



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:25 PM UTC

PDB ID : 4F9O / pdb_00004f9o
Title : Crystal Structure of recombinant human Hexokinase type I with 2-deoxy-Glucose 6-Phosphate
Authors : Shen, L.; Honzatko, R.B.
Deposited on : 2012-05-19
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

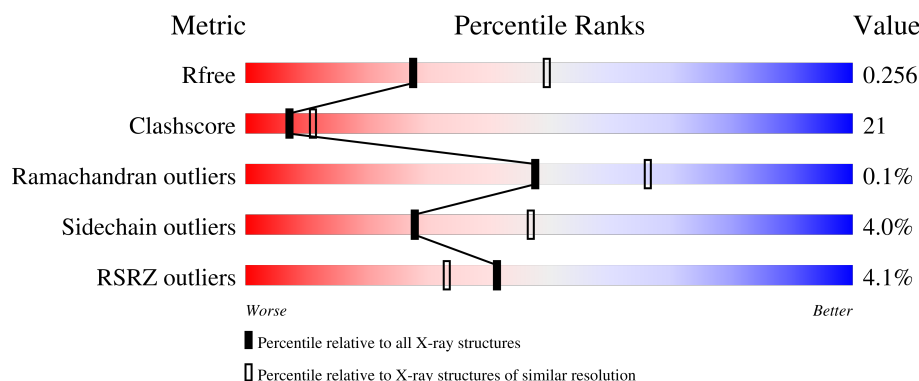
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	914	4% 66% 31% ..
1	B	914	4% 67% 28% ..

2 Entry composition [i](#)

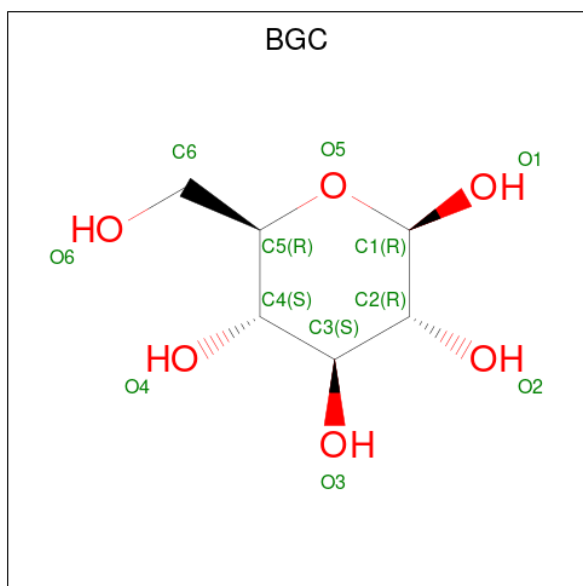
There are 6 unique types of molecules in this entry. The entry contains 14495 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hexokinase-1.

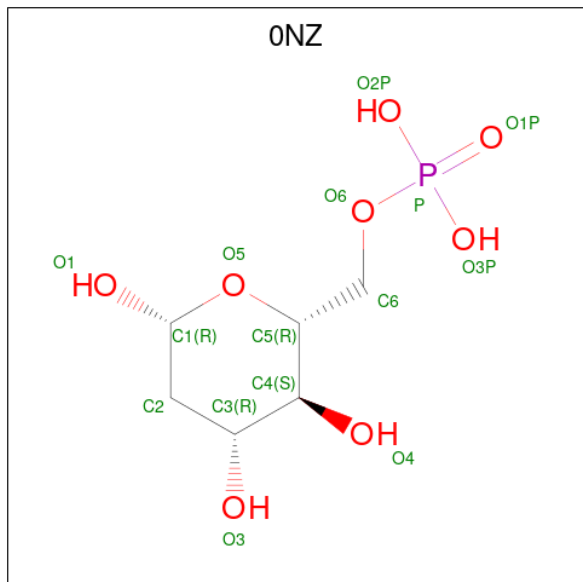
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	899	Total	C	N	O	S	0	0	0
			7033	4407	1240	1333	53			
1	B	899	Total	C	N	O	S	0	0	0
			7033	4407	1240	1333	53			

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



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	B	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is 2-deoxy-6-O-phosphono-beta-D-glucopyranose (CCD ID: 0NZ) (formula: $C_6H_{13}O_8P$).

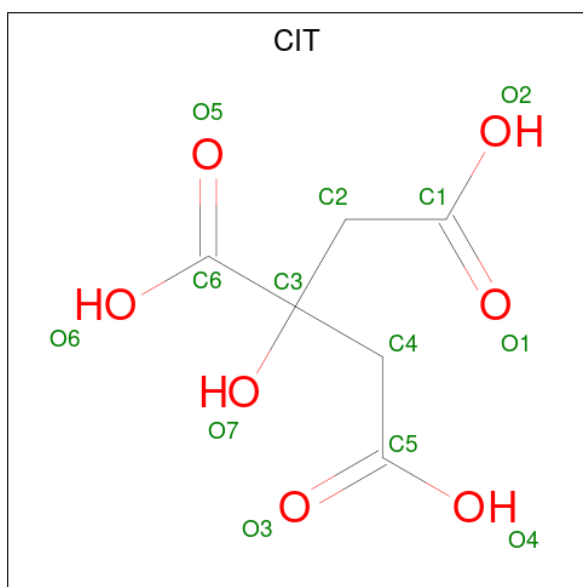


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			15	6	8	1		
3	A	1	Total	C	O	P	0	0
			15	6	8	1		
3	B	1	Total	C	O	P	0	0
			15	6	8	1		
3	B	1	Total	C	O	P	0	0
			15	6	8	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		
4	B	2	Total	Na	0	0
			2	2		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	6	7		

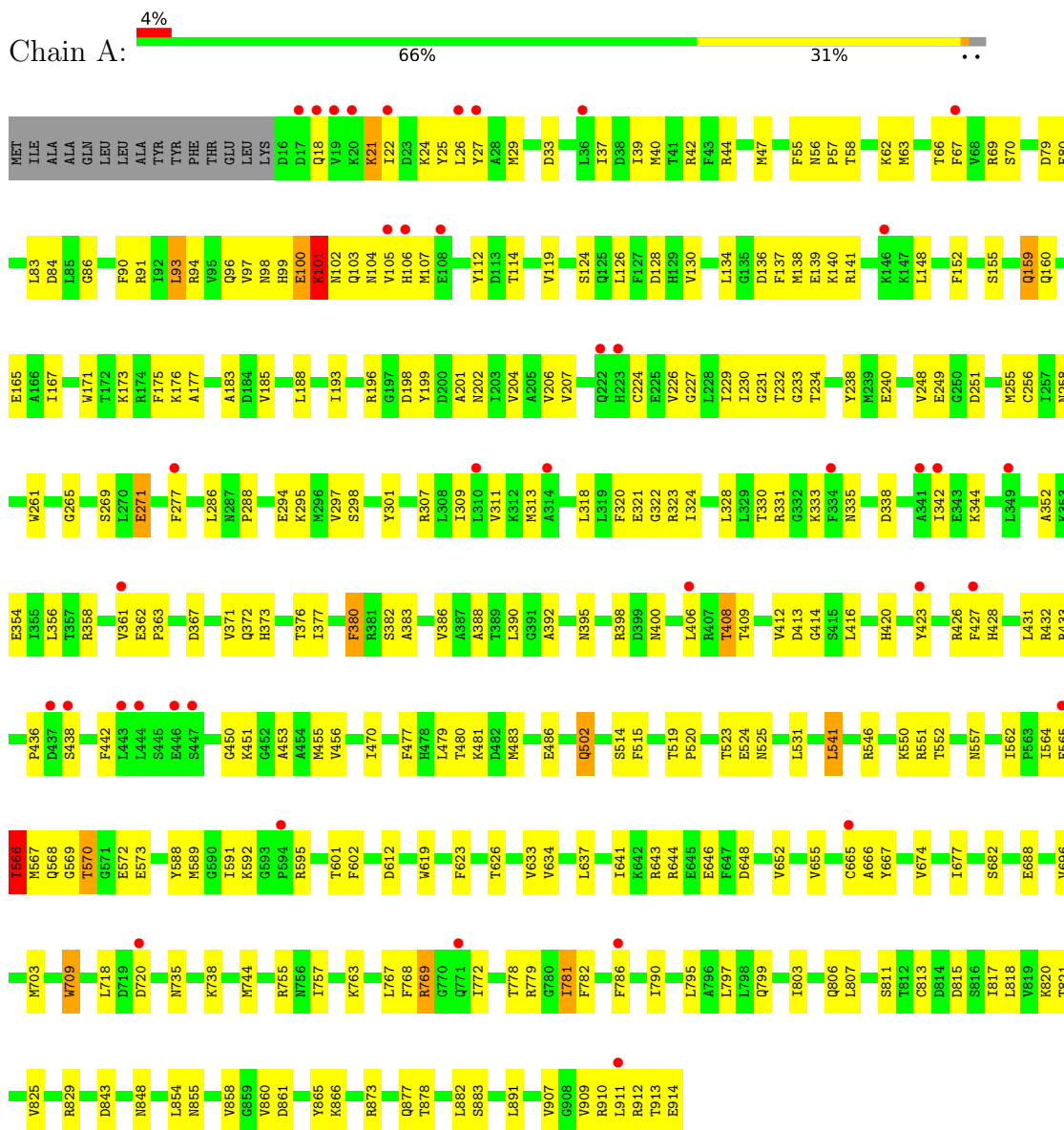
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	155	Total	O	0	0
			155	155		
6	B	149	Total	O	0	0
			149	149		

