	1.89	0.55
1:A:173:ASP:HA	1:A:595:ARG:HD2	1.89	0.55
1:B:637:PHE:CZ	1:B:661:ILE:HG13	2.42	0.55
1:A:93:PRO:HB2	1:A:135:LEU:HD12	1.88	0.55
1:A:385:LEU:O	1:A:385:LEU:HD22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TYR:CE2	1:B:298:LEU:HA	2.41	0.55
1:B:185:THR:O	1:B:196:ARG:HG3	2.06	0.55
1:B:218:THR:HG22	1:B:282:GLU:HB2	1.88	0.55
1:B:372:LEU:CD1	1:B:373:TYR:CA	2.76	0.55
1:A:565:TRP:CE3	1:A:565:TRP:N	2.74	0.55
1:B:437:LEU:HB2	1:B:442:ILE:HD11	1.88	0.55
1:A:18:TYR:C	1:A:18:TYR:CD1	2.80	0.55
1:A:371:GLU:HA	1:A:371:GLU:OE2	2.06	0.55
1:A:608:MET:HG3	1:A:643:VAL:HG22	1.89	0.55
1:B:186:LYS:HD3	1:B:565:TRP:CZ2	2.42	0.55
1:B:484:LYS:HD2	1:B:486:ASN:ND2	2.22	0.55
1:A:111:LYS:HD2	1:A:350:TYR:CE1	2.41	0.54
1:A:388:ASP:O	1:A:392:SER:HB3	2.06	0.54
1:B:683:ILE:HD12	1:B:684:SER:H	1.72	0.54
1:A:208:ILE:O	1:A:212:LYS:HG2	2.06	0.54
1:A:669:ASN:N	1:A:669:ASN:ND2	2.54	0.54
1:B:191:LEU:HD23	1:B:206:GLN:NE2	2.22	0.54
1:A:186:LYS:HG2	1:A:565:TRP:NE1	2.22	0.54
1:B:103:LYS:NZ	1:B:125:GLY:N	2.48	0.54
1:B:398:ALA:HB2	1:B:417:TRP:CE3	2.42	0.54
1:B:648:ASN:C	1:B:648:ASN:ND2	2.60	0.54
1:A:423:LYS:HE2	2:A:1719:GLC:H2	1.89	0.54
1:B:292:THR:HG22	1:B:294:GLU:N	2.20	0.54
1:B:432:TRP:HH2	1:B:710:ALA:HB2	1.71	0.54
1:A:158:TRP:HA	1:A:274:ASN:ND2	2.22	0.54
1:B:315:LEU:HB3	1:B:320:LYS:HA	1.90	0.54
1:B:570:LEU:HB3	1:B:574:LYS:HB2	1.90	0.54
1:B:46:LEU:O	1:B:83:TYR:HA	2.06	0.54
1:A:222:MET:HB3	1:A:223:PRO:CD	2.38	0.54
1:A:431:PHE:CD1	1:A:442:ILE:CD1	2.90	0.54
1:B:188:ARG:O	1:B:196:ARG:HD2	2.08	0.54
1:B:94:GLU:HA	1:B:321:ARG:HB3	1.89	0.54
1:B:291:HIS:HB3	1:B:327:THR:HG21	1.90	0.54
1:B:72:VAL:HG22	1:B:73:PHE:N	2.21	0.54
1:B:194:ASN:O	1:B:195:ILE:HG22	2.08	0.54
1:A:193:GLU:CG	1:A:194:ASN:N	2.71	0.54
1:B:172:LYS:HZ3	1:B:173:ASP:CG	2.11	0.54
1:B:220:GLU:HA	1:B:284:ILE:O	2.08	0.54
1:A:77:LEU:HD23	1:A:77:LEU:N	2.23	0.53
1:B:168:LYS:O	1:B:170:PRO:HD3	2.09	0.53
1:B:623:VAL:CG1	1:B:627:THR:HG23	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLY:O	1:A:168:LYS:N	2.41	0.53
1:A:353:THR:CG2	1:A:390:ILE:HD13	2.38	0.53
1:A:666:ASN:OD1	1:A:667:PRO:HD2	2.08	0.53
1:B:191:LEU:CB	1:B:195:ILE:HD11	2.39	0.53
1:B:486:ASN:HD21	1:B:554:ASN:HD21	1.56	0.53
1:B:475:LEU:HB3	1:B:544:ASP:OD1	2.08	0.53
1:B:648:ASN:ND2	1:B:652:GLU:H	2.06	0.53
1:A:469:SER:HA	1:A:541:LEU:HG	1.89	0.53
1:B:286:ASP:OD1	1:B:361:ARG:NH1	2.41	0.53
1:B:365:ALA:HB3	1:B:413:PHE:CZ	2.44	0.53
1:B:698:GLU:O	1:B:701:LYS:HB2	2.08	0.53
1:A:103:LYS:HE3	1:A:125:GLY:CA	2.38	0.53
1:A:185:THR:HG22	1:A:207:MET:CE	2.38	0.53
1:B:612:ASP:HA	1:B:643:VAL:HG23	1.91	0.53
1:A:191:LEU:HA	6:A:2069:HOH:O	2.09	0.53
1:A:468:THR:HB	1:A:541:LEU:HD12	1.90	0.53
1:A:674:PHE:CG	1:A:697:ILE:HG21	2.44	0.53
1:B:445:ARG:NH2	1:B:451:ASP:OD1	2.42	0.53
1:B:625:GLU:N	6:B:2165:HOH:O	2.42	0.53
1:B:641:GLY:O	1:B:655:ALA:HA	2.08	0.53
1:A:400:PRO:HG3	1:A:419:GLU:CB	2.39	0.53
1:A:595:ARG:HH11	1:A:595:ARG:HB2	1.74	0.53
1:A:613:VAL:HG22	1:A:614:THR:N	2.24	0.53
1:B:521:GLU:HB3	1:B:525:ARG:NH1	2.24	0.53
1:A:70:TRP:N	1:A:70:TRP:CD1	2.76	0.52
1:A:305:ARG:NH1	1:A:323:TYR:CZ	2.77	0.52
1:B:101:PRO:HD2	1:B:137:TYR:OH	2.08	0.52
1:A:121:ASP:HB3	1:A:140:ARG:HH22	1.74	0.52
1:A:188:ARG:HG3	1:A:190:ASP:HB3	1.91	0.52
1:A:376:ASN:C	1:A:378:LEU:H	2.12	0.52
1:A:611:LYS:O	1:A:640:GLU:HG2	2.09	0.52
1:A:78:ARG:HB3	1:A:79:PRO:CD	2.39	0.52
1:B:94:GLU:H	1:B:94:GLU:CD	2.10	0.52
1:A:104:VAL:CG1	1:A:143:GLY:HA2	2.31	0.52
1:A:146:VAL:CG1	1:A:147:PRO:HD2	2.39	0.52
1:A:415:TYR:O	1:A:416:GLN:CB	2.57	0.52
1:A:682:VAL:O	1:A:683:ILE:HB	2.08	0.52
1:B:505:CYS:CB	1:B:520:ARG:HD2	2.40	0.52
1:B:624:ASP:O	1:B:627:THR:CG2	2.56	0.52
1:B:688:ARG:HD2	1:B:689:GLU:O	2.09	0.52
1:A:319:ASN:O	1:A:320:LYS:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ASP:H	1:A:32:ASN:HD21	1.56	0.52
1:B:682:VAL:HG13	1:B:683:ILE:HG22	1.92	0.52
1:B:690:ILE:HG12	1:B:695:ARG:NH2	2.24	0.52
1:A:554:ASN:ND2	1:A:554:ASN:C	2.63	0.52
1:A:292:THR:HG21	1:A:294:GLU:HG3	1.92	0.52
1:A:633:GLN:HB3	6:A:2131:HOH:O	2.08	0.52
1:A:688:ARG:NH1	1:A:706:GLU:OE2	2.43	0.52
1:B:215:GLY:O	1:B:589:ARG:NH1	2.43	0.52
1:B:484:LYS:HE2	1:B:493:ASN:ND2	2.24	0.52
1:A:184:PHE:CG	1:A:185:THR:HG23	2.45	0.52
1:A:615:PHE:O	1:A:623:VAL:HG23	2.10	0.52
1:A:233:LEU:O	1:A:238:LEU:HB2	2.11	0.51
1:A:297:HIS:C	1:A:299:GLY:H	2.14	0.51
1:A:504:ASN:ND2	1:A:507:ALA:H	2.07	0.51
1:B:47:LEU:O	1:B:57:LYS:HB3	2.10	0.51
1:B:486:ASN:HD21	1:B:554:ASN:ND2	2.08	0.51
1:A:193:GLU:O	1:A:194:ASN:HB3	2.11	0.51
1:A:36:PHE:CD1	1:A:339:ARG:HG3	2.44	0.51
1:A:617:THR:CG2	1:A:618:LEU:N	2.64	0.51
1:B:377:MET:HG2	1:B:412:ASN:O	2.11	0.51
1:B:656:ASP:OD2	1:B:657:ASP:N	2.42	0.51
1:A:290:ASN:ND2	1:A:364:LEU:HB2	2.25	0.51
1:A:464:ILE:HD13	1:A:537:THR:HB	1.92	0.51
1:A:637:PHE:CZ	1:A:661:ILE:CB	2.94	0.51
1:B:600:PHE:HB3	1:B:613:VAL:HG11	1.93	0.51
1:B:635:VAL:C	1:B:636:ILE:HG13	2.30	0.51
1:A:312:TYR:HA	1:A:340:VAL:HG21	1.92	0.51
1:B:221:LEU:CD1	1:B:221:LEU:N	2.73	0.51
1:B:656:ASP:CG	1:B:657:ASP:H	2.13	0.51
1:B:709:THR:HG22	1:B:711:LEU:CD1	2.41	0.51
1:B:437:LEU:HD22	1:B:442:ILE:CD1	2.41	0.51
1:B:521:GLU:HB3	1:B:525:ARG:HH12	1.74	0.51
1:A:643:VAL:O	1:A:643:VAL:HG12	2.11	0.51
1:A:685:SER:O	1:A:687:LEU:HD12	2.11	0.51
