



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:27 PM UTC

PDB ID : 1OFH / pdb_00001ofh
Title : Asymmetric complex between HslV and I-domain deleted HslU (H. influenzae)
Authors : Kwon, A.R.; Kessler, B.M.; Overkleeft, H.S.; McKay, D.B.
Deposited on : 2003-04-14
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

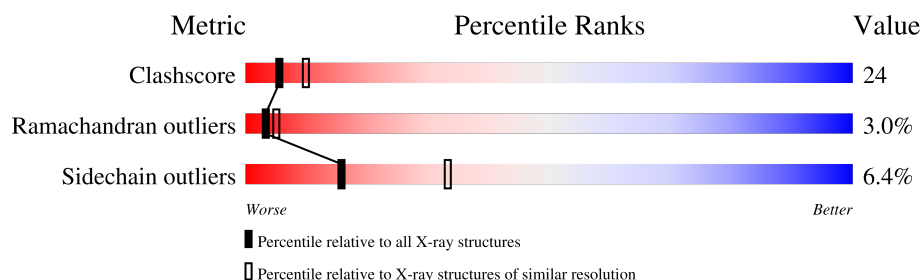
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	63% 28% 8%
1	B	310	64% 29% 7%
1	C	310	67% 28% 5%
2	G	174	55% 39% 6%
2	H	174	56% 39% 6%
2	I	174	65% 26% 8%
2	L	174	53% 42% 5%
2	M	174	55% 41% 5%

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Mol	Chain	Length	Quality of chain
2	N	174	52% 42% 5% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15254 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.

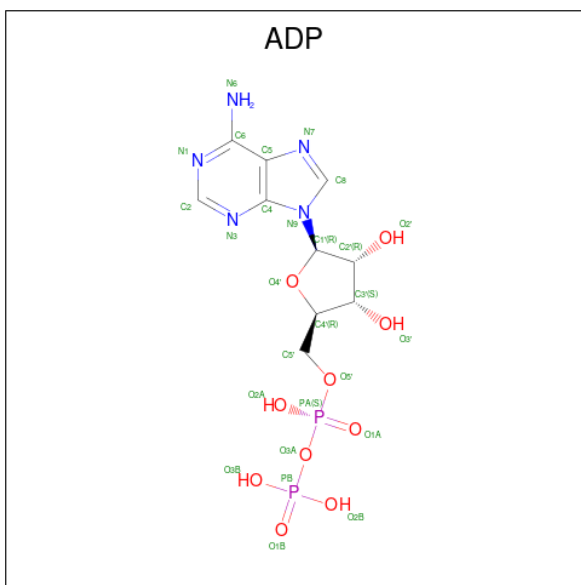
- Molecule 1 is a protein called ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2384	1492	422	461	9			
1	B	309	Total	C	N	O	S	0	0	0
			2384	1492	422	461	9			
1	C	309	Total	C	N	O	S	0	0	0
			2384	1492	422	461	9			

- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	H	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	I	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	L	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	M	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			
2	N	174	Total	C	N	O	S	0	0	1
			1319	826	236	253	4			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

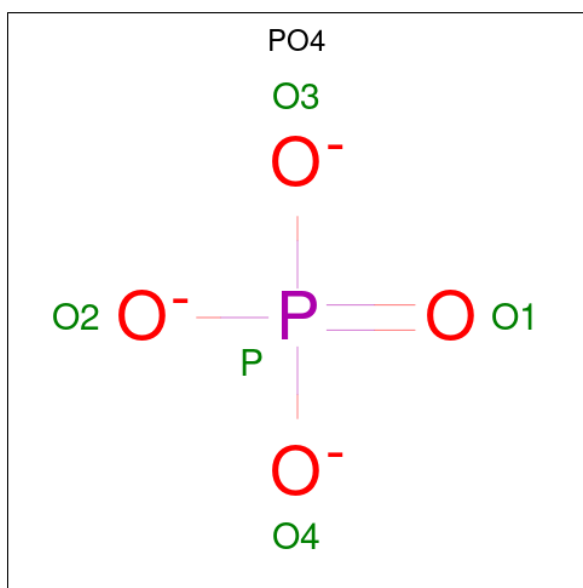


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total 2 Mg 2	0	0
4	B	2	Total 2 Mg 2	0	0
4	C	2	Total 2 Mg 2	0	0
4	G	1	Total 1 Mg 1	0	0
4	H	1	Total 1 Mg 1	0	0
4	I	1	Total 1 Mg 1	0	0
4	L	1	Total 1 Mg 1	0	0
4	M	1	Total 1 Mg 1	0	0
4	N	1	Total 1 Mg 1	0	0

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	20	Total	O	0	0
			20	20		
6	B	28	Total	O	0	0
			28	28		
6	C	31	Total	O	0	0
			31	31		
6	M	1	Total	O	0	0
			1	1		

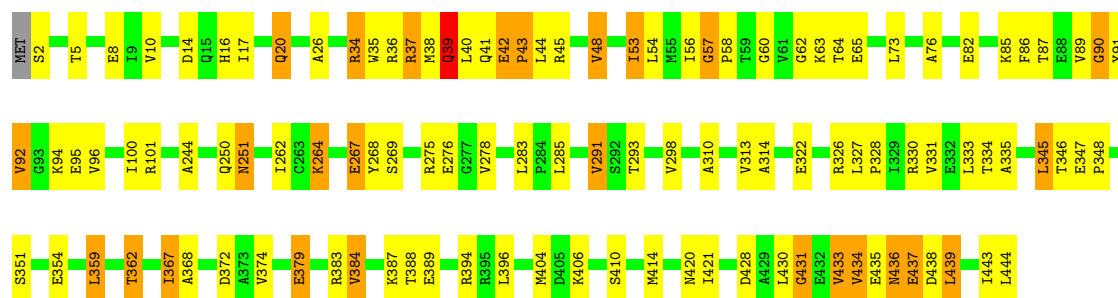
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

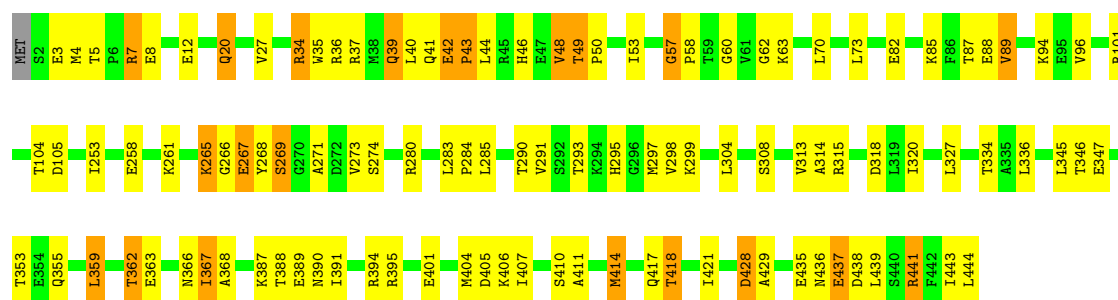
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

Chain A: 



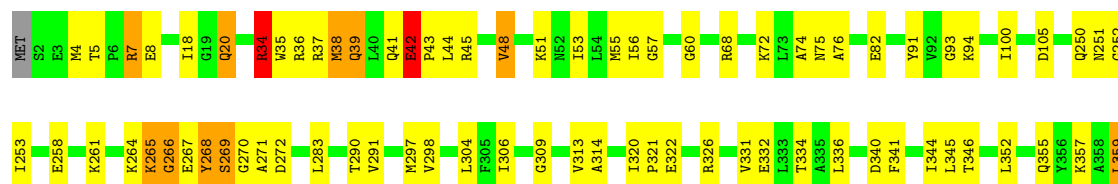
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

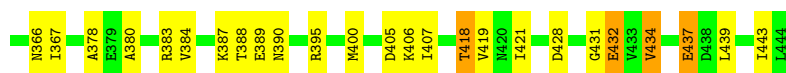
Chain B: 



• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

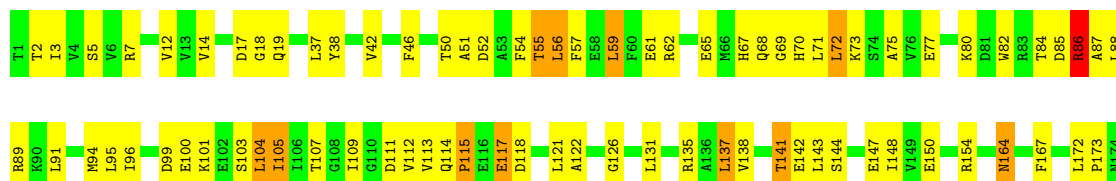
Chain C: 





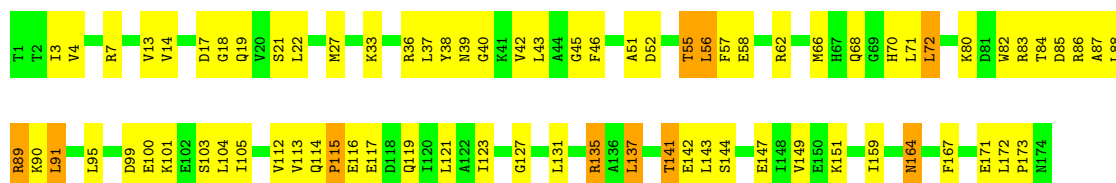
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain G: 55% 39% 6%