3 Residue-property plots

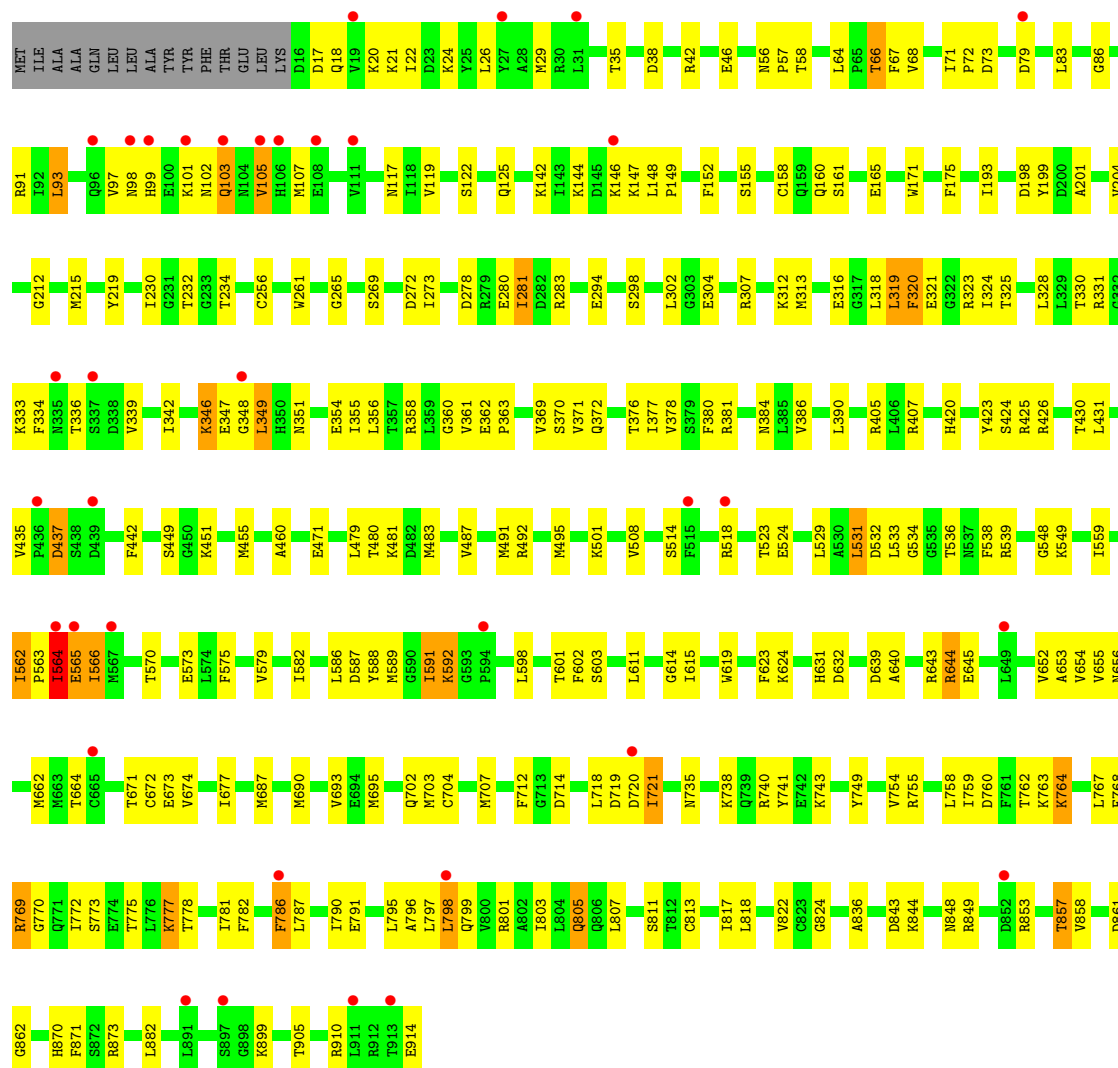
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Hexokinase-1



• Molecule 1: Hexokinase-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.98Å 122.09Å 120.35Å 90.00° 92.97° 90.00°	Depositor
Resolution (Å)	35.36 – 2.65 35.36 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.36-2.65) 98.9 (35.36-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.240 , 0.258 0.236 , 0.256	Depositor DCC
R_{free} test set	3466 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	51.5	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.002 for -h,-l,-k 0.000 for -h,l,k 0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14495	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CIT, 0NZ, 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	1/7139 (0.0%)	0.79	8/9606 (0.1%)
1	B	0.35	0/7139	0.79	3/9606 (0.0%)
All	All	0.36	1/14278 (0.0%)	0.79	11/19212 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	566	ILE	CG1-CD1	8.44	1.84	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	ILE	CA-C-N	9.39	129.45	119.78
1	A	562	ILE	C-N-CA	9.39	129.45	119.78
1	A	883	SER	CA-C-N	6.25	125.94	119.82
1	A	883	SER	C-N-CA	6.25	125.94	119.82
1	A	101	LYS	N-CA-C	-5.44	106.49	113.02
1	B	161	SER	N-CA-C	-5.27	107.02	113.50
1	A	569	GLY	N-CA-C	-5.15	103.64	111.42
1	B	199	TYR	N-CA-C	5.14	115.13	107.88
1	A	114	THR	CA-C-N	5.03	124.96	119.78
1	A	114	THR	C-N-CA	5.03	124.96	119.78
1	B	346	LYS	N-CA-C	5.03	116.57	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7033	0	7089	294	0
1	B	7033	0	7090	300	0
2	A	24	0	24	0	0
2	B	24	0	24	0	0
3	A	30	0	22	2	0
3	B	30	0	22	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	B	13	0	5	4	0
6	A	155	0	0	4	0
6	B	149	0	0	10	0
All	All	14495	0	14276	588	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 21.