1:B:482:ASN:ND2	1:B:504:ASN:HD21	1.87	0.51
1:A:159:ASP:C	1:A:159:ASP:OD2	2.48	0.51
1:A:177:TYR:O	1:A:179:VAL:HG22	2.11	0.51
1:A:182:LYS:HA	1:A:197:GLY:CA	2.40	0.51
1:B:165:LYS:HD3	1:B:165:LYS:H	1.75	0.51
1:B:624:ASP:N	1:B:627:THR:HG21	2.26	0.51
1:A:185:THR:HG22	1:A:207:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:PHE:O	1:A:580:PHE:N	2.42	0.50
1:A:218:THR:HG22	1:A:282:GLU:CB	2.37	0.50
1:B:372:LEU:CD1	1:B:373:TYR:HA	2.39	0.50
1:B:414:PRO:HB2	1:B:417:TRP:CD1	2.47	0.50
1:B:449:SER:N	1:B:450:PRO:CD	2.74	0.50
1:B:187:LEU:CD2	1:B:565:TRP:CD1	2.94	0.50
1:A:126:TYR:OH	1:A:298:LEU:HA	2.10	0.50
1:A:160:ASP:HB3	1:A:278:ASN:ND2	2.26	0.50
1:A:161:GLU:HG3	1:A:164:ILE:CG2	2.41	0.50
1:A:264:GLY:O	1:A:268:SER:HB2	2.11	0.50
1:B:482:ASN:OD1	1:B:504:ASN:OD1	2.28	0.50
1:B:191:LEU:HB3	1:B:192:PRO:HD2	1.94	0.50
1:B:105:LEU:HA	1:B:302:LEU:O	2.12	0.50
1:B:530:THR:O	1:B:533:VAL:HG12	2.12	0.50
1:A:189:LEU:CD1	1:A:189:LEU:N	2.69	0.50
1:A:650:TYR:HA	1:B:13:ARG:HD3	1.93	0.50
1:B:153:ASN:ND2	1:B:155:TYR:H	2.09	0.50
1:B:6:ARG:C	1:B:8:ARG:H	2.13	0.50
1:A:292:THR:HG23	1:A:293:ALA:H	1.76	0.50
1:A:87:VAL:HG21	1:A:307:ILE:HA	1.94	0.50
1:A:660:LEU:HB2	1:A:679:TRP:CZ3	2.47	0.50
1:B:285:ILE:O	1:B:285:ILE:HG13	2.12	0.50
1:A:193:GLU:HA	1:A:196:ARG:HD2	1.93	0.50
1:A:636:ILE:HD11	1:A:672:VAL:HG11	1.93	0.50
1:B:187:LEU:CD2	1:B:565:TRP:CB	2.78	0.50
1:B:694:GLU:HG2	1:B:703:LEU:HD11	1.93	0.50
1:A:222:MET:O	1:A:224:VAL:HG13	2.11	0.50
1:A:292:THR:CG2	1:A:294:GLU:H	2.16	0.50
1:A:369:ALA:CB	1:A:377:MET:HE2	2.41	0.50
1:B:126:TYR:OH	1:B:298:LEU:HA	2.11	0.50
1:B:442:ILE:O	1:B:446:LEU:HG	2.11	0.50
1:B:521:GLU:HB2	1:B:687:LEU:HD11	1.94	0.50
1:A:122:ALA:O	1:A:142:SER:HB3	2.12	0.50
1:A:189:LEU:HA	1:A:196:ARG:CZ	2.42	0.50
1:A:7:THR:HG22	4:A:1723:SO4:S	2.52	0.49
1:A:303:SER:O	1:A:307:ILE:CD1	2.44	0.49
1:A:78:ARG:CB	1:A:79:PRO:CD	2.90	0.49
1:A:24:TRP:CD2	1:A:79:PRO:HD3	2.46	0.49
1:B:350:TYR:O	1:B:354:GLU:CB	2.60	0.49
1:B:503:TRP:O	1:B:505:CYS:N	2.44	0.49
1:A:190:ASP:OD2	1:A:206:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLU:O	1:A:305:ARG:NH2	2.45	0.49
1:A:635:VAL:O	1:A:636:ILE:HG13	2.11	0.49
1:B:146:VAL:HG13	1:B:147:PRO:HD2	1.93	0.49
1:B:654:ILE:O	1:B:655:ALA:HB3	2.12	0.49
1:B:96:GLY:CA	1:B:320:LYS:O	2.60	0.49
1:A:530:THR:O	1:A:533:VAL:HG12	2.12	0.49
1:B:160:ASP:O	1:B:162:ASP:N	2.42	0.49
1:B:565:TRP:CE3	1:B:565:TRP:N	2.80	0.49
1:B:682:VAL:HG13	1:B:683:ILE:N	2.28	0.49
1:A:568:TRP:O	1:A:570:LEU:HG	2.13	0.49
1:B:111:LYS:HD2	1:B:350:TYR:CZ	2.46	0.49
1:B:261:CYS:HA	1:B:265:GLN:OE1	2.13	0.49
1:B:415:TYR:O	1:B:415:TYR:CD2	2.65	0.49
1:A:191:LEU:HB3	1:A:192:PRO:HD2	1.95	0.49
1:A:199:TYR:CZ	1:A:256:TYR:HB2	2.47	0.49
1:A:592:PRO:C	1:A:594:PHE:H	2.15	0.49
1:B:637:PHE:CE2	1:B:661:ILE:CB	2.93	0.49
1:A:630:SER:HB2	1:A:631:PRO:HD2	1.95	0.49
1:A:648:ASN:ND2	1:A:652:GLU:HB2	2.24	0.49
1:B:123:VAL:HG12	1:B:142:SER:HB2	1.94	0.49
1:A:10:ARG:NH1	1:A:10:ARG:CG	2.63	0.49
1:A:224:VAL:O	1:A:252:PRO:HA	2.13	0.49
1:A:682:VAL:CG2	1:A:683:ILE:HG13	2.42	0.49
1:A:357:VAL:HG12	1:A:359:GLY:H	1.78	0.49
1:A:376:ASN:ND2	1:A:378:LEU:H	2.10	0.49
1:A:584:MET:SD	1:A:683:ILE:HD13	2.53	0.49
1:A:132:ASN:O	1:A:133:GLN:C	2.52	0.48
1:A:183:GLY:O	1:A:566:PHE:CD1	2.66	0.48
1:A:617:THR:O	1:A:619:GLU:O	2.31	0.48
1:B:245:ASP:OD1	1:B:293:ALA:HA	2.12	0.48
1:B:16:ASP:N	1:B:32:ASN:HD21	2.05	0.48
1:B:431:PHE:CE2	1:B:665:ALA:HB2	2.48	0.48
1:B:669:ASN:HD22	1:B:669:ASN:N	2.10	0.48
1:A:377:MET:HG3	1:A:412:ASN:O	2.13	0.48
1:B:135:LEU:HG	1:B:321:ARG:HH12	1.71	0.48
1:B:334:ASN:CG	1:B:334:ASN:O	2.52	0.48
1:A:444:ASN:HD22	1:A:451:ASP:CG	2.17	0.48
1:A:709:THR:HG22	1:A:711:LEU:HD11	1.95	0.48
1:B:433:ARG:HG2	1:B:433:ARG:O	2.12	0.48
1:B:397:ILE:HG22	1:B:398:ALA:N	2.28	0.48
1:A:160:ASP:HB2	1:A:278:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ASN:O	1:B:457:ASN:CB	2.58	0.48
1:B:679:TRP:CE3	1:B:715:ARG:HB2	2.48	0.48
1:B:415:TYR:C	1:B:417:TRP:H	2.17	0.48
1:B:96:GLY:HA2	1:B:320:LYS:O	2.12	0.48
1:A:484:LYS:O	1:A:484:LYS:HD2	2.13	0.48
1:A:120:ASN:C	1:A:122:ALA:H	2.17	0.48
1:A:35:LEU:HD22	1:A:85:TYR:CD2	2.47	0.48
1:A:437:LEU:CB	1:A:438:PRO:HD2	2.37	0.48
1:B:290:ASN:ND2	1:B:364:LEU:HB2	2.28	0.48
1:B:460:PRO:O	1:B:536:GLY:HA2	2.14	0.48
1:A:424:TYR:HA	1:A:445:ARG:HD3	1.95	0.48
1:A:222:MET:CE	1:A:470:HIS:HB3	2.44	0.48
1:A:511:THR:CG2	1:A:512:ASN:N	2.76	0.48
1:A:138:ASP:OD1	1:A:138:ASP:C	2.51	0.48
1:A:24:TRP:CZ2	1:A:26:GLU:HA	2.49	0.48
1:A:400:PRO:O	1:A:409:GLN:HB2	2.14	0.48
1:A:682:VAL:HG22	1:A:682:VAL:O	2.12	0.48
1:B:402:ASP:OD1	1:B:402:ASP:N	2.47	0.48
1:A:250:PHE:CE2	1:A:347:SER:HA	2.49	0.47
1:B:513:ASP:C	1:B:513:ASP:OD2	2.52	0.47
1:A:108:PRO:HA	6:A:2085:HOH:O	2.13	0.47
1:A:134:ASP:HB3	1:A:298:LEU:HD23	1.95	0.47
1:A:186:LYS:HG2	1:A:565:TRP:CE2	2.49	0.47
1:A:379:ASN:ND2	1:A:381:PHE:HB3	2.26	0.47
1:A:415:TYR:HB2	6:B:2101:HOH:O	2.14	0.47
1:B:565:TRP:CE3	1:B:565:TRP:CA	2.97	0.47
1:B:350:TYR:O	1:B:354:GLU:HB3	2.14	0.47
1:A:133:GLN:C	1:A:135:LEU:H	2.16	0.47
1:B:103:LYS:HD3	1:B:103:LYS:N	2.28	0.47
1:B:172:LYS:HG2	1:B:595:ARG:O	2.14	0.47
1:B:232:PHE:CD1	1:B:233:LEU:HD13	2.50	0.47
1:A:364:LEU:HD22	1:A:402:ASP:HA	1.95	0.47
1:A:682:VAL:O	1:A:683:ILE:CB	2.62	0.47
