Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:02 am BST

PDB ID	:	1Z56
Title	:	Co-Crystal Structure of Lif1p-Lig4p
Authors	:	Dore, A.S.; Furnham, N.; Davies, O.R.; Sibanda, B.L.; Chirgadze, D.Y.; Jackson, S.P.; Pellegrini, L.; Blundell, T.L.
Deposited on	:	2005-03-17
Resolution	:	3.92 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:

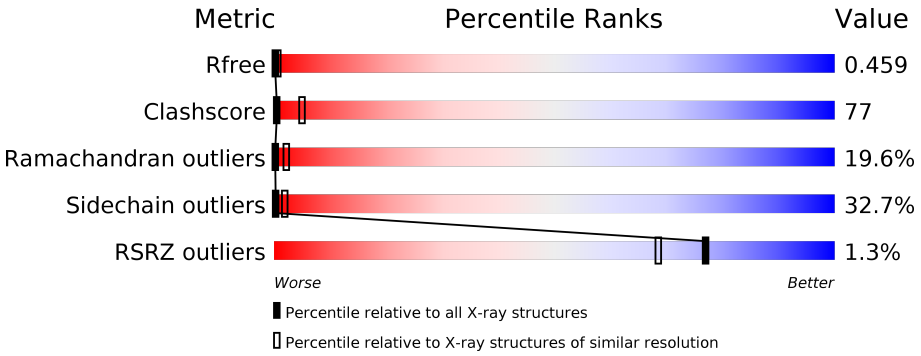
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.92 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}	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	246	8% 14% 9% 69%
1	B	246	% 7% 15% 7% • 69%
2	C	264	% 16% 39% 27% 8% 10%
3	D	8	38% 63%
4	E	7	71% 29%
4	H	7	57% 43%

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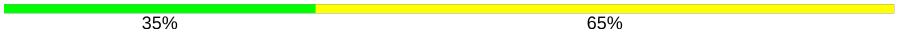
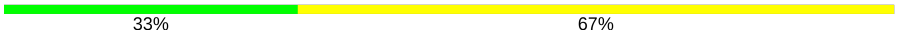
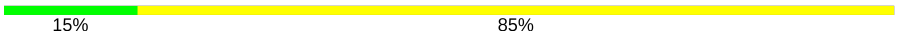
Mol	Chain	Length	Quality of chain
5	F	45	
6	G	37	
7	I	30	
8	J	20	
9	K	13	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4164 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 Ligase interacting factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	77	Total	C	N	O	S	0	0	0
			648	393	126	125	4			
1	B	76	Total	C	N	O	S	0	0	0
			643	393	122	123	5			

- Molecule 2 is a protein called DNA ligase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	237	Total	C	N	O	S	0	0	0
			1899	1209	319	359	12			

- Molecule 3 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	8	Total	C	N	O	0	0	0
			47	31	8	8			

- Molecule 4 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	7	Total	C	N	O	0	0	0
			42	28	7	7			
4	H	7	Total	C	N	O	0	0	0
			42	28	7	7			

- Molecule 5 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	45	Total	C	N	O	0	0	0
			258	168	45	45			

- Molecule 6 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	37	Total	C	N	O	0	0	0
			218	144	37	37			

- Molecule 7 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	I	30	Total	C	N	O	0	0	0
			173	113	30	30			

- Molecule 8 is a protein called Ligase interacting factor 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	J	20	Total	C	N	O	0	0	0
			118	78	20	20			

- Molecule 9 is a protein called Ligase interacting factor 1.

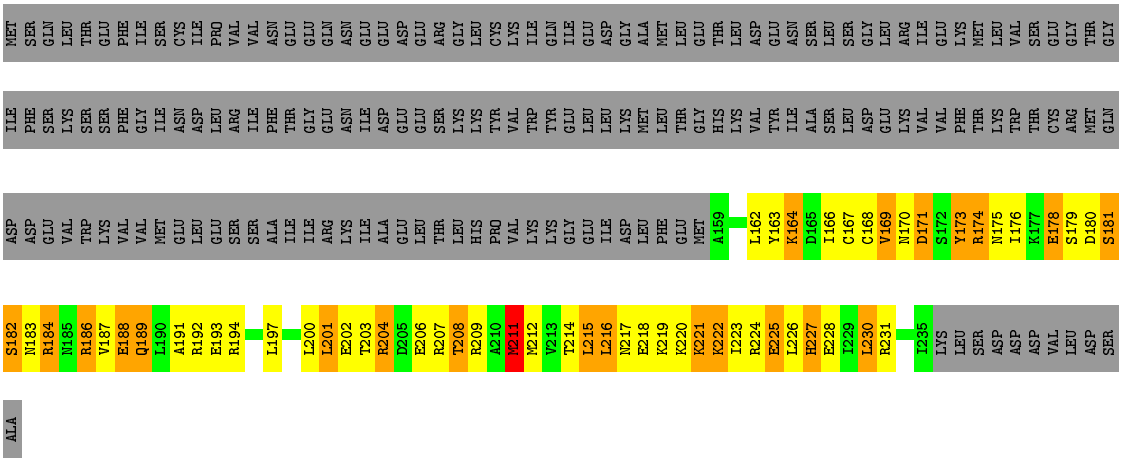
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	13	Total	C	N	O	0	0	0
			76	50	13	13			

3 Residue-property plots (i)

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

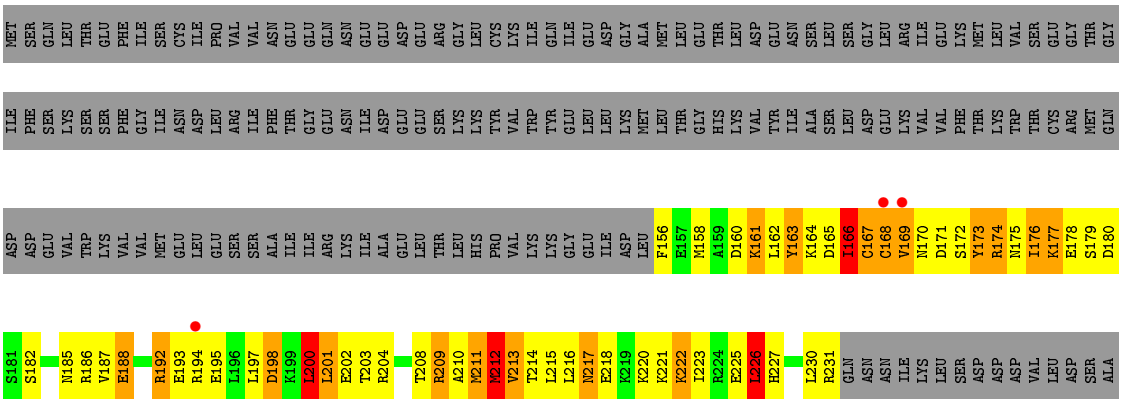
- Molecule 1: Ligase interacting factor 1

Chain A:



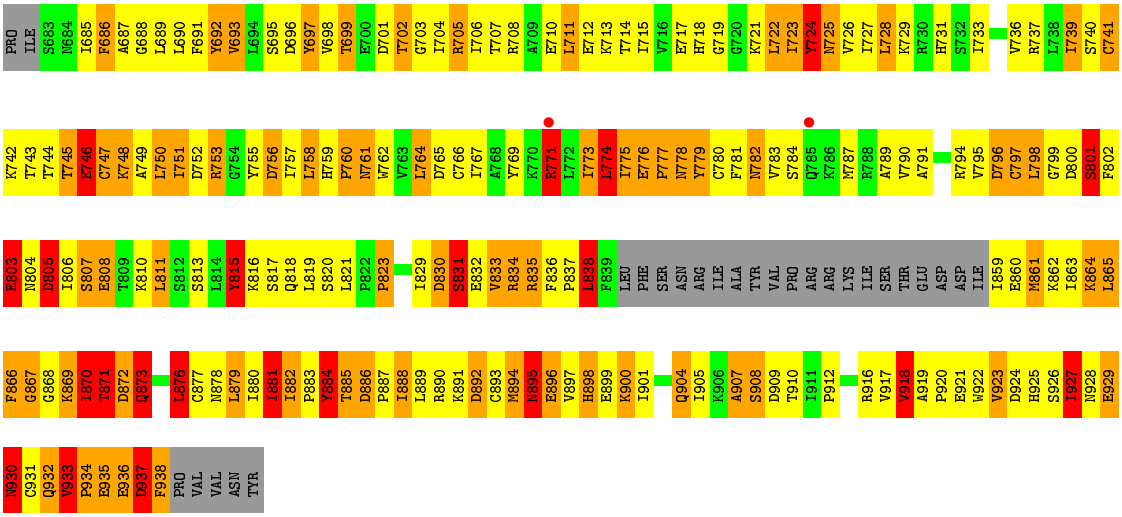
- Molecule 1: Ligase interacting factor 1

Chain B:



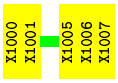
- Molecule 2: DNA ligase IV

Chain C:



• Molecule 3: Ligase interacting factor 1

Chain D:



• Molecule 4: Ligase interacting factor 1

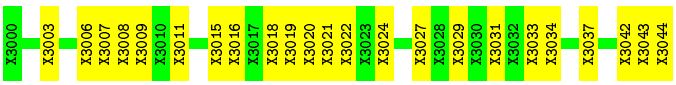
Chain E:

• Molecule 4: Ligase interacting factor 1

Chain H:

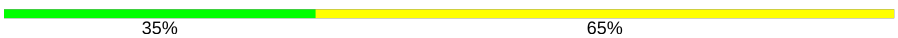
• Molecule 5: Ligase interacting factor 1

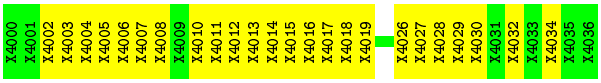
Chain F:



• Molecule 6: Ligase interacting factor 1

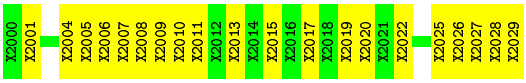
Chain G:





• Molecule 7: Ligase interacting factor 1

Chain I:

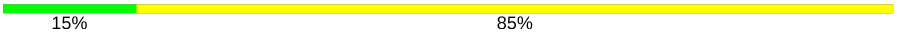


• Molecule 8: Ligase interacting factor 1

Chain J:

• Molecule 9: Ligase interacting factor 1

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	247.62Å 247.62Å 98.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.20 – 3.92 49.20 – 3.92	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.20-3.92) 99.9 (49.20-3.92)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.400 , 0.467 0.398 , 0.459	Depositor DCC
R_{free} test set	832 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	109.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 109.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	4164	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.69	0/650	0.85	0/865
1	B	0.77	0/646	0.90	1/858 (0.1%)
2	C	0.91	2/1931 (0.1%)	1.12	7/2609 (0.3%)
All	All	0.84	2/3227 (0.1%)	1.03	8/4332 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	5
8	J	0	18
All	All	0	23

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	835	ARG	CG-CD	5.18	1.64	1.51
2	C	803	GLU	CG-CD	5.16	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	835	ARG	NE-CZ-NH1	10.99	125.80	120.30
2	C	876	LEU	CA-CB-CG	7.73	133.09	115.30
1	B	200	LEU	CA-CB-CG	-7.50	98.04	115.30
2	C	758	LEU	CA-CB-CG	5.94	128.96	115.30
2	C	881	ILE	N-CA-C	-5.83	95.25	111.00
2	C	918	VAL	N-CA-C	5.19	125.00	111.00
2	C	774	LEU	CA-CB-CG	5.17	127.20	115.30
2	C	838	LEU	N-CA-C	5.02	124.55	111.00

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	724	TYR	Peptide
2	C	771	ARG	Peptide
2	C	805	ASP	Peptide
2	C	884	TYR	Peptide
2	C	895	ASN	Peptide
8	J	3001	UNK	Mainchain
8	J	3002	UNK	Mainchain
8	J	3003	UNK	Mainchain
8	J	3004	UNK	Mainchain
8	J	3005	UNK	Mainchain
8	J	3006	UNK	Mainchain
8	J	3007	UNK	Mainchain
8	J	3008	UNK	Mainchain
8	J	3009	UNK	Mainchain
8	J	3010	UNK	Mainchain
8	J	3011	UNK	Mainchain
8	J	3012	UNK	Mainchain
8	J	3013	UNK	Mainchain
8	J	3014	UNK	Mainchain
8	J	3015	UNK	Mainchain
8	J	3016	UNK	Mainchain
8	J	3017	UNK	Mainchain
8	J	3018	UNK	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	648	0	670	69	0
1	B	643	0	663	105	0
2	C	1899	0	1927	342	1
3	D	47	0	49	9	0
4	E	42	0	48	7	0
4	H	42	0	48	4	0
5	F	258	0	233	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	218	0	218	53	0
7	I	173	0	161	42	0
8	J	118	0	122	19	0
9	K	76	0	76	19	0
All	All	4164	0	4215	643	1

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 77.