All (588) 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:566:ILE:CD1	1:A:566:ILE:CG1	1.84	1.53
1:A:97:VAL:CG2	1:A:105:VAL:HA	1.47	1.41
1:B:319:LEU:HB2	1:B:320:PHE:CE1	1.67	1.29
1:A:79:ASP:OD1	1:A:96:GLN:HG2	1.32	1.28
1:B:319:LEU:C	1:B:320:PHE:HD1	1.41	1.26
1:B:319:LEU:CB	1:B:320:PHE:CE1	2.18	1.25
1:B:98:ASN:OD1	1:B:101:LYS:HG2	1.32	1.25
1:A:320:PHE:O	1:A:323:ARG:HG3	1.37	1.24
1:A:94:ARG:NE	1:A:96:GLN:OE1	1.73	1.21
1:A:323:ARG:NH2	1:A:362:GLU:O	1.75	1.20
1:B:775:THR:O	1:B:781:ILE:HD11	1.39	1.19
1:B:775:THR:O	1:B:781:ILE:CD1	1.94	1.15
1:B:480:THR:H	1:B:483:MET:HE3	1.12	1.14
1:A:480:THR:H	1:A:483:MET:HE3	1.11	1.12
1:B:319:LEU:C	1:B:320:PHE:CD1	2.27	1.12
1:A:97:VAL:HG21	1:A:105:VAL:HA	1.35	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:CZ	1:A:362:GLU:HB2	1.83	1.07
1:A:565:GLU:O	1:A:568:GLN:O	1.72	1.07
1:A:97:VAL:HG22	1:A:105:VAL:HA	1.27	1.07
1:A:323:ARG:NH2	1:A:362:GLU:HB2	1.67	1.06
1:A:570:THR:HG23	1:A:573:GLU:OE2	1.52	1.06
1:A:323:ARG:NH2	1:A:362:GLU:C	2.12	1.06
1:A:101:LYS:N	1:A:101:LYS:HD3	1.70	1.04
1:A:323:ARG:HH21	1:A:362:GLU:CA	1.70	1.04
1:B:319:LEU:HB2	1:B:320:PHE:HE1	1.04	1.02
1:B:319:LEU:HB3	1:B:320:PHE:CE1	1.90	1.02
1:B:853:ARG:HB3	1:B:853:ARG:HH11	1.25	1.01
1:A:101:LYS:N	1:A:101:LYS:CD	2.22	1.00
1:B:98:ASN:CG	1:B:101:LYS:HG2	1.86	1.00
1:A:66:THR:HG22	1:A:256:CYS:O	1.62	0.99
1:A:323:ARG:NH2	1:A:362:GLU:CA	2.25	0.99
1:A:592:LYS:NZ	1:A:646:GLU:OE1	1.94	0.99
1:A:480:THR:N	1:A:483:MET:HE3	1.76	0.99
1:A:323:ARG:HH21	1:A:362:GLU:N	1.60	0.98
1:A:101:LYS:HD3	1:A:101:LYS:H	1.28	0.97
1:A:97:VAL:CG2	1:A:105:VAL:CA	2.43	0.95
1:A:79:ASP:OD1	1:A:96:GLN:CG	2.13	0.95
1:A:323:ARG:NH2	1:A:362:GLU:CB	2.29	0.95
1:B:319:LEU:CB	1:B:320:PHE:CD1	2.47	0.95
1:B:319:LEU:CB	1:B:320:PHE:HE1	1.66	0.94
1:A:94:ARG:CZ	1:A:96:GLN:OE1	2.15	0.94
1:A:361:VAL:O	1:A:363:PRO:HD3	1.68	0.93
1:B:480:THR:N	1:B:483:MET:HE3	1.82	0.93
1:A:570:THR:CG2	1:A:573:GLU:OE2	2.16	0.92
1:A:100:GLU:HA	1:A:100:GLU:OE1	1.68	0.91
1:B:98:ASN:OD1	1:B:101:LYS:CG	2.18	0.91
1:A:480:THR:HG23	1:A:483:MET:HE2	1.51	0.90
1:B:662:MET:HE1	1:B:687:MET:HE3	1.53	0.90
1:B:797:LEU:HD11	1:B:817:ILE:HD11	1.54	0.90
1:B:853:ARG:HB3	1:B:853:ARG:NH1	1.85	0.89
1:B:431:LEU:HD22	1:B:442:PHE:HZ	1.37	0.88
1:B:66:THR:HG21	1:B:256:CYS:HB3	1.54	0.87
1:B:319:LEU:HB2	1:B:320:PHE:CD1	2.09	0.87
1:B:98:ASN:CG	1:B:101:LYS:CG	2.47	0.87
1:B:346:LYS:HG3	1:B:347:GLU:OE1	1.76	0.86
1:B:346:LYS:HB2	1:B:347:GLU:OE1	1.76	0.85
1:B:346:LYS:CG	1:B:347:GLU:OE1	2.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PHE:HD2	1:B:361:VAL:HB	1.42	0.84
1:B:356:LEU:HD11	1:B:371:VAL:HG21	1.58	0.84
1:A:98:ASN:OD1	1:A:100:GLU:HB2	1.77	0.83
1:B:97:VAL:HG21	1:B:455:MET:HE1	1.59	0.83
1:B:346:LYS:CB	1:B:347:GLU:OE1	2.27	0.83
1:B:320:PHE:CD1	1:B:320:PHE:N	2.44	0.82
1:B:420:HIS:HD2	1:B:423:TYR:H	1.23	0.82
1:B:764:LYS:HE2	6:B:1148:HOH:O	1.80	0.82
1:B:320:PHE:CE2	1:B:361:VAL:HG21	2.15	0.81
1:B:480:THR:H	1:B:483:MET:CE	1.93	0.81
1:A:66:THR:HG21	1:A:256:CYS:HB3	1.63	0.81
1:B:103:GLN:OE1	1:B:103:GLN:HA	1.78	0.81
1:B:531:LEU:HD21	1:B:582:ILE:HD11	1.62	0.81
1:B:426:ARG:HH21	5:B:1007:CIT:H41	1.46	0.80
1:A:763:LYS:HG3	1:A:772:ILE:HD11	1.63	0.80
1:A:323:ARG:HH21	1:A:362:GLU:C	1.83	0.80
1:A:570:THR:HG23	1:A:573:GLU:CD	2.06	0.79
1:B:98:ASN:ND2	1:B:101:LYS:HE3	1.98	0.79
1:A:97:VAL:HG22	1:A:105:VAL:CA	2.10	0.78
1:A:665:CYS:SG	1:A:891:LEU:HD23	2.23	0.78
1:B:320:PHE:HE2	1:B:361:VAL:HG21	1.48	0.78
1:A:480:THR:H	1:A:483:MET:CE	1.94	0.77
1:B:479:LEU:HA	1:B:483:MET:HE3	1.67	0.77
1:B:539:ARG:CZ	1:B:559:ILE:HD11	2.14	0.76
1:B:798:LEU:HB2	6:B:1114:HOH:O	1.85	0.76
1:B:98:ASN:HD21	1:B:101:LYS:HE3	1.51	0.76
1:A:93:LEU:HD22	1:A:450:GLY:HA3	1.67	0.76
1:B:768:PHE:HA	1:B:769:ARG:HH21	1.49	0.76
1:B:587:ASP:OD1	1:B:592:LYS:HD2	1.85	0.76
1:A:234:THR:HG22	1:A:294:GLU:HG3	1.68	0.75
1:B:405:ARG:HB3	1:B:405:ARG:NH1	2.01	0.75
1:A:323:ARG:HH21	1:A:362:GLU:H	1.33	0.75
1:A:354:GLU:O	1:A:358:ARG:HG3	1.85	0.75
1:A:160:GLN:HG2	1:A:165:GLU:O	1.88	0.74
1:A:767:LEU:HG	1:A:818:LEU:HD23	1.70	0.74
1:A:22:ILE:HD12	1:A:313:MET:HE1	1.67	0.74
1:B:405:ARG:HB3	1:B:405:ARG:HH11	1.53	0.74
1:B:562:ILE:O	1:B:562:ILE:HG22	1.86	0.74
1:A:79:ASP:CG	1:A:96:GLN:HG2	2.11	0.73
1:B:480:THR:HG23	1:B:483:MET:HE2	1.70	0.73
1:A:320:PHE:O	1:A:323:ARG:CG	2.29	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:ASP:O	1:B:764:LYS:HG2	1.89	0.73
1:B:778:THR:HB	1:B:781:ILE:HD11	1.71	0.73
1:A:98:ASN:O	1:A:103:GLN:N	2.19	0.72
1:A:786:PHE:CZ	1:A:790:ILE:HG13	2.24	0.72
1:B:103:GLN:OE1	1:B:103:GLN:CA	2.37	0.72
1:B:768:PHE:HE1	1:B:811:SER:HB3	1.53	0.72
1:A:98:ASN:ND2	1:A:101:LYS:HE3	2.05	0.71
1:A:97:VAL:HG21	1:A:105:VAL:CA	2.15	0.71
1:B:564:ILE:HG23	1:B:565:GLU:N	2.05	0.71
1:B:763:LYS:HG3	1:B:772:ILE:HD11	1.73	0.71
1:A:338:ASP:O	1:A:342:ILE:HD13	1.91	0.71
1:A:380:PHE:CD2	1:A:426:ARG:HD3	2.25	0.71
1:A:431:LEU:HD23	1:A:442:PHE:HZ	1.55	0.70
1:B:66:THR:CG2	1:B:256:CYS:HB3	2.22	0.70
1:B:320:PHE:CD2	1:B:361:VAL:HB	2.24	0.70
1:A:96:GLN:O	1:A:97:VAL:HG23	1.92	0.69
1:A:778:THR:HB	1:A:781:ILE:HD13	1.73	0.69
1:B:97:VAL:HG21	1:B:455:MET:CE	2.23	0.69
1:A:323:ARG:CZ	1:A:362:GLU:CB	2.64	0.69
1:B:644:ARG:O	1:B:644:ARG:NH1	2.25	0.69
1:A:265:GLY:HA2	1:A:269:SER:HB2	1.75	0.68
1:A:795:LEU:HD11	1:A:799:GLN:HG2	1.76	0.68
1:B:501:LYS:HB3	1:B:695:MET:SD	2.34	0.68
1:A:66:THR:CG2	1:A:256:CYS:HB3	2.22	0.68
1:B:319:LEU:O	1:B:320:PHE:HD1	1.75	0.68
1:B:319:LEU:HB3	1:B:320:PHE:CD1	2.22	0.68
1:A:94:ARG:NH2	1:A:96:GLN:OE1	2.27	0.67
1:A:502:GLN:OE1	1:A:502:GLN:N	2.26	0.67
1:B:21:LYS:NZ	1:B:21:LYS:HB3	2.10	0.67
1:A:331:ARG:HD2	1:B:588:TYR:CE2	2.30	0.67
1:A:390:LEU:HD23	1:A:431:LEU:HD22	1.77	0.67
1:B:575:PHE:O	1:B:579:VAL:HG23	1.94	0.67
1:B:281:ILE:HD12	1:B:304:GLU:HG3	1.76	0.67
1:A:356:LEU:HD11	1:A:371:VAL:HG21	1.76	0.66
1:A:910:ARG:O	1:A:914:GLU:HB2	1.95	0.66
1:A:480:THR:HG23	1:A:483:MET:CE	2.23	0.66
1:A:202:ASN:O	1:A:204:VAL:HG23	1.96	0.66
1:A:572:GLU:HB3	1:A:643:ARG:HH12	1.60	0.66
1:B:797:LEU:HD21	1:B:817:ILE:HD13	1.78	0.66
1:B:662:MET:CE	1:B:687:MET:HE3	2.26	0.65
1:A:324:ILE:HG23	1:A:328:LEU:HD23	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ARG:HB2	1:B:91:ARG:NH1	2.12	0.64
1:B:870:HIS:HD2	1:B:873:ARG:HH21	1.45	0.64
1:A:763:LYS:CG	1:A:772:ILE:HD11	2.27	0.64
1:B:768:PHE:CE1	1:B:811:SER:HB3	2.32	0.64
1:B:349:LEU:HD23	1:B:372:GLN:NE2	2.12	0.64
1:B:230:ILE:HD11	1:B:386:VAL:HG11	1.80	0.64
1:B:674:VAL:HB	1:B:858:VAL:HG22	1.78	0.64
