



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:42 pm GMT

PDB ID : 1SOJ
Title : CATALYTIC DOMAIN OF HUMAN PHOSPHODIESTERASE 3B IN COMPLEX WITH IBMX
Authors : Scapin, G.; Patel, S.B.; Chung, C.; Varnerin, J.P.; Edmondson, S.D.; Mastracchio, A.; Parmee, E.R.; Becker, J.W.; Singh, S.B.; Van Der Ploeg, L.H.; Tota, M.R.
Deposited on : 2004-03-15
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

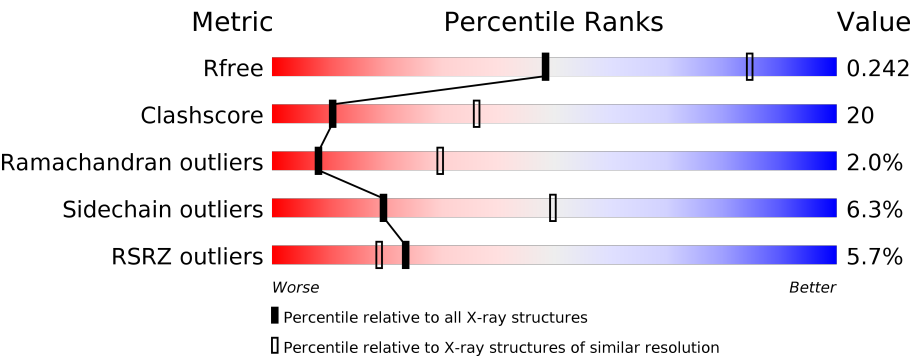
MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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}	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

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	420	<div><div>2%</div><div><div></div><div>56%</div><div>27%</div><div>•</div><div>13%</div></div></div>
1	B	420	<div><div>7%</div><div><div></div><div>55%</div><div>30%</div><div>5%</div><div>9%</div></div></div>
1	C	420	<div><div>3%</div><div><div></div><div>55%</div><div>29%</div><div>•</div><div>13%</div></div></div>
1	D	420	<div><div>6%</div><div><div></div><div>55%</div><div>31%</div><div>5%</div><div>9%</div></div></div>
1	E	420	<div><div>3%</div><div><div></div><div>55%</div><div>28%</div><div>•</div><div>13%</div></div></div>
1	F	420	<div><div>3%</div><div><div></div><div>58%</div><div>29%</div><div>5%</div><div>9%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	420	
1	H	420	
1	I	420	
1	J	420	
1	K	420	
1	L	420	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36048 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 cGMP-inhibited 3',5'-cyclic phosphodiesterase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	B	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	C	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	D	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	E	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	F	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	G	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	H	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	I	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	J	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			
1	K	364	Total	C	N	O	S	0	0	0
			2907	1862	496	535	14			
1	L	381	Total	C	N	O	S	0	0	0
			3017	1922	519	562	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

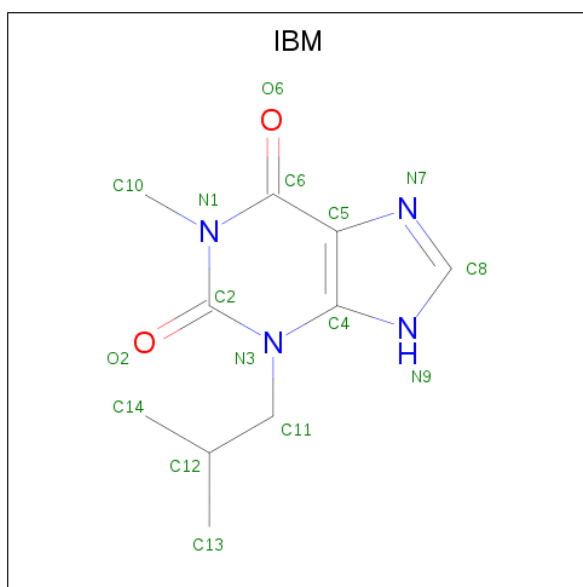
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mg	0	0
			2	2		
2	J	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mg	0	0
			2	2		
2	K	2	Total	Mg	0	0
			2	2		
2	E	2	Total	Mg	0	0
			2	2		
2	H	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	I	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		
2	L	2	Total	Mg	0	0
			2	2		
2	F	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 3-ISOBUTYL-1-METHYLNANTHINE (three-letter code: IBM) (formula: $C_{10}H_{14}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	10	4	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			16	10	4	2		
3	C	1	Total	C	N	O	0	0
			16	10	4	2		
3	D	1	Total	C	N	O	0	0
			16	10	4	2		
3	E	1	Total	C	N	O	0	0
			16	10	4	2		
3	F	1	Total	C	N	O	0	0
			16	10	4	2		
3	G	1	Total	C	N	O	0	0
			16	10	4	2		
3	H	1	Total	C	N	O	0	0
			16	10	4	2		
3	I	1	Total	C	N	O	0	0
			16	10	4	2		
3	J	1	Total	C	N	O	0	0
			16	10	4	2		
3	K	1	Total	C	N	O	0	0
			16	10	4	2		
3	L	1	Total	C	N	O	0	0
			16	10	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	24	Total	O	0	0
			24	24		
4	C	24	Total	O	0	0
			24	24		
4	D	24	Total	O	0	0
			24	24		
4	E	23	Total	O	0	0
			23	23		
4	F	25	Total	O	0	0
			25	25		
4	G	23	Total	O	0	0
			23	23		
4	H	25	Total	O	0	0
			25	25		

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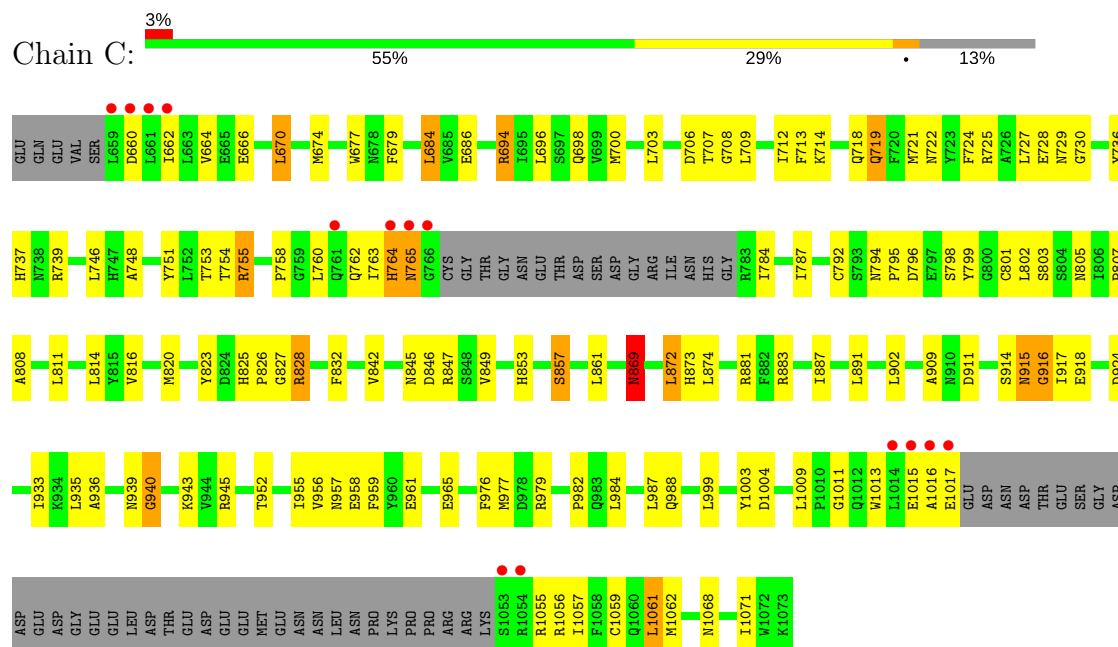
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	24	Total 24	O 24	0	0
4	J	24	Total 24	O 24	0	0
4	K	24	Total 24	O 24	0	0
4	L	24	Total 24	O 24	0	0

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.

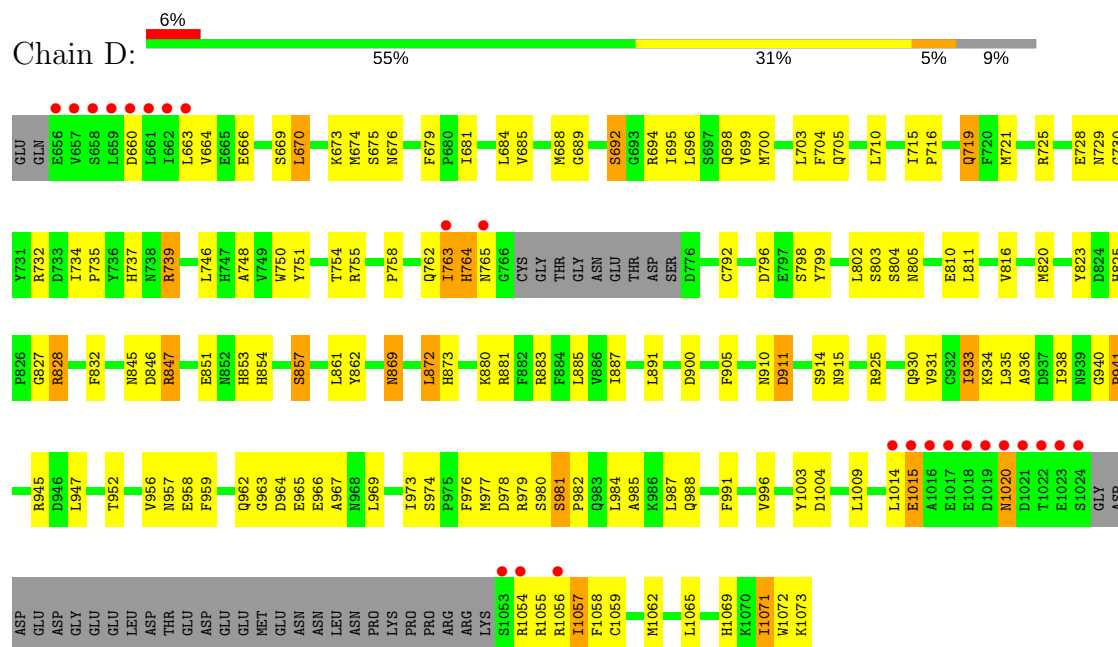
- Chain A:

- Chain B:
-
- 7% 55% 30% 5% 9%
- | Category | Value |
|----------|-------|
| Red | 7% |
| Green | 55% |
| Yellow | 30% |
| Grey | 9% |

- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

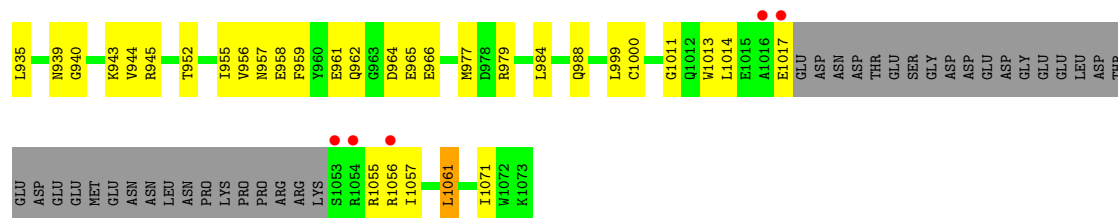


- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

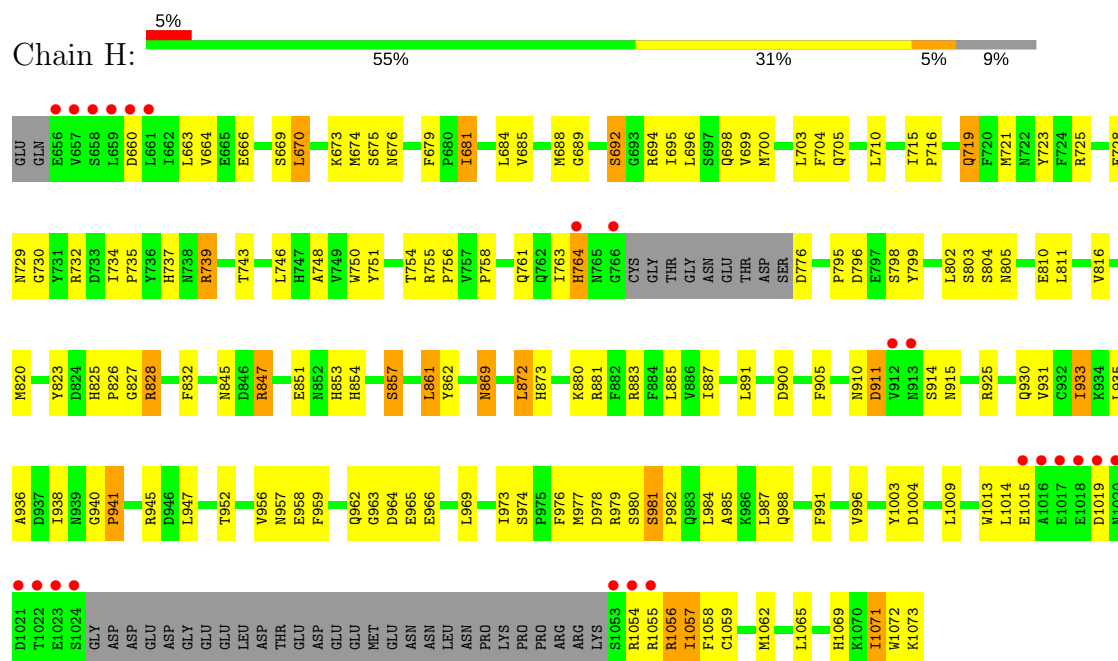


- Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

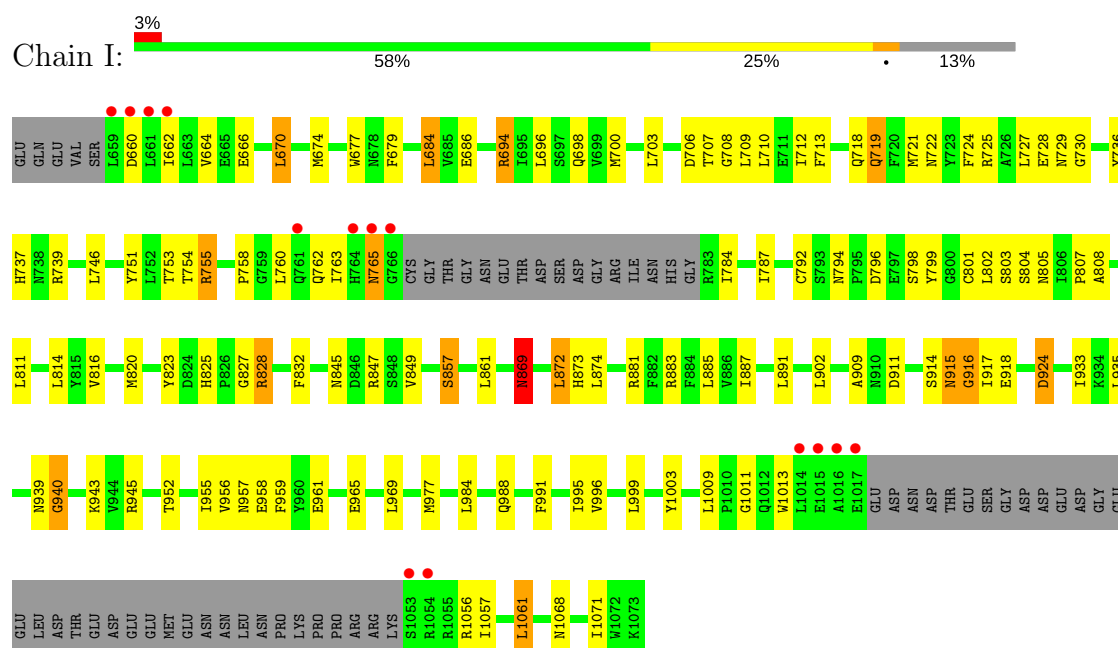




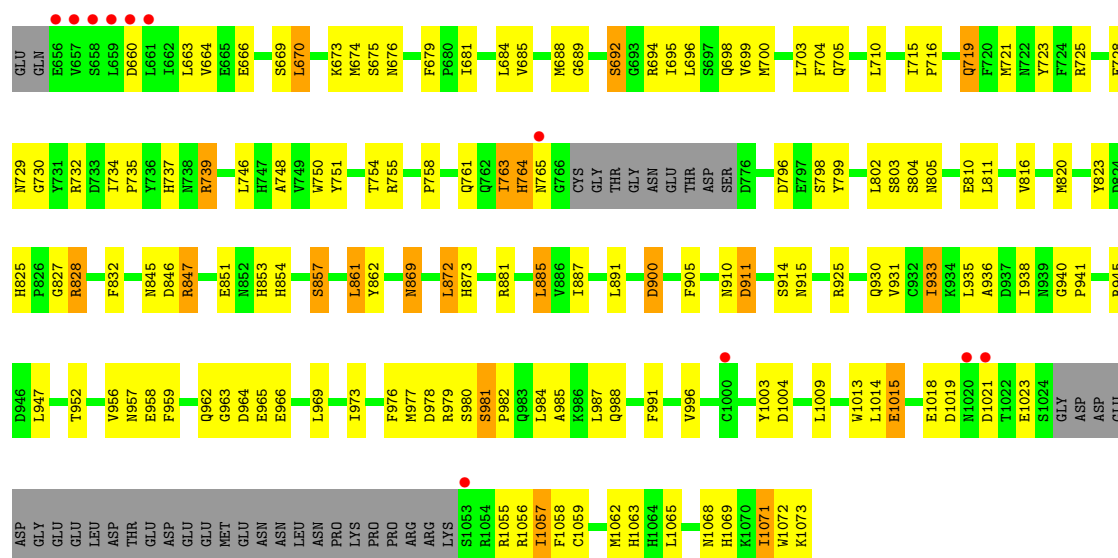
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



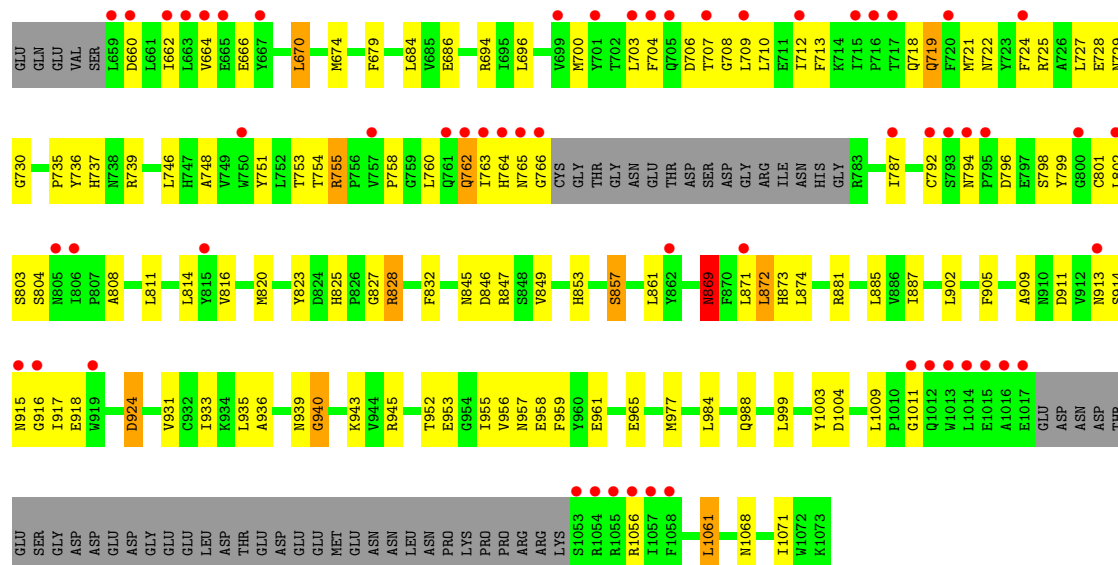
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



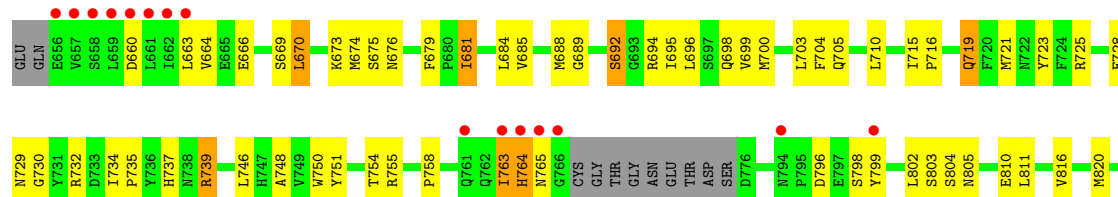
• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B

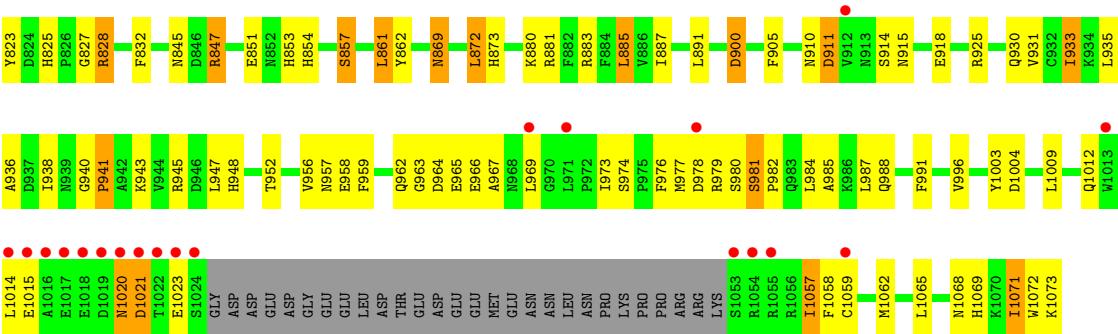


• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B



• Molecule 1: cGMP-inhibited 3',5'-cyclic phosphodiesterase B





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	275.05Å 147.08Å 253.49Å 90.00° 109.84° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 49.61 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.90) 96.6 (49.61-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.91Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.231 , 0.249 0.228 , 0.242	Depositor DCC
R_{free} test set	10128 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	36048	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: MG, IBM

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	0.45	0/2982	0.59	0/4053
1	B	0.44	0/3092	0.59	0/4203
1	C	0.45	0/2982	0.59	0/4053
1	D	0.47	0/3092	0.60	0/4203
1	E	0.47	1/2982 (0.0%)	0.59	0/4053
1	F	0.46	0/3092	0.59	0/4203
1	G	0.45	0/2982	0.59	0/4053
1	H	0.45	0/3092	0.59	1/4203 (0.0%)
1	I	0.45	0/2982	0.58	0/4053
1	J	0.46	0/3092	0.59	0/4203
1	K	0.47	0/2982	0.59	0/4053
1	L	0.47	0/3092	0.60	0/4203
All	All	0.46	1/36444 (0.0%)	0.59	1/49536 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1000	CYS	CB-SG	-5.15	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	795	PRO	N-CA-CB	5.03	109.34	103.30

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	2907	0	2772	110	0
1	B	3017	0	2834	132	0
1	C	2907	0	2772	124	0
1	D	3017	0	2834	134	0
1	E	2907	0	2772	114	0
1	F	3017	0	2834	119	0
1	G	2907	0	2772	109	0
1	H	3017	0	2834	126	0
1	I	2907	0	2772	108	0
1	J	3017	0	2834	143	0
1	K	2907	0	2772	108	0
1	L	3017	0	2834	125	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	16	0	14	0	0
3	B	16	0	14	0	0
3	C	16	0	14	0	0
3	D	16	0	14	0	0
3	E	16	0	14	0	0
3	F	16	0	14	0	0
3	G	16	0	14	0	0
3	H	16	0	14	0	0
3	I	16	0	14	0	0
3	J	16	0	14	0	0
3	K	16	0	14	0	0
3	L	16	0	14	0	0
4	A	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	3	0
4	C	24	0	0	1	0
4	D	24	0	0	1	0
4	E	23	0	0	2	0
4	F	25	0	0	1	0
4	G	23	0	0	1	0
4	H	25	0	0	0	0
4	I	24	0	0	1	0
4	J	24	0	0	0	0
4	K	24	0	0	1	0
4	L	24	0	0	1	0
All	All	36048	0	33804	1360	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 20.