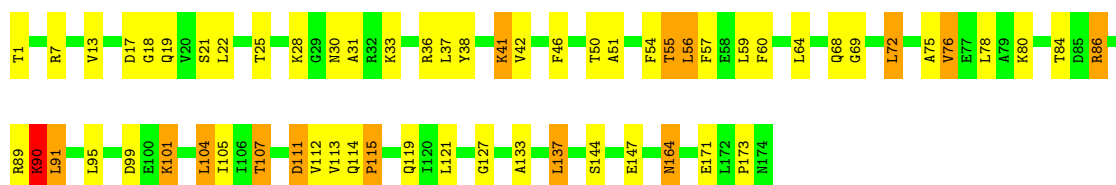
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain H: 56% 39% 6%



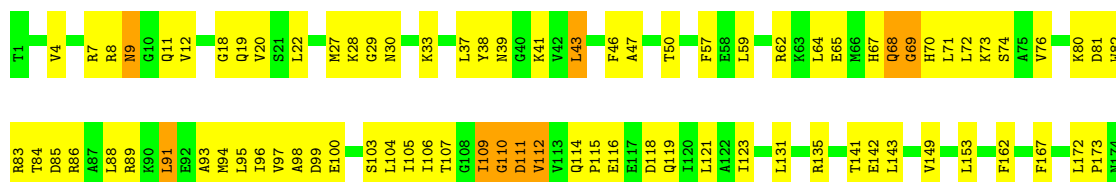
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain I: 65% 26% 8%



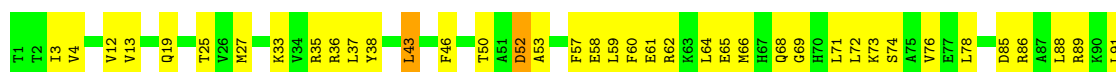
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

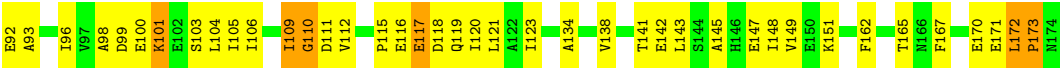
Chain L: 53% 42% 5%



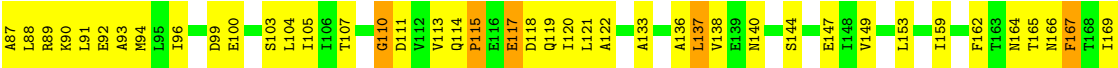
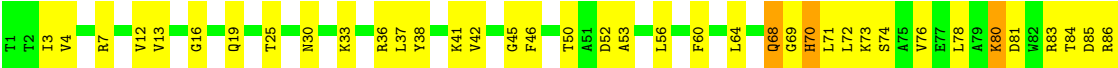
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain M: 55% 41% 5%





● Molecule 2: ATP-DEPENDENT PROTEASE HSLV



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	192.22Å 192.22Å 115.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.50	Depositor
% Data completeness (in resolution range)	97.0 (40.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15254	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, PO4

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	0.51	0/2415	1.05	14/3261 (0.4%)
1	B	0.54	0/2415	1.01	14/3261 (0.4%)
1	C	0.54	0/2415	0.98	11/3261 (0.3%)
2	G	0.42	1/1333 (0.1%)	0.85	0/1798
2	H	0.42	1/1333 (0.1%)	0.89	2/1798 (0.1%)
2	I	0.42	1/1333 (0.1%)	0.88	3/1798 (0.2%)
2	L	0.38	1/1333 (0.1%)	0.81	0/1798
2	M	0.38	1/1333 (0.1%)	0.83	1/1798 (0.1%)
2	N	0.37	1/1333 (0.1%)	0.87	3/1798 (0.2%)
All	All	0.47	6/15243 (0.0%)	0.93	48/20571 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	173	PRO	C-N	-6.02	1.25	1.33
2	I	173	PRO	C-N	-5.97	1.25	1.33
2	G	173	PRO	C-N	-5.94	1.25	1.33
2	L	173	PRO	C-N	-5.69	1.25	1.33
2	M	173	PRO	C-N	-5.63	1.25	1.33
2	N	173	PRO	C-N	-5.61	1.25	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	N-CA-C	-10.12	97.96	110.41
1	A	39	GLN	N-CA-C	-9.70	101.11	113.72
1	A	327	LEU	CA-C-N	9.05	128.66	119.24
1	A	327	LEU	C-N-CA	9.05	128.66	119.24
1	A	34	ARG	N-CA-C	-8.03	102.48	111.07
1	C	57	GLY	CA-C-N	7.45	127.89	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	GLY	C-N-CA	7.45	127.89	119.92
1	A	310	ALA	N-CA-C	-7.40	104.39	113.41
1	A	251	ASN	N-CA-C	7.07	118.75	110.41
1	B	414	MET	N-CA-C	-7.07	103.31	113.21
1	B	57	GLY	CA-C-N	6.83	126.80	120.03
1	B	57	GLY	C-N-CA	6.83	126.80	120.03
1	A	53	ILE	N-CA-C	6.78	119.28	108.85
1	A	276	GLU	N-CA-C	-6.65	104.03	111.28
1	B	62	GLY	N-CA-C	6.42	123.52	114.85
1	A	57	GLY	CA-C-N	6.36	127.79	119.84
1	A	57	GLY	C-N-CA	6.36	127.79	119.84
2	M	52	ASP	N-CA-C	-6.34	105.67	113.41
1	C	271	ALA	N-CA-C	-6.33	105.93	113.21
1	B	53	ILE	N-CA-C	6.14	117.43	108.53
2	I	127	GLY	N-CA-C	6.09	120.00	112.64
1	C	105	ASP	N-CA-C	-6.03	104.62	111.07
1	B	49	THR	CA-C-N	6.00	126.01	119.89
1	B	49	THR	C-N-CA	6.00	126.01	119.89
2	H	167	PHE	N-CA-C	6.00	119.40	110.52
2	I	90	LYS	N-CA-C	5.90	117.40	110.97
1	C	53	ILE	N-CA-C	5.84	117.84	108.85
1	C	346	THR	N-CA-C	5.83	121.97	114.56
1	C	34	ARG	N-CA-C	-5.82	105.02	111.36
1	B	34	ARG	N-CA-C	-5.78	104.89	111.07
2	N	169	ILE	N-CA-C	5.75	116.15	108.11
1	B	327	LEU	CA-C-N	5.60	125.27	119.05
1	B	327	LEU	C-N-CA	5.60	125.27	119.05
1	C	74	ALA	N-CA-C	-5.49	106.74	113.50
1	B	320	ILE	CA-C-N	5.47	126.68	119.84
1	B	320	ILE	C-N-CA	5.47	126.68	119.84
1	C	320	ILE	CA-C-N	5.47	125.55	119.32
1	C	320	ILE	C-N-CA	5.47	125.55	119.32
2	I	21	SER	N-CA-C	5.39	117.69	108.90
1	C	439	LEU	N-CA-C	-5.33	106.73	113.18
1	A	346	THR	N-CA-C	5.28	120.08	113.43
1	A	436	ASN	CB-CA-C	-5.21	109.01	115.89
2	H	127	GLY	N-CA-C	5.19	118.92	112.64
2	N	113	VAL	N-CA-C	5.17	115.42	107.77
1	B	105	ASP	N-CA-C	-5.09	105.38	111.03
1	A	62	GLY	N-CA-C	5.08	121.70	114.85
2	N	167	PHE	N-CA-C	5.07	118.27	110.42
1	B	347	GLU	N-CA-C	5.05	119.11	112.35

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	2384	0	2425	99	0
1	B	2384	0	2425	93	0
1	C	2384	0	2425	89	0
2	G	1319	0	1348	82	0
2	H	1319	0	1348	87	0
2	I	1319	0	1348	58	0
2	L	1319	0	1348	93	0
2	M	1319	0	1348	80	0
2	N	1319	0	1348	82	0
3	A	27	0	12	4	0
3	B	27	0	12	1	0
3	C	27	0	12	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	A	20	0	0	0	0
6	B	28	0	0	3	0
6	C	31	0	0	0	0
6	M	1	0	0	0	0
All	All	15254	0	15399	720	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 24.