1:B:415:TYR:O	1:B:415:TYR:HD2	1.97	0.47
1:A:17:PRO:HG3	1:A:66:THR:HB	1.96	0.47
1:B:193:GLU:O	1:B:194:ASN:OD1	2.33	0.47
1:B:437:LEU:CD1	1:B:437:LEU:N	2.78	0.47
1:A:127:LYS:HB3	1:A:130:ASP:HB2	1.97	0.47
1:A:430:ARG:O	1:A:435:GLU:HB2	2.15	0.47
1:B:180:HIS:O	1:B:181:VAL:C	2.51	0.47
1:B:397:ILE:CG2	1:B:464:ILE:CD1	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:LYS:HA	1:B:611:LYS:HA	1.96	0.47
1:A:112:ALA:HB1	1:A:265:GLN:NE2	2.30	0.47
1:A:211:LEU:HB3	1:A:216:ILE:HD11	1.96	0.47
1:A:160:ASP:HB3	1:A:278:ASN:HD21	1.79	0.47
1:A:547:SER:HA	6:A:2139:HOH:O	2.15	0.47
1:B:153:ASN:C	1:B:153:ASN:ND2	2.62	0.47
1:B:164:ILE:CG2	1:B:165:LYS:HE3	2.44	0.47
1:B:514:GLN:C	1:B:516:VAL:H	2.18	0.47
1:B:689:GLU:O	1:B:689:GLU:HG3	2.13	0.47
1:A:161:GLU:HG3	1:A:164:ILE:HG21	1.96	0.47
1:A:202:LEU:HD11	1:A:221:LEU:CD2	2.45	0.47
1:A:202:LEU:HD11	1:A:221:LEU:HD21	1.96	0.47
1:A:92:LYS:HE3	1:A:95:LEU:HD12	1.96	0.47
1:A:94:GLU:H	1:A:94:GLU:CD	2.18	0.47
1:B:103:LYS:HE3	1:B:125:GLY:HA2	1.97	0.47
1:A:398:ALA:HB2	1:A:417:TRP:HE3	1.75	0.47
1:B:468:THR:HG22	1:B:541:LEU:CB	2.44	0.47
1:A:193:GLU:HG2	1:A:194:ASN:N	2.31	0.46
1:A:146:VAL:HG13	1:A:147:PRO:HD2	1.97	0.46
1:A:210:TYR:OH	1:A:545:GLU:OE1	2.25	0.46
1:B:153:ASN:HD22	1:B:154:PRO:CD	2.27	0.46
1:B:688:ARG:NH1	1:B:706:GLU:OE2	2.38	0.46
1:A:562:GLU:N	1:A:562:GLU:OE1	2.48	0.46
1:B:290:ASN:OD1	1:B:291:HIS:HD2	1.99	0.46
1:A:30:GLY:HA3	1:A:73:PHE:CZ	2.51	0.46
1:A:561:ASN:O	1:A:565:TRP:CD2	2.69	0.46
1:B:193:GLU:H	1:B:196:ARG:NH1	2.13	0.46
1:A:204:SER:O	1:A:208:ILE:HG12	2.16	0.46
1:A:177:TYR:HE2	1:A:179:VAL:HG13	1.79	0.46
1:A:225:PHE:HD1	1:A:225:PHE:N	2.14	0.46
1:A:561:ASN:ND2	1:A:563:ILE:HG13	2.31	0.46
1:B:476:GLU:HB3	1:B:548:ARG:O	2.15	0.46
1:B:561:ASN:O	1:B:565:TRP:CD2	2.69	0.46
1:B:183:GLY:O	1:B:566:PHE:HB2	2.15	0.46
1:A:399:GLU:HA	1:A:400:PRO:HD3	1.72	0.46
1:A:419:GLU:CD	1:A:453:TYR:HE2	2.18	0.46
1:B:360:PHE:N	1:B:360:PHE:CD1	2.83	0.46
1:B:397:ILE:CG2	1:B:464:ILE:HD12	2.45	0.46
1:A:565:TRP:CA	1:A:565:TRP:CE3	2.99	0.46
1:A:199:TYR:O	1:A:202:LEU:N	2.47	0.46
1:A:225:PHE:CD1	1:A:225:PHE:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:PHE:HE2	1:A:661:ILE:CG2	2.29	0.46
1:A:714:ARG:HH11	1:A:714:ARG:HG3	1.81	0.46
1:B:180:HIS:O	1:B:182:LYS:N	2.49	0.46
1:B:673:LYS:CE	1:B:700:GLU:HB3	2.46	0.46
1:A:159:ASP:C	1:A:161:GLU:N	2.69	0.45
1:A:634:LEU:HD12	1:A:670:VAL:HG21	1.97	0.45
1:A:6:ARG:HG2	1:A:8:ARG:CG	2.46	0.45
1:B:247:ILE:HD12	1:B:247:ILE:N	2.17	0.45
1:B:425:ARG:HG2	1:B:429:ARG:NH1	2.31	0.45
1:B:503:TRP:C	1:B:505:CYS:H	2.19	0.45
1:B:682:VAL:HG12	1:B:712:VAL:C	2.36	0.45
1:A:314:MET:HE2	1:A:332:THR:HG21	1.97	0.45
1:A:619:GLU:HG2	1:A:620:GLY:H	1.80	0.45
1:A:636:ILE:HG12	1:A:662:ILE:HG12	1.99	0.45
1:B:530:THR:HA	1:B:533:VAL:HG12	1.98	0.45
1:B:624:ASP:C	6:B:2165:HOH:O	2.55	0.45
1:B:672:VAL:HG21	1:B:705:ILE:HD12	1.97	0.45
1:B:683:ILE:HG22	1:B:712:VAL:HB	1.98	0.45
1:A:443:ALA:HB1	1:A:615:PHE:CZ	2.51	0.45
1:B:532:LEU:HD12	1:B:584:MET:HB3	1.98	0.45
1:B:624:ASP:N	1:B:627:THR:CG2	2.80	0.45
1:A:134:ASP:OD1	1:A:134:ASP:C	2.55	0.45
1:A:232:PHE:O	1:A:236:LYS:HD2	2.16	0.45
1:A:606:PHE:CE1	1:A:653:ARG:HD3	2.52	0.45
1:B:217:THR:OG1	1:B:218:THR:HG23	2.16	0.45
1:B:681:LEU:C	1:B:681:LEU:HD13	2.36	0.45
1:A:161:GLU:O	1:A:161:GLU:CG	2.63	0.45
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.77	0.45
1:B:103:LYS:HZ2	1:B:125:GLY:N	2.06	0.45
1:B:523:GLN:NE2	1:B:708:ARG:HB3	2.32	0.45
1:B:55:TYR:CD2	1:B:55:TYR:N	2.83	0.45
1:B:162:ASP:O	1:B:163:PHE:HD2	1.99	0.45
1:B:294:GLU:HB3	1:B:305:ARG:NH1	2.31	0.45
1:B:297:HIS:C	1:B:299:GLY:H	2.20	0.45
1:B:604:LYS:HD3	1:B:609:PRO:O	2.17	0.45
1:A:209:SER:O	1:A:213:ASP:OD2	2.34	0.45
1:A:695:ARG:O	1:A:696:ILE:HG13	2.17	0.45
1:B:186:LYS:HG2	1:B:565:TRP:CE2	2.52	0.45
1:A:314:MET:HE2	1:A:332:THR:HG22	1.97	0.45
1:A:466:TYR:HD2	1:A:468:THR:O	2.00	0.45
1:A:554:ASN:C	1:A:554:ASN:HD22	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASN:ND2	1:B:154:PRO:HD2	2.32	0.45
1:B:160:ASP:O	1:B:162:ASP:OD1	2.35	0.45
1:B:398:ALA:HB2	1:B:417:TRP:HZ3	1.79	0.45
1:A:242:TRP:HB3	1:A:244:TYR:CD1	2.52	0.45
1:A:695:ARG:O	1:A:696:ILE:CG1	2.65	0.45
1:A:265:GLN:HG2	1:A:266:VAL:N	2.31	0.44
1:A:596:ARG:HE	1:A:646:GLU:HG2	1.82	0.44
1:B:108:PRO:HB2	1:B:343:MET:HE2	1.99	0.44
1:B:365:ALA:HB3	1:B:413:PHE:HZ	1.82	0.44
1:A:205:GLU:O	1:A:206:GLN:C	2.54	0.44
1:A:184:PHE:CE2	1:A:207:MET:HE2	2.52	0.44
1:A:247:ILE:O	1:A:247:ILE:HG13	2.17	0.44
1:A:441:GLU:O	1:A:445:ARG:HG2	2.17	0.44
1:A:5:PHE:N	1:A:5:PHE:CD1	2.86	0.44
1:B:425:ARG:CD	1:B:429:ARG:NH1	2.81	0.44
1:A:266:VAL:O	1:A:270:LYS:HG3	2.18	0.44
1:A:415:TYR:O	1:A:416:GLN:HB3	2.17	0.44
1:A:233:LEU:HD21	1:A:558:CYS:HB3	1.99	0.44
1:A:596:ARG:HD3	1:A:600:PHE:CE1	2.52	0.44
1:A:72:VAL:HG22	1:A:73:PHE:N	2.32	0.44
1:B:105:LEU:HD12	1:B:302:LEU:O	2.17	0.44
1:B:177:TYR:CD2	1:B:179:VAL:CG2	3.00	0.44
1:B:296:ASN:O	1:B:305:ARG:NH2	2.51	0.44
1:A:111:LYS:HB2	1:A:152:ILE:HD13	2.00	0.44
1:A:141:ASP:HB2	6:A:2032:HOH:O	2.17	0.44
1:A:326:PHE:O	1:A:403:VAL:CG2	2.57	0.44
1:B:261:CYS:HB2	1:B:265:GLN:CD	2.38	0.44
1:B:369:ALA:HB3	1:B:375:VAL:HG13	1.98	0.44
1:B:565:TRP:HE3	1:B:565:TRP:N	2.14	0.44
1:B:187:LEU:HD12	1:B:187:LEU:HA	1.77	0.44