All (1360) 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:719:GLN:H	1:A:719:GLN:HE21	1.04	1.00
1:E:825:HIS:HD2	1:E:827:GLY:H	1.10	1.00
1:I:719:GLN:H	1:I:719:GLN:HE21	1.06	0.98
1:K:762:GLN:HE22	1:K:804:SER:HB2	1.28	0.98
1:K:719:GLN:H	1:K:719:GLN:HE21	1.06	0.98
1:E:719:GLN:H	1:E:719:GLN:HE21	1.05	0.97
1:G:719:GLN:HE21	1:G:719:GLN:H	1.05	0.96
1:G:1014:LEU:HD12	1:G:1056:ARG:HB3	1.45	0.96
1:I:825:HIS:HD2	1:I:827:GLY:H	1.09	0.96
1:C:825:HIS:HD2	1:C:827:GLY:H	1.10	0.95
1:L:719:GLN:HE21	1:L:719:GLN:N	1.64	0.95
1:B:719:GLN:HE21	1:B:719:GLN:N	1.63	0.95
1:C:719:GLN:HE21	1:C:719:GLN:H	1.10	0.95
1:D:719:GLN:HE21	1:D:719:GLN:N	1.65	0.94
1:F:719:GLN:N	1:F:719:GLN:HE21	1.63	0.94
1:G:825:HIS:HD2	1:G:827:GLY:H	1.11	0.94
1:H:719:GLN:HE21	1:H:719:GLN:N	1.64	0.94
1:J:719:GLN:N	1:J:719:GLN:HE21	1.64	0.94
1:B:719:GLN:NE2	1:B:719:GLN:H	1.64	0.94
1:F:719:GLN:H	1:F:719:GLN:NE2	1.65	0.94
1:A:825:HIS:HD2	1:A:827:GLY:H	1.09	0.94
1:L:719:GLN:NE2	1:L:719:GLN:H	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:911:ASP:H	1:L:914:SER:HB3	1.34	0.93
1:H:719:GLN:NE2	1:H:719:GLN:H	1.66	0.93
1:J:719:GLN:H	1:J:719:GLN:NE2	1.65	0.93
1:B:911:ASP:H	1:B:914:SER:HB3	1.33	0.92
1:D:719:GLN:NE2	1:D:719:GLN:H	1.67	0.92
1:F:911:ASP:H	1:F:914:SER:HB3	1.33	0.92
1:K:825:HIS:HD2	1:K:827:GLY:H	1.10	0.91
1:D:911:ASP:H	1:D:914:SER:HB3	1.36	0.90
1:A:762:GLN:HE21	1:A:801:CYS:H	1.19	0.90
1:H:911:ASP:H	1:H:914:SER:HB3	1.34	0.89
1:J:911:ASP:H	1:J:914:SER:HB3	1.34	0.89
1:H:828:ARG:HG2	1:H:832:PHE:CD2	2.08	0.89
1:K:762:GLN:HA	1:K:762:GLN:HE21	1.37	0.88
1:F:828:ARG:HG2	1:F:832:PHE:CD2	2.08	0.88
1:K:730:GLY:HA3	1:K:823:TYR:CE1	2.08	0.88
1:A:730:GLY:HA3	1:A:823:TYR:CE1	2.09	0.87
1:J:828:ARG:HG2	1:J:832:PHE:CD2	2.09	0.87
1:B:828:ARG:HG2	1:B:832:PHE:CD2	2.09	0.86
1:E:730:GLY:HA3	1:E:823:TYR:CE1	2.11	0.86
1:G:730:GLY:HA3	1:G:823:TYR:CE1	2.11	0.86
1:I:754:THR:HG21	1:I:755:ARG:HH21	1.38	0.86
1:F:758:PRO:HG2	1:F:1057:ILE:HD13	1.56	0.86
1:D:828:ARG:HG2	1:D:832:PHE:CD2	2.10	0.86
1:L:828:ARG:HG2	1:L:832:PHE:CD2	2.11	0.85
1:G:754:THR:HG21	1:G:755:ARG:HH21	1.39	0.85
1:C:754:THR:HG21	1:C:755:ARG:HH21	1.39	0.85
1:J:758:PRO:HG2	1:J:1057:ILE:HD13	1.59	0.85
1:A:754:THR:HG21	1:A:755:ARG:HH21	1.41	0.84
1:A:719:GLN:N	1:A:719:GLN:HE21	1.74	0.84
1:C:730:GLY:HA3	1:C:823:TYR:CE1	2.11	0.84
1:D:825:HIS:HD2	1:D:827:GLY:H	1.25	0.84
1:I:730:GLY:HA3	1:I:823:TYR:CE1	2.11	0.84
1:K:754:THR:HG21	1:K:755:ARG:HH21	1.39	0.84
1:C:754:THR:HG22	1:C:755:ARG:HE	1.44	0.83
1:G:719:GLN:N	1:G:719:GLN:HE21	1.75	0.83
1:H:825:HIS:HD2	1:H:827:GLY:H	1.25	0.83
1:E:719:GLN:N	1:E:719:GLN:HE21	1.75	0.83
1:I:754:THR:HG22	1:I:755:ARG:HE	1.43	0.83
1:E:754:THR:HG21	1:E:755:ARG:HH21	1.41	0.83
1:I:719:GLN:HE21	1:I:719:GLN:N	1.76	0.83
1:F:825:HIS:HD2	1:F:827:GLY:H	1.25	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:719:GLN:HE21	1:K:719:GLN:N	1.75	0.82
1:B:1014:LEU:HD12	1:B:1056:ARG:HB3	1.61	0.82
1:A:754:THR:HG22	1:A:755:ARG:HE	1.44	0.82
1:L:825:HIS:HD2	1:L:827:GLY:H	1.25	0.82
1:G:754:THR:HG22	1:G:755:ARG:HE	1.45	0.81
1:C:828:ARG:HG2	1:C:832:PHE:CD2	2.16	0.81
1:A:705:GLN:HE22	1:J:1056:ARG:HH21	1.25	0.81
1:G:828:ARG:HG2	1:G:832:PHE:CD2	2.16	0.81
1:C:887:ILE:HD13	1:D:845:ASN:HB3	1.63	0.80
1:J:825:HIS:HD2	1:J:827:GLY:H	1.24	0.80
1:A:762:GLN:HE21	1:A:801:CYS:N	1.79	0.80
1:A:887:ILE:HD13	1:B:845:ASN:HB3	1.63	0.80
1:C:719:GLN:N	1:C:719:GLN:HE21	1.79	0.80
1:K:754:THR:HG22	1:K:755:ARG:HE	1.44	0.80
1:B:825:HIS:HD2	1:B:827:GLY:H	1.26	0.80
1:C:959:PHE:HB3	1:C:977:MET:HG2	1.64	0.79
1:E:828:ARG:HG2	1:E:832:PHE:CD2	2.17	0.79
1:L:739:ARG:HG2	1:L:739:ARG:HH11	1.48	0.79
1:E:754:THR:HG22	1:E:755:ARG:HE	1.47	0.79
1:I:737:HIS:HD2	1:I:958:GLU:OE2	1.66	0.78
1:A:828:ARG:HG2	1:A:832:PHE:CD2	2.18	0.78
1:A:959:PHE:HB3	1:A:977:MET:HG2	1.65	0.77
1:D:739:ARG:HH11	1:D:739:ARG:HG2	1.50	0.77
1:G:719:GLN:NE2	1:G:719:GLN:H	1.82	0.77
1:E:737:HIS:HD2	1:E:958:GLU:OE2	1.67	0.77
1:K:762:GLN:NE2	1:K:804:SER:HB2	1.98	0.77
1:K:828:ARG:HG2	1:K:832:PHE:CD2	2.20	0.77
1:I:883:ARG:NH1	1:J:846:ASP:OD2	2.18	0.77
1:G:959:PHE:HB3	1:G:977:MET:HG2	1.65	0.77
1:D:758:PRO:HG2	1:D:1057:ILE:HD13	1.66	0.77
1:A:737:HIS:HD2	1:A:958:GLU:OE2	1.66	0.76
1:G:913:ASN:ND2	1:K:1056:ARG:HH21	1.83	0.76
1:J:739:ARG:HG2	1:J:739:ARG:HH11	1.48	0.76
1:B:739:ARG:HG2	1:B:739:ARG:HH11	1.50	0.76
1:F:730:GLY:HA3	1:F:823:TYR:CE1	2.21	0.76
1:L:730:GLY:HA3	1:L:823:TYR:CE1	2.20	0.76
1:K:887:ILE:HD13	1:L:845:ASN:HB3	1.64	0.76
1:E:719:GLN:H	1:E:719:GLN:NE2	1.83	0.76
1:E:959:PHE:HB3	1:E:977:MET:HG2	1.67	0.76
1:C:737:HIS:HD2	1:C:958:GLU:OE2	1.67	0.75
1:I:828:ARG:HG2	1:I:832:PHE:CD2	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:730:GLY:HA3	1:J:823:TYR:CE1	2.21	0.75
1:D:754:THR:HG21	1:D:755:ARG:HH21	1.51	0.75
1:K:737:HIS:HD2	1:K:958:GLU:OE2	1.68	0.75
1:H:739:ARG:HG2	1:H:739:ARG:HH11	1.51	0.75
1:K:696:LEU:HB3	1:K:728:GLU:HG2	1.68	0.75
1:E:1014:LEU:HD12	1:E:1056:ARG:HB3	1.69	0.74
1:K:719:GLN:H	1:K:719:GLN:NE2	1.83	0.74
1:D:730:GLY:HA3	1:D:823:TYR:CE1	2.22	0.74
1:J:754:THR:HG21	1:J:755:ARG:HH21	1.52	0.74
1:I:696:LEU:HB3	1:I:728:GLU:HG2	1.70	0.74
1:H:754:THR:HG21	1:H:755:ARG:HH21	1.53	0.74
1:H:730:GLY:HA3	1:H:823:TYR:CE1	2.22	0.74
1:F:700:MET:HE2	1:F:746:LEU:HD21	1.70	0.73
1:I:959:PHE:HB3	1:I:977:MET:HG2	1.69	0.73
1:G:1014:LEU:HD12	1:G:1056:ARG:CB	2.18	0.73
1:F:739:ARG:HH11	1:F:739:ARG:HG2	1.51	0.73
1:F:911:ASP:N	1:F:914:SER:HB3	2.03	0.73
1:B:1057:ILE:HD12	1:B:1058:PHE:N	2.03	0.73
1:A:705:GLN:NE2	1:J:1056:ARG:HH21	1.87	0.73
1:F:754:THR:HG21	1:F:755:ARG:HH21	1.52	0.73
1:E:887:ILE:HD13	1:F:845:ASN:HB3	1.71	0.73
1:B:754:THR:HG21	1:B:755:ARG:HH21	1.54	0.72
1:C:696:LEU:HB3	1:C:728:GLU:HG2	1.70	0.72
1:A:719:GLN:H	1:A:719:GLN:NE2	1.82	0.72
1:B:911:ASP:N	1:B:914:SER:HB3	2.02	0.72
1:L:911:ASP:N	1:L:914:SER:HB3	2.04	0.72
1:B:730:GLY:HA3	1:B:823:TYR:CE1	2.24	0.72
1:H:696:LEU:HB3	1:H:728:GLU:HG2	1.70	0.72
1:F:1057:ILE:HD12	1:F:1058:PHE:N	2.03	0.72
1:K:959:PHE:HB3	1:K:977:MET:HG2	1.70	0.72
1:J:911:ASP:N	1:J:914:SER:HB3	2.03	0.72
1:A:696:LEU:HB3	1:A:728:GLU:HG2	1.71	0.72
1:G:1017:GLU:HB3	1:G:1055:ARG:HD3	1.72	0.72
1:G:737:HIS:HD2	1:G:958:GLU:OE2	1.71	0.72
1:E:696:LEU:HB3	1:E:728:GLU:HG2	1.71	0.72
1:F:696:LEU:HB3	1:F:728:GLU:HG2	1.71	0.72
1:F:1059:CYS:HB3	1:F:1062:MET:HB2	1.72	0.71
1:D:911:ASP:N	1:D:914:SER:HB3	2.05	0.71
1:L:696:LEU:HB3	1:L:728:GLU:HG2	1.70	0.71
1:G:696:LEU:HB3	1:G:728:GLU:HG2	1.72	0.71
1:H:956:VAL:HG11	1:H:984:LEU:HD13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1057:ILE:HD12	1:J:1058:PHE:N	2.06	0.71
1:B:696:LEU:HB3	1:B:728:GLU:HG2	1.71	0.71
1:C:1017:GLU:H	1:C:1055:ARG:HD3	1.55	0.71
1:L:956:VAL:HG11	1:L:984:LEU:HD13	1.72	0.71
1:E:1017:GLU:HB3	1:E:1055:ARG:HD3	1.73	0.70
1:D:956:VAL:HG11	1:D:984:LEU:HD13	1.72	0.70
1:B:915:ASN:CG	1:C:945:ARG:NH1	2.45	0.70
1:B:956:VAL:HG11	1:B:984:LEU:HD13	1.73	0.70
1:L:754:THR:HG21	1:L:755:ARG:HH21	1.56	0.70
1:H:1013:TRP:CE3	1:H:1057:ILE:HG22	2.27	0.70
1:I:891:LEU:HD13	1:J:847:ARG:NH2	2.06	0.70
1:H:911:ASP:N	1:H:914:SER:HB3	2.04	0.69
1:I:719:GLN:NE2	1:I:719:GLN:H	1.84	0.69
1:H:945:ARG:HH12	1:H:1071:ILE:HG21	1.57	0.69
1:F:956:VAL:HG11	1:F:984:LEU:HD13	1.73	0.69
1:J:696:LEU:HB3	1:J:728:GLU:HG2	1.73	0.69
1:D:696:LEU:HB3	1:D:728:GLU:HG2	1.73	0.69
1:J:956:VAL:HG11	1:J:984:LEU:HD13	1.73	0.69
1:I:762:GLN:NE2	1:I:801:CYS:H	1.91	0.68
1:C:719:GLN:NE2	1:C:719:GLN:H	1.87	0.68
1:L:853:HIS:O	1:L:857:SER:HB2	1.94	0.68
1:F:853:HIS:O	1:F:857:SER:HB2	1.93	0.68
1:F:945:ARG:HH12	1:F:1071:ILE:HG21	1.59	0.68
1:H:1056:ARG:HH11	1:H:1056:ARG:HB3	1.58	0.67
1:H:853:HIS:O	1:H:857:SER:HB2	1.94	0.67
1:H:816:VAL:O	1:H:820:MET:HG2	1.95	0.67
1:I:891:LEU:CD1	1:J:847:ARG:CZ	2.73	0.67
1:B:853:HIS:O	1:B:857:SER:HB2	1.94	0.67
1:D:853:HIS:O	1:D:857:SER:HB2	1.94	0.67
1:C:845:ASN:HB3	1:D:887:ILE:HD13	1.77	0.66
1:H:689:GLY:O	1:H:692:SER:HB3	1.95	0.66
1:B:915:ASN:ND2	1:C:945:ARG:HH11	1.92	0.66
1:D:945:ARG:HH12	1:D:1071:ILE:HG21	1.60	0.66
1:D:816:VAL:O	1:D:820:MET:HG2	1.96	0.66
1:L:734:ILE:HB	1:L:735:PRO:HD2	1.77	0.66
1:F:816:VAL:O	1:F:820:MET:HG2	1.96	0.66
1:B:689:GLY:O	1:B:692:SER:HB3	1.95	0.66
1:B:761:GLN:HG2	1:B:763:ILE:H	1.60	0.66
1:J:853:HIS:O	1:J:857:SER:HB2	1.96	0.66
1:J:945:ARG:HH12	1:J:1071:ILE:HG21	1.59	0.66
1:G:739:ARG:HG2	4:G:1423:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:816:VAL:O	1:L:820:MET:HG2	1.96	0.65
1:A:825:HIS:CD2	1:A:827:GLY:H	2.02	0.65
1:J:734:ILE:HB	1:J:735:PRO:HD2	1.77	0.65
1:B:979:ARG:O	1:B:982:PRO:HD3	1.96	0.65
1:L:700:MET:HE2	1:L:746:LEU:HD21	1.78	0.65
1:L:734:ILE:HD11	1:L:737:HIS:HB2	1.79	0.65
1:L:945:ARG:HH12	1:L:1071:ILE:HG21	1.60	0.65
1:C:700:MET:HE3	1:C:746:LEU:HD21	1.78	0.65
1:F:734:ILE:HB	1:F:735:PRO:HD2	1.78	0.65
1:A:700:MET:HE3	1:A:746:LEU:HD21	1.79	0.65
1:D:734:ILE:HD11	1:D:737:HIS:HB2	1.78	0.65
1:G:887:ILE:HD13	1:H:845:ASN:HB3	1.78	0.65
1:K:700:MET:HE3	1:K:746:LEU:HD21	1.79	0.65
1:H:734:ILE:HD11	1:H:737:HIS:HB2	1.79	0.65
1:B:734:ILE:HD11	1:B:737:HIS:HB2	1.79	0.65
1:D:689:GLY:O	1:D:692:SER:HB3	1.97	0.65
1:B:700:MET:HE2	1:B:746:LEU:HD21	1.77	0.64
1:I:825:HIS:CD2	1:I:827:GLY:H	2.01	0.64
1:B:816:VAL:O	1:B:820:MET:HG2	1.97	0.64
1:B:945:ARG:HH12	1:B:1071:ILE:HG21	1.61	0.64
1:A:845:ASN:HB3	1:B:887:ILE:HD13	1.79	0.64
1:E:700:MET:HE3	1:E:746:LEU:HD21	1.80	0.64
1:D:754:THR:HG22	1:D:755:ARG:HE	1.62	0.64
1:E:1017:GLU:H	1:E:1055:ARG:HD3	1.62	0.64
1:F:689:GLY:O	1:F:692:SER:HB3	1.97	0.64
1:E:1014:LEU:HD12	1:E:1056:ARG:CB	2.27	0.64
1:J:739:ARG:HG2	1:J:739:ARG:NH1	2.11	0.64
1:H:979:ARG:O	1:H:982:PRO:HD3	1.96	0.64
1:H:739:ARG:HG2	1:H:739:ARG:NH1	2.13	0.64
1:I:887:ILE:HD13	1:J:845:ASN:HB3	1.80	0.64
1:A:739:ARG:HG2	4:A:1123:HOH:O	1.98	0.63
1:B:734:ILE:HB	1:B:735:PRO:HD2	1.79	0.63
1:F:734:ILE:HD11	1:F:737:HIS:HB2	1.80	0.63
1:L:739:ARG:HG2	1:L:739:ARG:NH1	2.10	0.63
1:G:700:MET:HE3	1:G:746:LEU:HD21	1.79	0.63
1:J:1013:TRP:CZ3	1:J:1055:ARG:HB3	2.33	0.63
1:K:825:HIS:CD2	1:K:827:GLY:H	2.03	0.63
1:J:816:VAL:O	1:J:820:MET:HG2	1.99	0.63
1:I:762:GLN:HA	1:I:805:ASN:HD21	1.62	0.63
1:J:689:GLY:O	1:J:692:SER:HB3	1.98	0.63
1:L:689:GLY:O	1:L:692:SER:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:707:THR:HG23	1:I:787:ILE:HD12	1.81	0.63
1:B:739:ARG:HG2	1:B:739:ARG:NH1	2.12	0.63
1:E:902:LEU:HD11	1:E:999:LEU:HA	1.81	0.63
1:F:739:ARG:NH1	1:F:739:ARG:HG2	2.14	0.63
1:L:979:ARG:O	1:L:982:PRO:HD3	1.98	0.63
1:A:902:LEU:HD11	1:A:999:LEU:HA	1.80	0.63
1:L:758:PRO:HG2	1:L:1057:ILE:HG13	1.80	0.63
1:E:707:THR:HG23	1:E:787:ILE:HD12	1.81	0.62
1:I:700:MET:HE3	1:I:746:LEU:HD21	1.80	0.62
1:A:762:GLN:HA	1:A:805:ASN:HD21	1.63	0.62
1:J:734:ILE:HD11	1:J:737:HIS:HB2	1.82	0.62
1:A:945:ARG:HD3	1:D:915:ASN:HD21	1.63	0.62
1:L:825:HIS:CD2	1:L:827:GLY:H	2.14	0.62
1:I:902:LEU:HD11	1:I:999:LEU:HA	1.81	0.62
1:K:902:LEU:HD11	1:K:999:LEU:HA	1.81	0.62
1:B:934:LYS:HD3	4:B:1135:HOH:O	1.99	0.62
1:C:1056:ARG:HH11	1:C:1056:ARG:HG3	1.64	0.62
1:K:911:ASP:HB3	1:K:914:SER:HB3	1.82	0.62
1:C:911:ASP:HB3	1:C:914:SER:HB3	1.82	0.62
1:G:700:MET:HE3	1:G:746:LEU:CD2	2.30	0.62
1:L:692:SER:O	1:L:695:ILE:HG13	2.00	0.62
1:B:825:HIS:CD2	1:B:827:GLY:H	2.15	0.61
1:G:913:ASN:HD22	1:K:1056:ARG:HH21	1.47	0.61
1:C:718:GLN:HG3	1:C:722:ASN:HD21	1.65	0.61
1:C:707:THR:HG23	1:C:787:ILE:HD12	1.80	0.61
1:G:902:LEU:HD11	1:G:999:LEU:HA	1.82	0.61
1:H:734:ILE:HB	1:H:735:PRO:HD2	1.80	0.61
1:I:825:HIS:HD2	1:I:827:GLY:N	1.91	0.61
1:K:700:MET:HE3	1:K:746:LEU:CD2	2.31	0.61
1:C:902:LEU:HD11	1:C:999:LEU:HA	1.83	0.61
1:A:917:ILE:O	1:A:918:GLU:HB2	2.01	0.61
1:I:700:MET:HE3	1:I:746:LEU:CD2	2.30	0.61
1:G:707:THR:HG23	1:G:787:ILE:HD12	1.83	0.61
1:L:719:GLN:HE21	1:L:719:GLN:H	0.81	0.61
1:A:945:ARG:CD	1:D:915:ASN:HD21	2.13	0.61
1:C:700:MET:HE3	1:C:746:LEU:CD2	2.31	0.61
1:C:825:HIS:CD2	1:C:827:GLY:H	2.03	0.61
1:H:692:SER:O	1:H:695:ILE:HG13	2.00	0.61
1:K:707:THR:HG23	1:K:787:ILE:HD12	1.83	0.61
1:J:1058:PHE:CE1	1:J:1063:HIS:CE1	2.88	0.60
1:J:692:SER:O	1:J:695:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:THR:HG23	1:A:787:ILE:HD12	1.82	0.60
1:A:911:ASP:HB3	1:A:914:SER:HB3	1.83	0.60
1:E:825:HIS:CD2	1:E:827:GLY:H	2.03	0.60
1:E:845:ASN:HB3	1:F:887:ILE:HD13	1.82	0.60
1:J:1057:ILE:HD12	1:J:1058:PHE:H	1.65	0.60
1:J:700:MET:HE2	1:J:746:LEU:HD21	1.82	0.60
1:J:825:HIS:CD2	1:J:827:GLY:H	2.13	0.60
1:I:891:LEU:HD12	1:J:847:ARG:NH1	2.16	0.60
1:A:945:ARG:HH11	1:D:915:ASN:ND2	1.99	0.60
1:A:825:HIS:HD2	1:A:827:GLY:N	1.92	0.60
1:J:754:THR:HG22	1:J:755:ARG:HE	1.67	0.60
1:D:700:MET:HE2	1:D:746:LEU:HD21	1.83	0.60
1:F:692:SER:O	1:F:695:ILE:HG13	2.02	0.60
1:J:725:ARG:HH11	1:J:725:ARG:HG3	1.67	0.60
1:I:911:ASP:HB3	1:I:914:SER:HB3	1.83	0.60
1:J:1003:TYR:CD2	1:J:1009:LEU:HG	2.36	0.60
1:K:719:GLN:HA	1:K:722:ASN:HD22	1.67	0.60
1:K:679:PHE:HZ	1:K:684:LEU:HD12	1.67	0.60
1:D:734:ILE:HB	1:D:735:PRO:HD2	1.82	0.60
1:G:911:ASP:HB3	1:G:914:SER:HB3	1.82	0.60
1:I:891:LEU:HD12	1:J:847:ARG:CZ	2.32	0.60
1:I:845:ASN:HB3	1:J:887:ILE:HD13	1.83	0.59
1:A:945:ARG:NH1	1:D:915:ASN:CG	2.55	0.59
1:E:911:ASP:HB3	1:E:914:SER:HB3	1.84	0.59
1:A:707:THR:CG2	1:A:709:LEU:HG	2.33	0.59
1:D:692:SER:O	1:D:695:ILE:HG13	2.02	0.59
1:F:754:THR:HG22	1:F:755:ARG:HE	1.67	0.59
1:E:718:GLN:HG3	1:E:722:ASN:HD21	1.67	0.59
1:H:754:THR:HG22	1:H:755:ARG:HE	1.67	0.59
1:B:692:SER:O	1:B:695:ILE:HG13	2.02	0.59
1:G:825:HIS:CD2	1:G:827:GLY:H	2.04	0.59
1:E:700:MET:HE3	1:E:746:LEU:CD2	2.33	0.59
1:F:1003:TYR:CD2	1:F:1009:LEU:HG	2.38	0.59
1:L:754:THR:HG22	1:L:755:ARG:HE	1.68	0.59
1:B:725:ARG:HH11	1:B:725:ARG:HG3	1.67	0.59
1:H:679:PHE:HZ	1:H:684:LEU:HD12	1.68	0.59
1:L:725:ARG:HH11	1:L:725:ARG:HG3	1.66	0.59
1:K:707:THR:CG2	1:K:709:LEU:HG	2.32	0.58
1:F:979:ARG:O	1:F:982:PRO:HD3	2.02	0.58
1:H:751:TYR:CZ	1:H:755:ARG:HG3	2.37	0.58
1:K:730:GLY:HA3	1:K:823:TYR:HE1	1.64	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:917:ILE:O	1:C:918:GLU:HB2	2.03	0.58
1:D:739:ARG:HG2	1:D:739:ARG:NH1	2.13	0.58
1:F:748:ALA:HB3	1:F:936:ALA:HB1	1.86	0.58
1:B:1069:HIS:CE1	1:B:1073:LYS:HZ2	2.21	0.58
1:D:979:ARG:O	1:D:982:PRO:HD3	2.03	0.58
1:G:917:ILE:O	1:G:918:GLU:HB2	2.03	0.58
1:H:825:HIS:CD2	1:H:827:GLY:H	2.14	0.58
1:A:700:MET:HE3	1:A:746:LEU:CD2	2.33	0.58
1:B:941:PRO:O	1:B:1065:LEU:HD12	2.03	0.58
1:C:1017:GLU:HB3	1:C:1055:ARG:HD3	1.84	0.58
1:C:707:THR:CG2	1:C:709:LEU:HG	2.34	0.58
1:I:754:THR:CG2	1:I:755:ARG:HH21	2.15	0.58
1:L:1003:TYR:CD2	1:L:1009:LEU:HG	2.39	0.58
1:B:754:THR:HG22	1:B:755:ARG:HE	1.69	0.58
1:E:909:ALA:HB2	1:E:917:ILE:HD11	1.85	0.58
1:F:669:SER:HB3	1:F:673:LYS:NZ	2.19	0.58
1:J:1058:PHE:HE1	1:J:1063:HIS:ND1	2.01	0.58
1:J:962:GLN:O	1:J:966:GLU:HG3	2.04	0.58
1:C:883:ARG:NH1	1:D:846:ASP:OD2	2.36	0.58
1:E:1071:ILE:HG21	1:J:915:ASN:ND2	2.19	0.58
1:E:917:ILE:O	1:E:918:GLU:HB2	2.04	0.58
1:B:915:ASN:HD21	1:C:945:ARG:CD	2.16	0.58
1:I:707:THR:CG2	1:I:709:LEU:HG	2.34	0.58
1:I:883:ARG:HH12	1:J:846:ASP:CG	2.07	0.58
1:H:725:ARG:HG3	1:H:725:ARG:HH11	1.67	0.57
1:B:660:ASP:O	1:B:664:VAL:HG23	2.04	0.57
1:F:962:GLN:O	1:F:966:GLU:HG3	2.03	0.57
1:H:669:SER:HB3	1:H:673:LYS:NZ	2.19	0.57
1:K:909:ALA:HB2	1:K:917:ILE:HD11	1.85	0.57
1:E:679:PHE:HZ	1:E:684:LEU:HD12	1.69	0.57
1:F:1057:ILE:HD12	1:F:1058:PHE:H	1.67	0.57
1:K:825:HIS:HD2	1:K:827:GLY:N	1.93	0.57
1:L:748:ALA:HB3	1:L:936:ALA:HB1	1.86	0.57
1:E:719:GLN:HA	1:E:722:ASN:HD22	1.68	0.57
1:G:718:GLN:HG3	1:G:722:ASN:HD21	1.69	0.57
1:G:719:GLN:HA	1:G:722:ASN:HD22	1.69	0.57
1:G:909:ALA:HB2	1:G:917:ILE:HD11	1.85	0.57
1:I:1056:ARG:HG3	1:I:1056:ARG:HH11	1.69	0.57
1:K:718:GLN:HG3	1:K:722:ASN:HD21	1.68	0.57
1:B:1003:TYR:CD2	1:B:1009:LEU:HG	2.40	0.57
1:E:707:THR:CG2	1:E:709:LEU:HG	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1013:TRP:CE3	1:G:1057:ILE:HG22	2.40	0.57
1:G:679:PHE:HZ	1:G:684:LEU:HD12	1.69	0.57
1:E:751:TYR:CE2	1:E:755:ARG:HG3	2.40	0.57
1:L:679:PHE:HZ	1:L:684:LEU:HD12	1.70	0.57
1:F:825:HIS:CD2	1:F:827:GLY:H	2.15	0.57
1:B:751:TYR:CZ	1:B:755:ARG:HG3	2.40	0.57
1:D:725:ARG:HG3	1:D:725:ARG:HH11	1.69	0.57
1:H:1003:TYR:CD2	1:H:1009:LEU:HG	2.39	0.57
1:I:718:GLN:HG3	1:I:722:ASN:HD21	1.69	0.57
1:L:828:ARG:HG2	1:L:832:PHE:CG	2.40	0.57
1:H:660:ASP:O	1:H:664:VAL:HG23	2.05	0.57
1:I:1013:TRP:CE3	1:I:1057:ILE:HG22	2.40	0.57
1:I:802:LEU:HD22	1:I:802:LEU:H	1.70	0.57
1:D:952:THR:HG23	1:D:988:GLN:NE2	2.20	0.56
1:F:725:ARG:HG3	1:F:725:ARG:HH11	1.70	0.56
1:H:748:ALA:HB3	1:H:936:ALA:HB1	1.87	0.56
1:J:979:ARG:O	1:J:982:PRO:HD3	2.05	0.56
1:L:1012:GLN:O	1:L:1057:ILE:HG12	2.05	0.56
1:K:845:ASN:HB3	1:L:887:ILE:HD13	1.86	0.56
1:D:669:SER:HB3	1:D:673:LYS:NZ	2.20	0.56
1:G:802:LEU:HD22	1:G:802:LEU:H	1.71	0.56
1:K:762:GLN:CA	1:K:762:GLN:HE21	2.13	0.56
1:K:917:ILE:O	1:K:918:GLU:HB2	2.04	0.56
1:H:719:GLN:HE21	1:H:719:GLN:H	0.81	0.56
1:H:945:ARG:NH1	1:H:1071:ILE:HG21	2.20	0.56
1:C:719:GLN:HA	1:C:722:ASN:HD22	1.70	0.56
1:L:669:SER:HB3	1:L:673:LYS:NZ	2.20	0.56
1:D:941:PRO:O	1:D:1065:LEU:HD12	2.06	0.56
1:D:679:PHE:HZ	1:D:684:LEU:HD12	1.69	0.56
1:F:945:ARG:NH1	1:F:1071:ILE:HG21	2.20	0.56
1:I:969:LEU:HD23	1:L:873:HIS:CD2	2.41	0.56
1:L:962:GLN:O	1:L:966:GLU:HG3	2.06	0.56
1:C:679:PHE:HZ	1:C:684:LEU:HD12	1.71	0.56
1:C:909:ALA:HB2	1:C:917:ILE:HD11	1.88	0.56
1:D:962:GLN:O	1:D:966:GLU:HG3	2.05	0.56
1:E:802:LEU:HD22	1:E:802:LEU:H	1.70	0.56
1:K:935:LEU:O	1:K:935:LEU:HD23	2.06	0.56
1:L:941:PRO:O	1:L:1065:LEU:HD12	2.05	0.56
1:H:732:ARG:HD2	1:H:825:HIS:O	2.06	0.56
1:G:845:ASN:HB3	1:H:887:ILE:HD13	1.88	0.56
1:I:679:PHE:HZ	1:I:684:LEU:HD12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:754:THR:CG2	1:G:755:ARG:HH21	2.16	0.56
1:I:909:ALA:HB2	1:I:917:ILE:HD11	1.87	0.56
1:B:669:SER:HB3	1:B:673:LYS:NZ	2.21	0.55
1:C:1013:TRP:CE3	1:C:1057:ILE:HG22	2.40	0.55
1:C:935:LEU:O	1:C:935:LEU:HD23	2.06	0.55
1:D:862:TYR:OH	1:D:869:ASN:ND2	2.38	0.55
1:H:828:ARG:HG2	1:H:832:PHE:CG	2.40	0.55
1:J:945:ARG:NH1	1:J:1071:ILE:HG21	2.21	0.55
1:K:713:PHE:CD2	1:K:874:LEU:HD21	2.41	0.55
1:L:660:ASP:O	1:L:664:VAL:HG23	2.05	0.55
1:A:679:PHE:HZ	1:A:684:LEU:HD12	1.71	0.55
1:A:754:THR:CG2	1:A:755:ARG:HH21	2.17	0.55
1:D:1003:TYR:CD2	1:D:1009:LEU:HG	2.40	0.55
1:L:751:TYR:CZ	1:L:755:ARG:HG3	2.41	0.55
1:B:679:PHE:HZ	1:B:684:LEU:HD12	1.71	0.55
1:D:751:TYR:CZ	1:D:755:ARG:HG3	2.42	0.55
1:I:730:GLY:HA3	1:I:823:TYR:HE1	1.68	0.55
1:J:941:PRO:O	1:J:1065:LEU:HD12	2.06	0.55
1:C:1017:GLU:HB3	1:C:1055:ARG:HB2	1.88	0.55
1:F:660:ASP:O	1:F:664:VAL:HG23	2.07	0.55
1:G:708:GLY:O	1:G:712:ILE:HG13	2.06	0.55
1:A:730:GLY:HA3	1:A:823:TYR:HE1	1.66	0.55
1:D:825:HIS:CD2	1:D:827:GLY:H	2.14	0.55
1:F:828:ARG:HG2	1:F:832:PHE:CG	2.42	0.55
1:G:707:THR:CG2	1:G:709:LEU:HG	2.37	0.55
1:B:828:ARG:HG2	1:B:832:PHE:CG	2.41	0.55
1:C:751:TYR:CE2	1:C:755:ARG:HG3	2.42	0.55
1:F:679:PHE:HZ	1:F:684:LEU:HD12	1.72	0.55
1:I:719:GLN:HA	1:I:722:ASN:HD22	1.70	0.55
1:J:669:SER:HB3	1:J:673:LYS:NZ	2.22	0.55
1:K:760:LEU:HD23	1:K:801:CYS:N	2.22	0.55
1:L:945:ARG:NH1	1:L:1071:ILE:HG21	2.22	0.55
1:A:802:LEU:H	1:A:802:LEU:HD22	1.72	0.55
1:E:751:TYR:CZ	1:E:755:ARG:HG3	2.42	0.55
1:F:763:ILE:O	1:F:764:HIS:CB	2.53	0.55
1:F:911:ASP:H	1:F:914:SER:CB	2.15	0.55
1:H:700:MET:HE2	1:H:746:LEU:HD21	1.88	0.55
1:B:748:ALA:HB3	1:B:936:ALA:HB1	1.89	0.55
1:E:847:ARG:CZ	1:F:891:LEU:HD13	2.37	0.55
1:H:962:GLN:O	1:H:966:GLU:HG3	2.07	0.55
1:J:660:ASP:O	1:J:664:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1014:LEU:HD12	1:B:1056:ARG:CB	2.36	0.55
1:B:881:ARG:HH11	1:B:881:ARG:HG3	1.72	0.55
1:E:708:GLY:O	1:E:712:ILE:HG13	2.07	0.55
1:I:847:ARG:CZ	1:J:891:LEU:HD13	2.37	0.55
1:A:718:GLN:HG3	1:A:722:ASN:HD21	1.71	0.55
1:D:881:ARG:HH11	1:D:881:ARG:HG3	1.72	0.55
1:K:802:LEU:HD22	1:K:802:LEU:H	1.72	0.55
1:G:842:VAL:HA	1:H:883:ARG:HH22	1.71	0.54
1:I:917:ILE:O	1:I:918:GLU:HB2	2.05	0.54
1:J:862:TYR:OH	1:J:869:ASN:ND2	2.40	0.54
1:B:862:TYR:OH	1:B:869:ASN:ND2	2.37	0.54
1:D:737:HIS:HD2	1:D:958:GLU:OE2	1.90	0.54
1:G:945:ARG:HD3	1:L:915:ASN:HD21	1.72	0.54
1:C:754:THR:CG2	1:C:755:ARG:HH21	2.15	0.54
1:L:763:ILE:O	1:L:764:HIS:CB	2.55	0.54
1:C:825:HIS:HD2	1:C:827:GLY:N	1.93	0.54
1:I:751:TYR:CE2	1:I:755:ARG:HG3	2.42	0.54
1:A:751:TYR:CE2	1:A:755:ARG:HG3	2.42	0.54
1:D:945:ARG:NH1	1:D:1071:ILE:HG21	2.22	0.54
1:E:825:HIS:HD2	1:E:827:GLY:N	1.93	0.54
1:F:862:TYR:OH	1:F:869:ASN:ND2	2.39	0.54
1:G:751:TYR:CE2	1:G:755:ARG:HG3	2.41	0.54
1:A:721:MET:O	1:A:725:ARG:HG3	2.08	0.54
1:E:762:GLN:HA	1:E:805:ASN:HD21	1.73	0.54