All (720) 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:G:141:THR:HG23	2:G:143:LEU:H	1.17	1.08
1:A:406:LYS:H	1:A:406:LYS:HD2	1.21	1.04
2:H:83:ARG:HG3	2:I:55:THR:HG22	1.42	0.98
1:C:406:LYS:H	1:C:406:LYS:HD2	1.25	0.98
1:C:443:ILE:HD11	2:I:72:LEU:HD11	1.48	0.96
2:H:141:THR:HG23	2:H:143:LEU:H	1.33	0.94
1:A:267:GLU:HG3	2:G:62:ARG:HH12	1.32	0.91
1:A:20:GLN:HE21	1:A:20:GLN:HA	1.35	0.91
1:A:20:GLN:HE21	1:A:20:GLN:CA	1.83	0.90
1:B:406:LYS:H	1:B:406:LYS:HD2	1.37	0.90
2:N:105:ILE:HG13	2:N:121:LEU:HD13	1.55	0.89
2:G:18:GLY:H	2:G:164:ASN:HD21	1.17	0.89
1:A:443:ILE:HD11	2:G:72:LEU:HD11	1.54	0.89
1:C:20:GLN:HE21	1:C:20:GLN:HA	1.37	0.88
2:M:88:LEU:HA	2:M:91:LEU:HD13	1.54	0.87
1:C:383:ARG:O	1:C:387:LYS:HG2	1.75	0.87
2:M:109:ILE:HG13	2:M:110:GLY:H	1.42	0.84
1:B:20:GLN:HE21	1:B:20:GLN:HA	1.41	0.84
2:H:56:LEU:HD13	2:H:95:LEU:HG	1.57	0.83
1:C:406:LYS:HD2	1:C:406:LYS:N	1.94	0.82
2:L:12:VAL:HG21	2:L:98:ALA:HB1	1.63	0.80
2:I:89:ARG:HG2	2:I:90:LYS:HD3	1.62	0.80
1:C:38:MET:HE3	1:C:45:ARG:HD2	1.62	0.79
2:G:105:ILE:HG23	2:G:113:VAL:HG23	1.66	0.78
2:G:51:ALA:O	2:G:55:THR:HG22	1.84	0.78
2:G:56:LEU:HD13	2:G:95:LEU:HG	1.66	0.78
1:C:313:VAL:HG23	1:C:314:ALA:H	1.47	0.77
2:M:13:VAL:HG22	2:M:171:GLU:HG2	1.65	0.76
1:C:44:LEU:O	1:C:48:VAL:HG12	1.86	0.76
2:I:46:PHE:HB3	2:I:95:LEU:HD23	1.68	0.76
1:C:100:ILE:HG21	1:C:291:VAL:HG21	1.68	0.75
2:L:33:LYS:HA	2:L:46:PHE:CE1	2.22	0.75
1:A:267:GLU:HG3	2:G:62:ARG:NH1	2.00	0.75
2:G:86:ARG:HH11	2:G:86:ARG:HA	1.51	0.75
2:M:105:ILE:HG13	2:M:121:LEU:HD13	1.67	0.74
2:I:133:ALA:O	2:I:137:LEU:HD22	1.88	0.74
2:L:141:THR:HG21	2:L:143:LEU:HG	1.70	0.74
1:B:367:ILE:HD11	1:B:421:ILE:HD12	1.69	0.73
1:C:20:GLN:HE22	1:C:334:THR:H	1.33	0.73
2:I:144:SER:OG	2:I:147:GLU:HG3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:46:PHE:HB3	2:G:95:LEU:HD23	1.71	0.73
2:N:12:VAL:HG11	2:N:172:LEU:HD12	1.68	0.73
1:C:68:ARG:O	1:C:72:LYS:HD3	1.89	0.73
1:A:406:LYS:HD2	1:A:406:LYS:N	2.00	0.72
2:G:18:GLY:H	2:G:164:ASN:ND2	1.87	0.72
2:H:18:GLY:H	2:H:164:ASN:HD21	1.33	0.72
1:C:37:ARG:HH22	1:C:250:GLN:HE22	1.36	0.72
2:M:103:SER:C	2:M:104:LEU:HD12	2.15	0.72
2:G:37:LEU:HB2	2:G:42:VAL:HG23	1.70	0.71
2:G:141:THR:HG23	2:G:143:LEU:N	1.99	0.71
1:C:7:ARG:HG3	1:C:7:ARG:HH11	1.53	0.71
2:G:38:TYR:CE1	2:G:69:GLY:HA3	2.25	0.71
2:I:90:LYS:HD3	2:I:90:LYS:H	1.53	0.71
1:A:367:ILE:HD11	1:A:421:ILE:HD12	1.73	0.71
2:I:18:GLY:H	2:I:164:ASN:HD21	1.35	0.70
1:C:406:LYS:H	1:C:406:LYS:CD	2.04	0.70
2:N:72:LEU:O	2:N:76:VAL:HG23	1.92	0.70
1:B:20:GLN:HE22	1:B:334:THR:H	1.36	0.70
2:I:86:ARG:HD3	2:I:86:ARG:H	1.57	0.70
1:B:88:GLU:HB2	1:B:94:LYS:NZ	2.06	0.69
2:L:88:LEU:HA	2:L:91:LEU:HD13	1.72	0.69
1:A:439:LEU:HD23	2:G:72:LEU:HD12	1.74	0.69
1:B:362:THR:HG21	1:C:36:ARG:HG2	1.75	0.69
2:L:7:ARG:NH1	2:L:12:VAL:HB	2.06	0.69
2:L:110:GLY:O	2:L:111:ASP:HB2	1.93	0.69
1:A:406:LYS:H	1:A:406:LYS:CD	2.04	0.69
2:H:46:PHE:HB3	2:H:95:LEU:HD23	1.75	0.69
2:H:164:ASN:C	2:H:164:ASN:HD22	1.98	0.69
2:L:43:LEU:HD23	2:L:43:LEU:H	1.58	0.69
2:L:141:THR:HG22	2:L:142:GLU:N	2.07	0.68
2:M:27:MET:HE1	2:N:94:MET:HE1	1.73	0.68
2:M:43:LEU:HD23	2:M:43:LEU:H	1.58	0.68
2:G:100:GLU:OE2	2:G:172:LEU:HB3	1.93	0.68
2:L:71:LEU:HB2	2:L:99:ASP:OD2	1.94	0.68
2:L:131:LEU:HD11	2:L:135:ARG:NE	2.08	0.68
1:A:37:ARG:O	1:A:38:MET:HB3	1.93	0.68
2:L:7:ARG:HD2	2:L:119:GLN:HE21	1.59	0.67
2:L:22:LEU:HB2	2:L:27:MET:HE3	1.76	0.67
2:N:85:ASP:HB3	2:N:88:LEU:HD23	1.76	0.67
1:A:326:ARG:C	1:A:328:PRO:HD3	2.19	0.67
2:H:22:LEU:HD21	2:H:27:MET:HE3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:141:THR:HG22	2:L:143:LEU:H	1.59	0.67
1:A:439:LEU:HD21	2:G:73:LYS:HA	1.76	0.67
2:H:37:LEU:HD21	2:H:57:PHE:CZ	2.29	0.67
2:L:96:ILE:HG12	2:L:105:ILE:HG12	1.76	0.67
1:C:258:GLU:HB3	1:C:261:LYS:HG3	1.76	0.67
1:A:44:LEU:O	1:A:48:VAL:HG12	1.93	0.67
1:A:250:GLN:HA	1:A:250:GLN:HE21	1.59	0.67
2:I:38:TYR:CE1	2:I:69:GLY:HA3	2.30	0.67
1:B:406:LYS:HD2	1:B:406:LYS:N	2.09	0.67
1:B:443:ILE:HG22	1:B:444:LEU:N	2.09	0.67
1:B:367:ILE:HD12	1:B:404:MET:HE1	1.77	0.66
2:M:141:THR:CG2	2:M:143:LEU:HG	2.25	0.66
2:N:52:ASP:O	2:N:56:LEU:HD23	1.96	0.66
2:M:36:ARG:O	2:M:37:LEU:HD23	1.96	0.66
2:G:5:SER:HB2	2:G:14:VAL:HG22	1.77	0.66
2:L:91:LEU:HD12	2:L:91:LEU:H	1.60	0.66
2:G:101:LYS:HE2	2:G:101:LYS:HA	1.76	0.66
2:I:37:LEU:HB2	2:I:42:VAL:HG23	1.78	0.66
1:A:387:LYS:HG3	1:A:388:THR:HG23	1.77	0.65
2:H:115:PRO:HG3	2:H:121:LEU:HD11	1.78	0.65
1:C:7:ARG:HG3	1:C:7:ARG:NH1	2.11	0.65
1:C:20:GLN:HE21	1:C:20:GLN:CA	2.05	0.65
2:H:19:GLN:HE21	2:H:164:ASN:HB3	1.60	0.65
2:G:144:SER:HB3	2:G:147:GLU:HG3	1.78	0.65
1:A:345:LEU:HD23	1:A:374:VAL:HG13	1.78	0.65
2:M:72:LEU:O	2:M:76:VAL:HG23	1.97	0.65
2:M:109:ILE:HG13	2:M:110:GLY:N	2.10	0.65
2:G:46:PHE:HB3	2:G:95:LEU:CD2	2.27	0.64
1:A:100:ILE:HB	1:A:291:VAL:HG21	1.77	0.64
1:A:262:ILE:HD12	1:A:278:VAL:HG23	1.79	0.64
2:M:141:THR:HG21	2:M:143:LEU:HG	1.77	0.64
2:L:141:THR:HG22	2:L:142:GLU:H	1.60	0.64
1:A:20:GLN:HE21	1:A:20:GLN:N	1.96	0.64