All (643) 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)
2:C:922:TRP:HA	2:C:925:HIS:CE1	1.50	1.43
2:C:883:PRO:O	2:C:889:LEU:HB3	1.34	1.22
2:C:892:ASP:O	2:C:895:ASN:HB2	1.44	1.18
1:B:188:GLU:HA	1:B:192:ARG:HH21	1.08	1.17
2:C:834:ARG:HG2	2:C:869:LYS:CD	1.78	1.13
2:C:834:ARG:HG2	2:C:869:LYS:HE3	1.29	1.13
2:C:916:ARG:NH1	2:C:933:VAL:HG21	1.62	1.12
2:C:935:GLU:O	2:C:936:GLU:HG2	1.48	1.11
2:C:834:ARG:HG2	2:C:869:LYS:CE	1.79	1.11
2:C:916:ARG:HH11	2:C:933:VAL:HG21	1.11	1.10
2:C:776:GLU:OE1	2:C:777:PRO:HD3	1.52	1.09
7:I:2005:UNK:HG3	7:I:2006:UNK:N	1.50	1.08
7:I:2005:UNK:CG	7:I:2006:UNK:H	1.61	1.07
2:C:834:ARG:CG	2:C:869:LYS:HE3	1.85	1.06
8:J:3009:UNK:O	8:J:3010:UNK:HG2	1.56	1.04
2:C:866:PHE:HA	2:C:870:ILE:HG21	1.06	1.03
2:C:892:ASP:O	2:C:895:ASN:CB	2.05	1.03
2:C:866:PHE:HA	2:C:870:ILE:CG2	1.88	1.03
1:A:221:LYS:HE2	1:A:224:ARG:HH22	1.23	1.02
2:C:835:ARG:NH2	2:C:868:GLY:HA3	1.72	1.02
7:I:2017:UNK:HG2	7:I:2020:UNK:HG1	1.41	1.01
2:C:774:LEU:HD22	2:C:794:ARG:HG3	1.39	1.00
6:G:4002:UNK:O	6:G:4017:UNK:HG3	1.63	0.98
2:C:699:THR:O	2:C:741:CYS:HB2	1.62	0.98
2:C:870:ILE:HG13	2:C:871:THR:H	1.29	0.98
2:C:741:CYS:O	2:C:759:HIS:CD2	2.17	0.97
2:C:922:TRP:CA	2:C:925:HIS:CE1	2.47	0.97
7:I:2005:UNK:HG3	7:I:2006:UNK:H	0.80	0.96
1:B:188:GLU:HA	1:B:192:ARG:NH2	1.78	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:MET:HB2	2:C:832:GLU:OE2	1.63	0.96
2:C:895:ASN:O	2:C:897:VAL:N	1.99	0.96
1:B:211:MET:HB2	2:C:832:GLU:CD	1.87	0.95
6:G:4007:UNK:CG	6:G:4012:UNK:O	2.15	0.95
6:G:4013:UNK:O	6:G:4015:UNK:HG2	1.67	0.95
2:C:756:ASP:HB3	2:C:781:PHE:CD2	2.01	0.95
2:C:838:LEU:N	2:C:838:LEU:HD22	1.79	0.95
2:C:882:ILE:O	2:C:920:PRO:HD3	1.66	0.94
2:C:744:THR:O	2:C:747:CYS:HB2	1.68	0.92
7:I:2017:UNK:CG	7:I:2020:UNK:HG1	2.00	0.91
2:C:866:PHE:CA	2:C:870:ILE:HG21	1.99	0.91
2:C:883:PRO:HB2	2:C:889:LEU:HD22	1.52	0.91
9:K:4001:UNK:HG2	9:K:4002:UNK:H	1.36	0.91
2:C:774:LEU:CD2	2:C:794:ARG:HG3	1.99	0.90
6:G:4007:UNK:HG2	6:G:4012:UNK:O	1.72	0.90
7:I:2008:UNK:HG3	7:I:2009:UNK:N	1.83	0.90
2:C:922:TRP:HA	2:C:925:HIS:HE1	1.31	0.89
2:C:690:LEU:HA	2:C:722:LEU:HD23	1.52	0.89
7:I:2004:UNK:O	7:I:2004:UNK:HG3	1.72	0.89
2:C:888:ILE:HG13	2:C:889:LEU:N	1.85	0.89
2:C:783:VAL:HB	2:C:787:MET:HB3	1.51	0.89
2:C:888:ILE:HG13	2:C:889:LEU:H	1.38	0.88
2:C:883:PRO:O	2:C:889:LEU:CB	2.20	0.87
8:J:3007:UNK:HG3	8:J:3008:UNK:N	1.88	0.87
3:D:1005:UNK:O	4:E:2001:UNK:HG2	1.73	0.87
2:C:886:ASP:HB2	2:C:887:PRO:HD2	1.57	0.87
1:B:174:ARG:HG2	1:B:177:LYS:NZ	1.89	0.86
2:C:722:LEU:HB3	2:C:724:TYR:CE2	2.11	0.85
2:C:760:PRO:O	2:C:762:TRP:N	2.09	0.85
2:C:834:ARG:HG2	2:C:869:LYS:HD3	1.58	0.84
2:C:895:ASN:C	2:C:897:VAL:N	2.26	0.84
8:J:3013:UNK:HG3	8:J:3014:UNK:N	1.92	0.84
2:C:761:ASN:O	2:C:765:ASP:N	2.09	0.84
2:C:908:SER:HB3	2:C:912:PRO:HG3	1.58	0.84
1:A:227:HIS:O	1:A:230:LEU:HB2	1.78	0.84
2:C:766:CYS:SG	2:C:771:ARG:HG2	2.17	0.83
2:C:895:ASN:OD1	2:C:896:GLU:HB3	1.78	0.83
6:G:4008:UNK:HG3	6:G:4013:UNK:HG2	1.58	0.83
2:C:872:ASP:O	2:C:873:GLN:HB2	1.77	0.83
8:J:3013:UNK:HG3	8:J:3014:UNK:H	1.42	0.83
1:B:174:ARG:HG2	1:B:177:LYS:HZ1	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:756:ASP:HA	2:C:781:PHE:HB2	1.59	0.82
2:C:922:TRP:HA	2:C:925:HIS:ND1	1.94	0.82
5:F:3029:UNK:HB2	5:F:3033:UNK:HB2	1.60	0.82
2:C:896:GLU:O	2:C:899:GLU:HB3	1.79	0.82
6:G:4028:UNK:O	6:G:4029:UNK:HG2	1.79	0.82
2:C:781:PHE:CG	2:C:782:ASN:N	2.45	0.82
2:C:862:LYS:HG3	2:C:872:ASP:OD2	1.79	0.82
2:C:834:ARG:NE	2:C:835:ARG:O	2.11	0.82
6:G:4008:UNK:CG	6:G:4013:UNK:HG2	2.10	0.81
5:F:3006:UNK:HG3	5:F:3009:UNK:O	1.79	0.81
1:A:173:TYR:O	1:A:174:ARG:HD3	1.80	0.81
2:C:859:ILE:HG23	2:C:863:ILE:HB	1.63	0.81
2:C:838:LEU:CD2	2:C:872:ASP:HA	2.11	0.81
2:C:916:ARG:NH1	2:C:933:VAL:CG2	2.43	0.81
2:C:930:ASN:CG	2:C:931:CYS:H	1.83	0.80
2:C:870:ILE:CG1	2:C:871:THR:H	1.91	0.80
6:G:4018:UNK:O	6:G:4018:UNK:HG3	1.80	0.80
1:A:169:VAL:O	1:A:173:TYR:HB2	1.81	0.80
2:C:895:ASN:OD1	2:C:896:GLU:CB	2.30	0.80
7:I:2005:UNK:CG	7:I:2006:UNK:N	2.28	0.80
1:B:220:LYS:NZ	2:C:805:ASP:HB3	1.97	0.80
5:F:3027:UNK:HG3	5:F:3027:UNK:O	1.82	0.79
2:C:830:ASP:CG	2:C:831:SER:H	1.84	0.79
1:A:228:GLU:O	1:A:231:ARG:HD2	1.82	0.79
2:C:741:CYS:H	2:C:759:HIS:CB	1.96	0.79
2:C:866:PHE:O	2:C:868:GLY:N	2.16	0.79
2:C:904:GLN:HB3	2:C:912:PRO:HG2	1.64	0.79
1:B:201:LEU:O	1:B:204:ARG:HB2	1.83	0.78
9:K:4002:UNK:HG3	9:K:4003:UNK:N	1.97	0.78
2:C:739:ILE:HD13	2:C:739:ILE:H	1.47	0.78
2:C:935:GLU:O	2:C:936:GLU:CG	2.32	0.78
2:C:870:ILE:CG1	2:C:871:THR:N	2.47	0.77
2:C:834:ARG:HA	2:C:869:LYS:CG	2.14	0.77
2:C:925:HIS:CE1	2:C:936:GLU:CD	2.58	0.77
2:C:870:ILE:HG13	2:C:871:THR:N	2.00	0.77
1:B:211:MET:SD	2:C:832:GLU:HG3	2.25	0.76
1:A:219:LYS:HZ3	1:B:220:LYS:HE3	1.50	0.76
2:C:834:ARG:HE	2:C:835:ARG:C	1.88	0.76
2:C:932:GLN:H	2:C:932:GLN:CD	1.89	0.76
1:B:200:LEU:O	1:B:203:THR:HG22	1.85	0.76
7:I:2004:UNK:O	7:I:2011:UNK:HG2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:838:LEU:N	2:C:838:LEU:CD2	2.49	0.75
6:G:4007:UNK:HG3	6:G:4008:UNK:N	2.01	0.75
2:C:776:GLU:HA	2:C:776:GLU:OE1	1.82	0.75
2:C:887:PRO:HG2	2:C:888:ILE:HG23	1.67	0.75
2:C:835:ARG:CZ	2:C:868:GLY:HA3	2.16	0.75
7:I:2004:UNK:HG3	7:I:2011:UNK:CG	2.16	0.75
2:C:859:ILE:O	2:C:863:ILE:N	2.19	0.75
2:C:887:PRO:HG2	2:C:888:ILE:CG2	2.17	0.75
2:C:916:ARG:HH11	2:C:933:VAL:CG2	1.95	0.74
1:B:185:ASN:HA	1:B:188:GLU:CD	2.08	0.74
6:G:4007:UNK:HG3	6:G:4012:UNK:O	1.85	0.74
2:C:725:ASN:HB3	2:C:727:ILE:HG13	1.68	0.74
2:C:795:VAL:HA	2:C:801:SER:HA	1.70	0.74
7:I:2004:UNK:HG3	7:I:2011:UNK:HG1	1.70	0.73
2:C:725:ASN:HB3	2:C:727:ILE:CG1	2.18	0.73
1:A:211:MET:HG2	2:C:815:TYR:CE1	2.23	0.73
2:C:805:ASP:HB2	2:C:806:ILE:HG23	1.71	0.73
2:C:896:GLU:O	2:C:900:LYS:N	2.22	0.73
8:J:3015:UNK:HG3	8:J:3016:UNK:O	1.89	0.73
2:C:718:HIS:ND1	2:C:724:TYR:CE1	2.57	0.73
8:J:3007:UNK:CG	8:J:3008:UNK:N	2.52	0.73
2:C:838:LEU:H	2:C:838:LEU:HD22	1.52	0.72
2:C:884:TYR:O	2:C:889:LEU:HB2	1.88	0.72
5:F:3011:UNK:HG3	6:G:4034:UNK:CB	2.20	0.72
2:C:705:ARG:HD2	2:C:706:ILE:HG23	1.72	0.72
2:C:781:PHE:CE2	2:C:783:VAL:N	2.58	0.72
1:B:173:TYR:O	1:B:176:ILE:HG22	1.89	0.72
2:C:893:CYS:C	2:C:895:ASN:H	1.92	0.72
6:G:4008:UNK:HG3	6:G:4013:UNK:CG	2.19	0.72
2:C:745:THR:O	2:C:747:CYS:N	2.22	0.72
1:B:220:LYS:CE	2:C:805:ASP:HB3	2.18	0.72
2:C:933:VAL:H	2:C:934:PRO:HD3	1.55	0.72
2:C:723:ILE:O	2:C:724:TYR:CD2	2.42	0.71
2:C:886:ASP:CB	2:C:887:PRO:HD2	2.20	0.71
4:H:1000:UNK:O	4:H:1001:UNK:HG2	1.91	0.71
2:C:835:ARG:NE	2:C:868:GLY:O	2.23	0.71
8:J:3009:UNK:HG2	8:J:3010:UNK:O	1.90	0.71
1:A:219:LYS:O	1:A:223:ILE:HD13	1.91	0.71
1:A:221:LYS:CE	1:A:224:ARG:HH22	2.01	0.71
2:C:773:ILE:O	2:C:775:ILE:N	2.21	0.71
1:B:165:ASP:O	1:B:167:CYS:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:783:VAL:O	2:C:787:MET:N	2.21	0.70
2:C:750:LEU:HD12	2:C:755:TYR:HB2	1.72	0.70
2:C:795:VAL:CG1	2:C:796:ASP:N	2.53	0.70
7:I:2015:UNK:HB1	9:K:4006:UNK:HG3	1.71	0.70
2:C:696:ASP:H	2:C:724:TYR:HB2	1.56	0.70
2:C:925:HIS:NE2	2:C:936:GLU:OE2	2.25	0.70
2:C:757:ILE:HG22	2:C:759:HIS:ND1	2.06	0.69