1:H:862:TYR:OH	1:H:869:ASN:ND2	2.39	0.54
1:I:708:GLY:O	1:I:712:ILE:HG13	2.07	0.54
1:J:751:TYR:CZ	1:J:755:ARG:HG3	2.42	0.54
1:K:708:GLY:O	1:K:712:ILE:HG13	2.08	0.54
1:K:847:ARG:CZ	1:L:891:LEU:HD13	2.37	0.54
1:G:935:LEU:O	1:G:935:LEU:HD23	2.08	0.54
1:J:684:LEU:HD23	1:J:688:MET:HG3	1.89	0.54
1:C:713:PHE:CD2	1:C:874:LEU:HD21	2.43	0.54
1:C:881:ARG:HG3	1:C:881:ARG:HH11	1.73	0.54
1:D:748:ALA:HB3	1:D:936:ALA:HB1	1.90	0.54
1:B:962:GLN:O	1:B:966:GLU:HG3	2.07	0.54
1:D:660:ASP:O	1:D:664:VAL:HG23	2.07	0.54
1:F:934:LYS:HD3	4:F:1335:HOH:O	2.08	0.54
1:K:751:TYR:CE2	1:K:755:ARG:HG3	2.43	0.54
1:K:713:PHE:HD2	1:K:874:LEU:HD21	1.72	0.54
1:F:941:PRO:O	1:F:1065:LEU:HD12	2.08	0.53
1:A:790:LYS:NZ	1:J:1014:LEU:HD23	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:GLN:HE21	1:B:719:GLN:H	0.79	0.53
1:L:684:LEU:HD23	1:L:688:MET:HG3	1.91	0.53
1:L:735:PRO:HG2	1:L:958:GLU:HB2	1.90	0.53
1:A:737:HIS:CD2	1:A:958:GLU:OE2	2.56	0.53
1:C:730:GLY:HA3	1:C:823:TYR:HE1	1.69	0.53
1:G:760:LEU:HD23	1:G:801:CYS:N	2.23	0.53
1:J:761:GLN:HG2	1:J:763:ILE:H	1.72	0.53
1:K:753:THR:HA	1:K:802:LEU:HD23	1.90	0.53
1:L:862:TYR:OH	1:L:869:ASN:ND2	2.39	0.53
1:B:684:LEU:HD23	1:B:688:MET:HG3	1.89	0.53
1:B:945:ARG:NH1	1:B:1071:ILE:HG21	2.23	0.53
1:C:1017:GLU:CB	1:C:1055:ARG:HD3	2.39	0.53
1:C:708:GLY:O	1:C:712:ILE:HG13	2.08	0.53
1:C:802:LEU:H	1:C:802:LEU:HD22	1.73	0.53
1:F:751:TYR:CZ	1:F:755:ARG:HG3	2.44	0.53
1:H:737:HIS:HD2	1:H:958:GLU:OE2	1.91	0.53
1:I:765:ASN:HA	1:I:804:SER:HB3	1.90	0.53
1:F:700:MET:HE2	1:F:746:LEU:CD2	2.39	0.53
1:H:941:PRO:O	1:H:1065:LEU:HD12	2.08	0.53
1:I:721:MET:O	1:I:725:ARG:HG3	2.08	0.53
1:J:748:ALA:HB3	1:J:936:ALA:HB1	1.90	0.53
1:A:847:ARG:CZ	1:B:891:LEU:HD13	2.39	0.53
1:B:911:ASP:H	1:B:914:SER:CB	2.14	0.53
1:E:730:GLY:HA3	1:E:823:TYR:HE1	1.69	0.53
1:H:915:ASN:HD21	1:K:945:ARG:CD	2.22	0.53
1:J:1069:HIS:CE1	1:J:1073:LYS:HZ2	2.27	0.53
1:L:732:ARG:HD2	1:L:825:HIS:O	2.08	0.53
1:C:739:ARG:HG2	4:C:1223:HOH:O	2.08	0.53
1:F:1059:CYS:HB3	1:F:1062:MET:CB	2.38	0.53
1:F:735:PRO:HG2	1:F:958:GLU:HB2	1.91	0.53
1:H:1014:LEU:HD21	1:H:1058:PHE:HB2	1.91	0.53
1:J:679:PHE:HZ	1:J:684:LEU:HD12	1.73	0.53
1:J:828:ARG:HG2	1:J:832:PHE:CG	2.43	0.53
1:C:760:LEU:HD23	1:C:801:CYS:N	2.24	0.53
1:H:881:ARG:HH11	1:H:881:ARG:HG3	1.72	0.53
1:C:751:TYR:CZ	1:C:755:ARG:HG3	2.44	0.53
1:F:952:THR:HG23	1:F:988:GLN:NE2	2.24	0.53
1:G:881:ARG:HG3	1:G:881:ARG:HH11	1.74	0.53
1:J:704:PHE:HB3	1:J:710:LEU:HG	1.91	0.53
1:A:719:GLN:HA	1:A:722:ASN:HD22	1.73	0.53
1:E:753:THR:HA	1:E:802:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:881:ARG:HH11	1:F:881:ARG:HG3	1.73	0.53
1:G:753:THR:HA	1:G:802:LEU:HD23	1.91	0.53
1:I:713:PHE:CD2	1:I:874:LEU:HD21	2.44	0.53
1:J:763:ILE:O	1:J:764:HIS:CB	2.57	0.53
1:K:721:MET:O	1:K:725:ARG:HG3	2.09	0.53
1:H:915:ASN:HD21	1:K:945:ARG:HD3	1.74	0.53
1:H:828:ARG:NH1	1:H:965:GLU:OE1	2.43	0.52
1:J:1059:CYS:HB2	1:J:1062:MET:HB2	1.91	0.52
1:J:737:HIS:HD2	1:J:958:GLU:OE2	1.91	0.52
1:L:1069:HIS:CE1	1:L:1073:LYS:HZ2	2.27	0.52
1:L:881:ARG:HH11	1:L:881:ARG:HG3	1.74	0.52
1:A:909:ALA:HB2	1:A:917:ILE:HD11	1.89	0.52
1:F:685:VAL:HG22	1:F:695:ILE:CD1	2.39	0.52
1:I:754:THR:HG22	1:I:755:ARG:NE	2.21	0.52
1:C:1017:GLU:N	1:C:1055:ARG:HD3	2.22	0.52
1:D:762:GLN:HA	1:D:762:GLN:OE1	2.10	0.52
1:F:737:HIS:HD2	1:F:958:GLU:OE2	1.93	0.52
1:H:684:LEU:HD23	1:H:688:MET:HG3	1.92	0.52
1:E:1017:GLU:CB	1:E:1055:ARG:HD3	2.38	0.52
1:D:828:ARG:HG2	1:D:832:PHE:CG	2.43	0.52
1:E:662:ILE:O	1:E:666:GLU:HG3	2.08	0.52
1:E:763:ILE:H	1:E:805:ASN:ND2	2.07	0.52
1:F:1014:LEU:HD13	1:F:1056:ARG:NH2	2.25	0.52
1:L:737:HIS:HD2	1:L:958:GLU:OE2	1.92	0.52
1:G:751:TYR:CZ	1:G:755:ARG:HG3	2.44	0.52
1:J:732:ARG:HD2	1:J:825:HIS:O	2.10	0.52
1:C:753:THR:HA	1:C:802:LEU:HD23	1.91	0.52
1:E:713:PHE:CD2	1:E:874:LEU:HD21	2.45	0.52
1:I:891:LEU:CD1	1:J:847:ARG:NH2	2.70	0.52
1:K:707:THR:HG22	1:K:709:LEU:HG	1.91	0.52
1:B:737:HIS:HD2	1:B:958:GLU:OE2	1.93	0.52
1:C:1056:ARG:NH1	1:C:1056:ARG:HG3	2.25	0.52
1:L:704:PHE:HB3	1:L:710:LEU:HG	1.92	0.52
1:D:684:LEU:HD23	1:D:688:MET:HG3	1.90	0.52
1:F:804:SER:C	1:F:805:ASN:HD22	2.13	0.52
1:I:662:ILE:O	1:I:666:GLU:HG3	2.10	0.52
1:A:707:THR:HG22	1:A:709:LEU:HG	1.92	0.52
1:A:753:THR:HA	1:A:802:LEU:HD23	1.92	0.52
1:B:674:MET:C	1:B:676:ASN:H	2.13	0.51
1:B:915:ASN:HD21	1:C:945:ARG:HD3	1.75	0.51
1:D:1014:LEU:HD12	1:D:1056:ARG:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:915:ASN:CG	1:K:945:ARG:NH1	2.63	0.51
1:J:911:ASP:H	1:J:914:SER:CB	2.15	0.51
1:C:1061:LEU:C	1:C:1061:LEU:HD12	2.31	0.51
1:F:732:ARG:HD2	1:F:825:HIS:O	2.11	0.51
1:K:764:HIS:O	1:K:766:GLY:N	2.43	0.51
1:D:804:SER:C	1:D:805:ASN:HD22	2.13	0.51
1:D:828:ARG:NH1	1:D:965:GLU:OE1	2.44	0.51
1:G:911:ASP:HB3	1:G:914:SER:CB	2.41	0.51
1:J:881:ARG:HG3	1:J:881:ARG:HH11	1.75	0.51
1:A:1061:LEU:HD12	1:A:1061:LEU:C	2.31	0.51
1:G:721:MET:O	1:G:725:ARG:HG3	2.10	0.51
1:J:1058:PHE:CD1	1:J:1063:HIS:CE1	2.98	0.51
1:C:1017:GLU:HB3	1:C:1055:ARG:CD	2.41	0.51
1:E:1017:GLU:HB3	1:E:1055:ARG:CD	2.41	0.51
1:E:760:LEU:HD23	1:E:801:CYS:N	2.26	0.51
1:I:751:TYR:CZ	1:I:755:ARG:HG3	2.46	0.51
1:L:911:ASP:H	1:L:914:SER:CB	2.16	0.51
1:A:751:TYR:CZ	1:A:755:ARG:HG3	2.45	0.51
1:A:935:LEU:O	1:A:935:LEU:HD23	2.11	0.51
1:D:704:PHE:HB3	1:D:710:LEU:HG	1.91	0.51
1:D:732:ARG:HD2	1:D:825:HIS:O	2.10	0.51
1:I:737:HIS:CD2	1:I:958:GLU:OE2	2.56	0.51
1:K:754:THR:CG2	1:K:755:ARG:HH21	2.18	0.51
1:E:881:ARG:HH11	1:E:881:ARG:HG3	1.76	0.51
1:E:935:LEU:HD23	1:E:935:LEU:O	2.11	0.51
1:H:704:PHE:HB3	1:H:710:LEU:HG	1.92	0.51
1:K:881:ARG:HG3	1:K:881:ARG:HH11	1.76	0.51
1:F:684:LEU:HD23	1:F:688:MET:HG3	1.92	0.51
1:I:753:THR:HA	1:I:802:LEU:HD23	1.92	0.51
1:A:713:PHE:CD2	1:A:874:LEU:HD21	2.46	0.51
1:C:721:MET:O	1:C:725:ARG:HG3	2.10	0.51
1:F:704:PHE:HB3	1:F:710:LEU:HG	1.92	0.51
1:J:674:MET:C	1:J:676:ASN:H	2.13	0.51
1:K:911:ASP:HB3	1:K:914:SER:CB	2.40	0.51
1:C:713:PHE:HD2	1:C:874:LEU:HD21	1.76	0.51
1:F:674:MET:C	1:F:676:ASN:H	2.14	0.51
1:A:881:ARG:HG3	1:A:881:ARG:HH11	1.76	0.50
1:B:828:ARG:NH1	1:B:965:GLU:OE1	2.44	0.50
1:I:881:ARG:HG3	1:I:881:ARG:HH11	1.76	0.50
1:K:751:TYR:CZ	1:K:755:ARG:HG3	2.45	0.50
1:L:674:MET:C	1:L:676:ASN:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:THR:HG22	1:A:755:ARG:NE	2.22	0.50
1:D:763:ILE:O	1:D:764:HIS:CB	2.58	0.50
1:E:869:ASN:C	1:E:869:ASN:HD22	2.14	0.50
1:K:762:GLN:HA	1:K:762:GLN:NE2	2.18	0.50
1:A:708:GLY:O	1:A:712:ILE:HG13	2.12	0.50
1:B:952:THR:HG23	1:B:988:GLN:NE2	2.27	0.50
1:C:662:ILE:O	1:C:666:GLU:HG3	2.10	0.50
1:D:674:MET:C	1:D:676:ASN:H	2.13	0.50
1:A:1014:LEU:HD12	1:A:1056:ARG:CB	2.42	0.50
1:E:1071:ILE:CG2	1:J:915:ASN:ND2	2.75	0.50
1:H:685:VAL:HG22	1:H:695:ILE:CD1	2.41	0.50
1:H:803:SER:HA	1:H:811:LEU:HD11	1.94	0.50
1:J:685:VAL:HG22	1:J:695:ILE:CD1	2.41	0.50
1:B:735:PRO:HG2	1:B:958:GLU:HB2	1.94	0.50
1:D:735:PRO:HG2	1:D:958:GLU:HB2	1.92	0.50
1:E:713:PHE:HD2	1:E:874:LEU:HD21	1.77	0.50
1:H:674:MET:C	1:H:676:ASN:H	2.13	0.50
1:K:1061:LEU:C	1:K:1061:LEU:HD12	2.31	0.50
1:L:1020:ASN:CG	1:L:1021:ASP:H	2.15	0.50
1:D:719:GLN:HE21	1:D:719:GLN:H	0.81	0.50
1:F:828:ARG:NH1	1:F:965:GLU:OE1	2.44	0.50
1:J:735:PRO:HG2	1:J:958:GLU:HB2	1.92	0.50
1:J:739:ARG:CG	1:J:739:ARG:HH11	2.23	0.50
1:L:735:PRO:HG2	1:L:958:GLU:CB	2.41	0.50
1:L:976:PHE:CD2	1:L:987:LEU:HB2	2.47	0.50
1:A:911:ASP:HB3	1:A:914:SER:CB	2.41	0.50
1:I:1061:LEU:C	1:I:1061:LEU:HD12	2.32	0.50
1:L:828:ARG:NH1	1:L:965:GLU:OE1	2.45	0.50
1:L:964:ASP:OD2	1:L:979:ARG:NH1	2.45	0.50
1:C:869:ASN:HD22	1:C:869:ASN:C	2.14	0.50
1:D:965:GLU:O	1:D:969:LEU:HG	2.11	0.50
1:E:721:MET:O	1:E:725:ARG:HG3	2.11	0.50
1:F:1013:TRP:CZ3	1:F:1055:ARG:HB3	2.47	0.50
1:F:761:GLN:HG2	1:F:763:ILE:H	1.76	0.50
1:I:707:THR:HG22	1:I:709:LEU:HG	1.94	0.50
1:L:985:ALA:HA	1:L:1072:TRP:CE3	2.47	0.50
1:C:911:ASP:HB3	1:C:914:SER:CB	2.41	0.50
1:C:891:LEU:HD13	1:D:847:ARG:NH2	2.26	0.50
1:D:911:ASP:H	1:D:914:SER:CB	2.18	0.50
1:E:1061:LEU:C	1:E:1061:LEU:HD12	2.32	0.50
1:G:730:GLY:HA3	1:G:823:TYR:HE1	1.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:700:MET:HE3	1:H:746:LEU:CD1	2.42	0.50
1:K:660:ASP:O	1:K:664:VAL:HG23	2.12	0.50
1:C:737:HIS:CD2	1:C:958:GLU:OE2	2.58	0.49
1:H:763:ILE:O	1:H:764:HIS:CB	2.60	0.49
1:H:911:ASP:H	1:H:914:SER:CB	2.16	0.49
1:J:684:LEU:HD23	1:J:684:LEU:O	2.11	0.49
1:K:869:ASN:C	1:K:869:ASN:HD22	2.15	0.49
1:A:662:ILE:O	1:A:666:GLU:HG3	2.11	0.49
1:C:754:THR:HG22	1:C:755:ARG:NE	2.21	0.49
1:G:1061:LEU:HD12	1:G:1061:LEU:C	2.33	0.49
1:B:803:SER:HA	1:B:811:LEU:HD11	1.93	0.49
1:H:761:GLN:HG2	1:H:763:ILE:H	1.76	0.49
1:J:804:SER:C	1:J:805:ASN:HD22	2.15	0.49
1:E:739:ARG:HG2	4:E:1323:HOH:O	2.11	0.49
1:I:869:ASN:C	1:I:869:ASN:HD22	2.14	0.49
1:A:760:LEU:HD23	1:A:801:CYS:N	2.27	0.49
1:A:956:VAL:HG11	1:A:984:LEU:HD13	1.94	0.49
1:B:704:PHE:HB3	1:B:710:LEU:HG	1.93	0.49
1:C:754:THR:CG2	1:C:755:ARG:HE	2.21	0.49
1:K:736:TYR:CD1	1:K:955:ILE:HG13	2.47	0.49
1:B:732:ARG:HD2	1:B:825:HIS:O	2.12	0.49
1:G:713:PHE:CD2	1:G:874:LEU:HD21	2.48	0.49
1:I:713:PHE:HD2	1:I:874:LEU:HD21	1.76	0.49
1:B:1015:GLU:O	1:B:1055:ARG:HD2	2.12	0.49
1:B:804:SER:C	1:B:805:ASN:HD22	2.16	0.49
1:E:1059:CYS:SG	1:E:1062:MET:HB2	2.53	0.49
1:E:911:ASP:HB3	1:E:914:SER:CB	2.42	0.49
1:H:700:MET:HE3	1:H:746:LEU:HD13	1.95	0.49
1:K:794:ASN:HB3	1:K:799:TYR:HB2	1.94	0.49
1:K:956:VAL:HG11	1:K:984:LEU:HD13	1.95	0.49
1:L:685:VAL:HG22	1:L:695:ILE:CD1	2.42	0.49
1:C:660:ASP:O	1:C:664:VAL:HG23	2.13	0.49
1:I:911:ASP:HB3	1:I:914:SER:CB	2.42	0.49
1:K:662:ILE:O	1:K:666:GLU:HG3	2.12	0.49
1:L:803:SER:HA	1:L:811:LEU:HD11	1.95	0.49
1:A:736:TYR:CD1	1:A:955:ILE:HG13	2.48	0.49
1:A:869:ASN:C	1:A:869:ASN:HD22	2.16	0.49
1:G:660:ASP:O	1:G:664:VAL:HG23	2.13	0.49
1:H:804:SER:C	1:H:805:ASN:HD22	2.16	0.49
1:I:935:LEU:O	1:I:935:LEU:HD23	2.12	0.49
1:A:660:ASP:O	1:A:664:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:915:ASN:OD1	1:C:945:ARG:NH1	2.46	0.48
1:D:1069:HIS:CE1	1:D:1073:LYS:HZ2	2.28	0.48
1:E:707:THR:HG22	1:E:709:LEU:HG	1.94	0.48
1:B:810:GLU:OE1	1:B:925:ARG:HD2	2.13	0.48
1:C:736:TYR:CD1	1:C:955:ILE:HG13	2.48	0.48
1:B:685:VAL:HG22	1:B:695:ILE:CD1	2.43	0.48
1:C:816:VAL:O	1:C:820:MET:HG2	2.13	0.48
1:D:934:LYS:HD3	4:D:1235:HOH:O	2.14	0.48
1:F:1014:LEU:HD21	1:F:1058:PHE:HB2	1.95	0.48
1:K:729:ASN:HA	1:K:739:ARG:NH2	2.27	0.48
1:A:729:ASN:HA	1:A:739:ARG:NH2	2.28	0.48
1:B:991:PHE:CE2	1:B:996:VAL:HG23	2.48	0.48
1:D:700:MET:HE3	1:D:746:LEU:CD1	2.43	0.48
1:G:662:ILE:O	1:G:666:GLU:HG3	2.12	0.48
1:G:794:ASN:HB3	1:G:799:TYR:HB2	1.95	0.48
1:H:1069:HIS:CE1	1:H:1073:LYS:HZ2	2.29	0.48
1:J:1058:PHE:HE1	1:J:1063:HIS:CE1	2.30	0.48
1:K:729:ASN:HA	1:K:739:ARG:HH21	1.78	0.48
1:B:964:ASP:OD2	1:B:979:ARG:NH1	2.46	0.48
1:C:956:VAL:HG11	1:C:984:LEU:HD13	1.94	0.48
1:E:754:THR:CG2	1:E:755:ARG:HH21	2.18	0.48
1:F:735:PRO:HG2	1:F:958:GLU:CB	2.44	0.48
1:J:1058:PHE:CE1	1:J:1063:HIS:ND1	2.80	0.48
1:C:846:ASP:OD2	1:D:883:ARG:NH1	2.47	0.48
1:C:707:THR:HG22	1:C:709:LEU:HG	1.94	0.48
1:D:685:VAL:HG22	1:D:695:ILE:CD1	2.43	0.48
1:F:965:GLU:O	1:F:969:LEU:HG	2.13	0.48
1:H:985:ALA:HA	1:H:1072:TRP:CE3	2.49	0.48
1:J:828:ARG:NH1	1:J:965:GLU:OE1	2.46	0.48
1:L:952:THR:HG23	1:L:988:GLN:NE2	2.28	0.48
1:B:985:ALA:HA	1:B:1072:TRP:CE3	2.49	0.48
1:D:803:SER:HA	1:D:811:LEU:HD11	1.96	0.48
1:E:737:HIS:CD2	1:E:958:GLU:OE2	2.58	0.48
1:H:735:PRO:HG2	1:H:958:GLU:HB2	1.95	0.48
1:I:739:ARG:HG2	4:I:1523:HOH:O	2.13	0.48
1:J:965:GLU:O	1:J:969:LEU:HG	2.13	0.48
1:L:1059:CYS:HB3	1:L:1062:MET:HB2	1.96	0.48
1:F:964:ASP:OD2	1:F:979:ARG:NH1	2.47	0.48
1:G:825:HIS:HD2	1:G:827:GLY:N	1.94	0.48
1:H:716:PRO:HB2	1:H:719:GLN:HE22	1.79	0.48
1:G:847:ARG:CZ	1:H:891:LEU:HD13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:794:ASN:HB3	1:I:799:TYR:HB2	1.96	0.48
1:L:965:GLU:O	1:L:969:LEU:HG	2.14	0.48
1:C:1059:CYS:SG	1:C:1062:MET:HB2	2.54	0.48
1:D:739:ARG:HH11	1:D:739:ARG:CG	2.24	0.48
1:E:883:ARG:NH1	1:F:846:ASP:OD2	2.46	0.48
1:G:913:ASN:ND2	1:K:1056:ARG:HE	2.12	0.48
1:H:964:ASP:OD2	1:H:979:ARG:NH1	2.47	0.48
1:G:945:ARG:NH1	1:L:918:GLU:OE2	2.47	0.48
1:C:763:ILE:C	1:C:765:ASN:H	2.17	0.47
1:H:1013:TRP:CZ3	1:H:1057:ILE:HG22	2.48	0.47
1:H:952:THR:HG23	1:H:988:GLN:NE2	2.29	0.47
1:I:736:TYR:CD1	1:I:955:ILE:HG13	2.49	0.47
1:E:1071:ILE:HG21	1:J:915:ASN:HD21	1.79	0.47
1:E:891:LEU:CD1	1:F:847:ARG:CZ	2.93	0.47
1:E:891:LEU:HD13	1:F:847:ARG:NH2	2.28	0.47
1:B:965:GLU:O	1:B:969:LEU:HG	2.14	0.47
1:E:729:ASN:HA	1:E:739:ARG:HH21	1.79	0.47
1:H:1059:CYS:HB3	1:H:1062:MET:HB2	1.96	0.47
1:H:729:ASN:HA	1:H:739:ARG:HH22	1.79	0.47
1:H:991:PHE:CE2	1:H:996:VAL:HG23	2.49	0.47
1:I:762:GLN:HE22	1:I:801:CYS:H	1.60	0.47
1:J:735:PRO:HG2	1:J:958:GLU:CB	2.44	0.47
1:K:787:ILE:HG23	1:K:808:ALA:CB	2.44	0.47
1:L:670:LEU:O	1:L:674:MET:HG3	2.15	0.47
1:A:724:PHE:O	1:A:728:GLU:HG3	2.13	0.47
1:C:729:ASN:HA	1:C:739:ARG:NH2	2.28	0.47
1:D:796:ASP:OD1	1:D:798:SER:N	2.39	0.47
1:E:794:ASN:HB3	1:E:799:TYR:HB2	1.96	0.47
1:H:1056:ARG:NH1	1:H:1056:ARG:HB3	2.28	0.47
1:I:729:ASN:HA	1:I:739:ARG:NH2	2.29	0.47
1:J:803:SER:HA	1:J:811:LEU:HD11	1.96	0.47
1:L:810:GLU:OE1	1:L:925:ARG:HD2	2.15	0.47
1:D:700:MET:HE3	1:D:746:LEU:HD13	1.95	0.47
1:C:891:LEU:CD1	1:D:847:ARG:CZ	2.92	0.47
1:G:754:THR:HG22	1:G:755:ARG:NE	2.22	0.47
1:H:735:PRO:HG2	1:H:958:GLU:CB	2.45	0.47
1:I:847:ARG:NH2	1:J:891:LEU:HD13	2.30	0.47
1:L:674:MET:HE3	1:L:699:VAL:HG13	1.97	0.47
1:B:735:PRO:HG2	1:B:958:GLU:CB	2.44	0.47
1:D:716:PRO:HB2	1:D:719:GLN:HE22	1.80	0.47
1:E:846:ASP:HB2	4:E:1334:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:707:THR:HG22	1:G:709:LEU:HG	1.97	0.47
1:I:760:LEU:HD23	1:I:801:CYS:N	2.30	0.47
1:A:701:TYR:OH	1:J:1015:GLU:OE1	2.32	0.47
1:D:735:PRO:HG2	1:D:958:GLU:CB	2.44	0.47
1:E:952:THR:HG23	1:E:988:GLN:NE2	2.30	0.47
1:I:729:ASN:HA	1:I:739:ARG:HH21	1.79	0.47
1:J:810:GLU:OE1	1:J:925:ARG:HD2	2.14	0.47
1:K:670:LEU:HD22	1:K:674:MET:SD	2.54	0.47
1:K:727:LEU:HD21	1:K:820:MET:HB3	1.97	0.47
1:B:872:LEU:HD13	1:B:873:HIS:CG	2.50	0.47
1:G:796:ASP:OD1	1:G:798:SER:CB	2.63	0.47
1:A:1014:LEU:HD12	1:A:1056:ARG:HB3	1.97	0.47
1:B:1014:LEU:HD21	1:B:1058:PHE:HB2	1.97	0.47
1:B:729:ASN:HA	1:B:739:ARG:HH22	1.80	0.47
1:B:700:MET:HE3	1:B:746:LEU:HD13	1.97	0.47
1:C:729:ASN:HA	1:C:739:ARG:HH21	1.78	0.47
1:B:684:LEU:HD23	1:B:684:LEU:O	2.14	0.47
1:D:964:ASP:OD2	1:D:979:ARG:NH1	2.47	0.47
1:E:729:ASN:HA	1:E:739:ARG:NH2	2.29	0.47
1:G:816:VAL:O	1:G:820:MET:HG2	2.14	0.47
1:L:985:ALA:HA	1:L:1072:TRP:HE3	1.79	0.47
1:A:729:ASN:HA	1:A:739:ARG:HH21	1.79	0.47
1:B:845:ASN:O	1:B:847:ARG:HG2	2.15	0.47
1:B:981:SER:N	1:B:982:PRO:CD	2.78	0.47
1:C:794:ASN:HB3	1:C:799:TYR:HB2	1.97	0.47
1:D:985:ALA:HA	1:D:1072:TRP:CE3	2.49	0.47
1:E:816:VAL:O	1:E:820:MET:HG2	2.15	0.47
1:J:700:MET:HE3	1:J:746:LEU:CD1	2.45	0.47
1:J:985:ALA:HA	1:J:1072:TRP:CE3	2.50	0.47
1:D:1057:ILE:HD12	1:D:1058:PHE:N	2.30	0.46
1:B:700:MET:HE3	1:B:746:LEU:CD1	2.46	0.46
1:E:754:THR:HG22	1:E:755:ARG:NE	2.24	0.46
1:E:956:VAL:HG11	1:E:984:LEU:HD13	1.97	0.46
1:G:1056:ARG:HH11	1:G:1056:ARG:HG3	1.80	0.46
1:G:670:LEU:HD22	1:G:674:MET:SD	2.55	0.46
1:J:719:GLN:H	1:J:719:GLN:HE21	0.80	0.46
1:A:1056:ARG:HH11	1:A:1056:ARG:HG3	1.80	0.46
1:F:1069:HIS:ND1	1:F:1073:LYS:NZ	2.56	0.46
1:G:729:ASN:HA	1:G:739:ARG:NH2	2.31	0.46
1:H:965:GLU:O	1:H:969:LEU:HG	2.15	0.46
1:L:729:ASN:HA	1:L:739:ARG:HH22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:GLU:HB3	1:A:1055:ARG:CD	2.46	0.46
1:D:930:GLN:O	1:D:933:ILE:HG13	2.16	0.46
1:G:674:MET:CE	1:G:703:LEU:HD21	2.45	0.46
1:I:1056:ARG:NH1	1:I:1056:ARG:HG3	2.31	0.46
1:I:670:LEU:HD22	1:I:674:MET:SD	2.56	0.46
1:I:869:ASN:C	1:I:869:ASN:ND2	2.69	0.46
1:L:804:SER:C	1:L:805:ASN:HD22	2.19	0.46
1:L:991:PHE:CE2	1:L:996:VAL:HG23	2.50	0.46
1:C:869:ASN:C	1:C:869:ASN:ND2	2.69	0.46
1:B:915:ASN:OD1	1:C:945:ARG:CZ	2.64	0.46
1:E:869:ASN:ND2	1:E:869:ASN:C	2.68	0.46
1:G:727:LEU:HD21	1:G:820:MET:HB3	1.97	0.46
1:H:845:ASN:O	1:H:847:ARG:HG2	2.15	0.46
1:H:981:SER:N	1:H:982:PRO:CD	2.79	0.46
1:J:938:ILE:HD12	1:J:996:VAL:HG22	1.97	0.46
1:B:985:ALA:HA	1:B:1072:TRP:HE3	1.81	0.46
1:E:1071:ILE:CG2	1:J:915:ASN:HD22	2.29	0.46
1:E:846:ASP:OD2	1:F:883:ARG:NH1	2.48	0.46
1:F:700:MET:CE	1:F:746:LEU:CD2	2.94	0.46
1:F:976:PHE:CD2	1:F:987:LEU:HB2	2.50	0.46
1:I:660:ASP:O	1:I:664:VAL:HG23	2.15	0.46
1:K:823:TYR:CE2	1:K:857:SER:HB3	2.51	0.46
1:L:796:ASP:OD1	1:L:798:SER:N	2.43	0.46
1:A:939:ASN:ND2	1:A:943:LYS:HE3	2.31	0.46
1:C:1017:GLU:H	1:C:1055:ARG:CD	2.27	0.46
1:F:729:ASN:HA	1:F:739:ARG:HH22	1.81	0.46
1:B:974:SER:HB2	1:B:977:MET:SD	2.56	0.46
1:D:872:LEU:HD13	1:D:873:HIS:CG	2.51	0.46
1:E:787:ILE:HG23	1:E:808:ALA:CB	2.46	0.46
1:J:952:THR:HG23	1:J:988:GLN:NE2	2.31	0.46
1:L:1014:LEU:HD21	1:L:1058:PHE:HB2	1.97	0.46
1:L:725:ARG:NH1	1:L:725:ARG:HG3	2.30	0.46
1:K:707:THR:HG21	1:K:709:LEU:HG	1.98	0.46
1:G:1056:ARG:HE	1:K:913:ASN:ND2	2.13	0.46
1:B:716:PRO:HB2	1:B:719:GLN:HE22	1.81	0.46
1:H:872:LEU:HD13	1:H:873:HIS:CG	2.51	0.46
1:J:976:PHE:CD2	1:J:987:LEU:HB2	2.51	0.46
1:K:869:ASN:C	1:K:869:ASN:ND2	2.70	0.46
1:L:973:ILE:HG21	1:L:978:ASP:HB2	1.97	0.46
1:A:718:GLN:OE1	1:J:1021:ASP:HA	2.16	0.45
1:D:754:THR:CG2	1:D:755:ARG:HH21	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:973:ILE:HG21	1:D:978:ASP:HB2	1.98	0.45
1:F:754:THR:CG2	1:F:755:ARG:HH21	2.25	0.45
1:F:981:SER:N	1:F:982:PRO:CD	2.79	0.45
1:G:736:TYR:CD1	1:G:955:ILE:HG13	2.50	0.45
1:I:956:VAL:HG11	1:I:984:LEU:HD13	1.97	0.45
1:J:725:ARG:HG3	1:J:725:ARG:NH1	2.31	0.45
1:K:846:ASP:HB2	4:K:1634:HOH:O	2.15	0.45
1:K:871:LEU:HB3	1:K:874:LEU:HD12	1.98	0.45
1:B:915:ASN:HD21	1:C:945:ARG:HD2	1.81	0.45
1:D:1020:ASN:HA	1:D:1020:ASN:HD22	1.59	0.45
1:H:1057:ILE:HD12	1:H:1058:PHE:N	2.31	0.45
1:I:816:VAL:O	1:I:820:MET:HG2	2.16	0.45
1:A:727:LEU:HD21	1:A:820:MET:HB3	1.99	0.45
1:A:816:VAL:O	1:A:820:MET:HG2	2.15	0.45
1:D:1069:HIS:ND1	1:D:1073:LYS:NZ	2.54	0.45
1:E:754:THR:CG2	1:E:755:ARG:HE	2.24	0.45
1:K:754:THR:CG2	1:K:755:ARG:HE	2.21	0.45
1:D:703:LEU:HD22	1:D:750:TRP:CE2	2.52	0.45
1:D:810:GLU:OE1	1:D:925:ARG:HD2	2.16	0.45
1:F:985:ALA:HA	1:F:1072:TRP:CE3	2.51	0.45
1:G:939:ASN:ND2	1:G:943:LYS:HE3	2.32	0.45
1:K:816:VAL:O	1:K:820:MET:HG2	2.16	0.45
1:G:945:ARG:CD	1:L:915:ASN:HD21	2.28	0.45
1:A:707:THR:HG21	1:A:709:LEU:HG	1.98	0.45
1:B:976:PHE:CD2	1:B:987:LEU:HB2	2.51	0.45
1:B:915:ASN:CG	1:C:945:ARG:HH11	2.14	0.45
1:D:1014:LEU:HD12	1:D:1056:ARG:HB2	1.96	0.45
1:F:674:MET:HE3	1:F:699:VAL:HG13	1.99	0.45
1:G:787:ILE:HG23	1:G:808:ALA:CB	2.47	0.45
1:G:956:VAL:HG11	1:G:984:LEU:HD13	1.98	0.45
1:K:674:MET:CE	1:K:703:LEU:HD21	2.47	0.45
1:A:713:PHE:HD2	1:A:874:LEU:HD21	1.81	0.45
1:A:957:ASN:O	1:A:961:GLU:HG3	2.16	0.45
1:D:674:MET:HE3	1:D:699:VAL:HG13	1.98	0.45
1:D:700:MET:CE	1:D:746:LEU:CD2	2.94	0.45
1:E:660:ASP:O	1:E:664:VAL:HG23	2.17	0.45
1:F:1014:LEU:HD12	1:F:1056:ARG:HB3	1.99	0.45
1:H:725:ARG:HG3	1:H:725:ARG:NH1	2.30	0.45
1:J:670:LEU:O	1:J:674:MET:HG3	2.17	0.45
1:J:700:MET:HE3	1:J:746:LEU:HD13	1.99	0.45
1:L:938:ILE:HD12	1:L:996:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:872:LEU:HD13	1:B:873:HIS:CD2	2.52	0.45
1:C:764:HIS:O	1:C:765:ASN:O	2.35	0.45
1:D:938:ILE:HD12	1:D:996:VAL:HG22	1.98	0.45
1:E:957:ASN:O	1:E:961:GLU:HG3	2.17	0.45
1:F:719:GLN:H	1:F:719:GLN:HE21	0.79	0.45
1:F:739:ARG:HH11	1:F:739:ARG:CG	2.26	0.45
1:H:851:GLU:HA	1:H:854:HIS:HD2	1.82	0.45
1:B:670:LEU:O	1:B:674:MET:HG3	2.16	0.45
1:B:703:LEU:HD22	1:B:750:TRP:CE2	2.52	0.45
1:C:784:ILE:HG21	1:C:807:PRO:HB3	1.97	0.45
1:C:787:ILE:HG23	1:C:808:ALA:CB	2.47	0.45
1:D:1055:ARG:HG2	1:D:1056:ARG:H	1.81	0.45
1:H:976:PHE:CD2	1:H:987:LEU:HB2	2.51	0.45
1:J:1059:CYS:HB2	1:J:1062:MET:CB	2.47	0.45
1:A:762:GLN:NE2	1:A:800:GLY:HA2	2.31	0.45
1:B:694:ARG:O	1:B:698:GLN:HG2	2.17	0.45
1:B:700:MET:CE	1:B:746:LEU:CD2	2.95	0.45
1:H:985:ALA:HA	1:H:1072:TRP:HE3	1.81	0.45
1:A:869:ASN:C	1:A:869:ASN:ND2	2.71	0.45
1:E:784:ILE:HG22	1:E:786:TYR:CE1	2.52	0.45
1:F:796:ASP:OD1	1:F:798:SER:N	2.41	0.45
1:F:851:GLU:HA	1:F:854:HIS:HD2	1.81	0.45
1:J:754:THR:CG2	1:J:755:ARG:HH21	2.26	0.45
1:L:694:ARG:O	1:L:698:GLN:HG2	2.17	0.45
1:B:705:GLN:HG2	1:B:710:LEU:HD12	1.99	0.44
1:B:851:GLU:HA	1:B:854:HIS:HD2	1.82	0.44
1:E:763:ILE:H	1:E:805:ASN:HD21	1.64	0.44
1:E:796:ASP:OD1	1:E:798:SER:CB	2.66	0.44
1:F:700:MET:HE3	1:F:746:LEU:HD13	1.99	0.44
1:I:724:PHE:O	1:I:728:GLU:HG3	2.16	0.44
1:J:872:LEU:HD13	1:J:873:HIS:CG	2.52	0.44
1:G:1056:ARG:HH21	1:K:913:ASN:HD22	1.65	0.44