1:B:687:MET:HE1	1:B:704:CYS:HB2	1.80	0.63
1:B:160:GLN:HG2	1:B:165:GLU:O	1.98	0.63
1:A:79:ASP:O	1:A:148:LEU:HD22	1.98	0.63
1:A:479:LEU:HA	1:A:483:MET:HE3	1.81	0.63
1:A:56:ASN:N	1:A:57:PRO:HD2	2.14	0.63
1:A:595:ARG:NE	1:A:648:ASP:OD2	2.26	0.63
1:A:309:ILE:O	1:A:313:MET:HG3	1.99	0.63
1:A:39:ILE:HD13	1:A:42:ARG:HH21	1.64	0.63
1:B:471:GLU:HG3	6:B:1157:HOH:O	1.97	0.63
1:B:278:ASP:O	1:B:281:ILE:HG22	1.98	0.62
1:B:782:PHE:HD1	1:B:786:PHE:CE1	2.17	0.62
1:B:763:LYS:CG	1:B:772:ILE:HD11	2.29	0.62
1:A:431:LEU:CD2	1:A:442:PHE:HZ	2.11	0.62
1:A:398:ARG:HH11	1:A:398:ARG:HB3	1.65	0.62
1:A:786:PHE:O	1:A:790:ILE:HG12	2.00	0.62
1:A:398:ARG:HB3	1:A:398:ARG:NH1	2.15	0.61
1:B:420:HIS:CD2	1:B:423:TYR:H	2.13	0.61
1:B:437:ASP:OD1	1:B:437:ASP:N	2.32	0.61
1:A:124:SER:O	1:A:128:ASP:HB2	2.01	0.61
1:B:796:ALA:O	1:B:799:GLN:HB3	2.01	0.61
1:B:639:ASP:O	1:B:643:ARG:HG3	2.01	0.61
1:A:248:VAL:HG21	1:A:255:MET:HE1	1.81	0.61
1:A:431:LEU:HD23	1:A:442:PHE:CZ	2.36	0.61
1:B:320:PHE:HD2	1:B:361:VAL:CB	2.12	0.61
1:A:233:GLY:HA2	1:A:298:SER:CB	2.31	0.61
1:A:572:GLU:CB	1:A:643:ARG:HH12	2.14	0.60
1:B:479:LEU:HA	1:B:483:MET:CE	2.29	0.60
1:A:286:LEU:C	1:A:288:PRO:HD3	2.26	0.60
1:A:101:LYS:N	1:A:101:LYS:HD2	2.11	0.60
1:B:598:LEU:HD23	1:B:598:LEU:C	2.27	0.60
1:B:662:MET:HE1	1:B:687:MET:CE	2.29	0.60
1:B:320:PHE:CD2	1:B:361:VAL:CB	2.85	0.60
1:A:119:VAL:HG13	1:A:175:PHE:CD1	2.36	0.60
1:B:492:ARG:HD3	6:B:1128:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:PHE:CD2	1:A:807:LEU:HD11	2.37	0.60
1:B:431:LEU:HD22	1:B:442:PHE:CZ	2.29	0.60
1:B:539:ARG:HB3	1:B:559:ILE:HD13	1.83	0.60
1:A:271:GLU:OE1	1:A:271:GLU:HA	2.00	0.60
1:B:66:THR:HG23	1:B:68:VAL:HG23	1.85	0.59
1:A:176:LYS:NZ	1:A:286:LEU:O	2.29	0.59
1:B:495:MET:HE3	1:B:707:MET:HE3	1.84	0.59
1:B:767:LEU:HG	1:B:818:LEU:HD23	1.83	0.59
1:B:671:THR:OG1	1:B:857:THR:HG23	2.02	0.59
1:B:122:SER:OG	1:B:125:GLN:HG3	2.01	0.59
1:B:782:PHE:CD1	1:B:786:PHE:CE1	2.90	0.59
1:A:98:ASN:OD1	1:A:100:GLU:N	2.36	0.59
1:A:230:ILE:HD11	1:A:386:VAL:HG11	1.84	0.59
1:A:323:ARG:NH2	1:A:362:GLU:N	2.42	0.59
1:B:533:LEU:HD23	1:B:602:PHE:CE1	2.38	0.59
1:A:433:ARG:O	1:A:436:PRO:HD3	2.04	0.58
1:A:688:GLU:OE1	1:A:848:ASN:ND2	2.37	0.58
1:A:93:LEU:N	1:A:93:LEU:HD12	2.19	0.58
1:A:420:HIS:CD2	1:A:423:TYR:HB2	2.37	0.58
1:B:425:ARG:HH22	5:B:1007:CIT:H42	1.68	0.58
1:A:383:ALA:HB1	1:A:427:PHE:HB2	1.85	0.58
1:B:518:ARG:HG2	1:B:518:ARG:HH11	1.69	0.58
1:A:342:ILE:HG21	1:A:372:GLN:HA	1.84	0.57
1:A:755:ARG:NH2	1:A:779:ARG:HB3	2.19	0.57
1:B:323:ARG:NH2	1:B:362:GLU:HB2	2.19	0.57
1:B:426:ARG:HE	5:B:1007:CIT:H22	1.68	0.57
1:B:22:ILE:HD11	1:B:370:SER:HB3	1.86	0.57
1:B:601:THR:HA	1:B:655:VAL:O	2.04	0.57
1:A:97:VAL:HG21	1:A:105:VAL:HG22	1.87	0.57
1:A:295:LYS:HA	1:A:301:TYR:CD2	2.40	0.57
1:B:98:ASN:ND2	1:B:101:LYS:CE	2.66	0.57
1:A:26:LEU:HD21	1:A:309:ILE:CG2	2.34	0.57
1:B:26:LEU:HD12	1:B:377:ILE:HD12	1.85	0.57
1:B:870:HIS:CD2	1:B:873:ARG:HH21	2.23	0.57
1:A:565:GLU:HG3	1:A:566:ILE:HG12	1.87	0.57
1:B:735:ASN:HB2	1:B:738:LYS:HE3	1.87	0.57
1:A:406:LEU:HG	1:A:408:THR:HG22	1.87	0.57
1:B:354:GLU:O	1:B:358:ARG:HG3	2.04	0.56
1:B:565:GLU:HG2	1:B:566:ILE:N	2.19	0.56
1:B:35:THR:O	1:B:38:ASP:HB3	2.05	0.56
1:A:566:ILE:CD1	1:A:566:ILE:CG2	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:853:ARG:HH11	1:B:853:ARG:CB	2.10	0.56
1:A:134:LEU:O	1:A:138:MET:HG3	2.05	0.56
1:B:313:MET:HB2	1:B:319:LEU:HD12	1.88	0.56
1:B:319:LEU:CA	1:B:320:PHE:CD1	2.88	0.56
1:B:640:ALA:HA	1:B:643:ARG:HE	1.71	0.56
1:B:718:LEU:C	1:B:720:ASP:N	2.62	0.56
1:B:786:PHE:CD2	1:B:807:LEU:HD11	2.41	0.56
1:B:347:GLU:O	1:B:348:GLY:C	2.49	0.55
1:A:98:ASN:HB3	1:A:103:GLN:OE1	2.07	0.55
1:A:307:ARG:O	1:A:311:VAL:HG23	2.05	0.55
1:B:533:LEU:HD23	1:B:602:PHE:HE1	1.71	0.55
1:B:534:GLY:HA3	1:B:603:SER:HB2	1.87	0.55
1:B:795:LEU:HD11	1:B:799:GLN:HG2	1.87	0.55
1:A:913:THR:HG22	1:A:913:THR:O	2.07	0.55
1:A:813:CYS:O	1:A:817:ILE:HG13	2.06	0.55
1:B:347:GLU:OE1	1:B:347:GLU:N	2.39	0.55
1:B:349:LEU:HD11	1:B:369:VAL:HG22	1.89	0.55
1:A:644:ARG:NH1	1:A:646:GLU:OE2	2.39	0.55
1:B:56:ASN:N	1:B:57:PRO:HD2	2.22	0.55
1:B:813:CYS:O	1:B:817:ILE:HG12	2.06	0.55
1:A:107:MET:HE1	1:A:451:LYS:HB2	1.88	0.55
1:B:107:MET:HE1	1:B:451:LYS:HB2	1.89	0.55
1:B:614:GLY:O	1:B:632:ASP:HA	2.07	0.54
1:A:323:ARG:NH2	1:A:362:GLU:H	2.03	0.54
1:A:502:GLN:H	1:A:502:GLN:CD	2.15	0.54
1:B:797:LEU:HD21	1:B:817:ILE:CD1	2.37	0.54
1:A:44:ARG:HA	1:A:47:MET:CE	2.37	0.54
1:A:592:LYS:CE	1:A:646:GLU:OE1	2.55	0.54
1:A:408:THR:OG1	1:A:409:THR:N	2.40	0.54
1:B:20:LYS:HG3	1:B:24:LYS:HE3	1.87	0.54
1:A:428:HIS:O	1:A:432:ARG:HG3	2.07	0.54
1:B:564:ILE:CG2	1:B:565:GLU:N	2.70	0.54
1:A:26:LEU:HD22	1:A:29:MET:CE	2.37	0.54
1:B:103:GLN:OE1	1:B:103:GLN:O	2.26	0.54
1:A:480:THR:OG1	1:A:483:MET:HG3	2.08	0.54
1:A:612:ASP:O	1:A:634:VAL:HG21	2.08	0.53
1:B:425:ARG:NH2	5:B:1007:CIT:H42	2.23	0.53
1:B:29:MET:HE2	1:B:381:ARG:CZ	2.38	0.53
1:A:55:PHE:HA	1:B:799:GLN:NE2	2.23	0.53
1:A:232:THR:O	1:A:298:SER:HB2	2.09	0.53
1:B:265:GLY:HA2	1:B:269:SER:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:LEU:CA	1:B:483:MET:HE3	2.37	0.53
1:B:773:SER:O	1:B:777:LYS:HD2	2.08	0.53
1:A:790:ILE:O	1:A:820:LYS:NZ	2.42	0.53
1:B:351:ASN:O	1:B:355:ILE:HG12	2.08	0.53
1:B:193:ILE:HD13	1:B:201:ALA:HB3	1.90	0.53
1:B:232:THR:O	1:B:298:SER:HB2	2.09	0.53
1:A:140:LYS:HB2	1:A:141:ARG:HH11	1.74	0.53
1:B:390:LEU:HD23	1:B:431:LEU:HD13	1.92	0.52
1:B:588:TYR:HD2	1:B:589:MET:HE3	1.75	0.52
1:A:755:ARG:HH21	1:A:779:ARG:HB3	1.74	0.52
1:B:281:ILE:CD1	1:B:304:GLU:HG3	2.39	0.52
1:B:58:THR:HG22	1:B:58:THR:O	2.09	0.52
1:B:536:THR:HG22	6:B:1215:HOH:O	2.09	0.52
1:A:207:VAL:HA	6:A:1180:HOH:O	2.09	0.52
1:B:302:LEU:HD22	1:B:378:VAL:HG12	1.92	0.52
1:A:98:ASN:HD21	1:A:101:LYS:HE3	1.75	0.52
1:B:564:ILE:HG23	1:B:565:GLU:H	1.73	0.52
1:A:380:PHE:HE2	1:A:426:ARG:HB3	1.74	0.51
1:A:171:TRP:NE1	1:A:177:ALA:H	2.09	0.51
1:A:718:LEU:C	1:A:720:ASP:N	2.65	0.51
1:B:768:PHE:HA	1:B:769:ARG:NH2	2.24	0.51
1:B:501:LYS:CB	1:B:695:MET:SD	2.98	0.51
1:B:702:GLN:HB2	6:B:1173:HOH:O	2.11	0.51
1:B:799:GLN:O	1:B:803:ILE:HG13	2.11	0.51
1:A:25:TYR:HD2	1:A:313:MET:HE3	1.75	0.51
1:A:90:PHE:CZ	1:A:130:VAL:HG13	2.44	0.51
1:A:136:ASP:O	1:A:140:LYS:HG3	2.10	0.51
1:A:546:ARG:O	1:A:551:ARG:HA	2.11	0.51
1:A:361:VAL:C	1:A:363:PRO:HD3	2.36	0.51
1:B:142:LYS:HA	1:B:142:LYS:HE2	1.92	0.51
1:B:619:TRP:CD1	1:B:624:LYS:HA	2.46	0.51
1:B:144:LYS:NZ	1:B:198:ASP:HB3	2.26	0.51