2:G:107:THR:OG1	2:G:109:ILE:HG12	1.98	0.64
2:I:7:ARG:HD2	2:I:119:GLN:OE1	1.96	0.64
2:I:164:ASN:C	2:I:164:ASN:HD22	2.04	0.64
2:G:3:ILE:HG22	2:G:96:ILE:HD12	1.79	0.64
2:I:76:VAL:O	2:I:80:LYS:HG2	1.98	0.64
1:A:65:GLU:HG3	3:A:450:ADP:H2'	1.79	0.64
1:C:100:ILE:HG21	1:C:291:VAL:CG2	2.27	0.63
2:I:37:LEU:HD21	2:I:57:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:99:ASP:HA	2:G:172:LEU:HD12	1.80	0.63
2:L:104:LEU:CD2	2:L:114:GLN:HG2	2.28	0.63
2:N:144:SER:OG	2:N:147:GLU:HG3	1.99	0.63
1:B:3:GLU:HG3	1:B:4:MET:H	1.62	0.63
1:C:258:GLU:HB3	1:C:261:LYS:CG	2.29	0.63
2:N:33:LYS:HA	2:N:46:PHE:CE1	2.33	0.63
1:B:3:GLU:HG3	1:B:4:MET:N	2.14	0.63
2:N:4:VAL:HG13	2:N:149:VAL:HG13	1.79	0.63
2:N:80:LYS:HB2	2:N:80:LYS:NZ	2.13	0.63
2:G:117:GLU:HG3	2:G:118:ASP:N	2.13	0.63
1:B:443:ILE:CG2	1:B:444:LEU:N	2.62	0.63
2:H:42:VAL:HG12	2:H:99:ASP:HB3	1.80	0.62
1:C:322:GLU:O	1:C:326:ARG:HG2	1.99	0.62
2:L:141:THR:CG2	2:L:143:LEU:HG	2.29	0.62
1:B:280:ARG:HG3	1:B:280:ARG:HH11	1.65	0.62
2:M:115:PRO:HB2	2:M:119:GLN:OE1	2.00	0.62
1:A:359:LEU:O	1:A:362:THR:HB	1.98	0.62
1:C:38:MET:CE	1:C:45:ARG:HD2	2.30	0.62
2:L:59:LEU:HD12	2:L:62:ARG:HD3	1.82	0.61
1:C:357:LYS:HA	1:C:367:ILE:HD11	1.81	0.61
2:L:91:LEU:HD12	2:L:91:LEU:N	2.16	0.61
1:B:37:ARG:HA	1:B:40:LEU:HG	1.82	0.61
2:M:64:LEU:HD23	2:M:74:SER:OG	2.00	0.61
1:A:37:ARG:O	1:A:38:MET:CB	2.48	0.61
2:G:72:LEU:HD22	2:G:104:LEU:HD21	1.82	0.61
1:B:20:GLN:HE21	1:B:20:GLN:CA	2.08	0.61
2:N:133:ALA:O	2:N:137:LEU:HD22	2.00	0.61
2:M:62:ARG:O	2:M:65:GLU:HB2	2.01	0.61
1:C:290:THR:HG22	1:C:297:MET:HE3	1.83	0.61
1:C:37:ARG:HH22	1:C:250:GLN:NE2	1.99	0.60
1:C:355:GLN:O	1:C:359:LEU:HD22	2.01	0.60
1:B:313:VAL:HG23	1:B:314:ALA:N	2.16	0.60
2:M:96:ILE:HG12	2:M:105:ILE:HG12	1.82	0.60
2:G:137:LEU:O	2:G:141:THR:HG22	2.02	0.60
2:I:51:ALA:O	2:I:55:THR:HG23	2.01	0.60
2:I:90:LYS:HD3	2:I:90:LYS:N	2.15	0.60
2:N:94:MET:HE3	2:N:107:THR:CG2	2.32	0.60
1:B:313:VAL:HG23	1:B:314:ALA:H	1.66	0.60
1:B:39:GLN:HE21	1:B:39:GLN:N	1.98	0.60
2:H:58:GLU:O	2:H:62:ARG:HG2	2.00	0.60
1:A:20:GLN:HA	1:A:20:GLN:NE2	2.12	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ALA:HB1	1:A:251:ASN:O	2.02	0.59
1:C:270:GLY:C	1:C:272:ASP:H	2.09	0.59
2:M:104:LEU:HD23	2:M:112:VAL:HG11	1.84	0.59
2:N:103:SER:C	2:N:104:LEU:HD22	2.27	0.59
1:A:16:HIS:C	1:A:17:ILE:HD12	2.28	0.59
2:G:68:GLN:HB2	2:G:70:HIS:CE1	2.37	0.59
2:L:105:ILE:HG13	2:L:121:LEU:HD13	1.82	0.59
2:N:64:LEU:HD23	2:N:74:SER:OG	2.01	0.59
1:B:44:LEU:O	1:B:48:VAL:HG12	2.02	0.59
2:M:100:GLU:OE2	2:M:173:PRO:HG3	2.03	0.59
2:L:109:ILE:HG13	2:L:110:GLY:H	1.68	0.59
1:B:253:ILE:HD12	1:B:304:LEU:HD23	1.84	0.59
1:C:100:ILE:CG2	1:C:291:VAL:HG21	2.31	0.59
2:M:43:LEU:H	2:M:43:LEU:CD2	2.15	0.58
1:C:267:GLU:HB2	2:H:84:THR:HG21	1.84	0.58
2:H:46:PHE:HB3	2:H:95:LEU:CD2	2.32	0.58
1:A:16:HIS:HB2	1:A:17:ILE:HD12	1.83	0.58
1:B:346:THR:HG22	1:B:353:THR:OG1	2.03	0.58
1:C:18:ILE:CG1	1:C:344:ILE:HD13	2.33	0.58
2:H:144:SER:HB3	2:H:147:GLU:HG3	1.86	0.58
1:A:438:ASP:O	1:A:439:LEU:HB2	2.01	0.58
1:A:37:ARG:HA	1:A:40:LEU:HG	1.84	0.58
1:A:264:LYS:HE3	1:A:264:LYS:N	2.18	0.58
2:I:111:ASP:N	2:I:111:ASP:OD2	2.36	0.58
2:M:71:LEU:HD13	2:M:99:ASP:OD2	2.04	0.58
2:N:85:ASP:CB	2:N:88:LEU:HD23	2.34	0.58
2:M:59:LEU:HD23	2:M:88:LEU:HD21	1.86	0.58
1:B:406:LYS:H	1:B:406:LYS:CD	2.11	0.58
1:C:37:ARG:NH2	1:C:250:GLN:HE22	2.00	0.57
2:H:90:LYS:HD3	2:H:91:LEU:H	1.69	0.57
2:I:42:VAL:HG12	2:I:99:ASP:HB3	1.86	0.57
1:C:252:GLY:O	1:C:253:ILE:HD13	2.04	0.57
2:I:104:LEU:HD11	2:I:114:GLN:HG2	1.87	0.57
2:N:172:LEU:CB	2:N:173:PRO:HD3	2.34	0.57
2:G:37:LEU:HD21	2:G:57:PHE:CE1	2.40	0.57
1:A:42:GLU:HB3	1:A:43:PRO:HD3	1.87	0.57
1:A:91:TYR:CZ	1:A:94:LYS:HG2	2.39	0.57
1:A:101:ARG:HG2	1:A:293:THR:HG22	1.85	0.57
2:H:104:LEU:HD11	2:H:114:GLN:HG2	1.87	0.57
1:A:38:MET:HA	1:A:45:ARG:HD2	1.86	0.56
1:A:434:VAL:HG12	1:A:435:GLU:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HG12	1:A:368:ALA:N	2.19	0.56
2:I:25:THR:HA	2:N:159:ILE:O	2.05	0.56
2:I:41:LYS:HB2	2:I:41:LYS:NZ	2.20	0.56
2:I:56:LEU:HD13	2:I:95:LEU:HG	1.88	0.56
2:L:37:LEU:HD11	2:L:57:PHE:CD2	2.41	0.56
2:L:67:HIS:HB3	2:L:73:LYS:HE3	1.87	0.56
2:M:3:ILE:HB	2:M:123:ILE:CG1	2.35	0.56
1:C:37:ARG:HG3	1:C:48:VAL:HG13	1.87	0.56
2:L:38:TYR:CD2	2:L:64:LEU:HD13	2.40	0.56
2:N:80:LYS:HB2	2:N:80:LYS:HZ2	1.70	0.56
2:M:106:ILE:HD12	2:M:106:ILE:N	2.21	0.56
2:G:37:LEU:HB2	2:G:42:VAL:CG2	2.36	0.56
2:N:81:ASP:HA	2:N:84:THR:HB	1.87	0.56
2:N:115:PRO:HG3	2:N:121:LEU:HD11	1.87	0.56
1:A:92:VAL:O	1:A:95:GLU:HG2	2.06	0.56
2:M:86:ARG:HA	2:M:89:ARG:CZ	2.36	0.56
2:L:85:ASP:CG	2:L:88:LEU:HD13	2.31	0.55
2:L:95:LEU:O	2:L:105:ILE:HA	2.06	0.55
2:M:96:ILE:HG13	2:M:123:ILE:HD13	1.86	0.55
1:A:267:GLU:H	2:G:62:ARG:NH1	2.04	0.55
2:N:42:VAL:HG22	2:N:99:ASP:HB3	1.87	0.55
1:B:5:THR:OG1	1:B:8:GLU:HG3	2.07	0.55
2:I:13:VAL:HG22	2:I:171:GLU:HB3	1.87	0.55
1:B:266:GLY:O	1:B:267:GLU:C	2.49	0.55
2:H:90:LYS:CD	2:H:91:LEU:H	2.20	0.55