1:B:375:VAL:HG11	1:B:409:GLN:HG3	1.99	0.44
1:B:397:ILE:HG12	1:B:464:ILE:HD11	1.98	0.44
1:A:25:ILE:O	1:A:25:ILE:HG22	2.18	0.44
1:A:438:PRO:CA	1:A:631:PRO:HA	2.43	0.44
1:A:634:LEU:O	1:A:634:LEU:CD2	2.63	0.44
1:B:158:TRP:HE3	1:B:161:GLU:HG2	1.82	0.44
1:B:276:LEU:HD13	1:B:283:VAL:HG22	2.00	0.44
1:B:661:ILE:HD12	1:B:712:VAL:HG22	1.99	0.44
1:A:20:LEU:HA	1:A:34:SER:HB3	1.98	0.44
1:A:467:VAL:HG23	1:A:468:THR:N	2.32	0.44
1:A:579:GLU:OE2	1:A:583:LYS:NZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PHE:CE1	1:B:271:LYS:HG2	2.52	0.44
1:B:207:MET:HB3	1:B:207:MET:HE2	1.79	0.44
1:B:218:THR:CG2	1:B:282:GLU:HB2	2.47	0.44
1:B:454:LEU:O	1:B:454:LEU:HD12	2.18	0.44
1:A:242:TRP:HB3	1:A:244:TYR:HD1	1.83	0.44
1:A:6:ARG:HD2	4:A:1723:SO4:O3	2.18	0.44
1:B:158:TRP:CE3	1:B:161:GLU:HG2	2.53	0.44
1:B:285:ILE:HG12	1:B:357:VAL:HG11	1.99	0.44
1:B:367:ALA:HA	1:B:370:ARG:HG3	1.99	0.44
1:A:504:ASN:CB	1:A:507:ALA:O	2.65	0.44
1:B:194:ASN:C	1:B:195:ILE:CG2	2.87	0.44
1:A:141:ASP:OD1	1:A:141:ASP:C	2.56	0.43
1:A:253:GLU:OE2	1:A:253:GLU:HA	2.18	0.43
1:A:290:ASN:ND2	1:A:363:ASP:O	2.51	0.43
1:B:164:ILE:HG23	1:B:165:LYS:CE	2.43	0.43
1:B:290:ASN:ND2	1:B:363:ASP:O	2.51	0.43
1:B:400:PRO:O	1:B:401:TRP:HB3	2.18	0.43
1:B:464:ILE:HG22	1:B:464:ILE:O	2.18	0.43
1:B:541:LEU:HD13	1:B:542:GLY:O	2.18	0.43
1:A:532:LEU:HD12	1:A:584:MET:HB3	2.00	0.43
1:A:637:PHE:CE2	1:A:661:ILE:HG21	2.52	0.43
1:A:35:LEU:HD22	1:A:85:TYR:CE2	2.53	0.43
1:B:107:ASP:C	1:B:107:ASP:OD1	2.57	0.43
1:B:357:VAL:HG12	1:B:359:GLY:H	1.83	0.43
1:B:476:GLU:O	1:B:480:SER:HB2	2.18	0.43
1:A:177:TYR:HE2	1:A:179:VAL:CG1	2.31	0.43
1:A:311:ALA:HA	6:A:2097:HOH:O	2.18	0.43
1:A:500:ASN:O	1:A:501:TYR:C	2.56	0.43
1:B:514:GLN:C	1:B:516:VAL:N	2.71	0.43
1:A:6:ARG:HG2	1:A:8:ARG:HG2	2.00	0.43
1:B:230:GLN:HE22	3:B:1720:A16:C6B	2.31	0.43
1:B:379:ASN:O	1:B:383:ILE:HG13	2.18	0.43
1:B:666:ASN:CG	1:B:667:PRO:HD2	2.37	0.43
1:B:504:ASN:CG	1:B:507:ALA:O	2.57	0.43
1:A:126:TYR:OH	1:A:298:LEU:CA	2.67	0.43
1:A:449:SER:N	1:A:450:PRO:CD	2.81	0.43
1:B:596:ARG:HE	1:B:646:GLU:CG	2.32	0.43
1:A:126:TYR:CE2	1:A:298:LEU:HA	2.53	0.43
1:A:28:ASP:O	1:A:29:ASP:C	2.55	0.43
1:B:253:GLU:OE1	1:B:255:ARG:HB3	2.19	0.43
1:B:541:LEU:O	1:B:542:GLY:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:TRP:CE3	1:B:565:TRP:HA	2.53	0.43
1:B:439:TYR:CE2	1:B:623:VAL:HG21	2.53	0.43
1:A:357:VAL:CG1	1:A:358:ASP:N	2.82	0.43
1:A:561:ASN:HD21	1:A:563:ILE:HB	1.83	0.43
1:A:691:LYS:HB3	1:A:693:GLU:OE2	2.18	0.43
1:B:106:ILE:HA	6:B:2058:HOH:O	2.19	0.43
1:B:189:LEU:CD1	1:B:189:LEU:H	2.20	0.43
1:B:39:ASN:ND2	1:B:310:THR:OG1	2.52	0.43
1:B:461:PHE:HE1	1:B:597:GLU:HG3	1.84	0.43
1:B:486:ASN:O	1:B:487:GLU:C	2.56	0.43
1:B:608:MET:HB3	1:B:609:PRO:HD2	2.01	0.43
1:A:105:LEU:HA	1:A:302:LEU:O	2.18	0.43
1:A:659:PHE:HA	1:A:713:TYR:O	2.18	0.43
1:B:478:LEU:HD12	1:B:478:LEU:O	2.18	0.43
1:B:73:PHE:O	1:B:75:PRO:HD3	2.18	0.43
1:A:169:VAL:HA	1:A:170:PRO:HD2	1.83	0.43
1:A:334:ASN:HB3	6:A:2097:HOH:O	2.17	0.43
1:A:109:TYR:CE1	1:A:343:MET:HG3	2.54	0.43
1:A:583:LYS:HE2	1:A:583:LYS:HB2	1.91	0.43
1:A:673:LYS:HG2	1:A:700:GLU:O	2.19	0.43
1:B:164:ILE:C	1:B:165:LYS:HD3	2.39	0.43
1:B:222:MET:CE	1:B:470:HIS:HB3	2.49	0.43
1:B:291:HIS:CG	1:B:329:THR:HG1	2.37	0.43
1:B:379:ASN:HD21	1:B:382:PHE:H	1.67	0.43
1:A:222:MET:HE1	1:A:470:HIS:HB3	1.99	0.42
1:A:267:LEU:HD11	1:A:271:LYS:HE2	2.00	0.42
1:A:96:GLY:HA2	1:A:320:LYS:O	2.18	0.42
1:B:141:ASP:OD2	1:B:141:ASP:C	2.56	0.42
1:B:159:ASP:OD1	1:B:160:ASP:N	2.51	0.42
1:B:434:GLY:O	1:B:435:GLU:C	2.56	0.42
1:A:476:GLU:O	1:A:480:SER:HB2	2.19	0.42
1:A:65:LYS:HD2	1:A:70:TRP:CE2	2.54	0.42
1:B:174:THR:HG22	1:B:175:VAL:N	2.34	0.42
1:B:541:LEU:HD22	1:B:542:GLY:N	2.34	0.42
1:B:718:LEU:C	1:B:718:LEU:CD2	2.87	0.42
1:A:127:LYS:HD2	1:A:138:ASP:HA	2.00	0.42
1:A:480:SER:O	1:A:481:TYR:CG	2.72	0.42
1:A:504:ASN:O	1:A:505:CYS:HB2	2.19	0.42
1:A:588:TYR:CZ	1:A:595:ARG:HG2	2.54	0.42
1:B:257:SER:OG	1:B:260:GLY:O	2.31	0.42
1:B:351:TRP:O	1:B:357:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:C	1:B:8:ARG:N	2.72	0.42
1:A:46:LEU:HD11	1:A:86:ARG:HD2	2.00	0.42
1:A:446:LEU:HD11	1:A:663:LEU:HD12	2.01	0.42
1:B:325:ASP:OD1	1:B:328:GLY:N	2.43	0.42
1:B:636:ILE:CG1	1:B:662:ILE:HD13	2.44	0.42
1:B:690:ILE:H	1:B:690:ILE:CD1	2.02	0.42
1:A:377:MET:CE	1:A:409:GLN:HG3	2.46	0.42
1:A:414:PRO:HG2	1:A:417:TRP:CD1	2.55	0.42
1:A:623:VAL:CG1	1:A:628:TRP:HB2	2.50	0.42
1:A:696:ILE:HG22	1:A:697:ILE:N	2.34	0.42
1:B:177:TYR:O	1:B:179:VAL:HG23	2.20	0.42
1:B:194:ASN:ND2	1:B:195:ILE:CG2	2.82	0.42
1:B:361:ARG:C	1:B:361:ARG:HD3	2.39	0.42
1:B:617:THR:O	1:B:618:LEU:C	2.57	0.42
1:A:216:ILE:C	1:A:216:ILE:HD12	2.40	0.42
1:A:266:VAL:HG23	1:A:270:LYS:HE3	2.02	0.42
1:A:450:PRO:HG3	1:A:599:TYR:CD2	2.54	0.42
1:A:677:GLY:O	1:A:679:TRP:CD1	2.72	0.42
1:B:292:THR:CG2	1:B:293:ALA:H	2.30	0.42
1:B:601:GLN:O	1:B:612:ASP:OD1	2.36	0.42
1:B:659:PHE:HA	1:B:713:TYR:O	2.19	0.42
1:A:133:GLN:HB2	1:A:298:LEU:CD2	2.50	0.42
1:A:13:ARG:HH12	1:A:28:ASP:HB3	1.84	0.42
1:A:297:HIS:O	1:A:298:LEU:HB2	2.20	0.42
1:A:312:TYR:N	6:A:2097:HOH:O	2.51	0.42
1:A:504:ASN:HD22	1:A:507:ALA:H	1.59	0.42
1:A:596:ARG:HE	1:A:646:GLU:CG	2.32	0.42
1:A:86:ARG:NH1	1:A:86:ARG:HG2	2.33	0.42