1:L:981:SER:N	1:L:982:PRO:CD	2.79	0.44
1:C:670:LEU:HD22	1:C:674:MET:SD	2.57	0.44
1:C:707:THR:HG21	1:C:709:LEU:HG	1.98	0.44
1:I:915:ASN:HD22	1:I:915:ASN:HA	1.65	0.44
1:L:705:GLN:HG2	1:L:710:LEU:HD12	1.99	0.44
1:B:725:ARG:HG3	1:B:725:ARG:NH1	2.30	0.44
1:D:845:ASN:O	1:D:847:ARG:HG2	2.17	0.44
1:E:939:ASN:ND2	1:E:943:LYS:HE3	2.33	0.44
1:G:913:ASN:ND2	1:K:1056:ARG:NH2	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:823:TYR:CE2	1:I:857:SER:HB3	2.52	0.44
1:J:694:ARG:O	1:J:698:GLN:HG2	2.17	0.44
1:J:973:ILE:HG21	1:J:978:ASP:HB2	1.99	0.44
1:K:846:ASP:OD2	1:L:883:ARG:NH1	2.51	0.44
1:L:930:GLN:O	1:L:933:ILE:HG13	2.17	0.44
1:C:847:ARG:CZ	1:D:891:LEU:HD13	2.48	0.44
1:D:694:ARG:O	1:D:698:GLN:HG2	2.17	0.44
1:G:674:MET:HE1	1:G:703:LEU:HD21	2.00	0.44
1:G:823:TYR:CE2	1:G:857:SER:HB3	2.53	0.44
1:B:963:GLY:O	1:B:973:ILE:HD12	2.18	0.44
1:D:981:SER:N	1:D:982:PRO:CD	2.79	0.44
1:E:823:TYR:CE2	1:E:857:SER:HB3	2.52	0.44
1:F:684:LEU:O	1:F:684:LEU:HD23	2.17	0.44
1:G:762:GLN:HB3	1:G:765:ASN:CB	2.47	0.44
1:J:1003:TYR:HD2	1:J:1009:LEU:HG	1.81	0.44
1:A:814:LEU:HD11	1:A:933:ILE:HB	2.00	0.44
1:C:952:THR:O	1:C:956:VAL:HG22	2.18	0.44
1:E:727:LEU:HD21	1:E:820:MET:HB3	2.00	0.44
1:I:872:LEU:HD13	1:I:873:HIS:CD2	2.53	0.44
1:I:957:ASN:O	1:I:961:GLU:HG3	2.18	0.44
1:K:724:PHE:O	1:K:728:GLU:HG3	2.17	0.44
1:L:721:MET:O	1:L:725:ARG:HG2	2.18	0.44
1:L:905:PHE:CD1	1:L:931:VAL:HG21	2.52	0.44
1:A:787:ILE:HG23	1:A:808:ALA:CB	2.48	0.44
1:B:739:ARG:HH11	1:B:739:ARG:CG	2.23	0.44
1:C:939:ASN:ND2	1:C:943:LYS:HE3	2.33	0.44
1:D:684:LEU:O	1:D:684:LEU:HD23	2.18	0.44
1:D:729:ASN:HA	1:D:739:ARG:HH22	1.82	0.44
1:E:847:ARG:NH2	1:F:891:LEU:HD13	2.33	0.44
1:G:869:ASN:HD22	1:G:869:ASN:C	2.20	0.44
1:H:751:TYR:CE2	1:H:755:ARG:HG3	2.52	0.44
1:A:674:MET:CE	1:A:703:LEU:HD21	2.48	0.44
1:A:670:LEU:HD22	1:A:674:MET:SD	2.58	0.44
1:D:670:LEU:O	1:D:674:MET:HG3	2.18	0.44
1:D:976:PHE:CD2	1:D:987:LEU:HB2	2.53	0.44
1:F:803:SER:HA	1:F:811:LEU:HD11	1.99	0.44
1:G:729:ASN:HA	1:G:739:ARG:HH21	1.82	0.44
1:G:915:ASN:HD22	1:G:915:ASN:HA	1.65	0.44
1:H:1004:ASP:HA	1:H:1009:LEU:HD12	1.99	0.44
1:H:694:ARG:O	1:H:698:GLN:HG2	2.18	0.44
1:H:721:MET:O	1:H:725:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:974:SER:HB2	1:H:977:MET:SD	2.58	0.44
1:I:872:LEU:HD13	1:I:873:HIS:CG	2.53	0.44
1:J:845:ASN:O	1:J:847:ARG:HG2	2.17	0.44
1:F:805:ASN:N	1:F:805:ASN:HD22	2.16	0.44
1:F:810:GLU:OE1	1:F:925:ARG:HD2	2.18	0.44
1:F:930:GLN:O	1:F:933:ILE:HG13	2.18	0.44
1:G:957:ASN:O	1:G:961:GLU:HG3	2.17	0.44
1:H:825:HIS:CD2	1:H:826:PRO:HD2	2.53	0.44
1:J:796:ASP:OD1	1:J:798:SER:N	2.41	0.44
1:J:964:ASP:OD2	1:J:979:ARG:NH1	2.51	0.44
1:J:981:SER:N	1:J:982:PRO:CD	2.79	0.44
1:K:764:HIS:O	1:K:804:SER:O	2.36	0.44
1:L:681:ILE:H	1:L:681:ILE:HG13	1.45	0.44
1:E:872:LEU:HD13	1:E:873:HIS:CG	2.53	0.43
1:E:891:LEU:HD12	1:F:847:ARG:CZ	2.48	0.43
1:F:872:LEU:HD13	1:F:873:HIS:CG	2.53	0.43
1:F:973:ILE:HG21	1:F:978:ASP:HB2	1.98	0.43
1:G:724:PHE:O	1:G:728:GLU:HG3	2.17	0.43
1:G:713:PHE:HD2	1:G:874:LEU:HD21	1.82	0.43
1:I:707:THR:HG21	1:I:709:LEU:HG	1.99	0.43
1:L:872:LEU:HD13	1:L:873:HIS:CG	2.53	0.43
1:L:956:VAL:HG23	1:L:957:ASN:N	2.33	0.43
1:A:847:ARG:NH2	1:B:891:LEU:HD13	2.32	0.43
1:D:985:ALA:HA	1:D:1072:TRP:HE3	1.82	0.43
1:G:765:ASN:HA	1:G:804:SER:HB3	2.00	0.43
1:I:754:THR:CG2	1:I:755:ARG:HE	2.21	0.43
1:J:991:PHE:CE2	1:J:996:VAL:HG23	2.54	0.43
1:K:1004:ASP:CB	1:K:1009:LEU:HD12	2.48	0.43
1:K:939:ASN:ND2	1:K:943:LYS:HE3	2.33	0.43
1:L:670:LEU:HD22	1:L:674:MET:SD	2.58	0.43
1:L:959:PHE:HA	1:L:977:MET:HE2	2.00	0.43
1:A:914:SER:OG	1:A:915:ASN:N	2.51	0.43
1:B:881:ARG:HG3	1:B:881:ARG:NH1	2.33	0.43
1:D:725:ARG:HG3	1:D:725:ARG:NH1	2.32	0.43
1:E:917:ILE:O	1:E:924:ASP:OD2	2.36	0.43
1:H:810:GLU:OE1	1:H:925:ARG:HD2	2.18	0.43
1:J:670:LEU:HD22	1:J:674:MET:SD	2.58	0.43
1:J:729:ASN:HA	1:J:739:ARG:HH22	1.83	0.43
1:L:885:LEU:HA	1:L:885:LEU:HD12	1.78	0.43
1:B:694:ARG:HA	1:B:728:GLU:OE2	2.18	0.43
1:F:700:MET:HE3	1:F:746:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:930:GLN:O	1:H:933:ILE:HG13	2.17	0.43
1:J:851:GLU:HA	1:J:854:HIS:HD2	1.83	0.43
1:K:952:THR:HG23	1:K:988:GLN:NE2	2.34	0.43
1:L:963:GLY:O	1:L:973:ILE:HD12	2.18	0.43
1:C:677:TRP:NE1	1:C:943:LYS:HD3	2.34	0.43
1:C:842:VAL:HA	1:D:883:ARG:HH22	1.83	0.43
1:C:891:LEU:HD12	1:D:847:ARG:CZ	2.49	0.43
1:D:1004:ASP:HA	1:D:1009:LEU:HD12	2.00	0.43
1:D:881:ARG:NH1	1:D:881:ARG:HG3	2.34	0.43
1:E:1013:TRP:CE3	1:E:1057:ILE:HG22	2.53	0.43
1:F:985:ALA:HA	1:F:1072:TRP:HE3	1.84	0.43
1:H:872:LEU:HD13	1:H:873:HIS:CD2	2.53	0.43
1:L:974:SER:HB2	1:L:977:MET:SD	2.58	0.43
1:A:790:LYS:HZ3	1:J:1014:LEU:HD23	1.82	0.43
1:B:956:VAL:HG23	1:B:957:ASN:N	2.34	0.43
1:F:694:ARG:O	1:F:698:GLN:HG2	2.17	0.43
1:F:694:ARG:HA	1:F:728:GLU:OE2	2.18	0.43
1:G:914:SER:OG	1:G:915:ASN:N	2.49	0.43
1:G:964:ASP:OD2	1:G:979:ARG:NH1	2.52	0.43
1:B:670:LEU:HD22	1:B:674:MET:SD	2.58	0.43
1:C:823:TYR:CE2	1:C:857:SER:HB3	2.53	0.43
1:C:853:HIS:O	1:C:857:SER:HB2	2.19	0.43
1:D:754:THR:HG22	1:D:755:ARG:NE	2.31	0.43
1:E:677:TRP:NE1	1:E:943:LYS:HD3	2.33	0.43
1:E:724:PHE:O	1:E:728:GLU:HG3	2.18	0.43
1:E:939:ASN:O	1:E:940:GLY:C	2.57	0.43
1:G:758:PRO:HD3	1:G:1011:GLY:H	1.83	0.43
1:G:952:THR:HG23	1:G:988:GLN:NE2	2.34	0.43
1:H:956:VAL:HG23	1:H:957:ASN:N	2.34	0.43
1:I:787:ILE:HG23	1:I:808:ALA:CB	2.48	0.43
1:I:803:SER:HA	1:I:811:LEU:HD11	2.00	0.43
1:J:700:MET:CE	1:J:746:LEU:CD2	2.97	0.43
1:K:803:SER:HA	1:K:811:LEU:HD11	2.01	0.43
1:L:684:LEU:O	1:L:684:LEU:HD23	2.19	0.43
1:L:758:PRO:HG3	1:L:799:TYR:HE2	1.84	0.43
1:D:805:ASN:HD22	1:D:805:ASN:N	2.16	0.43
1:D:956:VAL:HG23	1:D:957:ASN:N	2.33	0.43
1:F:681:ILE:H	1:F:681:ILE:HG13	1.45	0.43
1:F:721:MET:O	1:F:725:ARG:HG2	2.18	0.43
1:G:677:TRP:NE1	1:G:943:LYS:HD3	2.34	0.43
1:H:684:LEU:O	1:H:684:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:723:TYR:CE1	1:H:861:LEU:HD13	2.53	0.43
1:H:959:PHE:HA	1:H:977:MET:HE2	1.99	0.43
1:I:914:SER:OG	1:I:915:ASN:N	2.51	0.43
1:J:1069:HIS:ND1	1:J:1073:LYS:NZ	2.54	0.43
1:K:847:ARG:NH2	1:L:891:LEU:HD13	2.33	0.43
1:L:700:MET:HE2	1:L:746:LEU:CD2	2.47	0.43
1:A:803:SER:HA	1:A:811:LEU:HD11	2.01	0.43
1:A:823:TYR:CE2	1:A:857:SER:HB3	2.54	0.43
1:B:684:LEU:CD2	1:B:688:MET:HG3	2.48	0.43
1:B:755:ARG:HD2	4:B:1131:HOH:O	2.18	0.43
1:B:973:ILE:HG21	1:B:978:ASP:HB2	2.01	0.43
1:C:724:PHE:O	1:C:728:GLU:HG3	2.19	0.43
1:C:758:PRO:HD3	1:C:1011:GLY:H	1.83	0.43
1:H:963:GLY:O	1:H:973:ILE:HD12	2.19	0.43
1:J:700:MET:HE2	1:J:700:MET:HA	2.01	0.43
1:J:959:PHE:CG	1:J:977:MET:HE2	2.53	0.43
1:K:1003:TYR:HD2	1:K:1009:LEU:HG	1.84	0.43
1:K:748:ALA:HB3	1:K:936:ALA:HB1	2.01	0.43
1:A:945:ARG:NH1	1:D:915:ASN:ND2	2.65	0.43
1:A:964:ASP:OD2	1:A:979:ARG:NH1	2.52	0.43
1:D:705:GLN:HG2	1:D:710:LEU:HD12	2.00	0.43
1:D:700:MET:CE	1:D:746:LEU:HD21	2.49	0.43
1:D:872:LEU:HD13	1:D:873:HIS:CD2	2.54	0.43
1:E:915:ASN:O	1:E:916:GLY:C	2.58	0.43
1:F:716:PRO:HB2	1:F:719:GLN:HE22	1.84	0.43
1:H:705:GLN:HG2	1:H:710:LEU:HD12	2.00	0.43
1:H:905:PHE:CD1	1:H:931:VAL:HG21	2.54	0.43
1:I:796:ASP:OD1	1:I:798:SER:CB	2.67	0.43
1:J:716:PRO:HB2	1:J:719:GLN:HE22	1.83	0.43
1:K:957:ASN:O	1:K:961:GLU:HG3	2.19	0.43
1:L:845:ASN:O	1:L:847:ARG:HG2	2.19	0.43
1:A:794:ASN:HB3	1:A:799:TYR:HB2	2.00	0.42
1:E:707:THR:HG21	1:E:709:LEU:HG	2.00	0.42
1:E:758:PRO:HD3	1:E:1011:GLY:H	1.84	0.42
1:E:964:ASP:OD2	1:E:979:ARG:NH1	2.52	0.42
1:F:705:GLN:HG2	1:F:710:LEU:HD12	2.02	0.42
1:A:758:PRO:HD3	1:A:1011:GLY:H	1.84	0.42
1:E:710:LEU:HD23	1:E:710:LEU:HA	1.87	0.42
1:F:845:ASN:O	1:F:847:ARG:HG2	2.19	0.42
1:G:803:SER:HA	1:G:811:LEU:HD11	2.01	0.42
1:H:700:MET:HA	1:H:700:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:881:ARG:NH1	1:H:881:ARG:HG3	2.33	0.42
1:I:727:LEU:HD21	1:I:820:MET:HB3	2.02	0.42
1:J:705:GLN:HG2	1:J:710:LEU:HD12	2.00	0.42
1:J:758:PRO:HG3	1:J:799:TYR:HE2	1.84	0.42
1:H:915:ASN:CG	1:K:945:ARG:HH11	2.23	0.42
1:K:737:HIS:CD2	1:K:958:GLU:OE2	2.59	0.42
1:B:1004:ASP:HA	1:B:1009:LEU:HD12	2.00	0.42
1:C:883:ARG:HH12	1:D:846:ASP:CG	2.21	0.42
1:C:957:ASN:O	1:C:961:GLU:HG3	2.20	0.42
1:D:700:MET:HE2	1:D:700:MET:HA	2.00	0.42
1:D:851:GLU:HA	1:D:854:HIS:HD2	1.83	0.42
1:D:952:THR:O	1:D:956:VAL:HG22	2.19	0.42
1:F:754:THR:HG22	1:F:755:ARG:NE	2.34	0.42
1:I:917:ILE:O	1:I:924:ASP:OD2	2.38	0.42
1:I:677:TRP:NE1	1:I:943:LYS:HD3	2.34	0.42
1:J:684:LEU:CD2	1:J:688:MET:HG3	2.49	0.42
1:B:721:MET:O	1:B:725:ARG:HG2	2.20	0.42
1:B:796:ASP:OD1	1:B:798:SER:N	2.41	0.42
1:C:796:ASP:OD1	1:C:798:SER:CB	2.68	0.42
1:F:764:HIS:O	1:F:766:GLY:N	2.52	0.42
1:F:952:THR:O	1:F:956:VAL:HG22	2.19	0.42
1:G:1014:LEU:N	1:G:1056:ARG:O	2.53	0.42
1:H:694:ARG:HA	1:H:728:GLU:OE2	2.19	0.42
1:I:684:LEU:HD23	1:I:684:LEU:O	2.20	0.42
1:J:985:ALA:HA	1:J:1072:TRP:HE3	1.84	0.42
1:J:663:LEU:HA	1:J:666:GLU:OE1	2.19	0.42
1:J:703:LEU:HD22	1:J:750:TRP:CE2	2.54	0.42
1:L:681:ILE:O	1:L:685:VAL:HG23	2.19	0.42
1:F:1014:LEU:HD13	1:F:1056:ARG:HH21	1.84	0.42
1:J:721:MET:O	1:J:725:ARG:HG2	2.19	0.42
1:J:956:VAL:HG23	1:J:957:ASN:N	2.34	0.42
1:A:871:LEU:HB3	1:A:874:LEU:HD12	2.01	0.42
1:D:758:PRO:HG3	1:D:799:TYR:HE2	1.84	0.42
1:F:915:ASN:CG	1:I:945:ARG:NH1	2.73	0.42
1:J:694:ARG:HA	1:J:728:GLU:OE2	2.19	0.42
1:J:952:THR:O	1:J:956:VAL:HG22	2.20	0.42
1:H:915:ASN:ND2	1:K:945:ARG:HH11	2.18	0.42
1:L:663:LEU:HA	1:L:666:GLU:OE1	2.20	0.42
1:L:703:LEU:HD22	1:L:750:TRP:CE2	2.54	0.42
1:L:755:ARG:HD2	4:L:1631:HOH:O	2.20	0.42
1:L:851:GLU:HA	1:L:854:HIS:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:LYS:HB3	1:A:934:LYS:HZ2	1.85	0.42
1:B:663:LEU:HA	1:B:666:GLU:OE1	2.19	0.42
1:A:842:VAL:HA	1:B:883:ARG:HH22	1.84	0.42
1:B:905:PHE:CD1	1:B:931:VAL:HG21	2.54	0.42
1:C:803:SER:HA	1:C:811:LEU:HD11	2.02	0.42
1:C:814:LEU:HD11	1:C:933:ILE:HB	2.02	0.42
1:E:969:LEU:HD23	1:H:873:HIS:CD2	2.54	0.42
1:F:725:ARG:HG3	1:F:725:ARG:NH1	2.33	0.42
1:G:814:LEU:HD11	1:G:933:ILE:HB	2.01	0.42
1:G:862:TYR:OH	1:G:869:ASN:ND2	2.52	0.42
1:G:737:HIS:CD2	1:G:958:GLU:OE2	2.60	0.42
1:H:710:LEU:HD23	1:H:715:ILE:HB	2.02	0.42
1:H:973:ILE:HG21	1:H:978:ASP:HB2	2.00	0.42
1:H:938:ILE:HD12	1:H:996:VAL:HG22	2.01	0.42
1:I:991:PHE:CD1	1:I:995:ILE:HD12	2.54	0.42
1:L:716:PRO:HB2	1:L:719:GLN:HE22	1.85	0.42
1:A:872:LEU:HD12	1:A:873:HIS:H	1.85	0.42
1:A:939:ASN:O	1:A:940:GLY:C	2.58	0.42
1:D:710:LEU:HD23	1:D:715:ILE:HB	2.02	0.42
1:D:880:LYS:HA	1:D:880:LYS:HD2	1.88	0.42
1:D:980:SER:O	1:D:981:SER:HB2	2.19	0.42
1:G:869:ASN:C	1:G:869:ASN:ND2	2.73	0.42
1:G:934:LYS:HZ2	1:G:934:LYS:HB3	1.85	0.42
1:G:962:GLN:O	1:G:966:GLU:HG3	2.20	0.42
1:I:969:LEU:HD23	1:L:873:HIS:HD2	1.82	0.42
1:J:723:TYR:CE1	1:J:861:LEU:HD13	2.55	0.42
1:L:1059:CYS:HB3	1:L:1062:MET:CB	2.49	0.42
1:A:674:MET:HE1	1:A:703:LEU:HD21	2.02	0.42
1:C:915:ASN:O	1:C:916:GLY:C	2.58	0.42
1:D:663:LEU:HA	1:D:666:GLU:OE1	2.20	0.42
1:H:695:ILE:HG22	1:H:743:THR:HG21	2.01	0.42
1:J:930:GLN:O	1:J:933:ILE:HG13	2.20	0.42
1:K:872:LEU:HD12	1:K:873:HIS:H	1.85	0.42
1:L:700:MET:HE3	1:L:746:LEU:HD13	2.02	0.42
1:L:881:ARG:NH1	1:L:881:ARG:HG3	2.34	0.42
1:B:763:ILE:O	1:B:764:HIS:CB	2.67	0.42
1:B:758:PRO:HG3	1:B:799:TYR:HE2	1.85	0.42
1:E:872:LEU:HD13	1:E:873:HIS:CD2	2.54	0.42
1:E:914:SER:OG	1:E:915:ASN:N	2.52	0.42
1:E:944:VAL:HG22	1:E:945:ARG:N	2.35	0.42
1:F:974:SER:HB2	1:F:977:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:784:ILE:HG21	1:G:807:PRO:HB3	2.00	0.42
1:J:1004:ASP:HA	1:J:1009:LEU:HD12	2.01	0.42
1:K:1004:ASP:HB2	1:K:1009:LEU:HD12	2.02	0.42
1:K:872:LEU:HD13	1:K:873:HIS:CG	2.54	0.42
1:L:1003:TYR:HD2	1:L:1009:LEU:HG	1.83	0.42
1:A:952:THR:O	1:A:956:VAL:HG22	2.20	0.41
1:B:952:THR:O	1:B:956:VAL:HG22	2.20	0.41
1:C:694:ARG:O	1:C:698:GLN:HG2	2.20	0.41
1:C:727:LEU:HD21	1:C:820:MET:HB3	2.02	0.41
1:C:915:ASN:HD22	1:C:915:ASN:HA	1.63	0.41
1:C:976:PHE:CG	1:C:987:LEU:HD13	2.55	0.41
1:D:974:SER:HB2	1:D:977:MET:SD	2.60	0.41
1:G:707:THR:HG21	1:G:709:LEU:HG	2.01	0.41
1:J:963:GLY:O	1:J:973:ILE:HD12	2.19	0.41
1:K:796:ASP:OD1	1:K:798:SER:CB	2.68	0.41
1:L:754:THR:HG22	1:L:755:ARG:NE	2.35	0.41
1:A:846:ASP:OD2	1:B:883:ARG:NH1	2.53	0.41
1:C:825:HIS:CD2	1:C:826:PRO:HD2	2.55	0.41
1:D:963:GLY:O	1:D:973:ILE:HD12	2.20	0.41
1:D:991:PHE:CE2	1:D:996:VAL:HG23	2.54	0.41
1:E:670:LEU:HD22	1:E:674:MET:SD	2.60	0.41
1:H:700:MET:CE	1:H:746:LEU:CD2	2.98	0.41
1:H:959:PHE:CB	1:H:977:MET:HE2	2.51	0.41
1:I:1068:ASN:O	1:I:1071:ILE:HG12	2.20	0.41
1:J:710:LEU:HD23	1:J:715:ILE:HB	2.03	0.41
1:L:1004:ASP:HA	1:L:1009:LEU:HD12	2.01	0.41
1:L:980:SER:O	1:L:981:SER:HB2	2.20	0.41
1:A:891:LEU:HD13	1:B:847:ARG:NH2	2.35	0.41
1:B:713:PHE:O	1:B:714:LYS:C	2.58	0.41
1:B:751:TYR:CE1	1:B:755:ARG:HG3	2.55	0.41
1:D:905:PHE:CD1	1:D:931:VAL:HG21	2.55	0.41
1:F:703:LEU:HD22	1:F:750:TRP:CE2	2.55	0.41
1:F:963:GLY:O	1:F:973:ILE:HD12	2.20	0.41
1:G:952:THR:O	1:G:956:VAL:HG22	2.20	0.41
1:H:670:LEU:HD22	1:H:674:MET:SD	2.60	0.41
1:H:755:ARG:HA	1:H:756:PRO:HD3	1.91	0.41
1:I:939:ASN:O	1:I:940:GLY:C	2.58	0.41
1:K:988:GLN:HA	1:K:988:GLN:OE1	2.21	0.41
1:L:694:ARG:HA	1:L:728:GLU:OE2	2.20	0.41
1:C:674:MET:CE	1:C:703:LEU:HD21	2.50	0.41
1:D:1059:CYS:HB3	1:D:1062:MET:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:663:LEU:HA	1:H:666:GLU:OE1	2.19	0.41
1:H:703:LEU:HD22	1:H:750:TRP:CE2	2.54	0.41
1:I:915:ASN:O	1:I:916:GLY:C	2.58	0.41
1:K:1068:ASN:O	1:K:1071:ILE:HG12	2.20	0.41
1:L:700:MET:CE	1:L:746:LEU:CD2	2.99	0.41
1:L:751:TYR:CE2	1:L:755:ARG:HG3	2.55	0.41
1:A:717:THR:OG1	1:J:1019:ASP:HA	2.20	0.41
1:A:796:ASP:OD1	1:A:798:SER:CB	2.69	0.41
1:B:751:TYR:CE2	1:B:755:ARG:HG3	2.55	0.41
1:B:812:MET:O	1:B:816:VAL:HG23	2.20	0.41
1:C:1003:TYR:HD2	1:C:1009:LEU:HG	1.85	0.41
1:E:736:TYR:CD1	1:E:955:ILE:HG13	2.55	0.41
1:G:762:GLN:CD	1:G:800:GLY:HA2	2.41	0.41
1:G:853:HIS:O	1:G:857:SER:HB2	2.21	0.41
1:G:915:ASN:O	1:G:916:GLY:C	2.58	0.41
1:H:796:ASP:OD1	1:H:798:SER:N	2.41	0.41
1:I:710:LEU:HA	1:I:710:LEU:HD23	1.87	0.41
1:L:723:TYR:CE1	1:L:861:LEU:HD13	2.56	0.41
1:A:902:LEU:HA	1:A:902:LEU:HD12	1.93	0.41
1:B:723:TYR:CE1	1:B:861:LEU:HD13	2.56	0.41
1:B:930:GLN:O	1:B:933:ILE:HG13	2.20	0.41
1:B:938:ILE:HD12	1:B:996:VAL:HG22	2.02	0.41
1:E:872:LEU:HD12	1:E:873:HIS:H	1.83	0.41
1:F:1003:TYR:HD2	1:F:1009:LEU:HG	1.82	0.41
1:F:881:ARG:NH1	1:F:881:ARG:HG3	2.35	0.41
1:G:1071:ILE:HG21	1:L:915:ASN:ND2	2.36	0.41
1:G:681:ILE:HG23	1:G:682:PHE:N	2.35	0.41
1:H:980:SER:O	1:H:981:SER:HB2	2.19	0.41
1:I:814:LEU:HD11	1:I:933:ILE:HB	2.02	0.41
1:L:880:LYS:HD2	1:L:880:LYS:HA	1.87	0.41
1:A:844:TYR:CE2	1:A:852:ASN:HB3	2.55	0.41
1:B:959:PHE:CG	1:B:977:MET:HE2	2.56	0.41
1:D:721:MET:O	1:D:725:ARG:HG2	2.19	0.41
1:E:953:GLU:O	1:E:957:ASN:ND2	2.54	0.41
1:F:663:LEU:HA	1:F:666:GLU:OE1	2.21	0.41
1:G:763:ILE:C	1:G:765:ASN:H	2.23	0.41
1:H:751:TYR:CE1	1:H:755:ARG:HG3	2.55	0.41
1:I:674:MET:CE	1:I:703:LEU:HD21	2.50	0.41
1:I:784:ILE:HG21	1:I:807:PRO:HB3	2.02	0.41
1:K:762:GLN:NE2	1:K:804:SER:CB	2.78	0.41
1:C:713:PHE:O	1:C:714:LYS:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:762:GLN:HA	1:C:805:ASN:HD21	1.86	0.41
1:C:917:ILE:O	1:C:924:ASP:OD2	2.38	0.41
1:D:716:PRO:HB2	1:D:719:GLN:NE2	2.35	0.41
1:D:959:PHE:CG	1:D:977:MET:HE2	2.56	0.41
1:F:670:LEU:O	1:F:674:MET:HG3	2.20	0.41
1:G:944:VAL:HG22	1:G:945:ARG:N	2.36	0.41
1:I:1003:TYR:HD2	1:I:1009:LEU:HG	1.86	0.41
1:I:939:ASN:ND2	1:I:943:LYS:HE3	2.36	0.41
1:I:952:THR:HG23	1:I:988:GLN:NE2	2.35	0.41
1:J:754:THR:HG22	1:J:755:ARG:NE	2.34	0.41
1:L:943:LYS:HG3	1:L:943:LYS:HZ2	1.76	0.41
1:B:681:ILE:H	1:B:681:ILE:HG13	1.46	0.41
1:B:885:LEU:HA	1:B:885:LEU:HD12	1.79	0.41
1:C:976:PHE:CD2	1:C:987:LEU:HB2	2.56	0.41
1:D:1014:LEU:HD21	1:D:1058:PHE:HB2	2.03	0.41
1:F:1004:ASP:HA	1:F:1009:LEU:HD12	2.02	0.41
1:F:685:VAL:HG22	1:F:695:ILE:HD11	2.03	0.41
1:G:872:LEU:HD13	1:G:873:HIS:CG	2.56	0.41
1:G:871:LEU:HB3	1:G:874:LEU:HD12	2.02	0.41
1:I:872:LEU:HD12	1:I:873:HIS:H	1.85	0.41
1:J:881:ARG:HG3	1:J:881:ARG:NH1	2.35	0.41
1:L:967:ALA:HB2	1:L:973:ILE:HD11	2.03	0.41
1:A:748:ALA:HB3	1:A:936:ALA:HB1	2.03	0.41
1:B:754:THR:HG22	1:B:755:ARG:NE	2.35	0.41
1:B:980:SER:O	1:B:981:SER:HB2	2.20	0.41
1:C:979:ARG:O	1:C:982:PRO:HD3	2.21	0.41
1:D:1015:GLU:HG3	1:D:1015:GLU:H	1.76	0.41
1:E:694:ARG:O	1:E:698:GLN:HG2	2.21	0.41
1:E:715:ILE:HA	1:E:716:PRO:HD2	1.96	0.41
1:E:803:SER:HA	1:E:811:LEU:HD11	2.02	0.41
1:E:976:PHE:CG	1:E:987:LEU:HD13	2.56	0.41
1:H:758:PRO:HG3	1:H:799:TYR:HE2	1.85	0.41
1:I:991:PHE:CE2	1:I:996:VAL:HG23	2.56	0.41
1:K:917:ILE:O	1:K:924:ASP:OD2	2.38	0.41
1:L:700:MET:HE3	1:L:746:LEU:CD1	2.50	0.41
1:B:828:ARG:NH2	4:B:1129:HOH:O	2.54	0.41
1:B:881:ARG:HG2	1:B:885:LEU:HD22	2.02	0.41
1:C:795:PRO:HD2	1:C:799:TYR:CD1	2.56	0.41
1:C:952:THR:HG23	1:C:988:GLN:NE2	2.36	0.41
1:E:871:LEU:HB3	1:E:874:LEU:HD12	2.03	0.41
1:G:713:PHE:O	1:G:714:LYS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:900:ASP:OD1	1:J:900:ASP:N	2.54	0.41
1:K:704:PHE:HB3	1:K:710:LEU:HG	2.03	0.41
1:K:953:GLU:O	1:K:957:ASN:ND2	2.54	0.41
1:L:710:LEU:HD23	1:L:715:ILE:HB	2.03	0.41
1:A:913:ASN:HA	1:C:1056:ARG:HE	1.85	0.40
1:A:915:ASN:O	1:A:916:GLY:C	2.59	0.40
1:B:825:HIS:CD2	1:B:826:PRO:HD2	2.56	0.40
1:C:872:LEU:HD13	1:C:873:HIS:CD2	2.57	0.40
1:C:872:LEU:HD13	1:C:873:HIS:CG	2.56	0.40
1:D:1003:TYR:HD2	1:D:1009:LEU:HG	1.85	0.40
1:E:814:LEU:HD11	1:E:933:ILE:HB	2.02	0.40
1:F:881:ARG:HG2	1:F:885:LEU:HD22	2.03	0.40
1:J:1015:GLU:OE1	1:J:1019:ASP:HB2	2.20	0.40
1:J:805:ASN:HD22	1:J:805:ASN:N	2.19	0.40
1:J:885:LEU:HA	1:J:885:LEU:HD12	1.81	0.40
1:J:905:PHE:CD1	1:J:931:VAL:HG21	2.56	0.40
1:A:962:GLN:O	1:A:966:GLU:HG3	2.22	0.40
1:C:1015:GLU:HB3	1:C:1016:ALA:H	1.77	0.40
1:D:694:ARG:HA	1:D:728:GLU:OE2	2.21	0.40
1:D:751:TYR:CE2	1:D:755:ARG:HG3	2.56	0.40
1:F:956:VAL:HG23	1:F:957:ASN:N	2.36	0.40
1:H:880:LYS:HA	1:H:880:LYS:HD2	1.86	0.40
1:I:758:PRO:HD3	1:I:1011:GLY:H	1.86	0.40
1:A:711:GLU:OE2	1:J:1013:TRP:HB2	2.21	0.40
1:J:674:MET:HE3	1:J:699:VAL:HG13	2.03	0.40
1:J:751:TYR:CE2	1:J:755:ARG:HG3	2.56	0.40
1:K:758:PRO:HD3	1:K:1011:GLY:H	1.85	0.40
1:K:853:HIS:O	1:K:857:SER:HB2	2.22	0.40
1:L:948:HIS:CD2	1:L:1068:ASN:HB3	2.56	0.40
1:L:952:THR:O	1:L:956:VAL:HG22	2.20	0.40
1:C:1068:ASN:O	1:C:1071:ILE:HG12	2.21	0.40
1:C:748:ALA:HB3	1:C:936:ALA:HB1	2.03	0.40
1:D:1069:HIS:CE1	1:D:1073:LYS:NZ	2.89	0.40
1:F:980:SER:O	1:F:981:SER:HB2	2.21	0.40
1:I:694:ARG:O	1:I:698:GLN:HG2	2.21	0.40
1:I:700:MET:HE3	1:I:746:LEU:CD1	2.51	0.40
1:I:802:LEU:HD22	1:I:802:LEU:N	2.36	0.40
1:J:1068:ASN:O	1:J:1071:ILE:HG12	2.21	0.40
1:E:1071:ILE:HG22	1:J:915:ASN:HD22	1.85	0.40
1:J:980:SER:O	1:J:981:SER:HB2	2.21	0.40
1:K:939:ASN:O	1:K:940:GLY:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:GLN:O	1:A:934:LYS:HG3	2.22	0.40
1:A:944:VAL:HG22	1:A:945:ARG:N	2.37	0.40
1:B:1069:HIS:CE1	1:B:1073:LYS:NZ	2.90	0.40
1:B:900:ASP:OD1	1:B:900:ASP:N	2.55	0.40
1:C:881:ARG:HG3	1:C:881:ARG:NH1	2.35	0.40
1:D:1059:CYS:HB3	1:D:1062:MET:HB2	2.03	0.40
1:H:1019:ASP:OD2	1:H:1055:ARG:HA	2.21	0.40
1:H:670:LEU:O	1:H:674:MET:HG3	2.21	0.40
1:H:674:MET:HE3	1:H:699:VAL:HG13	2.03	0.40
1:H:681:ILE:O	1:H:685:VAL:HG23	2.21	0.40
1:H:716:PRO:HB2	1:H:719:GLN:NE2	2.36	0.40
1:H:754:THR:HG22	1:H:755:ARG:NE	2.35	0.40
1:K:754:THR:HG22	1:K:755:ARG:NE	2.22	0.40
1:K:814:LEU:HD11	1:K:933:ILE:HB	2.02	0.40
1:K:905:PHE:CD1	1:K:931:VAL:HG21	2.56	0.40
1:L:900:ASP:N	1:L:900:ASP:OD1	2.55	0.40
1:B:1059:CYS:HB3	1:B:1062:MET:HB2	2.03	0.40
1:C:1004:ASP:CB	1:C:1009:LEU:HD12	2.52	0.40
1:C:939:ASN:O	1:C:940:GLY:C	2.60	0.40
1:D:967:ALA:HB2	1:D:973:ILE:HD11	2.04	0.40
1:E:712:ILE:H	1:E:712:ILE:HG13	1.77	0.40
1:E:743:THR:O	1:E:746:LEU:HB3	2.22	0.40
1:E:951:TRP:O	1:E:955:ILE:HD12	2.22	0.40
1:G:754:THR:CG2	1:G:755:ARG:HE	2.22	0.40
1:H:1004:ASP:CA	1:H:1009:LEU:HD12	2.51	0.40
1:K:735:PRO:HG2	1:K:958:GLU:HB2	2.03	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	358/420 (85%)	332 (93%)	21 (6%)	5 (1%)	12	39
1	B	375/420 (89%)	337 (90%)	28 (8%)	10 (3%)	5	22
1	C	358/420 (85%)	330 (92%)	22 (6%)	6 (2%)	10	34
1	D	375/420 (89%)	334 (89%)	31 (8%)	10 (3%)	5	22
1	E	358/420 (85%)	334 (93%)	18 (5%)	6 (2%)	10	34
1	F	375/420 (89%)	335 (89%)	31 (8%)	9 (2%)	6	25
1	G	358/420 (85%)	333 (93%)	22 (6%)	3 (1%)	21	54
1	H	375/420 (89%)	339 (90%)	28 (8%)	8 (2%)	8	29
1	I	358/420 (85%)	332 (93%)	20 (6%)	6 (2%)	10	34
1	J	375/420 (89%)	338 (90%)	28 (8%)	9 (2%)	6	25
1	K	358/420 (85%)	327 (91%)	25 (7%)	6 (2%)	10	34
1	L	375/420 (89%)	334 (89%)	30 (8%)	11 (3%)	5	20
All	All	4398/5040 (87%)	4005 (91%)	304 (7%)	89 (2%)	8	30