1:B:640:ALA:HA	1:B:643:ARG:NE	2.26	0.51
1:A:26:LEU:HD21	1:A:309:ILE:HG23	1.94	0.51
1:B:219:TYR:CD2	1:B:451:LYS:HD3	2.46	0.51
1:B:313:MET:HB2	1:B:319:LEU:CD1	2.41	0.51
1:A:565:GLU:CG	1:A:566:ILE:N	2.73	0.50
1:A:140:LYS:C	1:A:141:ARG:HD2	2.35	0.50
1:B:91:ARG:HH11	1:B:91:ARG:CB	2.25	0.50
1:B:193:ILE:HD13	1:B:201:ALA:CB	2.41	0.50
1:A:167:ILE:HA	1:A:183:ALA:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:TYR:CZ	1:B:331:ARG:HD2	2.46	0.50
1:A:25:TYR:CD2	1:A:313:MET:HE3	2.47	0.50
1:A:342:ILE:CG2	1:A:372:GLN:HA	2.41	0.50
1:A:797:LEU:HD11	1:A:817:ILE:HD11	1.93	0.50
1:A:376:THR:O	1:A:380:PHE:HB2	2.12	0.50
1:B:764:LYS:HB3	6:B:1148:HOH:O	2.11	0.50
1:A:119:VAL:HG12	1:A:175:PHE:HA	1.94	0.50
1:B:655:VAL:HG12	1:B:656:ASN:O	2.11	0.50
1:A:480:THR:CG2	1:A:483:MET:HE2	2.33	0.50
1:B:320:PHE:CD2	1:B:361:VAL:HG21	2.46	0.50
1:A:541:LEU:N	1:A:541:LEU:HD12	2.27	0.49
1:B:480:THR:HG23	1:B:483:MET:CE	2.42	0.49
1:B:102:ASN:O	1:B:102:ASN:OD1	2.30	0.49
1:A:767:LEU:HD23	1:A:815:ASP:OD1	2.12	0.49
1:A:854:LEU:HD12	1:A:855:ASN:N	2.27	0.49
1:A:907:VAL:O	1:A:911:LEU:HG	2.12	0.49
1:B:570:THR:OG1	1:B:573:GLU:HG3	2.12	0.49
1:A:514:SER:O	1:A:515:PHE:HB2	2.12	0.49
1:B:514:SER:OG	1:B:704:CYS:HB3	2.13	0.49
1:A:797:LEU:HD21	1:A:817:ILE:HG12	1.94	0.49
1:A:33:ASP:O	1:A:37:ILE:HG12	2.13	0.49
1:A:86:GLY:HA3	1:A:155:SER:OG	2.12	0.49
1:A:40:MET:HG3	1:A:388:ALA:O	2.13	0.49
1:B:623:PHE:O	1:B:624:LYS:CG	2.61	0.49
1:B:844:LYS:NZ	1:B:848:ASN:HD21	2.11	0.49
1:A:323:ARG:NE	1:A:362:GLU:HG2	2.28	0.49
1:B:870:HIS:CD2	1:B:873:ARG:NH2	2.80	0.49
1:A:565:GLU:HG2	1:A:566:ILE:H	1.78	0.48
1:B:66:THR:CG2	1:B:68:VAL:H	2.26	0.48
1:B:204:VAL:HG12	1:B:204:VAL:O	2.11	0.48
1:A:25:TYR:HE2	1:A:313:MET:HG2	1.78	0.48
1:A:412:VAL:HG12	1:A:413:ASP:N	2.27	0.48
1:A:566:ILE:CD1	1:A:566:ILE:CB	2.82	0.48
1:B:563:PRO:O	1:B:564:ILE:C	2.56	0.48
1:A:398:ARG:HH11	1:A:398:ARG:CB	2.27	0.48
1:A:541:LEU:HG	1:A:557:ASN:HB3	1.93	0.48
1:B:548:GLY:O	1:B:549:LYS:C	2.56	0.48
1:A:126:LEU:O	1:A:130:VAL:HG23	2.13	0.48
1:A:564:ILE:HD12	1:A:565:GLU:N	2.28	0.48
1:B:762:THR:O	1:B:770:GLY:HA2	2.13	0.48
1:A:56:ASN:N	1:A:57:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:LEU:O	1:A:641:ILE:HG13	2.14	0.48
1:B:325:THR:HG21	1:B:360:GLY:HA3	1.96	0.48
1:B:83:LEU:HB2	1:B:152:PHE:HD1	1.79	0.48
1:B:772:ILE:HG22	1:B:777:LYS:HD2	1.95	0.48
1:A:86:GLY:O	1:A:173:LYS:NZ	2.47	0.48
1:A:602:PHE:CE2	1:A:633:VAL:HG11	2.49	0.48
1:B:693:VAL:HG12	1:B:693:VAL:O	2.13	0.48
1:A:44:ARG:HG2	1:A:392:ALA:HB1	1.96	0.48
1:B:330:THR:HB	1:B:333:LYS:HG3	1.96	0.48
1:B:361:VAL:O	1:B:363:PRO:HD3	2.14	0.48
1:A:414:GLY:HA2	3:A:1002:ONZ:O6	2.14	0.47
1:A:564:ILE:HA	6:A:1231:HOH:O	2.12	0.47
1:B:862:GLY:HA2	3:B:1004:ONZ:O6	2.14	0.47
1:B:312:LYS:O	1:B:316:GLU:HG3	2.15	0.47
1:B:491:MET:O	1:B:495:MET:HG3	2.13	0.47
1:A:119:VAL:HG12	1:A:119:VAL:O	2.14	0.47
1:B:171:TRP:HB3	1:B:175:PHE:O	2.15	0.47
1:B:323:ARG:CZ	1:B:362:GLU:HB2	2.44	0.47
1:B:623:PHE:O	1:B:624:LYS:HG2	2.15	0.47
1:B:677:ILE:CD1	1:B:861:ASP:HB3	2.44	0.47
1:B:755:ARG:O	1:B:759:ILE:HG12	2.14	0.47
1:B:330:THR:HB	1:B:333:LYS:CG	2.44	0.47
1:A:416:LEU:HD21	1:A:423:TYR:CE2	2.50	0.47
1:A:480:THR:N	1:A:483:MET:CE	2.62	0.47
1:A:860:VAL:HG11	1:A:865:TYR:CE2	2.49	0.47
1:B:66:THR:HG23	1:B:68:VAL:H	1.79	0.47
1:B:743:LYS:HA	1:B:749:TYR:CD2	2.49	0.47
1:B:786:PHE:CZ	1:B:790:ILE:HG13	2.49	0.47
1:A:193:ILE:HD13	1:A:201:ALA:HB3	1.97	0.47
1:B:376:THR:O	1:B:380:PHE:HB2	2.14	0.47
1:A:24:LYS:O	1:A:27:TYR:HB3	2.15	0.46
1:A:67:PHE:HE2	1:A:160:GLN:O	1.99	0.46
1:A:134:LEU:HB3	1:A:199:TYR:OH	2.15	0.46
1:B:588:TYR:CD2	1:B:589:MET:HE3	2.51	0.46
1:B:589:MET:HE2	1:B:589:MET:HA	1.97	0.46
1:B:93:LEU:HD12	1:B:93:LEU:N	2.30	0.46
1:B:801:ARG:HG2	1:B:805:GLN:NE2	2.30	0.46
1:A:367:ASP:O	1:A:371:VAL:HG23	2.15	0.46
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.44	0.46
1:B:564:ILE:CG2	1:B:565:GLU:H	2.27	0.46
1:B:281:ILE:CD1	1:B:304:GLU:CG	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:THR:O	1:B:524:GLU:C	2.57	0.46
1:B:714:ASP:OD1	1:B:740:ARG:HG2	2.15	0.46
1:A:297:VAL:HG13	1:A:382:SER:OG	2.16	0.46
1:A:226:VAL:HG12	1:A:227:GLY:N	2.31	0.46
1:A:564:ILE:HG13	1:A:565:GLU:H	1.81	0.46
1:B:119:VAL:HG12	1:B:175:PHE:HA	1.98	0.46
1:B:778:THR:O	1:B:781:ILE:HG13	2.16	0.46
1:A:420:HIS:HD2	1:A:423:TYR:N	2.14	0.46
1:B:786:PHE:CD1	1:B:787:LEU:N	2.84	0.46
1:A:22:ILE:CD1	1:A:313:MET:HE1	2.41	0.46
1:A:453:ALA:O	1:A:456:VAL:HB	2.15	0.46
1:A:768:PHE:HE1	1:A:811:SER:HB3	1.81	0.46
1:A:873:ARG:HG2	1:A:873:ARG:HH11	1.81	0.46
1:B:281:ILE:HD11	1:B:304:GLU:HB3	1.98	0.46
1:B:718:LEU:C	1:B:720:ASP:H	2.23	0.46
1:B:786:PHE:CD1	1:B:786:PHE:C	2.94	0.46
1:A:21:LYS:HB2	1:A:21:LYS:NZ	2.30	0.45
1:A:313:MET:HB3	1:A:318:LEU:HB2	1.97	0.45
1:A:356:LEU:CD1	1:A:371:VAL:HG21	2.43	0.45
1:A:552:THR:HG22	1:B:117:ASN:ND2	2.31	0.45
1:A:674:VAL:HB	1:A:858:VAL:HG22	1.98	0.45
1:B:105:VAL:O	1:B:105:VAL:CG1	2.63	0.45
1:A:112:TYR:OH	1:A:137:PHE:HB2	2.16	0.45
1:A:767:LEU:HD13	1:A:768:PHE:CE2	2.52	0.45
1:A:821:THR:O	1:A:825:VAL:HG23	2.17	0.45
1:A:224:CYS:HA	1:A:409:THR:O	2.16	0.45
1:A:696:VAL:HG21	1:A:703:MET:HE3	1.98	0.45
1:A:744:MET:HE2	1:A:829:ARG:CZ	2.47	0.45
1:A:94:ARG:O	1:A:107:MET:HA	2.16	0.45
1:B:307:ARG:HB2	1:B:334:PHE:HB3	1.98	0.45
1:A:39:ILE:CD1	1:A:42:ARG:HH21	2.29	0.45
1:B:836:ALA:HA	1:B:882:LEU:HD12	1.99	0.45
1:A:55:PHE:C	1:A:57:PRO:HD2	2.41	0.45
1:B:99:HIS:C	1:B:102:ASN:H	2.25	0.45
1:B:673:GLU:CD	1:B:849:ARG:HH22	2.25	0.45
1:A:25:TYR:CE2	1:A:313:MET:HG2	2.52	0.45
1:B:664:THR:HG23	1:B:899:LYS:HB3	1.98	0.45
1:A:44:ARG:HA	1:A:47:MET:HE2	1.97	0.45
1:A:62:LYS:O	1:A:63:MET:C	2.60	0.45
1:A:323:ARG:HE	1:A:362:GLU:H	1.65	0.45
1:B:272:ASP:OD1	1:B:273:ILE:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD22	1:A:450:GLY:CA	2.42	0.45
1:A:238:TYR:CE2	1:A:240:GLU:HB2	2.52	0.45
1:A:619:TRP:HB3	1:A:623:PHE:O	2.17	0.45
1:B:64:LEU:HD13	1:B:158:CYS:O	2.16	0.45
1:B:563:PRO:HB2	1:B:566:ILE:HG13	1.99	0.45
1:A:66:THR:CG2	1:A:256:CYS:O	2.49	0.44
1:A:258:ASN:C	1:A:258:ASN:OD1	2.59	0.44
1:A:286:LEU:O	1:A:288:PRO:HD3	2.17	0.44
1:A:786:PHE:CE2	1:A:790:ILE:HG13	2.52	0.44
1:B:280:GLU:HG3	1:B:283:ARG:NH2	2.32	0.44
1:B:910:ARG:HG3	1:B:914:GLU:OE2	2.16	0.44
1:A:185:VAL:HA	1:A:188:LEU:HD12	1.99	0.44
1:A:342:ILE:CG2	1:A:372:GLN:HG3	2.48	0.44
1:B:21:LYS:HB3	1:B:21:LYS:HZ2	1.79	0.44
1:B:71:ILE:HB	1:B:72:PRO:HD2	1.99	0.44
1:B:73:ASP:OD1	1:B:73:ASP:C	2.60	0.44
1:B:591:ILE:H	1:B:591:ILE:HG13	1.61	0.44