2:N:86:ARG:HG3	2:N:87:ALA:N	2.22	0.55
2:H:51:ALA:O	2:H:55:THR:HG22	2.06	0.55
2:I:46:PHE:HB3	2:I:95:LEU:CD2	2.34	0.55
2:M:33:LYS:HA	2:M:46:PHE:CE1	2.42	0.55
2:M:52:ASP:OD1	2:N:83:ARG:HD3	2.06	0.55
1:A:267:GLU:C	1:A:269:SER:H	2.15	0.55
2:H:4:VAL:HG13	2:H:149:VAL:HG13	1.89	0.55
2:L:111:ASP:OD1	2:L:112:VAL:N	2.40	0.55
2:M:4:VAL:HG13	2:M:149:VAL:HG13	1.89	0.55
2:G:141:THR:HG21	2:G:143:LEU:HD12	1.88	0.54
2:N:19:GLN:NE2	2:N:162:PHE:HA	2.22	0.54
1:B:7:ARG:HG2	6:B:2001:HOH:O	2.07	0.54
2:H:83:ARG:CG	2:I:55:THR:HG22	2.27	0.54
2:L:172:LEU:C	2:L:172:LEU:HD23	2.32	0.54
1:B:41:GLN:HA	1:B:41:GLN:NE2	2.21	0.54
2:L:86:ARG:HG3	2:L:86:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:141:THR:HG23	2:H:143:LEU:N	2.13	0.54
2:L:43:LEU:HD23	2:L:98:ALA:O	2.06	0.54
2:L:43:LEU:H	2:L:43:LEU:CD2	2.20	0.54
2:M:145:ALA:O	2:M:149:VAL:HG23	2.08	0.54
2:H:103:SER:O	2:H:104:LEU:HD12	2.07	0.54
2:N:96:ILE:HG12	2:N:105:ILE:HG12	1.90	0.54
1:A:250:GLN:HE21	1:A:250:GLN:CA	2.19	0.54
2:H:89:ARG:HG2	2:H:90:LYS:HD3	1.88	0.54
2:I:105:ILE:HG22	2:I:113:VAL:O	2.08	0.54
1:B:89:VAL:HG13	1:B:89:VAL:O	2.07	0.54
1:C:340:ASP:O	1:C:344:ILE:HG12	2.08	0.54
2:L:115:PRO:HG3	2:L:121:LEU:HG	1.90	0.54
2:M:116:GLU:O	2:M:118:ASP:N	2.41	0.54
2:M:85:ASP:CG	2:M:88:LEU:HD13	2.33	0.54
1:B:96:VAL:CG1	1:B:285:LEU:HD22	2.38	0.53
2:G:141:THR:HG23	2:G:142:GLU:N	2.23	0.53
2:L:7:ARG:HB3	2:L:119:GLN:HB3	1.90	0.53
1:C:267:GLU:HB2	2:H:84:THR:CG2	2.38	0.53
2:N:71:LEU:HB2	2:N:99:ASP:OD2	2.07	0.53
1:A:250:GLN:HA	1:A:250:GLN:NE2	2.23	0.53
2:G:164:ASN:C	2:G:164:ASN:HD22	2.15	0.53
2:H:37:LEU:HB2	2:H:42:VAL:HG23	1.91	0.53
2:M:59:LEU:CD2	2:M:88:LEU:HD21	2.39	0.53
2:L:104:LEU:HD21	2:L:114:GLN:HG2	1.91	0.53
2:M:86:ARG:HG3	2:M:86:ARG:HH11	1.74	0.53
2:I:17:ASP:HB2	2:I:164:ASN:ND2	2.24	0.53
2:L:28:LYS:HE3	2:L:30:ASN:O	2.08	0.53
2:L:65:GLU:OE1	2:L:65:GLU:HA	2.08	0.53
2:N:104:LEU:HD11	2:N:114:GLN:HG2	1.90	0.53
1:A:351:SER:OG	1:A:354:GLU:HG3	2.09	0.53
2:L:72:LEU:O	2:L:76:VAL:HG22	2.09	0.53
2:L:94:MET:HB3	2:L:123:ILE:HD12	1.90	0.53
2:N:86:ARG:HA	2:N:89:ARG:NH1	2.23	0.53
1:A:410:SER:O	1:A:414:MET:HG3	2.09	0.53
2:M:99:ASP:OD1	2:M:101:LYS:N	2.42	0.53
1:A:262:ILE:HG21	1:A:278:VAL:HG21	1.90	0.53
2:H:52:ASP:OD2	2:H:91:LEU:HA	2.09	0.53
2:M:120:ILE:HD13	2:M:134:ALA:HB1	1.91	0.53
2:N:19:GLN:HB2	2:N:164:ASN:ND2	2.24	0.53
2:N:94:MET:HE3	2:N:107:THR:HG21	1.91	0.53
2:L:38:TYR:HD2	2:L:64:LEU:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LYS:HD2	1:B:308:SER:HB2	1.90	0.52
2:G:85:ASP:OD2	2:G:86:ARG:N	2.43	0.52
2:H:100:GLU:CD	2:H:100:GLU:H	2.17	0.52
2:I:90:LYS:HG2	2:I:91:LEU:N	2.24	0.52
1:B:42:GLU:HB3	1:B:43:PRO:HD3	1.92	0.52
2:L:96:ILE:HG13	2:L:123:ILE:HD13	1.91	0.52
2:N:3:ILE:HD13	2:N:16:GLY:HA3	1.92	0.52
2:H:71:LEU:C	2:H:71:LEU:HD13	2.35	0.52
2:H:131:LEU:HG	2:H:135:ARG:NH1	2.25	0.52
1:B:12:GLU:HB3	1:B:73:LEU:HD22	1.91	0.52
2:N:13:VAL:HG22	2:N:171:GLU:HG3	1.92	0.52
1:C:367:ILE:HG22	1:C:419:VAL:HB	1.92	0.52
2:N:85:ASP:O	2:N:89:ARG:HG3	2.10	0.52
1:A:384:VAL:HA	1:A:387:LYS:HG2	1.91	0.52
2:H:84:THR:O	2:I:89:ARG:NH2	2.42	0.52
2:M:85:ASP:O	2:M:89:ARG:HG3	2.09	0.52
1:C:388:THR:OG1	1:C:389:GLU:N	2.43	0.51
2:I:55:THR:O	2:I:59:LEU:HB2	2.10	0.51
1:B:414:MET:O	1:B:417:GLN:HG3	2.11	0.51
2:G:99:ASP:HA	2:G:172:LEU:CD1	2.41	0.51
1:B:27:VAL:HB	1:B:70:LEU:HD22	1.92	0.51
1:C:290:THR:CG2	1:C:297:MET:HE3	2.40	0.51
2:G:164:ASN:ND2	2:G:164:ASN:C	2.69	0.51
2:H:141:THR:HG23	2:H:142:GLU:N	2.25	0.51
2:L:83:ARG:O	2:L:89:ARG:HD3	2.11	0.51
1:B:88:GLU:HB2	1:B:94:LYS:HZ1	1.75	0.51
1:C:344:ILE:HD12	3:C:450:ADP:C2	2.46	0.51
2:I:105:ILE:CG2	2:I:113:VAL:HB	2.40	0.51
1:B:315:ARG:O	1:B:318:ASP:HB2	2.10	0.51
2:H:131:LEU:HD21	2:H:135:ARG:HH12	1.76	0.51
2:N:30:ASN:HA	2:N:166:ASN:HD22	1.75	0.51
1:A:60:GLY:HA2	3:A:450:ADP:O3A	2.11	0.50
2:G:7:ARG:HG3	2:G:12:VAL:HG22	1.93	0.50
2:H:151:LYS:CE	2:N:140:ASN:HD21	2.23	0.50
1:B:268:TYR:CD1	1:B:269:SER:N	2.75	0.50
1:A:56:ILE:HD12	1:A:56:ILE:N	2.27	0.50
2:G:82:TRP:HZ2	2:G:91:LEU:HD23	1.75	0.50
2:G:3:ILE:O	2:G:122:ALA:HA	2.12	0.50
2:H:22:LEU:HD13	2:H:27:MET:HB2	1.93	0.50
2:M:116:GLU:C	2:M:118:ASP:H	2.19	0.50
2:L:64:LEU:HD22	2:L:69:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:138:VAL:HG23	2:M:148:ILE:HD13	1.94	0.50
1:B:101:ARG:HG2	1:B:293:THR:HG22	1.94	0.50
1:C:35:TRP:O	1:C:39:GLN:NE2	2.45	0.50
2:N:46:PHE:CZ	2:N:50:THR:HG22	2.47	0.50
1:B:441:ARG:NH2	2:I:37:LEU:HD23	2.25	0.50
1:C:267:GLU:CB	2:H:84:THR:HG21	2.40	0.50
1:C:443:ILE:HD11	2:I:72:LEU:CD1	2.32	0.50
2:H:164:ASN:C	2:H:164:ASN:ND2	2.65	0.50
2:L:141:THR:CG2	2:L:142:GLU:N	2.75	0.50
2:M:71:LEU:HD22	2:M:99:ASP:OD2	2.12	0.50
2:N:36:ARG:O	2:N:37:LEU:HD23	2.12	0.49
2:M:88:LEU:CA	2:M:91:LEU:HD13	2.35	0.49
1:A:64:THR:N	3:A:450:ADP:O2B	2.46	0.49
1:B:366:ASN:O	1:B:418:THR:HA	2.11	0.49
2:H:85:ASP:OD1	2:H:86:ARG:N	2.46	0.49
2:N:83:ARG:O	2:N:89:ARG:HD3	2.12	0.49
2:G:94:MET:HG2	2:G:107:THR:HG22	1.95	0.49
1:A:444:LEU:HD23	1:A:444:LEU:C	2.38	0.49