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	869	ASN
1	C	765	ASN
1	C	869	ASN
1	D	764	HIS
1	E	763	ILE
1	E	869	ASN
1	F	764	HIS
1	F	765	ASN
1	H	764	HIS
1	I	763	ILE
1	I	765	ASN
1	I	869	ASN
1	J	764	HIS
1	K	763	ILE
1	K	765	ASN
1	K	869	ASN
1	L	764	HIS
1	A	916	GLY
1	B	764	HIS
1	B	1071	ILE
1	C	916	GLY
1	D	763	ILE

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Mol	Chain	Res	Type
1	D	765	ASN
1	D	1054	ARG
1	D	1071	ILE
1	E	765	ASN
1	E	916	GLY
1	F	1054	ARG
1	F	1071	ILE
1	G	869	ASN
1	G	916	GLY
1	H	1071	ILE
1	I	916	GLY
1	J	763	ILE
1	J	1023	GLU
1	J	1071	ILE
1	K	916	GLY
1	L	1020	ASN
1	L	1071	ILE
1	A	765	ASN
1	B	675	SER
1	C	764	HIS
1	J	675	SER
1	J	765	ASN
1	L	763	ILE
1	L	765	ASN
1	L	869	ASN
1	A	940	GLY
1	B	869	ASN
1	B	940	GLY
1	B	981	SER
1	D	869	ASN
1	D	981	SER
1	E	940	GLY
1	F	675	SER
1	F	869	ASN
1	F	981	SER
1	H	675	SER
1	H	869	ASN
1	H	981	SER
1	J	869	ASN
1	J	981	SER
1	K	940	GLY
1	L	675	SER