1:B:158:TRP:CD2	1:B:356:HIS:CE1	3.07	0.42
1:B:370:ARG:HA	1:B:374:SER:O	2.19	0.42
1:A:242:TRP:CD2	1:A:557:PHE:HA	2.55	0.42
1:A:613:VAL:HG23	1:A:639:LEU:HD23	2.01	0.42
1:A:711:LEU:HB3	1:A:713:TYR:HE1	1.84	0.42
1:B:290:ASN:OD1	1:B:291:HIS:CD2	2.73	0.42
1:B:134:ASP:OD2	1:B:297:HIS:HD2	2.01	0.42
1:A:244:TYR:CD2	3:A:1722:A16:H2C	2.55	0.42
1:A:209:SER:O	1:A:213:ASP:CG	2.58	0.42
1:A:468:THR:O	1:A:469:SER:HB2	2.20	0.42
2:A:1721:GLC:O1	2:B:1719:GLC:H61	2.20	0.42
1:B:33:PHE:O	1:B:71:HIS:HA	2.20	0.42
1:A:485:HIS:HE1	1:A:508:GLU:OE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LYS:HD3	6:A:2174:HOH:O	2.20	0.42
1:A:709:THR:HG22	1:A:711:LEU:CD1	2.49	0.42
1:B:191:LEU:CB	1:B:192:PRO:HD2	2.48	0.42
1:B:638:VAL:CG2	1:B:660:LEU:HD13	2.49	0.42
1:A:158:TRP:HA	1:A:274:ASN:HD21	1.83	0.41
1:A:168:LYS:HB2	1:A:168:LYS:HE3	1.44	0.41
1:A:184:PHE:CD2	1:A:185:THR:CG2	3.01	0.41
1:A:222:MET:O	1:A:223:PRO:C	2.58	0.41
1:A:543:GLY:O	1:A:546:LEU:N	2.42	0.41
1:B:453:TYR:O	1:B:458:LYS:HB2	2.20	0.41
1:B:681:LEU:HD22	1:B:682:VAL:N	2.34	0.41
1:B:90:PRO:HG2	1:B:97:LEU:HD13	2.01	0.41
1:A:182:LYS:O	1:A:184:PHE:N	2.53	0.41
1:A:198:THR:CB	1:A:256:TYR:O	2.66	0.41
1:A:316:GLN:O	1:A:320:LYS:N	2.47	0.41
1:A:419:GLU:HG3	1:A:453:TYR:CE2	2.55	0.41
1:A:661:ILE:CD1	1:A:661:ILE:N	2.83	0.41
1:A:716:ILE:O	1:A:717:GLU:HB2	2.19	0.41
1:B:39:ASN:ND2	1:B:308:ASP:OD2	2.44	0.41
1:A:529:ILE:HD12	1:A:710:ALA:HB3	2.02	0.41
1:B:20:LEU:HB2	1:B:109:TYR:CD2	2.55	0.41
1:B:232:PHE:O	1:B:236:LYS:HD2	2.20	0.41
1:A:228:ILE:CG2	1:A:229:ASP:N	2.83	0.41
1:A:357:VAL:HG12	1:A:358:ASP:N	2.33	0.41
1:A:487:GLU:HG3	1:A:493:ASN:HB2	2.02	0.41
1:B:232:PHE:CD1	1:B:232:PHE:C	2.92	0.41
1:B:661:ILE:HD13	1:B:712:VAL:HG22	2.00	0.41
1:A:120:ASN:C	1:A:122:ALA:N	2.71	0.41
1:A:291:HIS:HB3	1:A:327:THR:HG21	2.02	0.41
1:A:703:LEU:HA	6:A:2207:HOH:O	2.21	0.41
1:B:174:THR:HG23	1:B:218:THR:HG23	2.01	0.41
1:B:308:ASP:O	1:B:312:TYR:HD1	2.04	0.41
1:B:335:LEU:O	1:B:341:ILE:HD11	2.20	0.41
1:A:376:ASN:C	1:A:378:LEU:N	2.74	0.41
1:A:613:VAL:HA	1:A:638:VAL:O	2.21	0.41
1:A:636:ILE:CD1	1:A:672:VAL:HG11	2.50	0.41
1:B:221:LEU:HD13	1:B:221:LEU:N	2.36	0.41
1:B:372:LEU:O	1:B:372:LEU:CD1	2.67	0.41
1:B:524:LYS:NZ	1:B:547:SER:HB3	2.36	0.41
1:A:232:PHE:C	1:A:232:PHE:CD1	2.94	0.41
1:A:225:PHE:CD2	1:A:249:PHE:HD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:THR:CB	1:A:460:PRO:CD	2.72	0.41
1:A:460:PRO:O	1:A:536:GLY:HA2	2.21	0.41
1:A:611:LYS:O	1:A:640:GLU:HG3	2.19	0.41
1:A:638:VAL:CG2	1:A:660:LEU:HD13	2.51	0.41
1:B:152:ILE:HD13	6:B:2009:HOH:O	2.21	0.41
1:B:541:LEU:C	1:B:541:LEU:HD22	2.41	0.41
1:B:202:LEU:HD23	1:B:202:LEU:C	2.41	0.41
1:B:296:ASN:C	1:B:296:ASN:HD22	2.24	0.41
1:B:314:MET:CG	1:B:334:ASN:CB	2.93	0.41
1:B:445:ARG:HA	1:B:445:ARG:HE	1.86	0.41
1:B:578:LEU:O	1:B:582:LYS:HG3	2.21	0.41
1:A:160:ASP:CB	1:A:278:ASN:ND2	2.83	0.41
1:A:16:ASP:HA	1:A:17:PRO:HD3	1.89	0.41
1:A:371:GLU:O	1:A:372:LEU:HD22	2.21	0.41
1:B:242:TRP:HB3	1:B:244:TYR:CD1	2.55	0.41
1:A:135:LEU:HA	1:A:135:LEU:HD12	1.77	0.41
1:A:337:HIS:HB2	6:A:2097:HOH:O	2.19	0.41
1:B:400:PRO:CA	1:B:413:PHE:HE1	2.29	0.41
1:A:267:LEU:HD13	1:A:271:LYS:HE2	1.99	0.41
1:A:396:LEU:HG	1:A:416:GLN:NE2	2.36	0.41
1:A:571:ASP:OD1	1:A:574:LYS:HG3	2.21	0.41
1:B:295:GLY:O	1:B:331:ASN:HB3	2.21	0.41
1:B:600:PHE:CZ	1:B:639:LEU:HD22	2.56	0.41
1:B:672:VAL:CG2	1:B:705:ILE:HD12	2.50	0.41
1:A:100:ASN:HB3	1:A:103:LYS:HG2	2.03	0.40
1:A:124:PHE:C	1:A:126:TYR:H	2.25	0.40
1:A:154:PRO:O	5:A:1724:GOL:H2	2.21	0.40
1:A:391:LEU:C	1:A:393:GLN:H	2.23	0.40
1:A:550:GLN:NE2	1:A:556:ALA:CB	2.84	0.40
1:A:575:SER:O	1:A:578:LEU:HB3	2.20	0.40
1:B:187:LEU:HB2	6:B:2069:HOH:O	2.20	0.40
1:B:18:TYR:HA	1:B:19:PRO:HA	1.73	0.40
1:B:335:LEU:CD1	1:B:335:LEU:N	2.83	0.40
1:B:525:ARG:NH1	1:B:687:LEU:HD21	2.36	0.40
1:B:101:PRO:HD2	1:B:137:TYR:HH	1.85	0.40
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.81	0.40
1:B:646:GLU:O	1:B:653:ARG:HA	2.21	0.40
1:B:718:LEU:C	1:B:718:LEU:HD22	2.41	0.40
1:A:385:LEU:HD23	1:A:391:LEU:CD1	2.48	0.40
1:A:514:GLN:O	1:A:518:ILE:HG13	2.21	0.40
1:A:676:LYS:HG2	1:A:676:LYS:H	1.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:LEU:HD23	1:A:713:TYR:CZ	2.56	0.40
1:B:308:ASP:HB3	1:B:311:ALA:HB3	2.03	0.40
1:B:316:GLN:OE1	1:B:319:ASN:HB2	2.21	0.40
1:B:635:VAL:HB	1:B:663:LEU:HB2	2.03	0.40
1:B:92:LYS:HB3	1:B:95:LEU:HD12	2.04	0.40
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.84	0.40
1:A:550:GLN:NE2	1:A:556:ALA:HB3	2.36	0.40
1:A:624:ASP:CG	1:A:627:THR:HG22	2.42	0.40
1:A:701:LYS:HG2	1:A:702:GLU:N	2.35	0.40
1:B:227:PHE:HA	1:B:246:PRO:HA	2.04	0.40
1:B:25:ILE:HG22	1:B:25:ILE:O	2.20	0.40
1:B:133:GLN:HB3	1:B:298:LEU:HD21	2.04	0.40
1:B:42:LYS:HB3	1:B:88:TYR:CB	2.44	0.40
1:B:624:ASP:CG	6:B:2165:HOH:O	2.45	0.40
1:B:72:VAL:CG2	1:B:73:PHE:N	2.84	0.40
1:A:364:LEU:HD23	1:A:364:LEU:HA	1.92	0.40
1:B:227:PHE:CE2	1:B:243:GLY:HA3	2.56	0.40
1:B:319:ASN:O	1:B:320:LYS:HB2	2.21	0.40
1:B:337:HIS:ND1	1:B:338:PRO:HD2	2.37	0.40
1:B:440:SER:HB2	1:B:628:TRP:NE1	2.37	0.40
1:B:444:ASN:O	1:B:449:SER:N	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:ARG:O	1:B:654:ILE:O[2_565]	1.79	0.41
1:A:653:ARG:NH2	1:B:656:ASP:O[2_565]	2.18	0.02