1:B:401:GLU:OE1	1:C:51:LYS:HG3	2.12	0.49
1:B:444:LEU:HD22	2:I:31:ALA:HB1	1.94	0.49
2:G:61:GLU:O	2:G:65:GLU:HG2	2.13	0.49
2:G:91:LEU:N	2:G:91:LEU:HD22	2.27	0.49
2:L:141:THR:CG2	2:L:142:GLU:H	2.26	0.49
2:G:104:LEU:CD1	2:G:114:GLN:HG2	2.42	0.49
2:H:22:LEU:CD2	2:H:27:MET:HE3	2.42	0.49
2:L:99:ASP:OD1	2:L:100:GLU:N	2.40	0.49
2:N:12:VAL:CG1	2:N:172:LEU:HB2	2.43	0.49
2:H:90:LYS:CG	2:H:91:LEU:N	2.76	0.49
2:I:90:LYS:H	2:I:90:LYS:CD	2.24	0.49
2:N:104:LEU:CD1	2:N:114:GLN:HG2	2.43	0.49
1:B:407:ILE:HG13	6:B:2026:HOH:O	2.12	0.49
1:C:264:LYS:O	1:C:266:GLY:N	2.46	0.49
2:G:138:VAL:HG23	2:G:148:ILE:HD13	1.95	0.49
1:A:384:VAL:HB	1:A:434:VAL:HG21	1.95	0.48
2:L:106:ILE:N	2:L:106:ILE:HD12	2.27	0.48
2:N:85:ASP:CG	2:N:88:LEU:HD23	2.38	0.48
1:B:362:THR:CG2	1:C:36:ARG:HG2	2.41	0.48
1:C:265:LYS:O	1:C:267:GLU:N	2.46	0.48
2:G:50:THR:O	2:G:54:PHE:HD1	1.96	0.48
2:N:172:LEU:HB2	2:N:173:PRO:HD3	1.94	0.48
1:B:60:GLY:HA2	3:B:450:ADP:O3A	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:19:GLN:HE21	2:G:164:ASN:HB3	1.78	0.48
2:G:73:LYS:HE2	2:G:77:GLU:HG2	1.96	0.48
2:H:90:LYS:HG2	2:H:91:LEU:N	2.27	0.48
2:I:164:ASN:C	2:I:164:ASN:ND2	2.68	0.48
2:M:172:LEU:CB	2:M:173:PRO:HD3	2.43	0.48
1:B:436:ASN:O	1:B:437:GLU:C	2.56	0.48
1:C:60:GLY:HA2	3:C:450:ADP:O3A	2.13	0.48
1:C:407:ILE:HD13	1:C:419:VAL:HG11	1.96	0.48
2:H:17:ASP:HB2	2:H:164:ASN:ND2	2.28	0.48
2:L:43:LEU:HD22	2:L:172:LEU:HD13	1.93	0.48
2:N:100:GLU:OE2	2:N:173:PRO:HG3	2.12	0.48
2:H:101:LYS:HA	2:H:101:LYS:HE2	1.96	0.48
2:I:1:THR:HG23	2:I:33:LYS:NZ	2.29	0.48
2:L:64:LEU:HD23	2:L:74:SER:OG	2.12	0.48
2:L:82:TRP:HA	2:L:88:LEU:HB3	1.96	0.48
2:N:68:GLN:O	2:N:70:HIS:N	2.46	0.48
2:L:8:ARG:O	2:L:9:ASN:HB2	2.14	0.48
2:L:18:GLY:O	2:L:29:GLY:C	2.56	0.48
2:N:86:ARG:NH2	2:N:90:LYS:HE2	2.29	0.48
2:I:19:GLN:HE21	2:I:164:ASN:HB3	1.78	0.48
2:M:86:ARG:HA	2:M:89:ARG:NH1	2.29	0.48
1:B:367:ILE:HG22	6:B:2023:HOH:O	2.12	0.48
2:L:38:TYR:HE2	2:L:64:LEU:HB3	1.78	0.48
2:N:91:LEU:HD12	2:N:91:LEU:N	2.29	0.48
2:L:116:GLU:C	2:L:118:ASP:H	2.21	0.48
2:H:38:TYR:C	2:H:40:GLY:H	2.22	0.48
2:L:71:LEU:HD11	2:L:97:VAL:HB	1.96	0.48
1:C:366:ASN:O	1:C:418:THR:HA	2.14	0.47
2:H:100:GLU:O	2:H:101:LYS:HE2	2.14	0.47
2:H:100:GLU:OE2	2:H:172:LEU:HD13	2.14	0.47
2:L:9:ASN:C	2:L:11:GLN:H	2.22	0.47
2:N:103:SER:O	2:N:104:LEU:HD13	2.13	0.47
2:G:52:ASP:HA	2:G:55:THR:CG2	2.44	0.47
2:H:99:ASP:HA	2:H:172:LEU:CD1	2.44	0.47
2:H:151:LYS:HE2	2:N:140:ASN:HD21	1.79	0.47
2:M:43:LEU:HD12	2:M:170:GLU:HB2	1.95	0.47
2:M:58:GLU:O	2:M:61:GLU:HB2	2.14	0.47
2:M:91:LEU:N	2:M:91:LEU:HD12	2.29	0.47
1:A:5:THR:N	1:A:8:GLU:OE1	2.45	0.47
1:C:269:SER:HA	1:C:272:ASP:HB3	1.95	0.47
1:C:443:ILE:CD1	2:I:72:LEU:HD11	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:103:SER:O	2:G:104:LEU:HD12	2.14	0.47
2:H:4:VAL:CG1	2:H:149:VAL:HG13	2.44	0.47
1:A:367:ILE:HD12	1:A:404:MET:HE1	1.96	0.47
1:A:433:VAL:O	1:A:434:VAL:C	2.57	0.47
1:B:367:ILE:HG12	1:B:368:ALA:N	2.28	0.47
1:B:443:ILE:CG2	1:B:444:LEU:H	2.27	0.47
2:L:94:MET:HE1	2:L:107:THR:HG22	1.94	0.47
1:C:421:ILE:N	1:C:421:ILE:HD12	2.30	0.47
2:I:90:LYS:HG2	2:I:91:LEU:H	1.79	0.47
2:L:12:VAL:HG13	2:L:12:VAL:O	2.15	0.47
2:L:38:TYR:CE2	2:L:64:LEU:HB3	2.50	0.47
2:N:94:MET:HE3	2:N:107:THR:HG22	1.95	0.47
1:A:326:ARG:O	1:A:328:PRO:HD3	2.13	0.47
1:B:258:GLU:HB3	1:B:261:LYS:HG2	1.96	0.47
2:L:47:ALA:HB3	2:L:94:MET:HB2	1.96	0.47
2:H:36:ARG:HG2	2:H:43:LEU:CD2	2.44	0.47
2:H:82:TRP:NE1	2:H:88:LEU:HD12	2.30	0.47
1:A:267:GLU:N	2:G:62:ARG:NH1	2.62	0.47
2:L:91:LEU:H	2:L:91:LEU:CD1	2.27	0.47
1:B:390:ASN:HB2	2:H:68:GLN:OE1	2.15	0.47
2:G:114:GLN:O	2:G:115:PRO:O	2.33	0.47
1:A:433:VAL:O	1:A:433:VAL:HG23	2.15	0.46
2:G:154:ARG:HA	2:G:167:PHE:HZ	1.80	0.46
1:A:54:LEU:HD23	1:A:330:ARG:HD2	1.97	0.46
1:A:267:GLU:H	2:G:62:ARG:HH12	1.62	0.46
1:B:388:THR:OG1	1:B:389:GLU:N	2.48	0.46
2:G:80:LYS:NZ	2:G:84:THR:HG22	2.31	0.46
2:G:95:LEU:O	2:G:105:ILE:HA	2.14	0.46
2:I:17:ASP:HB2	2:I:164:ASN:HD22	1.80	0.46
2:M:104:LEU:HD23	2:M:112:VAL:CG1	2.45	0.46
2:N:30:ASN:HA	2:N:166:ASN:ND2	2.30	0.46
2:N:33:LYS:O	2:N:45:GLY:HA2	2.15	0.46
1:A:89:VAL:HG22	1:A:90:GLY:N	2.31	0.46
1:A:347:GLU:HB2	1:A:348:PRO:HD3	1.96	0.46
1:B:94:LYS:O	1:B:94:LYS:HG2	2.16	0.46
1:C:91:TYR:CE1	1:C:93:GLY:HA3	2.50	0.46
2:G:52:ASP:O	2:G:55:THR:HG23	2.16	0.46
2:G:86:ARG:HH11	2:G:86:ARG:CA	2.26	0.46
2:I:50:THR:O	2:I:54:PHE:HD1	1.98	0.46
2:L:81:ASP:HA	2:L:84:THR:OG1	2.15	0.46
1:B:268:TYR:HD1	1:B:269:SER:H	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:115:PRO:HG3	2:M:121:LEU:CG	2.46	0.46
1:B:439:LEU:HD12	2:H:72:LEU:HD12	1.98	0.46
2:G:18:GLY:N	2:G:164:ASN:HD21	1.99	0.46
2:G:86:ARG:O	2:G:88:LEU:N	2.48	0.46
2:G:117:GLU:HG3	2:G:118:ASP:H	1.81	0.46
2:H:36:ARG:HG2	2:H:43:LEU:HD23	1.97	0.46
2:H:38:TYR:O	2:H:39:ASN:HB2	2.15	0.46
2:M:141:THR:HG22	2:M:142:GLU:N	2.29	0.46
1:A:17:ILE:HD12	1:A:17:ILE:N	2.31	0.46
1:B:96:VAL:HG12	1:B:285:LEU:HD22	1.98	0.46
2:L:80:LYS:O	2:L:80:LYS:HD3	2.16	0.46