2:C:930:ASN:ND2	2:C:931:CYS:H	1.89	0.69
2:C:830:ASP:CG	2:C:831:SER:N	2.44	0.69
2:C:795:VAL:HG12	2:C:796:ASP:N	2.07	0.69
2:C:930:ASN:CG	2:C:931:CYS:N	2.46	0.69
2:C:834:ARG:NH2	2:C:835:ARG:O	2.25	0.69
1:B:170:ASN:HD21	6:G:4010:UNK:CG	2.06	0.69
8:J:3007:UNK:HG3	8:J:3008:UNK:C	2.22	0.69
6:G:4017:UNK:CG	6:G:4018:UNK:N	2.55	0.68
2:C:692:TYR:HB2	2:C:722:LEU:HD12	1.74	0.68
6:G:4017:UNK:HG2	6:G:4018:UNK:N	2.07	0.68
2:C:796:ASP:CG	2:C:797:CYS:N	2.46	0.68
5:F:3006:UNK:HG2	5:F:3007:UNK:N	2.07	0.68
6:G:4007:UNK:HG2	6:G:4014:UNK:N	2.09	0.68
2:C:896:GLU:HA	2:C:899:GLU:HB3	1.76	0.68
2:C:931:CYS:HA	2:C:932:GLN:OE1	1.94	0.68
2:C:718:HIS:O	2:C:722:LEU:N	2.25	0.67
2:C:879:LEU:HD22	2:C:916:ARG:O	1.93	0.67
1:B:156:PHE:HB3	1:B:158:MET:HB2	1.75	0.67
2:C:722:LEU:HB3	2:C:724:TYR:CZ	2.28	0.67
2:C:722:LEU:HD13	2:C:723:ILE:N	2.09	0.67
2:C:893:CYS:C	2:C:895:ASN:N	2.47	0.67
1:B:210:ALA:O	1:B:214:THR:HG22	1.95	0.67
1:A:183:ASN:O	1:A:187:VAL:HG23	1.95	0.66
1:B:162:LEU:C	1:B:164:LYS:H	1.96	0.66
1:A:162:LEU:C	1:A:164:LYS:H	1.96	0.66
2:C:739:ILE:HD13	2:C:739:ILE:N	2.11	0.66
2:C:811:LEU:O	2:C:815:TYR:HB2	1.95	0.66
2:C:748:LYS:O	2:C:750:LEU:N	2.29	0.66
7:I:2005:UNK:HG3	7:I:2007:UNK:N	2.11	0.66
5:F:3024:UNK:HA	5:F:3034:UNK:HG1	1.76	0.66
2:C:838:LEU:HB3	2:C:879:LEU:HB3	1.76	0.66
2:C:834:ARG:HA	2:C:869:LYS:HG2	1.76	0.66
1:A:217:ASN:O	1:A:220:LYS:HG2	1.95	0.65
2:C:932:GLN:N	2:C:932:GLN:CD	2.48	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:2004:UNK:O	7:I:2004:UNK:CG	2.42	0.65
1:A:162:LEU:C	1:A:164:LYS:N	2.49	0.65
2:C:886:ASP:HB2	2:C:887:PRO:CD	2.25	0.65
2:C:690:LEU:CA	2:C:722:LEU:HD23	2.24	0.65
2:C:894:MET:O	2:C:895:ASN:C	2.34	0.65
2:C:895:ASN:O	2:C:898:HIS:N	2.30	0.65
2:C:706:ILE:HG13	2:C:707:THR:HG22	1.79	0.65
5:F:3008:UNK:O	5:F:3008:UNK:HG3	1.97	0.65
1:A:182:SER:HB3	1:A:186:ARG:NH2	2.12	0.65
2:C:866:PHE:C	2:C:868:GLY:H	2.00	0.65
1:B:220:LYS:HZ1	2:C:805:ASP:HB3	1.62	0.65
1:B:212:MET:O	1:B:216:LEU:N	2.30	0.64
2:C:834:ARG:HA	2:C:869:LYS:HB3	1.79	0.64
2:C:781:PHE:CZ	2:C:787:MET:HG2	2.33	0.64
2:C:870:ILE:O	2:C:871:THR:HG23	1.98	0.64
1:A:203:THR:HG23	1:A:207:ARG:HH22	1.62	0.64
2:C:718:HIS:ND1	2:C:724:TYR:HE1	1.93	0.64
1:B:170:ASN:HD21	6:G:4010:UNK:HG1	1.62	0.64
2:C:834:ARG:HA	2:C:869:LYS:CB	2.28	0.64
2:C:889:LEU:O	2:C:890:ARG:C	2.35	0.64
2:C:702:THR:H	2:C:742:LYS:HD3	1.63	0.64
5:F:3029:UNK:HG1	5:F:3033:UNK:O	1.98	0.64
2:C:741:CYS:H	2:C:759:HIS:HB2	1.61	0.64
2:C:776:GLU:OE1	2:C:791:ALA:HB1	1.97	0.63
1:A:168:CYS:SG	1:B:169:VAL:HG12	2.39	0.63
5:F:3037:UNK:HG3	5:F:3037:UNK:O	1.97	0.63
3:D:1005:UNK:HB1	4:E:2002:UNK:HG2	1.80	0.63
1:A:189:GLN:HA	1:A:189:GLN:HE21	1.64	0.63
2:C:781:PHE:CD1	2:C:782:ASN:N	2.64	0.63
4:E:2001:UNK:CG	4:E:2002:UNK:H	2.12	0.63
2:C:744:THR:OG1	2:C:745:THR:N	2.30	0.63
9:K:4006:UNK:HB2	9:K:4008:UNK:HG2	1.81	0.63
6:G:4007:UNK:HB2	6:G:4014:UNK:HA	1.80	0.62
6:G:4008:UNK:CG	6:G:4013:UNK:CG	2.75	0.62
2:C:795:VAL:HG12	2:C:796:ASP:O	2.00	0.62
1:A:217:ASN:HA	1:A:220:LYS:CE	2.29	0.62
1:B:210:ALA:O	1:B:214:THR:N	2.32	0.62
5:F:3015:UNK:HG1	6:G:4030:UNK:HG3	1.81	0.62
2:C:692:TYR:H	2:C:722:LEU:HG	1.65	0.62
8:J:3009:UNK:C	8:J:3010:UNK:HG2	2.29	0.62
2:C:896:GLU:HG2	2:C:899:GLU:OE1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:HA	1:B:188:GLU:OE1	2.00	0.61
5:F:3006:UNK:HG2	5:F:3007:UNK:H	1.64	0.61
4:E:2001:UNK:HG3	4:E:2002:UNK:N	2.14	0.61
1:B:166:ILE:O	1:B:170:ASN:HB2	2.00	0.61
2:C:701:ASP:HA	2:C:742:LYS:HB2	1.81	0.61
5:F:3006:UNK:CG	5:F:3009:UNK:O	2.49	0.61
6:G:4010:UNK:O	6:G:4011:UNK:C	2.48	0.61
1:B:156:PHE:HB3	1:B:158:MET:H	1.66	0.60
8:J:3014:UNK:HG3	9:K:4005:UNK:HG3	1.82	0.60
2:C:740:SER:HA	2:C:759:HIS:HB3	1.82	0.60
9:K:4004:UNK:O	9:K:4005:UNK:HG2	2.01	0.60
7:I:2004:UNK:HB1	7:I:2011:UNK:HB2	1.82	0.60
9:K:4003:UNK:HG3	9:K:4003:UNK:O	2.01	0.60
3:D:1005:UNK:HB1	4:E:2002:UNK:CG	2.31	0.60
2:C:866:PHE:C	2:C:868:GLY:N	2.55	0.60
1:A:224:ARG:HB3	1:A:228:GLU:OE1	2.02	0.60
1:A:162:LEU:HB3	1:B:162:LEU:HD13	1.83	0.60
6:G:4004:UNK:O	6:G:4006:UNK:HG2	2.02	0.60
1:B:220:LYS:HE3	2:C:805:ASP:HB3	1.82	0.60
2:C:834:ARG:CG	2:C:869:LYS:HD3	2.29	0.60
2:C:879:LEU:CD2	2:C:916:ARG:O	2.50	0.60
5:F:3021:UNK:HG3	5:F:3021:UNK:O	2.00	0.60
2:C:933:VAL:N	2:C:934:PRO:HD3	2.16	0.60
5:F:3016:UNK:HB1	5:F:3019:UNK:HG2	1.83	0.59
6:G:4008:UNK:O	6:G:4008:UNK:HG2	2.01	0.59
2:C:756:ASP:CA	2:C:781:PHE:HB2	2.32	0.59
1:B:173:TYR:C	1:B:175:ASN:N	2.54	0.59
2:C:722:LEU:HD13	2:C:723:ILE:H	1.67	0.59
1:B:204:ARG:NH1	2:C:927:ILE:HG12	2.17	0.59
2:C:884:TYR:HB3	2:C:885:THR:HG23	1.83	0.59
1:B:173:TYR:C	1:B:175:ASN:H	2.06	0.59
2:C:834:ARG:HG2	2:C:869:LYS:CG	2.32	0.59
2:C:925:HIS:CE1	2:C:936:GLU:OE2	2.56	0.59
2:C:776:GLU:O	2:C:778:ASN:CG	2.41	0.59
1:A:200:LEU:O	1:A:203:THR:N	2.36	0.58
2:C:757:ILE:O	2:C:779:TYR:HB3	2.03	0.58
1:B:213:VAL:HG12	1:B:214:THR:N	2.19	0.58
5:F:3003:UNK:O	5:F:3003:UNK:HG2	2.02	0.58
1:B:164:LYS:HA	1:B:166:ILE:HD11	1.84	0.58
7:I:2017:UNK:CG	7:I:2020:UNK:CG	2.78	0.58
1:A:191:ALA:C	1:A:193:GLU:H	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:2001:UNK:HG2	7:I:2013:UNK:C	2.34	0.58
1:A:176:ILE:HD11	1:B:176:ILE:HB	1.85	0.58
2:C:753:ARG:HE	2:C:755:TYR:HE1	1.49	0.58
2:C:795:VAL:CG1	2:C:796:ASP:H	2.16	0.58
1:B:197:LEU:HG	1:B:198:ASP:N	2.19	0.58
6:G:4004:UNK:N	6:G:4017:UNK:HB1	2.19	0.58
9:K:4001:UNK:HG2	9:K:4002:UNK:N	2.12	0.58
6:G:4007:UNK:HA	6:G:4013:UNK:C	2.33	0.57
7:I:2028:UNK:O	7:I:2029:UNK:HG2	2.04	0.57
2:C:727:ILE:HB	2:C:728:LEU:HD23	1.86	0.57
1:B:197:LEU:O	1:B:200:LEU:N	2.30	0.57
2:C:834:ARG:CZ	2:C:835:ARG:O	2.52	0.57
8:J:3009:UNK:C	8:J:3010:UNK:CG	2.82	0.57
2:C:687:ALA:HB3	2:C:690:LEU:HG	1.86	0.57
2:C:783:VAL:HB	2:C:787:MET:CB	2.30	0.57
2:C:815:TYR:C	2:C:817:SER:H	2.06	0.57
2:C:715:ILE:O	2:C:719:GLY:N	2.34	0.57
2:C:924:ASP:O	2:C:927:ILE:HG22	2.05	0.57
7:I:2008:UNK:CG	7:I:2009:UNK:N	2.58	0.57
6:G:4018:UNK:O	6:G:4018:UNK:CG	2.51	0.57
1:B:156:PHE:C	1:B:158:MET:H	2.07	0.56
1:B:212:MET:O	1:B:213:VAL:C	2.42	0.56
6:G:4008:UNK:N	6:G:4013:UNK:HB2	2.20	0.56
2:C:879:LEU:HD22	2:C:880:ILE:H	1.69	0.56
7:I:2010:UNK:N	9:K:4011:UNK:CG	2.68	0.56
1:B:194:ARG:HA	1:B:197:LEU:HB3	1.86	0.56
1:B:217:ASN:HD22	1:B:217:ASN:H	1.52	0.56
2:C:710:GLU:H	2:C:713:LYS:HB2	1.70	0.56
2:C:834:ARG:O	2:C:835:ARG:HG3	2.05	0.56
2:C:835:ARG:HH11	2:C:927:ILE:HD11	1.69	0.56
2:C:896:GLU:C	2:C:899:GLU:HB3	2.26	0.56
1:B:214:THR:HG23	1:B:215:LEU:HG	1.88	0.56
2:C:834:ARG:NH1	2:C:836:PHE:CZ	2.74	0.56
4:E:2001:UNK:HG3	4:E:2002:UNK:H	1.69	0.56
2:C:759:HIS:CE1	2:C:779:TYR:HA	2.41	0.55
9:K:4002:UNK:CG	9:K:4003:UNK:N	2.67	0.55
2:C:741:CYS:O	2:C:759:HIS:HD2	1.80	0.55
2:C:933:VAL:H	2:C:934:PRO:CD	2.19	0.55
2:C:774:LEU:HD22	2:C:794:ARG:CG	2.26	0.55
1:A:217:ASN:HA	1:A:220:LYS:HE2	1.90	0.54
2:C:697:TYR:HB2	2:C:726:VAL:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:896:GLU:CA	2:C:899:GLU:HB3	2.36	0.54
2:C:777:PRO:HA	2:C:779:TYR:CE1	2.42	0.54
2:C:834:ARG:NE	2:C:835:ARG:C	2.60	0.54
3:D:1005:UNK:HG3	3:D:1006:UNK:H	1.72	0.54