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	713/718 (99%)	589 (83%)	113 (16%)	11 (2%)	12	37
1	B	712/718 (99%)	612 (86%)	92 (13%)	8 (1%)	17	47
All	All	1425/1436 (99%)	1201 (84%)	205 (14%)	19 (1%)	14	41

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	683	ILE
1	A	121	ASP
1	A	164	ILE
1	B	195	ILE
1	B	515	ASN
1	A	230	GLN
1	B	517	VAL
1	A	193	GLU
1	A	415	TYR
1	B	160	ASP
1	B	193	GLU
1	A	160	ASP
1	A	676	LYS
1	B	623	VAL
1	A	707	GLY
1	A	295	GLY
1	B	181	VAL
1	A	643	VAL
1	B	542	GLY

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	631/636 (99%)	559 (89%)	72 (11%)	7	20
1	B	630/636 (99%)	572 (91%)	58 (9%)	11	30
All	All	1261/1272 (99%)	1131 (90%)	130 (10%)	8	24

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	10	ARG
1	A	70	TRP
1	A	78	ARG
1	A	82	LEU
1	A	86	ARG
1	A	88	TYR
1	A	105	LEU
1	A	127	LYS
1	A	134	ASP
1	A	135	LEU
1	A	138	ASP
1	A	159	ASP
1	A	162	ASP
1	A	164	ILE
1	A	165	LYS
1	A	168	LYS
1	A	171	LEU
1	A	172	LYS
1	A	173	ASP
1	A	179	VAL
1	A	186	LYS
1	A	189	LEU
1	A	191	LEU
1	A	194	ASN
1	A	206	GLN
1	A	222	MET
1	A	233	LEU
1	A	239	THR
1	A	245	ASP
1	A	254	CYS
1	A	257	SER
1	A	258	SER
1	A	261	CYS
1	A	266	VAL
1	A	267	LEU
1	A	286	ASP
1	A	287	VAL
1	A	334	ASN
1	A	335	LEU
1	A	354	GLU
1	A	376	ASN