2:N:50:THR:O	2:N:53:ALA:HB3	2.16	0.46
2:N:115:PRO:HG3	2:N:121:LEU:CD1	2.46	0.46
1:C:268:TYR:O	1:C:270:GLY:N	2.48	0.46
2:H:36:ARG:NH2	2:H:172:LEU:HD23	2.31	0.46
1:C:20:GLN:CA	1:C:20:GLN:NE2	2.75	0.46
1:C:405:ASP:HB3	1:C:406:LYS:HD2	1.98	0.46
2:L:93:ALA:O	2:L:94:MET:HE2	2.15	0.46
2:L:110:GLY:O	2:L:111:ASP:CB	2.62	0.46
2:M:118:ASP:OD2	2:M:120:ILE:HD12	2.16	0.46
2:N:86:ARG:O	2:N:90:LYS:HD3	2.16	0.46
2:N:92:GLU:O	2:N:93:ALA:HB2	2.15	0.46
1:A:20:GLN:CA	1:A:20:GLN:NE2	2.58	0.46
1:A:283:LEU:HD21	1:A:322:GLU:HB3	1.97	0.46
1:A:430:LEU:O	1:A:431:GLY:C	2.58	0.46
1:B:104:THR:HG22	1:B:295:HIS:CD2	2.51	0.46
1:A:283:LEU:HD11	1:A:322:GLU:HB2	1.99	0.45
1:B:362:THR:HG21	1:C:36:ARG:CG	2.46	0.45
2:G:5:SER:CB	2:G:14:VAL:HG22	2.45	0.45
2:H:99:ASP:HA	2:H:172:LEU:HD12	1.97	0.45
2:N:38:TYR:CD1	2:N:41:LYS:HD3	2.51	0.45
1:A:86:PHE:O	1:A:87:THR:C	2.60	0.45
1:C:313:VAL:HG23	1:C:314:ALA:N	2.22	0.45
2:L:70:HIS:CD2	2:L:73:LYS:HD3	2.51	0.45
2:L:83:ARG:NH1	2:L:83:ARG:HG3	2.31	0.45
2:M:62:ARG:O	2:M:66:MET:HG2	2.16	0.45
1:B:4:MET:HB3	1:B:8:GLU:HB2	1.98	0.45
1:B:355:GLN:O	1:B:359:LEU:HD22	2.16	0.45
2:L:103:SER:C	2:L:104:LEU:HG	2.41	0.45
2:M:109:ILE:CG1	2:M:110:GLY:H	2.11	0.45
2:M:115:PRO:HG3	2:M:121:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ARG:HG3	1:C:48:VAL:CG1	2.46	0.45
2:H:56:LEU:HD13	2:H:95:LEU:CG	2.39	0.45
2:I:42:VAL:HG21	2:I:64:LEU:HD13	1.97	0.45
2:L:64:LEU:HA	2:L:74:SER:OG	2.16	0.45
2:M:147:GLU:O	2:M:151:LYS:HG3	2.16	0.45
1:B:444:LEU:OXT	2:H:113:VAL:HA	2.17	0.45
2:G:80:LYS:HD2	2:G:80:LYS:O	2.17	0.45
2:G:105:ILE:HG22	2:G:121:LEU:HD13	1.98	0.45
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.80	0.45
2:G:67:HIS:C	2:G:69:GLY:H	2.24	0.45
2:L:4:VAL:HG13	2:L:149:VAL:HG13	1.99	0.45
2:L:19:GLN:NE2	2:L:162:PHE:HA	2.31	0.45
2:L:104:LEU:HD22	2:L:112:VAL:CG1	2.47	0.45
2:H:13:VAL:HG22	2:H:171:GLU:HB3	1.97	0.45
2:N:117:GLU:H	2:N:117:GLU:HG3	1.56	0.45
1:A:53:ILE:HG22	1:A:54:LEU:N	2.31	0.45
1:C:72:LYS:N	1:C:72:LYS:CD	2.80	0.45
1:C:270:GLY:C	1:C:272:ASP:N	2.75	0.45
1:C:437:GLU:OE1	1:C:437:GLU:N	2.48	0.45
2:H:70:HIS:O	2:H:71:LEU:C	2.60	0.45
2:L:68:GLN:O	2:L:70:HIS:N	2.49	0.45
1:A:2:SER:HB3	1:A:35:TRP:HE1	1.81	0.45
2:L:95:LEU:HB2	2:L:106:ILE:HB	1.99	0.45
1:A:63:LYS:HG2	1:A:333:LEU:HD13	1.99	0.44
1:B:87:THR:HB	1:B:88:GLU:OE2	2.16	0.44
2:G:104:LEU:HD11	2:G:114:GLN:HG2	1.98	0.44
2:L:153:LEU:HB3	2:L:167:PHE:CE2	2.52	0.44
2:M:3:ILE:HB	2:M:123:ILE:HG12	1.98	0.44
2:N:104:LEU:HD22	2:N:104:LEU:N	2.32	0.44
1:A:20:GLN:HE21	1:A:20:GLN:H	1.64	0.44
1:B:35:TRP:O	1:B:39:GLN:NE2	2.50	0.44
2:H:3:ILE:HB	2:H:123:ILE:CG1	2.48	0.44
2:H:62:ARG:O	2:H:66:MET:HG3	2.17	0.44
2:H:90:LYS:HD3	2:H:90:LYS:N	2.32	0.44
2:I:86:ARG:HD3	2:I:86:ARG:N	2.27	0.44
2:L:83:ARG:HG3	2:L:83:ARG:HH11	1.82	0.44
2:M:19:GLN:NE2	2:M:162:PHE:HA	2.33	0.44
2:M:43:LEU:HD23	2:M:43:LEU:N	2.29	0.44
2:N:105:ILE:HD11	2:N:121:LEU:HB3	1.99	0.44
1:C:352:LEU:HD13	1:C:400:MET:HG3	1.99	0.44
1:B:41:GLN:HA	1:B:41:GLN:HE21	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:116:GLU:C	2:M:118:ASP:N	2.75	0.44
1:A:41:GLN:HA	1:A:41:GLN:NE2	2.33	0.44
2:H:131:LEU:CG	2:H:135:ARG:NH1	2.81	0.44
2:H:137:LEU:HG	2:H:143:LEU:HD12	1.99	0.44
2:I:115:PRO:HG3	2:I:121:LEU:CG	2.48	0.44
2:L:141:THR:HG21	2:L:143:LEU:CG	2.45	0.44
1:A:41:GLN:HA	1:A:41:GLN:HE21	1.81	0.44
1:C:18:ILE:HG13	1:C:344:ILE:HD13	1.98	0.44
2:N:120:ILE:O	2:N:121:LEU:HD23	2.17	0.44
1:A:73:LEU:HD12	1:A:73:LEU:C	2.43	0.44
2:L:82:TRP:HA	2:L:88:LEU:HD23	1.98	0.44
2:N:71:LEU:HD22	2:N:99:ASP:OD2	2.17	0.44
1:A:334:THR:OG1	1:A:335:ALA:N	2.49	0.44
1:B:441:ARG:NH2	2:I:36:ARG:O	2.45	0.44
2:H:19:GLN:NE2	2:H:164:ASN:HB3	2.32	0.44
2:I:38:TYR:CD1	2:I:41:LYS:HD3	2.52	0.44
1:C:55:MET:HE3	1:C:306:ILE:HG21	1.99	0.44
1:C:390:ASN:HB2	2:I:68:GLN:OE1	2.18	0.44
2:G:75:ALA:HB1	2:G:112:VAL:HG11	2.00	0.44
2:M:37:LEU:O	2:M:38:TYR:C	2.60	0.44
1:A:313:VAL:HG23	1:A:314:ALA:N	2.33	0.43
2:N:36:ARG:NH1	2:N:36:ARG:HG2	2.31	0.43
1:A:345:LEU:HD13	1:A:396:LEU:HD13	2.01	0.43
2:G:19:GLN:HB2	2:G:164:ASN:HB3	2.00	0.43
2:H:80:LYS:O	2:H:84:THR:HG23	2.18	0.43
2:N:12:VAL:CG1	2:N:172:LEU:HD12	2.45	0.43
2:N:86:ARG:HA	2:N:89:ARG:CZ	2.48	0.43
1:A:20:GLN:N	1:A:20:GLN:NE2	2.64	0.43
1:A:267:GLU:CG	2:G:62:ARG:HH12	2.18	0.43
1:A:379:GLU:O	1:A:383:ARG:HB2	2.17	0.43
1:A:388:THR:OG1	1:A:389:GLU:N	2.51	0.43
2:G:37:LEU:HD21	2:G:57:PHE:CZ	2.53	0.43
2:H:116:GLU:O	2:H:117:GLU:C	2.62	0.43
2:N:7:ARG:HB3	2:N:119:GLN:HB3	2.00	0.43
2:N:46:PHE:CE2	2:N:50:THR:HG22	2.53	0.43
1:A:359:LEU:HD13	1:A:359:LEU:HA	1.80	0.43
1:B:85:LYS:O	1:B:85:LYS:HG3	2.17	0.43
2:M:88:LEU:HD12	2:M:88:LEU:N	2.33	0.43
1:B:280:ARG:HH11	1:B:280:ARG:CG	2.31	0.43
2:G:2:THR:OG1	2:G:126:GLY:HA3	2.18	0.43
2:H:13:VAL:HG22	2:H:171:GLU:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:94:MET:CB	2:L:123:ILE:HD12	2.48	0.43
2:N:4:VAL:HG12	2:N:153:LEU:HD21	2.01	0.43
2:N:115:PRO:HG3	2:N:121:LEU:CG	2.48	0.43
1:A:36:ARG:O	1:A:39:GLN:HB2	2.19	0.43