2:C:924:ASP:C	2:C:926:SER:H	2.09	0.54
1:B:160:ASP:HA	1:B:163:TYR:HB2	1.90	0.54
1:B:217:ASN:ND2	1:B:217:ASN:H	2.06	0.54
5:F:3029:UNK:CB	5:F:3033:UNK:HB2	2.35	0.54
9:K:4007:UNK:HG3	9:K:4007:UNK:O	2.06	0.54
2:C:835:ARG:NH2	2:C:868:GLY:CA	2.61	0.54
2:C:892:ASP:O	2:C:895:ASN:HB3	2.04	0.54
5:F:3011:UNK:HG3	6:G:4034:UNK:HB1	1.89	0.54
7:I:2017:UNK:HG2	7:I:2020:UNK:CG	2.25	0.54
1:A:222:LYS:HG2	2:C:802:PHE:CE2	2.43	0.54
5:F:3015:UNK:HG2	6:G:4030:UNK:HA	1.89	0.54
7:I:2017:UNK:HG3	7:I:2020:UNK:HG1	1.88	0.54
1:A:192:ARG:HG2	1:A:192:ARG:O	2.08	0.53
2:C:798:LEU:C	2:C:798:LEU:HD12	2.29	0.53
6:G:4005:UNK:HA	6:G:4015:UNK:C	2.38	0.53
4:H:1005:UNK:O	4:H:1005:UNK:HG2	2.08	0.53
6:G:4008:UNK:HG1	6:G:4013:UNK:HG2	1.89	0.53
1:B:213:VAL:O	1:B:215:LEU:N	2.41	0.53
2:C:745:THR:O	2:C:746:GLU:C	2.47	0.53
2:C:835:ARG:H	2:C:869:LYS:HG2	1.74	0.53
6:G:4008:UNK:HG3	6:G:4012:UNK:C	2.38	0.53
7:I:2025:UNK:O	7:I:2025:UNK:HG3	2.07	0.53
4:E:2001:UNK:CG	4:E:2002:UNK:N	2.71	0.53
1:A:222:LYS:HG2	2:C:802:PHE:HE2	1.74	0.53
2:C:802:PHE:CD1	2:C:802:PHE:N	2.74	0.53
2:C:904:GLN:HB3	2:C:912:PRO:CG	2.37	0.53
5:F:3022:UNK:O	5:F:3022:UNK:HG3	2.07	0.53
6:G:4008:UNK:HG3	6:G:4013:UNK:CB	2.39	0.53
2:C:801:SER:C	2:C:802:PHE:HD1	2.13	0.52
2:C:859:ILE:HA	2:C:862:LYS:HB3	1.91	0.52
2:C:870:ILE:HG23	2:C:871:THR:H	1.74	0.52
2:C:925:HIS:NE2	2:C:936:GLU:CD	2.61	0.52
8:J:3004:UNK:HB1	8:J:3018:UNK:O	2.10	0.52
2:C:896:GLU:HA	2:C:899:GLU:CB	2.38	0.52
1:B:162:LEU:C	1:B:164:LYS:N	2.63	0.52
5:F:3016:UNK:HB1	5:F:3019:UNK:CG	2.39	0.52
5:F:3042:UNK:O	5:F:3043:UNK:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:829:ILE:HD12	2:C:829:ILE:O	2.10	0.52
2:C:926:SER:O	2:C:928:ASN:N	2.43	0.52
2:C:761:ASN:O	2:C:764:LEU:N	2.43	0.52
6:G:4007:UNK:CG	6:G:4008:UNK:N	2.70	0.52
2:C:687:ALA:O	2:C:688:GLY:C	2.48	0.52
2:C:759:HIS:CE1	2:C:780:CYS:N	2.78	0.52
2:C:725:ASN:O	2:C:737:ARG:NH2	2.34	0.52
2:C:926:SER:C	2:C:928:ASN:N	2.64	0.51
5:F:3015:UNK:CG	6:G:4030:UNK:HG3	2.40	0.51
1:B:176:ILE:O	1:B:180:ASP:N	2.34	0.51
2:C:725:ASN:HB3	2:C:727:ILE:HG12	1.92	0.51
2:C:834:ARG:HG3	2:C:869:LYS:HE3	1.83	0.51
2:C:795:VAL:HG13	2:C:796:ASP:H	1.75	0.51
2:C:861:MET:HB2	2:C:881:ILE:CD1	2.40	0.51
2:C:718:HIS:CG	2:C:719:GLY:N	2.78	0.51
3:D:1000:UNK:C	3:D:1001:UNK:HG2	2.40	0.51
8:J:3008:UNK:C	8:J:3010:UNK:HG2	2.35	0.51
1:A:168:CYS:SG	1:B:169:VAL:CG1	2.99	0.51
1:B:178:GLU:O	1:B:182:SER:HB2	2.10	0.51
2:C:771:ARG:HD3	2:C:771:ARG:C	2.30	0.51
2:C:863:ILE:O	2:C:867:GLY:N	2.38	0.51
7:I:2004:UNK:CG	7:I:2011:UNK:HG1	2.40	0.51
8:J:3007:UNK:O	8:J:3007:UNK:HB2	2.09	0.51
6:G:4026:UNK:C	6:G:4027:UNK:HG2	2.40	0.51
2:C:859:ILE:O	2:C:860:GLU:C	2.48	0.51
2:C:926:SER:C	2:C:928:ASN:H	2.13	0.51
1:B:220:LYS:CE	2:C:800:ASP:OD2	2.59	0.51
2:C:743:THR:HG22	2:C:744:THR:H	1.75	0.51
1:B:201:LEU:HG	1:B:202:GLU:N	2.26	0.51
1:A:175:ASN:OD1	1:A:176:ILE:N	2.43	0.50
1:A:230:LEU:HD21	1:B:230:LEU:HD21	1.93	0.50
2:C:705:ARG:CD	2:C:706:ILE:HG23	2.40	0.50
3:D:1005:UNK:HG3	3:D:1006:UNK:N	2.25	0.50
6:G:4003:UNK:HG3	6:G:4017:UNK:O	2.11	0.50
2:C:704:ILE:HG22	2:C:705:ARG:HG3	1.92	0.50
2:C:714:THR:O	2:C:718:HIS:HD2	1.94	0.50
2:C:886:ASP:CB	2:C:887:PRO:CD	2.88	0.50
2:C:714:THR:O	2:C:715:ILE:C	2.49	0.50
7:I:2010:UNK:N	9:K:4011:UNK:HG1	2.26	0.50
1:A:187:VAL:O	1:A:187:VAL:HG12	2.12	0.50
2:C:861:MET:HB2	2:C:881:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:803:GLU:CD	2:C:804:ASN:H	2.15	0.50
2:C:820:SER:O	2:C:821:LEU:HG	2.12	0.50
3:D:1005:UNK:CG	3:D:1006:UNK:H	2.24	0.50
2:C:859:ILE:O	2:C:862:LYS:N	2.45	0.50
2:C:884:TYR:OH	2:C:938:PHE:HA	2.11	0.50
2:C:705:ARG:HD2	2:C:706:ILE:N	2.26	0.50
2:C:917:VAL:HG23	2:C:917:VAL:O	2.12	0.50
8:J:3009:UNK:CG	8:J:3010:UNK:O	2.57	0.50
1:A:179:SER:HB3	1:B:180:ASP:OD1	2.12	0.49
1:B:156:PHE:HB3	1:B:158:MET:CB	2.42	0.49
2:C:870:ILE:HG23	2:C:871:THR:N	2.27	0.49
2:C:760:PRO:HD2	2:C:761:ASN:ND2	2.28	0.49
2:C:777:PRO:HA	2:C:779:TYR:CZ	2.47	0.49
2:C:894:MET:O	2:C:895:ASN:O	2.30	0.49
5:F:3027:UNK:HG2	6:G:4027:UNK:HG3	1.94	0.49
7:I:2027:UNK:HG3	7:I:2027:UNK:O	2.12	0.49
1:A:217:ASN:HA	1:A:220:LYS:CD	2.42	0.49
1:B:174:ARG:HG2	1:B:177:LYS:HZ2	1.71	0.49
2:C:870:ILE:HD12	2:C:871:THR:OG1	2.13	0.49
2:C:887:PRO:HG2	2:C:888:ILE:HG22	1.93	0.49
3:D:1007:UNK:O	3:D:1007:UNK:HG2	2.12	0.49
1:A:168:CYS:O	1:A:171:ASP:HB2	2.12	0.49
5:F:3006:UNK:CG	5:F:3007:UNK:H	2.26	0.49
2:C:935:GLU:HG3	2:C:935:GLU:O	2.13	0.49
2:C:705:ARG:HD2	2:C:706:ILE:H	1.77	0.49
5:F:3016:UNK:HG3	5:F:3018:UNK:N	2.27	0.49
7:I:2004:UNK:O	7:I:2011:UNK:CG	2.60	0.49
7:I:2028:UNK:C	7:I:2029:UNK:HG2	2.43	0.49
2:C:865:LEU:HB3	2:C:870:ILE:HG12	1.95	0.48
2:C:757:ILE:O	2:C:781:PHE:HB3	2.13	0.48
2:C:779:TYR:HB2	2:C:781:PHE:HD1	1.77	0.48
7:I:2005:UNK:HG2	7:I:2010:UNK:HA	1.94	0.48
1:B:170:ASN:HD21	6:G:4010:UNK:HG2	1.79	0.48
2:C:834:ARG:CZ	2:C:869:LYS:HZ2	2.26	0.48
2:C:899:GLU:C	2:C:901:ILE:H	2.17	0.48
1:A:166:ILE:C	1:A:168:CYS:N	2.65	0.48
1:A:230:LEU:HD21	1:B:230:LEU:HD11	1.95	0.48
2:C:886:ASP:OD1	2:C:888:ILE:HG12	2.13	0.48
1:A:203:THR:HG23	1:A:207:ARG:NH2	2.29	0.48
1:B:222:LYS:HB3	1:B:222:LYS:NZ	2.29	0.48
1:B:222:LYS:CB	1:B:222:LYS:NZ	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HB3	1:B:162:LEU:CD1	2.44	0.47
2:C:703:GLY:HA3	2:C:707:THR:O	2.14	0.47
1:B:161:LYS:O	1:B:164:LYS:HB2	2.14	0.47
1:B:171:ASP:C	1:B:173:TYR:N	2.67	0.47
2:C:837:PRO:C	2:C:838:LEU:HD13	2.35	0.47
5:F:3024:UNK:CB	5:F:3031:UNK:HG2	2.43	0.47
2:C:728:LEU:N	2:C:728:LEU:HD23	2.29	0.47
2:C:889:LEU:HA	2:C:893:CYS:SG	2.55	0.47
1:A:178:GLU:O	1:A:182:SER:N	2.48	0.47
1:B:172:SER:O	1:B:175:ASN:HB3	2.14	0.47
7:I:2005:UNK:HG1	7:I:2010:UNK:CB	2.44	0.47
2:C:876:LEU:O	2:C:876:LEU:HD13	2.15	0.47
1:B:197:LEU:CG	1:B:198:ASP:N	2.77	0.47
1:A:168:CYS:C	1:A:170:ASN:H	2.17	0.47
5:F:3024:UNK:HA	5:F:3034:UNK:CG	2.44	0.47
1:A:178:GLU:N	1:A:181:SER:HB3	2.30	0.47
2:C:702:THR:OG1	2:C:742:LYS:HG2	2.15	0.47
2:C:872:ASP:O	2:C:873:GLN:CB	2.52	0.47
2:C:920:PRO:O	2:C:922:TRP:N	2.48	0.47
2:C:757:ILE:N	2:C:781:PHE:HB3	2.30	0.46
2:C:821:LEU:O	2:C:823:PRO:HD3	2.14	0.46
1:A:226:LEU:HD21	1:B:227:HIS:ND1	2.30	0.46
2:C:723:ILE:C	2:C:724:TYR:CG	2.88	0.46
2:C:802:PHE:HD1	2:C:802:PHE:N	2.13	0.46
1:B:185:ASN:O	1:B:188:GLU:HB2	2.15	0.46
2:C:918:VAL:O	2:C:919:ALA:C	2.51	0.46
5:F:3027:UNK:CG	6:G:4027:UNK:HG3	2.46	0.46
1:A:215:LEU:HD11	2:C:798:LEU:HD23	1.98	0.46
2:C:722:LEU:HB3	2:C:724:TYR:HE2	1.76	0.46
2:C:723:ILE:O	2:C:724:TYR:CG	2.68	0.46
2:C:776:GLU:OE1	2:C:777:PRO:CD	2.44	0.46
2:C:897:VAL:HA	2:C:900:LYS:HB2	1.96	0.46
2:C:924:ASP:C	2:C:926:SER:N	2.68	0.46
2:C:796:ASP:CG	2:C:797:CYS:H	2.19	0.46
1:A:194:ARG:HE	1:B:194:ARG:NH2	2.13	0.46
2:C:715:ILE:O	2:C:718:HIS:CD2	2.69	0.46
3:D:1000:UNK:O	3:D:1001:UNK:HG2	2.15	0.46
1:A:191:ALA:C	1:A:193:GLU:N	2.67	0.46
1:A:224:ARG:O	1:A:225:GLU:C	2.54	0.46
1:B:204:ARG:HH12	2:C:927:ILE:HG23	1.81	0.46
2:C:932:GLN:N	2:C:932:GLN:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:4005:UNK:HA	6:G:4015:UNK:O	2.16	0.46
6:G:4007:UNK:HA	6:G:4013:UNK:O	2.16	0.46
1:A:204:ARG:HH11	1:A:204:ARG:HB3	1.81	0.46