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Mol	Chain	Res	Type
1	A	378	LEU
1	A	415	TYR
1	A	480	SER
1	A	484	LYS
1	A	486	ASN
1	A	493	ASN
1	A	508	GLU
1	A	522	LYS
1	A	541	LEU
1	A	545	GLU
1	A	554	ASN
1	A	559	GLN
1	A	561	ASN
1	A	565	TRP
1	A	583	LYS
1	A	601	GLN
1	A	603	LYS
1	A	618	LEU
1	A	619	GLU
1	A	657	ASP
1	A	664	ASN
1	A	669	ASN
1	A	671	LYS
1	A	676	LYS
1	A	681	LEU
1	A	682	VAL
1	A	688	ARG
1	A	693	GLU
1	A	695	ARG
1	A	701	LYS
1	B	7	THR
1	B	10	ARG
1	B	94	GLU
1	B	105	LEU
1	B	148	LYS
1	B	152	ILE
1	B	153	ASN
1	B	159	ASP
1	B	161	GLU
1	B	165	LYS
1	B	186	LYS
1	B	187	LEU

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Mol	Chain	Res	Type
1	B	188	ARG
1	B	189	LEU
1	B	190	ASP
1	B	191	LEU
1	B	193	GLU
1	B	195	ILE
1	B	218	THR
1	B	221	LEU
1	B	222	MET
1	B	233	LEU
1	B	245	ASP
1	B	247	ILE
1	B	255	ARG
1	B	267	LEU
1	B	286	ASP
1	B	296	ASN
1	B	319	ASN
1	B	321	ARG
1	B	331	ASN
1	B	354	GLU
1	B	360	PHE
1	B	373	TYR
1	B	415	TYR
1	B	416	GLN
1	B	425	ARG
1	B	433	ARG
1	B	445	ARG
1	B	447	LEU
1	B	480	SER
1	B	493	ASN
1	B	504	ASN
1	B	505	CYS
1	B	520	ARG
1	B	545	GLU
1	B	546	LEU
1	B	547	SER
1	B	554	ASN
1	B	565	TRP
1	B	584	MET
1	B	648	ASN
1	B	653	ARG
1	B	654	ILE