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Mol	Chain	Res	Type
1	L	940	GLY
1	L	981	SER
1	L	1023	GLU
1	B	763	ILE
1	B	765	ASN
1	C	940	GLY
1	D	675	SER
1	D	940	GLY
1	F	763	ILE
1	H	940	GLY
1	I	940	GLY
1	B	1017	GLU
1	G	940	GLY
1	H	1054	ARG
1	J	940	GLY
1	F	940	GLY
1	E	849	VAL
1	I	849	VAL
1	K	849	VAL
1	B	941	PRO
1	C	849	VAL
1	L	941	PRO
1	A	849	VAL
1	D	941	PRO
1	H	941	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/370 (83%)	288 (94%)	18 (6%)	21	53
1	B	313/370 (85%)	291 (93%)	22 (7%)	16	44
1	C	306/370 (83%)	290 (95%)	16 (5%)	25	59
1	D	313/370 (85%)	291 (93%)	22 (7%)	16	44
1	E	306/370 (83%)	291 (95%)	15 (5%)	27	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	313/370 (85%)	292 (93%)	21 (7%)	18	46
1	G	306/370 (83%)	287 (94%)	19 (6%)	20	51
1	H	313/370 (85%)	291 (93%)	22 (7%)	16	44
1	I	306/370 (83%)	288 (94%)	18 (6%)	21	53
1	J	313/370 (85%)	292 (93%)	21 (7%)	18	46
1	K	306/370 (83%)	288 (94%)	18 (6%)	21	53
1	L	313/370 (85%)	292 (93%)	21 (7%)	18	46
All	All	3714/4440 (84%)	3481 (94%)	233 (6%)	20	50