1:B:223:ILE:O	1:B:226:LEU:HB2	2.16	0.46
2:C:756:ASP:HB3	2:C:781:PHE:HD2	1.65	0.45
2:C:759:HIS:HE1	2:C:780:CYS:H	1.64	0.45
2:C:886:ASP:OD2	2:C:887:PRO:HD2	2.16	0.45
5:F:3011:UNK:HG3	6:G:4034:UNK:HA	1.98	0.45
1:A:211:MET:HG2	2:C:815:TYR:HE1	1.73	0.45
2:C:725:ASN:CB	2:C:727:ILE:HG13	2.42	0.45
4:H:1000:UNK:C	4:H:1001:UNK:HG2	2.46	0.45
2:C:787:MET:C	2:C:789:ALA:N	2.65	0.45
2:C:836:PHE:HD1	2:C:837:PRO:HD2	1.81	0.45
2:C:888:ILE:CG1	2:C:889:LEU:N	2.70	0.45
2:C:838:LEU:HD11	2:C:865:LEU:HG	1.99	0.45
1:B:158:MET:HE3	9:K:4010:UNK:O	2.17	0.45
1:B:165:ASP:C	1:B:167:CYS:N	2.69	0.45
2:C:722:LEU:HB3	2:C:724:TYR:OH	2.17	0.45
2:C:870:ILE:C	2:C:870:ILE:HD12	2.36	0.45
2:C:884:TYR:C	2:C:885:THR:HG23	2.36	0.45
2:C:922:TRP:O	2:C:923:VAL:C	2.55	0.45
2:C:692:TYR:HB2	2:C:724:TYR:HE2	1.81	0.45
2:C:726:VAL:HA	2:C:737:ARG:NH2	2.31	0.45
2:C:779:TYR:CB	2:C:781:PHE:HD1	2.30	0.45
2:C:796:ASP:OD2	2:C:797:CYS:N	2.48	0.45
2:C:722:LEU:HD12	2:C:724:TYR:CE2	2.52	0.45
6:G:4002:UNK:CG	6:G:4019:UNK:HB2	2.47	0.45
1:B:222:LYS:HB3	1:B:222:LYS:HZ3	1.82	0.45
2:C:741:CYS:N	2:C:759:HIS:HB2	2.30	0.45
2:C:837:PRO:HB3	2:C:871:THR:OG1	2.17	0.45
2:C:925:HIS:CE1	2:C:936:GLU:OE1	2.69	0.45
1:A:223:ILE:O	1:A:227:HIS:HB2	2.16	0.44
1:B:217:ASN:HD21	2:C:806:ILE:HG13	1.82	0.44
2:C:798:LEU:HD12	2:C:798:LEU:O	2.17	0.44
2:C:887:PRO:O	2:C:891:LYS:HB2	2.18	0.44
2:C:924:ASP:O	2:C:926:SER:N	2.50	0.44
2:C:838:LEU:HD23	2:C:872:ASP:HA	1.94	0.44
7:I:2008:UNK:O	9:K:4011:UNK:HG1	2.17	0.44
1:A:179:SER:HA	1:A:183:ASN:HB2	1.99	0.44
5:F:3006:UNK:CG	5:F:3007:UNK:N	2.76	0.44
1:A:222:LYS:HB2	1:A:222:LYS:HE3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:PHE:HB3	1:B:158:MET:N	2.30	0.44
2:C:713:LYS:O	2:C:717:GLU:HB2	2.18	0.44
2:C:886:ASP:CG	2:C:887:PRO:HD2	2.37	0.44
1:A:208:THR:OG1	1:A:208:THR:O	2.36	0.44
1:B:215:LEU:HA	1:B:218:GLU:HB2	2.00	0.44
2:C:718:HIS:CE1	2:C:724:TYR:CE1	3.05	0.44
2:C:745:THR:C	2:C:747:CYS:N	2.71	0.44
2:C:807:SER:H	2:C:810:LYS:HB2	1.82	0.44
2:C:890:ARG:O	2:C:894:MET:HB2	2.18	0.44
2:C:895:ASN:OD1	2:C:896:GLU:HB2	2.11	0.44
7:I:2028:UNK:O	7:I:2029:UNK:CG	2.66	0.44
2:C:697:TYR:HB2	2:C:726:VAL:HA	1.99	0.44
2:C:746:GLU:HG3	2:C:747:CYS:N	2.33	0.44
7:I:2009:UNK:HA	9:K:4011:UNK:CG	2.48	0.44
1:A:200:LEU:O	1:A:202:GLU:N	2.51	0.43
1:A:189:GLN:O	1:A:193:GLU:HG3	2.17	0.43
1:A:204:ARG:O	1:A:208:THR:HG22	2.18	0.43
7:I:2004:UNK:CB	7:I:2011:UNK:HB2	2.47	0.43
1:B:197:LEU:O	1:B:198:ASP:C	2.56	0.43
2:C:907:ALA:O	2:C:908:SER:C	2.56	0.43
1:B:158:MET:CE	9:K:4010:UNK:O	2.66	0.43
1:A:214:THR:HA	1:A:217:ASN:HB3	2.00	0.43
2:C:818:GLN:OE1	2:C:821:LEU:HD11	2.18	0.43
2:C:862:LYS:CG	2:C:872:ASP:OD2	2.59	0.43
6:G:4008:UNK:N	6:G:4012:UNK:O	2.52	0.43
1:A:221:LYS:HE2	1:A:224:ARG:NH2	2.08	0.43
1:B:166:ILE:HG22	1:B:170:ASN:HD22	1.84	0.43
2:C:757:ILE:HB	2:C:759:HIS:CE1	2.53	0.43
7:I:2026:UNK:O	7:I:2026:UNK:HG3	2.18	0.43
2:C:804:ASN:O	2:C:805:ASP:C	2.56	0.43
1:B:161:LYS:HB2	1:B:161:LYS:HE3	1.77	0.43
1:A:194:ARG:HB2	1:B:194:ARG:NH1	2.34	0.43
1:B:198:ASP:HA	1:B:201:LEU:HD21	2.00	0.43
1:B:221:LYS:HD3	1:B:225:GLU:OE2	2.18	0.43
2:C:916:ARG:HH12	2:C:933:VAL:HG21	1.70	0.43
5:F:3043:UNK:C	5:F:3044:UNK:HG3	2.49	0.43
6:G:4008:UNK:HG2	6:G:4012:UNK:H	1.83	0.43
1:A:180:ASP:OD1	1:B:179:SER:HB3	2.19	0.43
1:A:187:VAL:HG22	1:B:187:VAL:HG23	1.99	0.43
2:C:710:GLU:O	2:C:712:GLU:N	2.52	0.43
2:C:756:ASP:OD1	2:C:756:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:3042:UNK:HG1	6:G:4016:UNK:HG1	1.99	0.43
8:J:3015:UNK:O	9:K:4005:UNK:CG	2.66	0.43
1:B:177:LYS:C	1:B:179:SER:H	2.22	0.42
2:C:800:ASP:C	2:C:801:SER:O	2.57	0.42
7:I:2005:UNK:CG	7:I:2010:UNK:CB	2.96	0.42
1:B:162:LEU:O	1:B:164:LYS:N	2.51	0.42
1:B:165:ASP:C	1:B:167:CYS:H	2.22	0.42
2:C:705:ARG:HH11	2:C:706:ILE:H	1.65	0.42
2:C:811:LEU:HD22	2:C:815:TYR:CZ	2.55	0.42
6:G:4008:UNK:HG3	6:G:4013:UNK:HB2	2.01	0.42
7:I:2017:UNK:HG3	7:I:2020:UNK:CG	2.48	0.42
2:C:860:GLU:O	2:C:864:LYS:HD3	2.20	0.42
2:C:751:ILE:CG2	2:C:781:PHE:HA	2.49	0.42
1:B:220:LYS:HD3	2:C:802:PHE:HA	2.02	0.42
7:I:2005:UNK:CG	7:I:2010:UNK:HA	2.50	0.42
1:B:167:CYS:O	1:B:168:CYS:C	2.57	0.42
1:B:212:MET:O	1:B:213:VAL:O	2.38	0.42
2:C:751:ILE:HG23	2:C:757:ILE:HG13	2.01	0.42
2:C:937:ASP:OD2	2:C:938:PHE:CZ	2.72	0.42
5:F:3029:UNK:CG	5:F:3033:UNK:HB2	2.50	0.42
7:I:2001:UNK:HG2	7:I:2013:UNK:O	2.20	0.42
1:B:209:ARG:O	1:B:212:MET:N	2.53	0.42
1:A:188:GLU:OE1	1:A:189:GLN:HG2	2.20	0.42
4:H:1000:UNK:O	4:H:1001:UNK:CG	2.65	0.42
2:C:741:CYS:H	2:C:759:HIS:CG	2.38	0.41
1:B:211:MET:CB	2:C:832:GLU:CD	2.73	0.41
2:C:834:ARG:HG2	2:C:869:LYS:HG2	2.01	0.41
2:C:866:PHE:CG	2:C:870:ILE:HG21	2.54	0.41
5:F:3027:UNK:HG2	6:G:4026:UNK:O	2.19	0.41
9:K:4006:UNK:HB2	9:K:4008:UNK:CG	2.50	0.41
2:C:705:ARG:NH1	2:C:706:ILE:HG12	2.35	0.41
2:C:759:HIS:CE1	2:C:780:CYS:H	2.36	0.41
2:C:834:ARG:NH1	2:C:836:PHE:CE2	2.88	0.41
1:A:162:LEU:O	1:A:164:LYS:N	2.53	0.41
2:C:807:SER:O	2:C:810:LYS:N	2.53	0.41
5:F:3016:UNK:O	5:F:3020:UNK:HG2	2.20	0.41
6:G:4007:UNK:CB	6:G:4014:UNK:HA	2.50	0.41
1:A:197:LEU:HA	1:A:200:LEU:HD12	2.02	0.41
1:B:163:TYR:HA	1:B:163:TYR:HD1	1.65	0.41
1:B:221:LYS:C	1:B:223:ILE:H	2.23	0.41
2:C:865:LEU:HA	2:C:865:LEU:HD13	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:3010:UNK:C	8:J:3011:UNK:HG2	2.51	0.41
1:A:209:ARG:HA	1:A:209:ARG:HD2	1.81	0.41
1:B:174:ARG:HA	1:B:177:LYS:CD	2.51	0.41
1:B:213:VAL:O	1:B:217:ASN:ND2	2.46	0.41
1:B:217:ASN:OD1	2:C:805:ASP:OD1	2.38	0.41
2:C:832:GLU:O	2:C:833:VAL:HG23	2.20	0.41
5:F:3011:UNK:HG3	6:G:4034:UNK:CA	2.51	0.41
1:B:197:LEU:HD23	1:B:198:ASP:OD1	2.19	0.41
1:A:223:ILE:HD11	1:B:223:ILE:HG12	2.02	0.41
2:C:892:ASP:C	2:C:895:ASN:H	2.24	0.41
1:A:226:LEU:O	1:A:230:LEU:HD23	2.21	0.41
2:C:695:SER:HA	2:C:724:TYR:CB	2.50	0.41
9:K:4012:UNK:HG3	9:K:4012:UNK:O	2.20	0.41
1:A:184:ARG:HD3	1:A:184:ARG:C	2.41	0.41
1:B:166:ILE:HG13	1:B:166:ILE:H	1.65	0.41
2:C:920:PRO:C	2:C:922:TRP:N	2.72	0.41
1:B:173:TYR:O	1:B:175:ASN:N	2.54	0.41
1:B:213:VAL:C	1:B:215:LEU:H	2.25	0.41
6:G:4032:UNK:HG2	6:G:4032:UNK:O	2.20	0.41
8:J:3004:UNK:CG	8:J:3005:UNK:N	2.84	0.41
1:A:212:MET:O	1:A:216:LEU:HD12	2.20	0.40
6:G:4008:UNK:O	6:G:4008:UNK:CG	2.69	0.40
2:C:778:ASN:C	2:C:779:TYR:CG	2.95	0.40
2:C:815:TYR:HD1	2:C:815:TYR:HA	1.80	0.40
2:C:884:TYR:HB3	2:C:885:THR:CG2	2.51	0.40
2:C:896:GLU:O	2:C:900:LYS:HG2	2.21	0.40
7:I:2008:UNK:O	7:I:2010:UNK:N	2.53	0.40
7:I:2017:UNK:HA	7:I:2020:UNK:HG2	2.02	0.40
7:I:2019:UNK:HA	7:I:2022:UNK:HB1	2.02	0.40
1:A:208:THR:O	1:A:212:MET:HG3	2.21	0.40
2:C:743:THR:HG22	2:C:744:THR:N	2.36	0.40
2:C:815:TYR:C	2:C:817:SER:N	2.74	0.40
1:B:170:ASN:O	1:B:174:ARG:HG3	2.21	0.40
1:B:211:MET:SD	2:C:832:GLU:CG	3.06	0.40
2:C:715:ILE:HA	2:C:718:HIS:NE2	2.37	0.40
2:C:739:ILE:O	2:C:739:ILE:HG12	2.21	0.40
2:C:764:LEU:O	2:C:767:ILE:HB	2.21	0.40
1:B:220:LYS:HD3	2:C:802:PHE:C	2.42	0.40
2:C:922:TRP:CA	2:C:925:HIS:ND1	2.75	0.40
8:J:3010:UNK:CG	8:J:3010:UNK:O	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:727:ILE:CG2	2:C:916:ARG:NE[5_555]	1.96	0.24