1:A:436:PRO:C	1:A:438:SER:H	2.25	0.44
1:A:768:PHE:HA	1:A:769:ARG:CZ	2.47	0.44
1:B:380:PHE:CD2	1:B:426:ARG:HD3	2.53	0.44
1:B:384:ASN:HD22	1:B:384:ASN:HA	1.62	0.44
1:B:801:ARG:HG2	1:B:805:GLN:HE22	1.82	0.44
1:A:25:TYR:C	1:A:27:TYR:H	2.25	0.44
1:A:373:HIS:O	1:A:377:ILE:HG12	2.16	0.44
1:A:84:ASP:OD2	3:A:1002:ONZ:O3	2.35	0.44
1:A:106:HIS:ND1	1:A:107:MET:N	2.65	0.44
1:B:320:PHE:CD2	1:B:361:VAL:CG2	3.00	0.44
1:B:342:ILE:O	1:B:372:GLN:HG3	2.16	0.44
1:B:712:PHE:HB3	1:B:741:TYR:HB2	2.00	0.44
1:B:791:GLU:OE1	1:B:824:GLY:HA2	2.18	0.44
1:B:42:ARG:O	1:B:46:GLU:HG2	2.18	0.44
1:B:204:VAL:HG12	1:B:460:ALA:HB1	1.99	0.44
1:A:297:VAL:HA	1:A:382:SER:OG	2.18	0.44
1:A:479:LEU:HA	1:A:483:MET:CE	2.47	0.44
1:A:565:GLU:CG	1:A:566:ILE:HG12	2.47	0.44
1:A:479:LEU:CA	1:A:483:MET:HE3	2.45	0.44
1:A:99:HIS:O	1:A:102:ASN:N	2.48	0.44
1:A:551:ARG:NH1	1:A:551:ARG:HG3	2.32	0.44
1:A:589:MET:HB2	1:A:591:ILE:HG12	2.00	0.44
1:B:148:LEU:HA	1:B:149:PRO:HD3	1.75	0.44
1:B:718:LEU:O	1:B:720:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:THR:O	1:B:339:VAL:HB	2.18	0.43
1:B:471:GLU:OE1	1:B:471:GLU:O	2.35	0.43
1:A:229:ILE:O	1:A:234:THR:HA	2.19	0.43
1:A:735:ASN:HB2	1:A:738:LYS:HE3	2.00	0.43
1:A:100:GLU:HB3	1:A:101:LYS:CD	2.49	0.43
1:A:420:HIS:HB3	1:A:423:TYR:HB2	2.01	0.43
1:A:790:ILE:HD11	1:A:803:ILE:CG2	2.48	0.43
1:A:486:GLU:HG2	6:A:1141:HOH:O	2.17	0.43
1:B:71:ILE:HA	1:B:215:MET:SD	2.57	0.43
1:B:91:ARG:NH1	1:B:91:ARG:CB	2.80	0.43
1:A:320:PHE:C	1:A:322:GLY:N	2.75	0.43
1:B:644:ARG:HA	1:B:644:ARG:HD2	1.31	0.43
1:B:539:ARG:NH1	1:B:559:ILE:HD11	2.33	0.43
1:B:775:THR:O	1:B:781:ILE:HD13	2.04	0.43
1:A:400:ASN:HD22	1:A:400:ASN:HA	1.62	0.43
1:A:551:ARG:HG3	1:A:551:ARG:HH11	1.83	0.43
1:A:26:LEU:HD21	1:A:309:ILE:HG21	2.01	0.43
1:A:204:VAL:HG12	1:A:204:VAL:O	2.17	0.43
1:B:508:VAL:HG22	6:B:1223:HOH:O	2.19	0.43
1:B:611:LEU:HG	1:B:653:ALA:CB	2.49	0.43
1:B:662:MET:HG3	1:B:674:VAL:C	2.44	0.43
1:A:58:THR:OG1	1:B:799:GLN:NE2	2.52	0.43
1:A:98:ASN:ND2	1:A:101:LYS:CE	2.80	0.43
1:A:251:ASP:N	1:A:251:ASP:OD1	2.50	0.43
1:A:666:ALA:O	1:A:667:TYR:C	2.61	0.43
1:B:349:LEU:HD11	1:B:369:VAL:CG2	2.49	0.43
1:B:672:CYS:HA	1:B:857:THR:O	2.19	0.43
1:B:798:LEU:O	1:B:798:LEU:CD2	2.67	0.43
1:B:662:MET:SD	1:B:687:MET:HE3	2.59	0.42
1:A:79:ASP:OD2	1:A:148:LEU:HD21	2.19	0.42
1:A:159:GLN:HB3	1:A:167:ILE:HB	2.01	0.42
1:A:265:GLY:HA2	1:A:269:SER:CB	2.46	0.42
1:A:420:HIS:HD2	1:A:423:TYR:HB2	1.82	0.42
1:A:525:ASN:OD1	1:A:546:ARG:HA	2.19	0.42
1:A:709:TRP:C	1:A:709:TRP:CD1	2.96	0.42
1:B:529:LEU:O	1:B:598:LEU:HA	2.19	0.42
1:B:871:PHE:CD2	1:B:871:PHE:C	2.97	0.42
1:A:83:LEU:HB2	1:A:152:PHE:HD1	1.84	0.42
1:A:861:ASP:OD1	1:A:866:LYS:HE3	2.19	0.42
1:A:69:ARG:O	1:A:70:SER:HB3	2.19	0.42
1:B:384:ASN:ND2	1:B:430:THR:HG21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ILE:HG13	1:A:352:ALA:HB2	2.02	0.42
1:A:451:LYS:O	1:A:455:MET:HG2	2.19	0.42
1:A:477:PHE:CZ	1:A:757:ILE:HD11	2.54	0.42
1:B:67:PHE:HE2	1:B:160:GLN:O	2.03	0.42
1:B:405:ARG:HH11	1:B:405:ARG:CB	2.27	0.42
1:A:44:ARG:NH1	1:A:395:ASN:HB3	2.35	0.42
1:B:212:GLY:HA3	1:B:449:SER:HB2	2.00	0.42
1:B:492:ARG:CZ	1:B:844:LYS:HG3	2.49	0.42
1:B:524:GLU:CD	1:B:524:GLU:H	2.27	0.42
1:B:738:LYS:HE3	6:B:1129:HOH:O	2.18	0.42
1:A:519:THR:HB	1:A:520:PRO:HD2	2.01	0.42
1:B:22:ILE:HD11	1:B:370:SER:CB	2.48	0.42
1:B:83:LEU:HB2	1:B:152:PHE:CD1	2.54	0.42
1:B:718:LEU:O	1:B:719:ASP:C	2.63	0.42
1:B:818:LEU:O	1:B:822:VAL:HG23	2.20	0.42
1:A:523:THR:O	1:A:524:GLU:C	2.63	0.42
1:A:652:VAL:HG21	1:A:909:VAL:HG22	2.01	0.42
1:A:718:LEU:C	1:A:720:ASP:H	2.27	0.42
1:A:786:PHE:CD1	1:A:786:PHE:C	2.96	0.42
1:A:803:ILE:O	1:A:806:GLN:HB2	2.20	0.42
1:A:911:LEU:O	1:A:914:GLU:HB3	2.20	0.42
1:B:261:TRP:CD1	1:B:261:TRP:C	2.98	0.42
1:A:479:LEU:C	1:A:483:MET:HE3	2.41	0.42
1:B:324:ILE:HG23	1:B:328:LEU:HD23	2.01	0.42
1:B:775:THR:HG22	1:B:781:ILE:HD13	2.01	0.42
1:B:518:ARG:HH11	1:B:518:ARG:CG	2.32	0.41
1:A:57:PRO:HG2	1:B:799:GLN:HE21	1.84	0.41
1:B:79:ASP:O	1:B:149:PRO:HD2	2.20	0.41
1:B:523:THR:OG1	1:B:910:ARG:NH1	2.53	0.41
1:A:100:GLU:C	1:A:101:LYS:HD2	2.45	0.41
1:A:277:PHE:CE1	1:A:309:ILE:HA	2.55	0.41
1:A:601:THR:HA	1:A:655:VAL:O	2.20	0.41
1:B:21:LYS:HB3	1:B:21:LYS:HZ3	1.83	0.41
1:B:347:GLU:O	1:B:351:ASN:N	2.43	0.41
1:B:347:GLU:HB2	1:B:351:ASN:ND2	2.36	0.41
1:B:349:LEU:HD22	1:B:349:LEU:HA	1.76	0.41
1:B:690:MET:SD	1:B:703:MET:HB2	2.60	0.41
1:B:589:MET:CB	1:B:591:ILE:HG12	2.50	0.41
1:B:563:PRO:O	1:B:566:ILE:N	2.41	0.41
1:B:654:VAL:HG13	1:B:654:VAL:O	2.20	0.41
1:B:754:VAL:O	1:B:758:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:THR:HG22	1:B:294:GLU:HG3	2.03	0.41
1:A:97:VAL:HG21	1:A:105:VAL:CG2	2.51	0.41
1:A:380:PHE:HD2	1:A:426:ARG:HD3	1.76	0.41
1:A:878:THR:O	1:A:882:LEU:HG	2.20	0.41
1:B:86:GLY:HA3	1:B:155:SER:OG	2.21	0.41
1:A:152:PHE:O	1:A:206:VAL:HA	2.21	0.41
1:A:196:ARG:C	1:A:198:ASP:N	2.78	0.41
1:A:295:LYS:HB2	6:A:1228:HOH:O	2.21	0.41
1:A:524:GLU:H	1:A:524:GLU:CD	2.29	0.41
1:A:564:ILE:CG1	1:A:565:GLU:N	2.84	0.41
1:B:20:LYS:HE3	1:B:24:LYS:CE	2.51	0.41
1:B:615:ILE:HA	1:B:631:HIS:O	2.21	0.41
1:B:652:VAL:HB	1:B:905:THR:HG23	2.03	0.41
1:A:99:HIS:C	1:A:102:ASN:H	2.27	0.41
1:A:330:THR:HB	1:A:333:LYS:CG	2.51	0.41
1:B:105:VAL:O	1:B:105:VAL:HG13	2.21	0.41
1:A:91:ARG:CB	1:A:91:ARG:NH1	2.84	0.40
1:A:98:ASN:H	1:A:103:GLN:HB2	1.87	0.40
1:B:687:MET:CE	1:B:704:CYS:HB2	2.49	0.40
1:B:798:LEU:HG	6:B:1114:HOH:O	2.20	0.40
1:A:323:ARG:NE	1:A:362:GLU:CG	2.85	0.40
1:A:912:ARG:C	1:A:914:GLU:H	2.29	0.40
1:B:532:ASP:O	1:B:538:PHE:HA	2.21	0.40
1:A:139:GLU:HA	1:A:139:GLU:OE1	2.21	0.40
1:A:261:TRP:CD1	1:A:261:TRP:C	2.99	0.40
1:A:782:PHE:CD1	1:A:786:PHE:CE1	3.09	0.40
1:B:17:ASP:O	1:B:21:LYS:HG3	2.21	0.40
1:B:712:PHE:HB3	1:B:741:TYR:CB	2.51	0.40
1:B:718:LEU:HD22	1:B:721:ILE:HD11	2.04	0.40
1:A:44:ARG:HA	1:A:47:MET:HE3	2.03	0.40
1:A:231:GLY:O	1:A:232:THR:C	2.63	0.40
1:A:677:ILE:O	1:A:682:SER:HA	2.21	0.40
1:B:18:GLN:HA	1:B:18:GLN:OE1	2.21	0.40
1:B:103:GLN:OE1	1:B:103:GLN:C	2.64	0.40
1:B:483:MET:O	1:B:487:VAL:HG23	2.21	0.40
1:B:586:LEU:HB3	1:B:592:LYS:HB3	2.03	0.40
1:B:778:THR:HB	1:B:781:ILE:CD1	2.48	0.40
1:A:570:THR:HA	1:A:626:THR:OG1	2.22	0.40
1:B:431:LEU:CD2	1:B:442:PHE:HZ	2.21	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	897/914 (98%)	838 (93%)	58 (6%)	1 (0%)	48	66
1	B	897/914 (98%)	843 (94%)	53 (6%)	1 (0%)	48	66
All	All	1794/1828 (98%)	1681 (94%)	111 (6%)	2 (0%)	48	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	B	564	ILE