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	670	LEU
1	A	684	LEU
1	A	686	GLU
1	A	694	ARG
1	A	706	ASP
1	A	719	GLN
1	A	755	ARG
1	A	792	CYS
1	A	828	ARG
1	A	857	SER
1	A	861	LEU
1	A	869	ASN
1	A	872	LEU
1	A	885	LEU
1	A	915	ASN
1	A	924	ASP
1	A	965	GLU
1	A	1061	LEU
1	B	670	LEU
1	B	681	ILE
1	B	692	SER
1	B	719	GLN
1	B	739	ARG
1	B	792	CYS
1	B	802	LEU
1	B	828	ARG
1	B	847	ARG
1	B	857	SER

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Mol	Chain	Res	Type
1	B	861	LEU
1	B	872	LEU
1	B	885	LEU
1	B	900	ASP
1	B	910	ASN
1	B	911	ASP
1	B	933	ILE
1	B	935	LEU
1	B	947	LEU
1	B	1015	GLU
1	B	1019	ASP
1	B	1057	ILE
1	C	670	LEU
1	C	684	LEU
1	C	686	GLU
1	C	694	ARG
1	C	706	ASP
1	C	719	GLN
1	C	755	ARG
1	C	792	CYS
1	C	828	ARG
1	C	857	SER
1	C	861	LEU
1	C	869	ASN
1	C	872	LEU
1	C	915	ASN
1	C	965	GLU
1	C	1061	LEU
1	D	670	LEU
1	D	681	ILE
1	D	692	SER
1	D	719	GLN
1	D	739	ARG
1	D	792	CYS
1	D	802	LEU
1	D	828	ARG
1	D	847	ARG
1	D	857	SER
1	D	861	LEU
1	D	872	LEU
1	D	885	LEU
1	D	900	ASP

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Mol	Chain	Res	Type
1	D	910	ASN
1	D	911	ASP
1	D	933	ILE
1	D	935	LEU
1	D	947	LEU
1	D	1015	GLU
1	D	1020	ASN
1	D	1057	ILE
1	E	670	LEU
1	E	684	LEU
1	E	686	GLU
1	E	694	ARG
1	E	706	ASP
1	E	719	GLN
1	E	792	CYS
1	E	828	ARG
1	E	857	SER
1	E	861	LEU
1	E	869	ASN
1	E	872	LEU
1	E	915	ASN
1	E	965	GLU
1	E	1061	LEU
1	F	670	LEU
1	F	681	ILE
1	F	692	SER
1	F	719	GLN
1	F	739	ARG
1	F	802	LEU
1	F	828	ARG
1	F	847	ARG
1	F	857	SER
1	F	861	LEU
1	F	872	LEU
1	F	885	LEU
1	F	900	ASP
1	F	910	ASN
1	F	911	ASP
1	F	933	ILE
1	F	935	LEU
1	F	947	LEU
1	F	1015	GLU

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Mol	Chain	Res	Type
1	F	1057	ILE
1	F	1059	CYS
1	G	670	LEU
1	G	684	LEU
1	G	686	GLU
1	G	694	ARG
1	G	706	ASP
1	G	719	GLN
1	G	755	ARG
1	G	792	CYS
1	G	828	ARG
1	G	857	SER
1	G	861	LEU
1	G	869	ASN
1	G	872	LEU
1	G	885	LEU
1	G	915	ASN
1	G	924	ASP
1	G	965	GLU
1	G	1000	CYS
1	G	1061	LEU
1	H	670	LEU
1	H	681	ILE
1	H	692	SER
1	H	719	GLN
1	H	739	ARG
1	H	776	ASP
1	H	802	LEU
1	H	828	ARG
1	H	847	ARG
1	H	857	SER
1	H	861	LEU
1	H	872	LEU
1	H	885	LEU
1	H	900	ASP
1	H	910	ASN
1	H	911	ASP
1	H	933	ILE
1	H	935	LEU
1	H	947	LEU
1	H	1015	GLU
1	H	1056	ARG

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Mol	Chain	Res	Type
1	H	1057	ILE
1	I	670	LEU
1	I	684	LEU
1	I	686	GLU
1	I	694	ARG
1	I	706	ASP
1	I	719	GLN
1	I	755	ARG
1	I	792	CYS
1	I	828	ARG
1	I	857	SER
1	I	861	LEU
1	I	869	ASN
1	I	872	LEU
1	I	885	LEU
1	I	915	ASN
1	I	924	ASP
1	I	965	GLU
1	I	1061	LEU
1	J	670	LEU
1	J	681	ILE
1	J	692	SER
1	J	719	GLN
1	J	739	ARG
1	J	802	LEU
1	J	828	ARG
1	J	847	ARG
1	J	857	SER
1	J	861	LEU
1	J	872	LEU
1	J	885	LEU
1	J	900	ASP
1	J	910	ASN
1	J	911	ASP
1	J	933	ILE
1	J	935	LEU
1	J	947	LEU
1	J	1015	GLU
1	J	1018	GLU
1	J	1057	ILE
1	K	670	LEU
1	K	686	GLU

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Mol	Chain	Res	Type
1	K	694	ARG
1	K	706	ASP
1	K	719	GLN
1	K	755	ARG
1	K	762	GLN
1	K	792	CYS
1	K	828	ARG
1	K	857	SER
1	K	861	LEU
1	K	869	ASN
1	K	872	LEU
1	K	885	LEU
1	K	915	ASN
1	K	924	ASP
1	K	965	GLU
1	K	1061	LEU
1	L	670	LEU
1	L	681	ILE
1	L	692	SER
1	L	719	GLN
1	L	739	ARG
1	L	802	LEU
1	L	828	ARG
1	L	847	ARG
1	L	857	SER
1	L	861	LEU
1	L	872	LEU
1	L	885	LEU
1	L	900	ASP
1	L	910	ASN
1	L	911	ASP
1	L	933	ILE
1	L	935	LEU
1	L	947	LEU
1	L	1015	GLU
1	L	1021	ASP
1	L	1057	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	705	GLN

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Mol	Chain	Res	Type
1	A	719	GLN
1	A	722	ASN
1	A	737	HIS
1	A	762	GLN
1	A	805	ASN
1	A	825	HIS
1	A	869	ASN
1	A	915	ASN
1	A	923	ASN
1	A	939	ASN
1	A	957	ASN
1	A	988	GLN
1	A	994	HIS
1	B	719	GLN
1	B	737	HIS
1	B	805	ASN
1	B	825	HIS
1	B	869	ASN
1	B	915	ASN
1	B	923	ASN
1	B	939	ASN
1	C	718	GLN
1	C	719	GLN
1	C	722	ASN
1	C	737	HIS
1	C	762	GLN
1	C	805	ASN
1	C	825	HIS
1	C	869	ASN
1	C	915	ASN
1	C	923	ASN
1	C	939	ASN
1	C	957	ASN
1	C	988	GLN
1	C	994	HIS
1	D	719	GLN
1	D	737	HIS
1	D	805	ASN
1	D	825	HIS
1	D	869	ASN
1	D	915	ASN
1	D	923	ASN

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Mol	Chain	Res	Type
1	D	939	ASN
1	D	1020	ASN
1	E	718	GLN
1	E	719	GLN
1	E	722	ASN
1	E	737	HIS
1	E	762	GLN
1	E	805	ASN
1	E	825	HIS
1	E	869	ASN
1	E	915	ASN
1	E	923	ASN
1	E	939	ASN
1	E	957	ASN
1	E	988	GLN
1	F	719	GLN
1	F	737	HIS
1	F	805	ASN
1	F	825	HIS
1	F	869	ASN
1	F	923	ASN
1	F	939	ASN
1	G	718	GLN
1	G	719	GLN
1	G	722	ASN
1	G	737	HIS
1	G	762	GLN
1	G	805	ASN
1	G	825	HIS
1	G	869	ASN
1	G	913	ASN
1	G	915	ASN
1	G	923	ASN
1	G	939	ASN
1	G	957	ASN
1	G	988	GLN
1	H	719	GLN
1	H	737	HIS
1	H	794	ASN
1	H	805	ASN
1	H	825	HIS
1	H	869	ASN

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Mol	Chain	Res	Type
1	H	923	ASN
1	H	939	ASN
1	I	718	GLN
1	I	719	GLN
1	I	722	ASN
1	I	737	HIS
1	I	762	GLN
1	I	805	ASN
1	I	825	HIS
1	I	869	ASN
1	I	915	ASN
1	I	923	ASN
1	I	939	ASN
1	I	957	ASN
1	I	988	GLN
1	J	719	GLN
1	J	737	HIS
1	J	805	ASN
1	J	825	HIS
1	J	869	ASN
1	J	923	ASN
1	J	939	ASN
1	J	1063	HIS
1	K	718	GLN
1	K	719	GLN
1	K	722	ASN
1	K	737	HIS
1	K	762	GLN
1	K	794	ASN
1	K	805	ASN
1	K	825	HIS
1	K	869	ASN
1	K	913	ASN
1	K	915	ASN
1	K	923	ASN
1	K	939	ASN
1	K	957	ASN
1	K	988	GLN
1	L	719	GLN
1	L	737	HIS
1	L	805	ASN
1	L	825	HIS

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Mol	Chain	Res	Type
1	L	869	ASN
1	L	915	ASN
1	L	923	ASN
1	L	939	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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	$\# Z > 2$
3	IBM	A	2111	-	13,17,17	1.75	3 (23%)	19,25,25	2.63	6 (31%)
3	IBM	B	2112	-	13,17,17	1.66	3 (23%)	19,25,25	2.67	6 (31%)
3	IBM	C	2113	-	13,17,17	1.53	3 (23%)	19,25,25	2.59	6 (31%)
3	IBM	D	2114	-	13,17,17	1.65	3 (23%)	19,25,25	2.69	7 (36%)
3	IBM	E	2115	-	13,17,17	1.52	2 (15%)	19,25,25	2.57	6 (31%)
3	IBM	F	2116	-	13,17,17	1.49	2 (15%)	19,25,25	2.67	7 (36%)
3	IBM	G	2117	-	13,17,17	1.48	3 (23%)	19,25,25	2.64	6 (31%)
3	IBM	H	2118	-	13,17,17	1.51	3 (23%)	19,25,25	2.58	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IBM	I	2119	-	13,17,17	1.43	3 (23%)	19,25,25	2.61	7 (36%)
3	IBM	J	2120	-	13,17,17	1.46	3 (23%)	19,25,25	2.60	6 (31%)
3	IBM	K	2121	-	13,17,17	1.66	3 (23%)	19,25,25	2.59	6 (31%)
3	IBM	L	2122	-	13,17,17	1.66	3 (23%)	19,25,25	2.65	7 (36%)