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	75/246 (30%)	51 (68%)	18 (24%)	6 (8%)	1 15
1	B	74/246 (30%)	41 (55%)	21 (28%)	12 (16%)	0 3
2	C	233/264 (88%)	120 (52%)	56 (24%)	57 (24%)	0 1
All	All	382/756 (50%)	212 (56%)	95 (25%)	75 (20%)	0 2

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	ILE
2	C	693	VAL
2	C	711	LEU
2	C	745	THR
2	C	748	LYS
2	C	749	ALA
2	C	760	PRO
2	C	761	ASN
2	C	774	LEU
2	C	784	SER
2	C	803	GLU
2	C	823	PRO
2	C	867	GLY
2	C	870	ILE
2	C	871	THR
2	C	878	ASN
2	C	885	THR

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Mol	Chain	Res	Type
2	C	886	ASP
2	C	896	GLU
2	C	921	GLU
2	C	933	VAL
2	C	936	GLU
1	A	167	CYS
1	B	167	CYS
1	B	177	LYS
1	B	188	GLU
1	B	193	GLU
1	B	213	VAL
2	C	746	GLU
2	C	773	ILE
2	C	799	GLY
2	C	805	ASP
2	C	813	SER
2	C	831	SER
2	C	872	ASP
2	C	876	LEU
2	C	884	TYR
2	C	895	ASN
2	C	907	ALA
2	C	927	ILE
2	C	929	GLU
2	C	935	GLU
2	C	937	ASP
1	B	163	TYR
1	B	174	ARG
1	B	195	GLU
1	B	198	ASP
1	B	226	LEU
2	C	686	PHE
2	C	724	TYR
2	C	728	LEU
2	C	731	HIS
2	C	769	TYR
2	C	778	ASN
2	C	801	SER
2	C	808	GLU
2	C	815	TYR
2	C	873	GLN
2	C	908	SER