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	774/786 (98%)	746 (96%)	28 (4%)	31	51
1	B	774/786 (98%)	740 (96%)	34 (4%)	25	43
All	All	1548/1572 (98%)	1486 (96%)	62 (4%)	28	47

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	21	LYS
1	A	80	PHE
1	A	93	LEU

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Mol	Chain	Res	Type
1	A	100	GLU
1	A	101	LYS
1	A	159	GLN
1	A	249	GLU
1	A	271	GLU
1	A	321	GLU
1	A	335	ASN
1	A	344	LYS
1	A	380	PHE
1	A	408	THR
1	A	470	ILE
1	A	481	LYS
1	A	502	GLN
1	A	531	LEU
1	A	541	LEU
1	A	550	LYS
1	A	566	ILE
1	A	567	MET
1	A	570	THR
1	A	709	TRP
1	A	769	ARG
1	A	781	ILE
1	A	843	ASP
1	A	877	GLN
1	B	66	THR
1	B	93	LEU
1	B	103	GLN
1	B	105	VAL
1	B	146	LYS
1	B	147	LYS
1	B	281	ILE
1	B	319	LEU
1	B	320	PHE
1	B	321	GLU
1	B	349	LEU
1	B	407	ARG
1	B	424	SER
1	B	435	VAL
1	B	437	ASP
1	B	481	LYS
1	B	531	LEU
1	B	562	ILE