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
3	IBM	A	2111	-	-	0/4/4/4	0/2/2/2
3	IBM	B	2112	-	-	0/4/4/4	0/2/2/2
3	IBM	C	2113	-	-	0/4/4/4	0/2/2/2
3	IBM	D	2114	-	-	0/4/4/4	0/2/2/2
3	IBM	E	2115	-	-	0/4/4/4	0/2/2/2
3	IBM	F	2116	-	-	0/4/4/4	0/2/2/2
3	IBM	G	2117	-	-	0/4/4/4	0/2/2/2
3	IBM	H	2118	-	-	0/4/4/4	0/2/2/2
3	IBM	I	2119	-	-	0/4/4/4	0/2/2/2
3	IBM	J	2120	-	-	0/4/4/4	0/2/2/2
3	IBM	K	2121	-	-	0/4/4/4	0/2/2/2
3	IBM	L	2122	-	-	0/4/4/4	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2113	IBM	C5-C4	-3.07	1.33	1.52
3	A	2111	IBM	C5-C4	-3.07	1.33	1.52
3	J	2120	IBM	C5-C4	-3.03	1.33	1.52
3	B	2112	IBM	C5-C4	-3.02	1.33	1.52
3	I	2119	IBM	C5-C4	-3.01	1.33	1.52
3	K	2121	IBM	C5-C4	-2.97	1.34	1.52
3	F	2116	IBM	C5-C4	-2.96	1.34	1.52
3	H	2118	IBM	C5-C4	-2.96	1.34	1.52
3	D	2114	IBM	C5-C4	-2.95	1.34	1.52
3	L	2122	IBM	C5-C4	-2.89	1.34	1.52
3	G	2117	IBM	C5-C4	-2.87	1.34	1.52
3	E	2115	IBM	C5-C4	-2.81	1.34	1.52
3	I	2119	IBM	C2-N3	2.24	1.40	1.37
3	J	2120	IBM	C4-N3	2.27	1.47	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2118	IBM	C4-N3	2.30	1.47	1.45
3	I	2119	IBM	C4-N3	2.37	1.48	1.45
3	B	2112	IBM	C4-N3	2.46	1.48	1.45
3	G	2117	IBM	C2-N3	2.47	1.40	1.37
3	A	2111	IBM	C2-N3	2.57	1.40	1.37
3	G	2117	IBM	C4-N3	2.66	1.48	1.45
3	H	2118	IBM	C2-N3	2.74	1.40	1.37
3	D	2114	IBM	C4-N3	2.77	1.48	1.45
3	J	2120	IBM	C2-N3	2.81	1.40	1.37
3	C	2113	IBM	C2-N3	2.81	1.40	1.37
3	L	2122	IBM	C2-N3	2.91	1.41	1.37
3	C	2113	IBM	C4-N3	2.91	1.48	1.45
3	K	2121	IBM	C2-N3	3.02	1.41	1.37
3	F	2116	IBM	C2-N3	3.06	1.41	1.37
3	E	2115	IBM	C4-N3	3.14	1.48	1.45
3	L	2122	IBM	C4-N3	3.20	1.48	1.45
3	B	2112	IBM	C2-N3	3.28	1.41	1.37
3	D	2114	IBM	C2-N3	3.37	1.41	1.37
3	K	2121	IBM	C4-N3	3.40	1.49	1.45
3	A	2111	IBM	C4-N3	4.10	1.49	1.45

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2116	IBM	O6-C6-C5	-2.64	115.66	121.37
3	B	2112	IBM	O6-C6-C5	-2.62	115.69	121.37
3	A	2111	IBM	O6-C6-C5	-2.53	115.88	121.37
3	D	2114	IBM	O6-C6-C5	-2.44	116.08	121.37
3	K	2121	IBM	O6-C6-C5	-2.41	116.16	121.37
3	I	2119	IBM	O6-C6-C5	-2.36	116.25	121.37
3	G	2117	IBM	O6-C6-C5	-2.32	116.33	121.37
3	L	2122	IBM	O6-C6-C5	-2.30	116.38	121.37
3	E	2115	IBM	O6-C6-C5	-2.30	116.38	121.37
3	H	2118	IBM	O6-C6-C5	-2.28	116.43	121.37
3	C	2113	IBM	O6-C6-C5	-2.26	116.47	121.37
3	J	2120	IBM	O6-C6-C5	-2.20	116.61	121.37
3	F	2116	IBM	C11-N3-C2	2.14	120.71	117.56
3	I	2119	IBM	C11-N3-C2	2.14	120.71	117.56
3	L	2122	IBM	C11-N3-C2	2.30	120.95	117.56
3	C	2113	IBM	O6-C6-N1	2.49	125.62	121.13
3	K	2121	IBM	O6-C6-N1	2.52	125.67	121.13
3	H	2118	IBM	O6-C6-N1	2.61	125.84	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	2120	IBM	O6-C6-N1	2.62	125.86	121.13
3	D	2114	IBM	O6-C6-N1	2.63	125.87	121.13
3	L	2122	IBM	O6-C6-N1	2.63	125.88	121.13
3	I	2119	IBM	O6-C6-N1	2.74	126.08	121.13
3	A	2111	IBM	O6-C6-N1	2.77	126.13	121.13
3	E	2115	IBM	O6-C6-N1	2.84	126.26	121.13
3	G	2117	IBM	O6-C6-N1	2.86	126.29	121.13
3	I	2119	IBM	N7-C8-N9	2.97	114.27	104.73
3	B	2112	IBM	O6-C6-N1	2.98	126.50	121.13
3	A	2111	IBM	N7-C8-N9	3.02	114.44	104.73
3	D	2114	IBM	N7-C8-N9	3.02	114.44	104.73
3	H	2118	IBM	N7-C8-N9	3.03	114.47	104.73
3	F	2116	IBM	O6-C6-N1	3.04	126.61	121.13
3	L	2122	IBM	N7-C8-N9	3.05	114.52	104.73
3	J	2120	IBM	N7-C8-N9	3.10	114.69	104.73
3	K	2121	IBM	N7-C8-N9	3.11	114.70	104.73
3	D	2114	IBM	C11-N3-C2	3.12	122.15	117.56
3	B	2112	IBM	N7-C8-N9	3.13	114.78	104.73
3	F	2116	IBM	N7-C8-N9	3.13	114.78	104.73
3	C	2113	IBM	N7-C8-N9	3.15	114.86	104.73
3	G	2117	IBM	N7-C8-N9	3.16	114.87	104.73
3	E	2115	IBM	N7-C8-N9	3.24	115.14	104.73
3	K	2121	IBM	C5-C4-N9	4.24	108.72	103.23
3	C	2113	IBM	C4-C5-N7	4.36	108.24	102.46
3	G	2117	IBM	C4-C5-N7	4.40	108.29	102.46
3	D	2114	IBM	C5-C4-N9	4.40	108.93	103.23
3	A	2111	IBM	C5-C4-N9	4.42	108.95	103.23
3	L	2122	IBM	C5-C4-N9	4.42	108.95	103.23
3	E	2115	IBM	C5-C4-N9	4.45	108.99	103.23
3	I	2119	IBM	C4-C5-N7	4.46	108.36	102.46
3	H	2118	IBM	C4-C5-N7	4.47	108.39	102.46
3	I	2119	IBM	C5-C4-N9	4.50	109.06	103.23
3	J	2120	IBM	C5-C4-N9	4.53	109.10	103.23
3	A	2111	IBM	C4-C5-N7	4.57	108.51	102.46
3	L	2122	IBM	C4-C5-N7	4.58	108.53	102.46
3	F	2116	IBM	C5-C4-N9	4.61	109.20	103.23
3	H	2118	IBM	C5-C4-N9	4.61	109.20	103.23
3	G	2117	IBM	C5-C4-N9	4.61	109.21	103.23
3	E	2115	IBM	C4-C5-N7	4.62	108.59	102.46
3	J	2120	IBM	C4-C5-N7	4.65	108.62	102.46
3	B	2112	IBM	C5-C4-N9	4.65	109.26	103.23
3	F	2116	IBM	C4-C5-N7	4.66	108.64	102.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2114	IBM	C4-C5-N7	4.66	108.64	102.46
3	B	2112	IBM	C4-C5-N7	4.67	108.65	102.46
3	C	2113	IBM	C5-C4-N9	4.76	109.40	103.23
3	K	2121	IBM	C4-C5-N7	4.88	108.93	102.46
3	E	2115	IBM	C5-C4-N3	7.15	119.23	110.33
3	C	2113	IBM	C5-C4-N3	7.40	119.54	110.33
3	K	2121	IBM	C5-C4-N3	7.41	119.55	110.33
3	A	2111	IBM	C5-C4-N3	7.47	119.63	110.33
3	H	2118	IBM	C5-C4-N3	7.50	119.67	110.33
3	F	2116	IBM	C5-C4-N3	7.51	119.68	110.33
3	B	2112	IBM	C5-C4-N3	7.55	119.72	110.33
3	G	2117	IBM	C5-C4-N3	7.55	119.72	110.33
3	L	2122	IBM	C5-C4-N3	7.58	119.77	110.33
3	I	2119	IBM	C5-C4-N3	7.61	119.80	110.33
3	J	2120	IBM	C5-C4-N3	7.64	119.83	110.33
3	D	2114	IBM	C5-C4-N3	7.72	119.94	110.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	364/420 (86%)	-0.00	9 (2%) 57 54	24, 42, 80, 100	0
1	B	381/420 (90%)	0.33	29 (7%) 14 10	25, 50, 92, 100	0
1	C	364/420 (86%)	0.09	14 (3%) 40 35	26, 43, 81, 100	0
1	D	381/420 (90%)	0.34	24 (6%) 20 15	22, 47, 89, 100	0
1	E	364/420 (86%)	0.07	12 (3%) 46 40	23, 42, 81, 100	0
1	F	381/420 (90%)	0.15	14 (3%) 41 36	21, 45, 79, 100	0
1	G	364/420 (86%)	-0.02	14 (3%) 40 35	24, 44, 83, 100	0
1	H	381/420 (90%)	0.28	23 (6%) 22 17	29, 52, 92, 100	0
1	I	364/420 (86%)	0.07	14 (3%) 40 35	23, 42, 81, 100	0
1	J	381/420 (90%)	0.11	11 (2%) 51 46	22, 46, 77, 100	0
1	K	364/420 (86%)	0.64	57 (15%) 2 1	28, 51, 87, 100	0
1	L	381/420 (90%)	0.55	35 (9%) 9 6	29, 54, 91, 100	0
All	All	4470/5040 (88%)	0.22	256 (5%) 24 19	21, 46, 85, 100	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	659	LEU	11.8
1	H	1022	THR	11.4
1	B	1024	SER	11.3
1	D	1021	ASP	10.7
1	H	1020	ASN	10.4
1	B	1022	THR	10.4
1	K	1053	SER	10.4
1	L	1053	SER	10.2
1	B	1053	SER	10.0
1	L	1016	ALA	10.0
1	H	1016	ALA	9.9

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Mol	Chain	Res	Type	RSRZ
1	H	1018	GLU	9.9
1	B	1021	ASP	9.7
1	L	1021	ASP	9.7
1	D	1024	SER	9.5
1	C	1016	ALA	9.4
1	D	1053	SER	8.9
1	B	1018	GLU	8.9
1	E	1016	ALA	8.8
1	B	1019	ASP	8.8
1	D	1016	ALA	8.7
1	H	1021	ASP	8.6
1	D	1020	ASN	8.5
1	B	1020	ASN	8.5
1	I	1016	ALA	8.5
1	H	1024	SER	8.5
1	B	1023	GLU	8.5
1	L	1020	ASN	8.4
1	D	1019	ASP	8.3
1	D	1022	THR	8.1
1	B	1016	ALA	8.1
1	H	1019	ASP	8.0
1	D	1018	GLU	7.9
1	D	1023	GLU	7.9
1	A	1016	ALA	7.8
1	L	1019	ASP	7.7
1	L	1022	THR	7.7
1	D	1017	GLU	7.7
1	L	1018	GLU	7.6
1	L	1017	GLU	7.5
1	C	1017	GLU	7.5
1	A	1017	GLU	7.4
1	F	658	SER	7.3
1	H	658	SER	7.2
1	B	657	VAL	7.2
1	D	657	VAL	7.2
1	I	1053	SER	7.2
1	L	1023	GLU	7.1
1	G	1053	SER	7.0
1	F	656	GLU	6.9
1	C	1053	SER	6.9
1	B	1054	ARG	6.8
1	D	658	SER	6.7

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Mol	Chain	Res	Type	RSRZ
1	L	1024	SER	6.7
1	A	1053	SER	6.7
1	L	1054	ARG	6.4
1	H	1053	SER	6.4
1	B	1017	GLU	6.3
1	I	1017	GLU	6.3
1	K	1017	GLU	6.2
1	B	658	SER	6.2
1	J	657	VAL	6.1
1	H	656	GLU	6.0
1	H	1017	GLU	6.0
1	E	1017	GLU	5.9
1	L	656	GLU	5.9
1	L	657	VAL	5.9
1	D	660	ASP	5.9
1	J	660	ASP	5.8
1	A	766	GLY	5.8
1	L	658	SER	5.8
1	G	1016	ALA	5.7
1	H	1023	GLU	5.7
1	H	659	LEU	5.6
1	L	659	LEU	5.5
1	I	1054	ARG	5.4
1	B	656	GLU	5.3
1	F	659	LEU	5.2
1	E	659	LEU	5.1
1	J	658	SER	5.1
1	F	657	VAL	5.1
1	D	1054	ARG	5.1
1	D	659	LEU	5.0
1	K	1016	ALA	4.9
1	J	656	GLU	4.9
1	H	1015	GLU	4.8
1	D	1015	GLU	4.8
1	E	1053	SER	4.8
1	L	1015	GLU	4.8
1	H	1054	ARG	4.7
1	H	657	VAL	4.7
1	G	1017	GLU	4.5
1	K	701	TYR	4.5
1	L	765	ASN	4.4
1	L	660	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	765	ASN	4.4
1	E	765	ASN	4.4
1	D	662	ILE	4.3
1	J	765	ASN	4.3
1	G	913	ASN	4.3
1	D	661	LEU	4.3
1	I	659	LEU	4.2
1	K	1014	LEU	4.2
1	B	660	ASP	4.2
1	C	660	ASP	4.2
1	C	764	HIS	4.1
1	I	764	HIS	4.1
1	K	761	GLN	4.1
1	K	1056	ARG	4.1
1	K	659	LEU	4.1
1	J	659	LEU	4.0
1	G	764	HIS	4.0
1	B	659	LEU	3.9
1	E	764	HIS	3.9
1	F	1019	ASP	3.9
1	C	766	GLY	3.9
1	G	765	ASN	3.9
1	A	1054	ARG	3.8
1	K	660	ASP	3.8
1	L	1055	ARG	3.8
1	E	660	ASP	3.8
1	I	660	ASP	3.8
1	H	660	ASP	3.8
1	F	660	ASP	3.7
1	E	766	GLY	3.7
1	K	720	PHE	3.6
1	K	764	HIS	3.6
1	B	1015	GLU	3.6
1	K	1054	ARG	3.6
1	D	656	GLU	3.5
1	K	1055	ARG	3.5
1	K	1012	GLN	3.5
1	K	795	PRO	3.4
1	L	764	HIS	3.4
1	L	763	ILE	3.4
1	G	1054	ARG	3.4
1	K	1057	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	1013	TRP	3.4
1	K	787	ILE	3.3
1	B	1055	ARG	3.3
1	H	766	GLY	3.3
1	K	802	LEU	3.2
1	A	765	ASN	3.2
1	F	662	ILE	3.2
1	I	766	GLY	3.1
1	G	912	VAL	3.1
1	L	912	VAL	3.1
1	L	1014	LEU	3.1
1	C	661	LEU	3.0
1	F	912	VAL	3.0
1	H	913	ASN	3.0
1	B	765	ASN	3.0
1	L	661	LEU	3.0
1	K	717	THR	3.0
1	K	704	PHE	2.9
1	B	766	GLY	2.9
1	F	1053	SER	2.9
1	K	913	ASN	2.9
1	C	761	GLN	2.8
1	D	765	ASN	2.8
1	K	862	TYR	2.8
1	H	1055	ARG	2.8
1	K	800	GLY	2.8
1	F	661	LEU	2.8
1	G	1056	ARG	2.8
1	B	663	LEU	2.8
1	G	663	LEU	2.8
1	G	784	ILE	2.7
1	F	1020	ASN	2.7
1	C	1015	GLU	2.7
1	K	763	ILE	2.7
1	K	662	ILE	2.7
1	L	794	ASN	2.7
1	E	661	LEU	2.7
1	K	815	TYR	2.7
1	B	661	LEU	2.7
1	K	916	GLY	2.6
1	L	766	GLY	2.6
1	B	764	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	763	ILE	2.6
1	E	1054	ARG	2.6
1	K	709	LEU	2.6
1	K	705	GLN	2.6
1	K	699	VAL	2.6
1	C	662	ILE	2.6
1	B	1056	ARG	2.6
1	K	762	GLN	2.6
1	H	764	HIS	2.6
1	D	663	LEU	2.5
1	G	664	VAL	2.5
1	I	662	ILE	2.5
1	H	661	LEU	2.5
1	K	663	LEU	2.5
1	B	667	TYR	2.5
1	J	1053	SER	2.5
1	K	757	VAL	2.5
1	L	799	TYR	2.5
1	D	1014	LEU	2.5
1	K	703	LEU	2.5
1	F	1018	GLU	2.4
1	K	806	ILE	2.4
1	K	765	ASN	2.4
1	K	1015	GLU	2.4
1	A	659	LEU	2.4
1	K	665	GLU	2.4
1	K	794	ASN	2.4
1	B	1014	LEU	2.4
1	L	663	LEU	2.4
1	G	766	GLY	2.3
1	L	1059	CYS	2.3
1	C	1054	ARG	2.3
1	L	662	ILE	2.3
1	K	1013	TRP	2.3
1	K	805	ASN	2.3
1	F	1021	ASP	2.3
1	K	667	TYR	2.3
1	D	1056	ARG	2.3
1	B	912	VAL	2.3
1	J	661	LEU	2.3
1	K	716	PRO	2.2
1	L	971	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	978	ASP	2.2
1	K	792	CYS	2.2
1	G	661	LEU	2.2
1	L	969	LEU	2.2
1	K	715	ILE	2.2
1	K	793	SER	2.2
1	L	761	GLN	2.2
1	K	664	VAL	2.2
1	J	1021	ASP	2.2
1	I	761	GLN	2.1
1	E	916	GLY	2.1
1	K	1058	PHE	2.1
1	A	916	GLY	2.1
1	K	915	ASN	2.1
1	K	707	THR	2.1
1	I	1014	LEU	2.1
1	K	766	GLY	2.1
1	B	1013	TRP	2.1
1	K	750	TRP	2.1
1	K	871	LEU	2.1
1	B	662	ILE	2.1
1	H	912	VAL	2.1
1	J	1020	ASN	2.1
1	I	1015	GLU	2.1
1	K	1011	GLY	2.1
1	C	1014	LEU	2.0
1	K	919	TRP	2.0
1	K	712	ILE	2.0
1	J	1000	CYS	2.0
1	F	664	VAL	2.0
1	I	765	ASN	2.0
1	A	784	ILE	2.0
1	E	662	ILE	2.0
1	K	724	PHE	2.0
1	I	661	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
2	MG	B	2126	1/1	0.93	0.11	56,56,56,56	0
3	IBM	H	2118	16/16	0.93	0.25	72,78,79,80	0
3	IBM	L	2122	16/16	0.94	0.22	68,77,78,79	0
2	MG	I	2140	1/1	0.95	0.12	27,27,27,27	0
3	IBM	B	2112	16/16	0.95	0.24	54,56,59,59	0
3	IBM	D	2114	16/16	0.96	0.20	35,53,56,57	0
3	IBM	G	2117	16/16	0.96	0.21	44,49,50,51	0
2	MG	L	2146	1/1	0.97	0.07	30,30,30,30	0
3	IBM	A	2111	16/16	0.97	0.18	36,38,42,42	0
2	MG	H	2138	1/1	0.97	0.06	32,32,32,32	0
2	MG	H	2137	1/1	0.97	0.13	12,12,12,12	0
3	IBM	E	2115	16/16	0.97	0.19	28,32,35,37	0
3	IBM	K	2121	16/16	0.97	0.19	54,59,60,61	0
2	MG	B	2125	1/1	0.98	0.10	4,4,4,4	0
3	IBM	C	2113	16/16	0.98	0.19	36,42,48,48	0
2	MG	L	2145	1/1	0.98	0.12	23,23,23,23	0
3	IBM	J	2120	16/16	0.98	0.23	31,35,40,41	0
2	MG	F	2134	1/1	0.98	0.07	19,19,19,19	0
3	IBM	I	2119	16/16	0.98	0.19	35,38,39,39	0
3	IBM	F	2116	16/16	0.98	0.17	28,37,40,40	0
2	MG	K	2143	1/1	0.98	0.12	20,20,20,20	0
2	MG	J	2142	1/1	0.99	0.11	39,39,39,39	0
2	MG	A	2124	1/1	0.99	0.11	41,41,41,41	0
2	MG	K	2144	1/1	0.99	0.12	40,40,40,40	0
2	MG	I	2139	1/1	0.99	0.15	5,5,5,5	0
2	MG	C	2128	1/1	0.99	0.10	29,29,29,29	0
2	MG	E	2132	1/1	0.99	0.14	29,29,29,29	0
2	MG	A	2123	1/1	0.99	0.13	2,2,2,2	0
2	MG	E	2131	1/1	0.99	0.15	1,1,1,1	0
2	MG	D	2129	1/1	0.99	0.16	9,9,9,9	0
2	MG	J	2141	1/1	0.99	0.14	6,6,6,6	0
2	MG	F	2133	1/1	0.99	0.16	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	G	2136	1/1	0.99	0.10	28,28,28,28	0
2	MG	G	2135	1/1	0.99	0.12	1,1,1,1	0
2	MG	D	2130	1/1	0.99	0.11	22,22,22,22	0
2	MG	C	2127	1/1	1.00	0.14	5,5,5,5	0

6.5 Other polymers [i](#)

There are no such residues in this entry.