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Mol	Chain	Res	Type
2	C	923	VAL
1	A	178	GLU
1	A	201	LEU
1	B	212	MET
2	C	777	PRO
2	C	782	ASN
2	C	869	LYS
1	A	181	SER
2	C	819	LEU
2	C	900	LYS
2	C	934	PRO
1	A	169	VAL
1	A	211	MET
2	C	930	ASN
2	C	833	VAL
2	C	733	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	74/229 (32%)	51 (69%)	23 (31%)	0 2
1	B	73/229 (32%)	55 (75%)	18 (25%)	0 5
2	C	217/244 (89%)	139 (64%)	78 (36%)	0 1
All	All	364/702 (52%)	245 (67%)	119 (33%)	0 2

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	TYR
1	A	164	LYS
1	A	171	ASP
1	A	173	TYR
1	A	174	ARG
1	A	182	SER

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Mol	Chain	Res	Type
1	A	184	ARG
1	A	186	ARG
1	A	188	GLU
1	A	189	GLN
1	A	201	LEU
1	A	204	ARG
1	A	206	GLU
1	A	208	THR
1	A	211	MET
1	A	215	LEU
1	A	216	LEU
1	A	218	GLU
1	A	221	LYS
1	A	222	LYS
1	A	225	GLU
1	A	227	HIS
1	A	230	LEU
1	B	161	LYS
1	B	166	ILE
1	B	168	CYS
1	B	169	VAL
1	B	173	TYR
1	B	176	ILE
1	B	186	ARG
1	B	192	ARG
1	B	200	LEU
1	B	201	LEU
1	B	208	THR
1	B	209	ARG
1	B	211	MET
1	B	212	MET
1	B	217	ASN
1	B	222	LYS
1	B	226	LEU
1	B	231	ARG
2	C	685	ILE
2	C	686	PHE
2	C	689	LEU
2	C	691	PHE
2	C	692	TYR
2	C	693	VAL
2	C	697	TYR

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Mol	Chain	Res	Type
2	C	698	VAL
2	C	699	THR
2	C	702	THR
2	C	705	ARG
2	C	708	ARG
2	C	711	LEU
2	C	721	LYS
2	C	722	LEU
2	C	723	ILE
2	C	724	TYR
2	C	725	ASN
2	C	729	LYS
2	C	736	VAL
2	C	739	ILE
2	C	741	CYS
2	C	746	GLU
2	C	747	CYS
2	C	750	LEU
2	C	751	ILE
2	C	752	ASP
2	C	753	ARG
2	C	756	ASP
2	C	758	LEU
2	C	764	LEU
2	C	771	ARG
2	C	775	ILE
2	C	776	GLU
2	C	779	TYR
2	C	790	VAL
2	C	796	ASP
2	C	797	CYS
2	C	798	LEU
2	C	801	SER
2	C	807	SER
2	C	808	GLU
2	C	811	LEU
2	C	815	TYR
2	C	816	LYS
2	C	830	ASP
2	C	831	SER
2	C	834	ARG
2	C	838	LEU

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Mol	Chain	Res	Type
2	C	861	MET
2	C	864	LYS
2	C	865	LEU
2	C	866	PHE
2	C	870	ILE
2	C	871	THR
2	C	873	GLN
2	C	876	LEU
2	C	877	CYS
2	C	879	LEU
2	C	881	ILE
2	C	882	ILE
2	C	884	TYR
2	C	888	ILE
2	C	892	ASP
2	C	894	MET
2	C	898	HIS
2	C	904	GLN
2	C	905	ILE
2	C	909	ASP
2	C	910	THR
2	C	918	VAL
2	C	927	ILE
2	C	929	GLU
2	C	930	ASN
2	C	932	GLN
2	C	933	VAL
2	C	937	ASP
2	C	938	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	183	ASN
1	A	189	GLN
1	B	170	ASN
1	B	217	ASN
2	C	878	ASN
2	C	928	ASN
2	C	930	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	77/246 (31%)	-0.07	0 100 100	53, 88, 113, 115	0
1	B	76/246 (30%)	0.14	3 (3%) 39 31	49, 89, 100, 105	0
2	C	237/264 (89%)	-0.10	2 (0%) 86 80	23, 76, 104, 114	0
3	D	0/8	-	-	-	-
4	E	0/7	-	-	-	-
4	H	0/7	-	-	-	-
5	F	0/45	-	-	-	-
6	G	0/37	-	-	-	-
7	I	0/30	-	-	-	-
8	J	0/20	-	-	-	-
9	K	0/13	-	-	-	-
All	All	390/923 (42%)	-0.04	5 (1%) 77 68	23, 81, 110, 115	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	169	VAL	2.8
2	C	771	ARG	2.2
1	B	194	ARG	2.1
1	B	168	CYS	2.1
2	C	785	GLN	2.1

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.