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Mol	Chain	Res	Type
1	B	564	ILE
1	B	565	GLU
1	B	566	ILE
1	B	591	ILE
1	B	592	LYS
1	B	644	ARG
1	B	645	GLU
1	B	721	ILE
1	B	764	LYS
1	B	769	ARG
1	B	777	LYS
1	B	786	PHE
1	B	798	LEU
1	B	805	GLN
1	B	843	ASP
1	B	857	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	102	ASN
1	A	104	ASN
1	A	125	GLN
1	A	129	HIS
1	A	159	GLN
1	A	202	ASN
1	A	222	GLN
1	A	335	ASN
1	A	384	ASN
1	A	400	ASN
1	A	466	GLN
1	A	467	HIS
1	A	506	ASN
1	A	700	GLN
1	A	724	HIS
1	A	771	GLN
1	A	799	GLN
1	A	805	GLN
1	A	806	GLN
1	A	810	ASN
1	A	832	GLN

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Mol	Chain	Res	Type
1	A	877	GLN
1	A	887	ASN
1	B	96	GLN
1	B	125	GLN
1	B	202	ASN
1	B	291	GLN
1	B	345	ASN
1	B	372	GLN
1	B	384	ASN
1	B	400	ASN
1	B	420	HIS
1	B	466	GLN
1	B	469	GLN
1	B	502	GLN
1	B	506	ASN
1	B	557	ASN
1	B	771	GLN
1	B	799	GLN
1	B	805	GLN
1	B	806	GLN
1	B	832	GLN
1	B	848	ASN
1	B	870	HIS
1	B	887	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	BGC	B	1003	-	12,12,12	0.38	0	17,17,17	0.83	0
2	BGC	B	1001	-	12,12,12	0.46	0	17,17,17	1.06	2 (11%)
2	BGC	A	1003	-	12,12,12	0.34	0	17,17,17	1.22	2 (11%)
3	0NZ	B	1004	-	15,15,15	1.15	1 (6%)	19,22,22	0.81	1 (5%)
3	0NZ	B	1002	-	15,15,15	1.21	1 (6%)	19,22,22	0.84	1 (5%)
2	BGC	A	1001	-	12,12,12	0.55	0	17,17,17	1.05	2 (11%)
3	0NZ	A	1002	-	15,15,15	0.88	1 (6%)	19,22,22	0.68	1 (5%)
5	CIT	B	1007	-	12,12,12	1.06	0	17,17,17	1.45	2 (11%)
3	0NZ	A	1004	-	15,15,15	1.21	1 (6%)	19,22,22	0.98	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	B	1003	-	-	0/2/22/22	0/1/1/1
2	BGC	B	1001	-	-	0/2/22/22	0/1/1/1
2	BGC	A	1003	-	-	0/2/22/22	0/1/1/1
3	0NZ	B	1004	-	-	3/6/22/22	0/1/1/1
3	0NZ	B	1002	-	-	1/6/22/22	0/1/1/1
2	BGC	A	1001	-	-	0/2/22/22	0/1/1/1
3	0NZ	A	1002	-	-	1/6/22/22	0/1/1/1
5	CIT	B	1007	-	-	7/16/16/16	-
3	0NZ	A	1004	-	-	2/6/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	0NZ	P-O1P	3.49	1.61	1.50
3	A	1004	0NZ	P-O1P	3.36	1.60	1.50
3	B	1004	0NZ	P-O1P	3.33	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	0NZ	P-O2P	2.02	1.62	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1007	CIT	O6-C6-C3	3.80	120.42	113.14
2	A	1003	BGC	O5-C1-C2	-3.42	104.29	110.30
3	A	1004	0NZ	O3P-P-O6	3.25	115.15	106.67
2	B	1001	BGC	O5-C1-C2	-2.85	105.28	110.30
3	B	1004	0NZ	O2P-P-O6	2.72	113.75	106.67
2	B	1001	BGC	C1-O5-C5	-2.70	108.43	113.65
3	B	1002	0NZ	O2P-P-O6	2.53	113.27	106.67
3	A	1002	0NZ	O6-P-O1P	2.43	113.00	106.44
2	A	1003	BGC	C1-O5-C5	-2.39	109.02	113.65
2	A	1001	BGC	O5-C1-C2	-2.21	106.42	110.30
2	A	1001	BGC	C1-O5-C5	-2.18	109.43	113.65
5	B	1007	CIT	O4-C5-C4	2.07	120.90	114.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	0NZ	C6-O6-P-O1P
3	B	1004	0NZ	C6-O6-P-O3P
5	B	1007	CIT	C1-C2-C3-O7
5	B	1007	CIT	C1-C2-C3-C6
5	B	1007	CIT	O7-C3-C6-O5
5	B	1007	CIT	O7-C3-C6-O6
5	B	1007	CIT	C4-C3-C6-O5
5	B	1007	CIT	C4-C3-C6-O6
5	B	1007	CIT	C1-C2-C3-C4
3	A	1002	0NZ	C5-C6-O6-P
3	A	1004	0NZ	C5-C6-O6-P
3	B	1002	0NZ	C5-C6-O6-P
3	B	1004	0NZ	C5-C6-O6-P
3	B	1004	0NZ	C6-O6-P-O2P

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1004	ONZ	1	0
3	A	1002	ONZ	2	0
5	B	1007	CIT	4	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, 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	899/914 (98%)	0.45	39 (4%) 40 32	27, 53, 81, 122	0
1	B	899/914 (98%)	0.44	35 (3%) 43 35	27, 53, 81, 122	0
All	All	1798/1828 (98%)	0.44	74 (4%) 41 33	27, 53, 81, 122	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	911	LEU	4.3
1	A	786	PHE	3.8
1	A	447	SER	3.6
1	B	786	PHE	3.6
1	A	406	LEU	3.5
1	B	103	GLN	3.4
1	A	19	VAL	3.2
1	B	335	ASN	3.1
1	B	79	ASP	3.1
1	A	443	LEU	3.1
1	B	99	HIS	3.1
1	B	101	LYS	3.1
1	A	18	GLN	3.0
1	B	911	LEU	3.0
1	A	310	LEU	2.9
1	A	223	HIS	2.9
1	A	665	CYS	2.9
1	A	361	VAL	2.8
1	B	852	ASP	2.7
1	A	108	GLU	2.7
1	B	19	VAL	2.7
1	A	314	ALA	2.6
1	A	427	PHE	2.6
1	B	98	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	105	VAL	2.5
1	A	342	ILE	2.5
1	B	649	LEU	2.5
1	B	594	PRO	2.5
1	B	111	VAL	2.4
1	A	334	PHE	2.4
1	B	146	LYS	2.4
1	A	444	LEU	2.4
1	B	891	LEU	2.4
1	B	565	GLU	2.4
1	A	423	TYR	2.4
1	B	518	ARG	2.4
1	B	515	PHE	2.4
1	B	564	ILE	2.3
1	B	897	SER	2.3
1	A	105	VAL	2.3
1	B	108	GLU	2.3
1	A	22	ILE	2.3
1	B	665	CYS	2.3
1	A	437	ASP	2.3
1	A	26	LEU	2.3
1	A	36	LEU	2.3
1	A	565	GLU	2.2
1	A	222	GLN	2.2
1	A	146	LYS	2.2
1	A	341	ALA	2.2
1	B	567	MET	2.2
1	A	720	ASP	2.2
1	A	27	TYR	2.1
1	B	27	TYR	2.1
1	B	348	GLY	2.1
1	A	17	ASP	2.1
1	B	337	SER	2.1
1	A	20	LYS	2.1
1	B	96	GLN	2.1
1	B	31	LEU	2.1
1	B	106	HIS	2.1
1	B	439	ASP	2.1
1	B	436	PRO	2.1
1	A	349	LEU	2.1
1	B	798	LEU	2.1
1	A	106	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	720	ASP	2.0
1	A	446	GLU	2.0
1	A	67	PHE	2.0
1	A	277	PHE	2.0
1	A	438	SER	2.0
1	A	594	PRO	2.0
1	B	913	THR	2.0
1	A	771	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CIT	B	1007	13/13	0.76	0.17	104,104,105,105	0
4	NA	B	1005	1/1	0.78	0.11	56,56,56,56	0
2	BGC	A	1001	12/12	0.87	0.10	40,43,44,45	0
2	BGC	B	1003	12/12	0.91	0.08	30,33,34,36	0
2	BGC	B	1001	12/12	0.92	0.12	43,46,49,49	0
2	BGC	A	1003	12/12	0.93	0.09	29,34,35,38	0
3	0NZ	A	1002	15/15	0.93	0.08	48,49,50,50	0
4	NA	A	1005	1/1	0.94	0.06	58,58,58,58	0
4	NA	A	1006	1/1	0.94	0.06	46,46,46,46	0
3	0NZ	B	1002	15/15	0.95	0.11	53,55,57,58	0
3	0NZ	B	1004	15/15	0.95	0.09	29,34,38,38	0
4	NA	B	1006	1/1	0.96	0.05	47,47,47,47	0
3	0NZ	A	1004	15/15	0.96	0.09	27,35,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.