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Mol	Chain	Res	Type
1	B	688	ARG
1	B	690	ILE
1	B	704	GLU
1	B	718	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	53	GLN
1	A	131	GLN
1	A	194	ASN
1	A	206	GLN
1	A	226	HIS
1	A	274	ASN
1	A	277	HIS
1	A	278	ASN
1	A	334	ASN
1	A	342	GLN
1	A	376	ASN
1	A	379	ASN
1	A	386	GLN
1	A	393	GLN
1	A	412	ASN
1	A	416	GLN
1	A	444	ASN
1	A	485	HIS
1	A	493	ASN
1	A	500	ASN
1	A	504	ASN
1	A	523	GLN
1	A	535	GLN
1	A	554	ASN
1	A	561	ASN
1	A	633	GLN
1	A	664	ASN
1	A	668	ASN
1	A	669	ASN
1	B	32	ASN
1	B	81	GLN
1	B	133	GLN
1	B	153	ASN

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Mol	Chain	Res	Type
1	B	194	ASN
1	B	226	HIS
1	B	248	ASN
1	B	278	ASN
1	B	296	ASN
1	B	297	HIS
1	B	331	ASN
1	B	342	GLN
1	B	379	ASN
1	B	412	ASN
1	B	416	GLN
1	B	456	ASN
1	B	457	ASN
1	B	482	ASN
1	B	492	ASN
1	B	493	ASN
1	B	494	GLN
1	B	500	ASN
1	B	523	GLN
1	B	535	GLN
1	B	550	GLN
1	B	554	ASN
1	B	648	ASN
1	B	669	ASN

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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	A	1719	-	12,12,12	1.03	0	17,17,17	0.74	0
2	GLC	A	1720	-	12,12,12	1.06	0	17,17,17	0.74	0
2	GLC	A	1721	-	12,12,12	1.04	0	17,17,17	0.73	0
3	A16	A	1722	1	33,34,35	2.10	12 (36%)	43,50,52	2.06	6 (13%)
4	SO4	A	1723	-	4,4,4	0.53	0	6,6,6	0.15	0
5	GOL	A	1724	-	5,5,5	0.44	0	5,5,5	0.29	0
2	GLC	B	1719	-	12,12,12	1.01	0	17,17,17	0.74	0
3	A16	B	1720	1	33,34,35	2.10	13 (39%)	43,50,52	2.07	6 (13%)

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	1719	-	-	0/2/22/22	0/1/1/1
2	GLC	A	1720	-	-	0/2/22/22	0/1/1/1
2	GLC	A	1721	-	-	0/2/22/22	0/1/1/1
3	A16	A	1722	1	1/1/14/16	0/12/69/72	0/3/3/3
4	SO4	A	1723	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1724	-	-	0/4/4/4	0/0/0/0
2	GLC	B	1719	-	-	0/2/22/22	0/1/1/1
3	A16	B	1720	1	1/1/14/16	0/12/69/72	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1722	A16	C7A-C5A	-5.97	1.38	1.53
3	B	1720	A16	C7A-C5A	-5.75	1.39	1.53
3	B	1720	A16	C1B-C2B	2.07	1.58	1.52
3	A	1722	A16	C4A-C3A	2.08	1.57	1.52
3	B	1720	A16	C4A-C3A	2.11	1.57	1.52
3	B	1720	A16	C5A-C4A	2.15	1.55	1.53
3	A	1722	A16	C5A-C4A	2.16	1.55	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1722	A16	C2C-C3C	2.20	1.55	1.52
3	A	1722	A16	C4B-N4B	2.22	1.51	1.47
3	B	1720	A16	O5C-C1C	2.29	1.47	1.43
3	A	1722	A16	O5C-C1C	2.34	1.47	1.43
3	A	1722	A16	O4C-C1B	2.42	1.48	1.41
3	B	1720	A16	O4C-C1B	2.42	1.48	1.41
3	B	1720	A16	C4B-N4B	2.47	1.51	1.47
3	B	1720	A16	C2C-C3C	2.55	1.56	1.52
3	B	1720	A16	C3C-C4C	2.84	1.60	1.52
3	A	1722	A16	C7A-C1A	2.85	1.58	1.53
3	B	1720	A16	C7A-C1A	2.91	1.58	1.53
3	A	1722	A16	C3C-C4C	2.95	1.60	1.52
3	B	1720	A16	C3B-C4B	2.99	1.59	1.53
3	A	1722	A16	C3B-C4B	3.09	1.59	1.53
3	B	1720	A16	O5B-C1B	3.33	1.50	1.41
3	A	1722	A16	O5B-C1B	3.42	1.50	1.41
3	A	1722	A16	C2A-C1A	3.98	1.61	1.52
3	B	1720	A16	C2A-C1A	4.02	1.61	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1722	A16	C1B-O4C-C4C	2.30	123.59	118.00
3	B	1720	A16	C1B-O4C-C4C	2.68	124.53	118.00
3	A	1722	A16	C1C-O5C-C5C	2.75	115.96	112.17
3	B	1720	A16	C1C-O5C-C5C	2.78	115.99	112.17
3	A	1722	A16	O4C-C4C-C3C	3.03	114.49	107.19
3	B	1720	A16	O4C-C4C-C3C	3.10	114.64	107.19
3	A	1722	A16	C7A-C5A-C6A	5.39	121.64	111.99
3	B	1720	A16	C7A-C5A-C6A	5.44	121.74	111.99
3	B	1720	A16	C5A-C7A-C1A	7.21	117.62	108.54
3	A	1722	A16	C5A-C7A-C1A	7.37	117.83	108.54
3	B	1720	A16	C7A-C5A-C4A	7.66	118.30	109.99
3	A	1722	A16	C7A-C5A-C4A	7.66	118.30	109.99

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1722	A16	C5A
3	B	1720	A16	C5A

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1719	GLC	1	0
2	A	1721	GLC	1	0
3	A	1722	A16	1	0
4	A	1723	SO4	3	0
5	A	1724	GOL	3	0
2	B	1719	GLC	1	0
3	B	1720	A16	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	715/718 (99%)	-0.31	3 (0%)	92 90	19, 50, 80, 110	0
1	B	714/718 (99%)	-0.36	3 (0%)	92 90	23, 47, 80, 106	1 (0%)
All	All	1429/1436 (99%)	-0.33	6 (0%)	92 90	19, 49, 80, 110	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	PHE	3.5
1	B	621	ARG	2.5
1	A	135	LEU	2.3
1	B	18	TYR	2.2
1	B	373	TYR	2.2
1	A	160	ASP	2.1

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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GLC	A	1721	12/12	0.63	0.43	13.16	93,99,107,108	0
2	GLC	A	1720	12/12	0.83	0.40	11.78	80,104,110,111	0
3	A16	B	1720	32/33	0.66	0.44	8.57	85,134,146,148	0
5	GOL	A	1724	6/6	0.77	0.43	7.42	78,82,90,90	0
2	GLC	A	1719	12/12	0.68	0.45	4.79	85,101,105,110	0
3	A16	A	1722	32/33	0.77	0.32	2.85	94,124,132,140	0
2	GLC	B	1719	12/12	0.79	0.32	-	85,102,104,105	0
4	SO4	A	1723	5/5	0.64	0.28	-	112,118,133,135	0

6.5 Other polymers [i](#)

There are no such residues in this entry.