1:A:283:LEU:HD11	1:A:322:GLU:CB	2.49	0.43
1:B:88:GLU:N	1:B:88:GLU:CD	2.77	0.43
1:B:283:LEU:HB2	1:B:284:PRO:HD3	2.00	0.43
1:B:443:ILE:HD11	2:H:72:LEU:HD11	2.00	0.43
1:C:266:GLY:O	1:C:267:GLU:HG2	2.18	0.43
1:C:341:PHE:HB2	1:C:378:ALA:HB1	2.01	0.43
2:G:150:GLU:C	2:G:150:GLU:CD	2.86	0.43
2:M:53:ALA:O	2:M:57:PHE:HB2	2.18	0.43
1:A:89:VAL:HG23	1:A:94:LYS:HB2	2.00	0.43
1:C:4:MET:HE2	1:C:8:GLU:HB3	1.99	0.43
2:H:88:LEU:O	2:H:89:ARG:C	2.61	0.43
2:I:75:ALA:HB1	2:I:112:VAL:HG11	1.99	0.43
2:L:18:GLY:O	2:L:29:GLY:O	2.36	0.43
2:L:46:PHE:CZ	2:L:50:THR:HG22	2.54	0.43
2:M:43:LEU:HD23	2:M:98:ALA:O	2.19	0.43
2:M:71:LEU:HD12	2:M:71:LEU:H	1.82	0.43
1:A:85:LYS:O	1:A:85:LYS:HG2	2.18	0.43
1:B:36:ARG:O	1:B:39:GLN:HB2	2.18	0.43
1:B:428:ASP:OD1	1:B:429:ALA:N	2.52	0.43
1:C:41:GLN:HE21	1:C:41:GLN:HA	1.84	0.43
2:L:43:LEU:HD22	2:L:172:LEU:CD1	2.48	0.43
1:A:34:ARG:CZ	1:A:251:ASN:HA	2.49	0.43
1:A:91:TYR:OH	1:A:94:LYS:HE3	2.19	0.43
1:C:250:GLN:NE2	1:C:250:GLN:HA	2.34	0.43
2:L:20:VAL:O	2:L:27:MET:HB3	2.19	0.43
1:A:267:GLU:N	2:G:62:ARG:HH12	2.16	0.42
1:B:439:LEU:CD1	2:H:72:LEU:HD12	2.49	0.42
1:C:34:ARG:HG3	1:C:34:ARG:HH11	1.84	0.42
2:H:52:ASP:HA	2:H:55:THR:HG23	2.00	0.42
2:H:159:ILE:O	2:M:25:THR:HA	2.19	0.42
2:I:18:GLY:H	2:I:164:ASN:ND2	2.11	0.42
1:B:290:THR:HG22	1:B:297:MET:HE3	2.01	0.42
2:H:100:GLU:C	2:H:101:LYS:HE2	2.44	0.42
2:N:19:GLN:HE22	2:N:162:PHE:HA	1.83	0.42
1:B:410:SER:O	1:B:411:ALA:C	2.60	0.42
1:C:42:GLU:OE2	1:C:45:ARG:NH2	2.50	0.42
2:H:52:ASP:O	2:H:55:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:19:GLN:HE22	2:M:162:PHE:HA	1.84	0.42
2:M:60:PHE:HB2	2:M:78:LEU:HD22	2.01	0.42
2:N:68:GLN:C	2:N:70:HIS:H	2.26	0.42
1:A:275:ARG:O	1:A:278:VAL:HG22	2.18	0.42
1:C:395:ARG:HA	1:C:395:ARG:HD3	1.82	0.42
2:H:36:ARG:HH22	2:H:172:LEU:HD23	1.84	0.42
2:I:60:PHE:HA	2:I:78:LEU:HD22	2.01	0.42
2:L:39:ASN:O	2:L:41:LYS:HG2	2.19	0.42
2:N:60:PHE:CD1	2:N:78:LEU:HD22	2.55	0.42
2:N:83:ARG:NH1	2:N:110:GLY:HA2	2.34	0.42
2:N:84:THR:O	2:N:89:ARG:NH1	2.52	0.42
1:B:359:LEU:O	1:B:362:THR:HB	2.20	0.42
1:B:417:GLN:HE21	1:B:417:GLN:HB3	1.64	0.42
2:M:72:LEU:HA	2:M:104:LEU:HD21	2.01	0.42
2:M:172:LEU:HB2	2:M:173:PRO:HD3	2.01	0.42
1:B:387:LYS:HD2	1:B:435:GLU:OE2	2.19	0.42
2:G:131:LEU:HD21	2:G:135:ARG:NH2	2.35	0.42
2:L:70:HIS:CB	2:L:73:LYS:HD3	2.50	0.42
2:M:105:ILE:HD11	2:M:121:LEU:HB3	2.01	0.42
1:A:436:ASN:HB3	1:A:437:GLU:H	1.62	0.42
1:C:380:ALA:O	1:C:384:VAL:HG12	2.20	0.42
2:L:109:ILE:HG13	2:L:110:GLY:N	2.33	0.42
2:L:22:LEU:HB2	2:L:27:MET:CE	2.47	0.42
1:A:16:HIS:CB	1:A:17:ILE:HD12	2.47	0.42
1:C:56:ILE:HA	1:C:309:GLY:O	2.19	0.42
1:C:72:LYS:N	1:C:72:LYS:HD2	2.34	0.42
1:C:253:ILE:HD12	1:C:304:LEU:HD23	2.01	0.42
2:H:99:ASP:OD2	2:H:99:ASP:C	2.63	0.42
2:I:28:LYS:HG2	2:I:30:ASN:H	1.84	0.42
1:A:53:ILE:CG2	1:A:54:LEU:N	2.83	0.42
1:B:387:LYS:HD3	1:B:387:LYS:HA	1.87	0.42
1:A:26:ALA:CB	1:A:331:VAL:HG11	2.50	0.41
2:N:71:LEU:HD23	2:N:104:LEU:HD23	2.02	0.41
1:C:283:LEU:HD21	1:C:322:GLU:HB3	2.01	0.41
1:C:283:LEU:HD11	1:C:322:GLU:CB	2.50	0.41
1:C:443:ILE:HG21	2:I:114:GLN:HG3	2.02	0.41
2:G:117:GLU:CG	2:G:118:ASP:N	2.82	0.41
2:H:7:ARG:HB3	2:H:119:GLN:HB3	2.02	0.41
2:M:92:GLU:O	2:M:93:ALA:HB2	2.20	0.41
2:M:104:LEU:HD12	2:M:104:LEU:N	2.35	0.41
2:N:165:THR:HA	2:N:167:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLN:CA	1:B:20:GLN:NE2	2.79	0.41
1:B:395:ARG:HA	1:B:395:ARG:HD3	1.78	0.41
1:C:434:VAL:HG23	1:C:434:VAL:O	2.20	0.41
2:G:105:ILE:HG22	2:G:121:LEU:HD22	2.02	0.41
2:G:105:ILE:CG2	2:G:121:LEU:HD22	2.50	0.41
2:H:33:LYS:O	2:H:45:GLY:HA2	2.20	0.41
2:L:88:LEU:HA	2:L:91:LEU:CD1	2.45	0.41
2:N:3:ILE:O	2:N:122:ALA:HA	2.20	0.41
1:A:65:GLU:CG	3:A:450:ADP:H2'	2.48	0.41
1:B:57:GLY:HA2	1:B:58:PRO:HD3	1.86	0.41
1:B:444:LEU:HD23	1:B:444:LEU:HA	1.90	0.41
1:C:76:ALA:HB1	1:C:251:ASN:O	2.21	0.41
2:I:105:ILE:O	2:I:105:ILE:HG23	2.19	0.41
2:L:85:ASP:HB3	2:L:88:LEU:HD13	2.02	0.41
2:M:12:VAL:HG11	2:M:172:LEU:HD12	2.02	0.41
2:M:35:ARG:HB2	2:M:57:PHE:HE2	1.86	0.41
1:A:57:GLY:HA2	1:A:58:PRO:HD3	1.87	0.41
2:L:9:ASN:C	2:L:11:GLN:N	2.75	0.41
2:M:119:GLN:OE1	2:M:119:GLN:HA	2.20	0.41
2:M:165:THR:HA	2:M:167:PHE:CE2	2.55	0.41
2:N:12:VAL:HG13	2:N:12:VAL:O	2.21	0.41
1:B:437:GLU:O	1:B:439:LEU:N	2.53	0.41
2:G:17:ASP:HB2	2:G:164:ASN:HD22	1.86	0.41
2:L:7:ARG:HD2	2:L:119:GLN:NE2	2.31	0.41
2:M:36:ARG:HG2	2:M:36:ARG:NH1	2.36	0.41
2:N:118:ASP:O	2:N:119:GLN:HB2	2.20	0.41
1:A:2:SER:CB	1:A:35:TRP:HE1	2.34	0.41
1:B:391:ILE:HG22	1:C:321:PRO:HB3	2.03	0.41
1:B:405:ASP:HB3	1:B:406:LYS:HD2	2.03	0.41
1:C:91:TYR:CE2	1:C:94:LYS:HG3	2.56	0.41
1:C:100:ILE:CB	1:C:291:VAL:HG21	2.51	0.41
2:G:88:LEU:O	2:G:89:ARG:C	2.63	0.41
2:H:90:LYS:CG	2:H:91:LEU:H	2.34	0.41
2:I:101:LYS:NZ	2:I:101:LYS:HB2	2.36	0.41
2:L:131:LEU:HD11	2:L:135:ARG:HE	1.84	0.41
2:M:46:PHE:CD2	2:M:53:ALA:HB2	2.56	0.41
2:N:120:ILE:HD11	2:N:138:VAL:HG21	2.02	0.41
1:B:443:ILE:HG21	2:H:114:GLN:HG3	2.02	0.41
1:C:41:GLN:HA	1:C:41:GLN:NE2	2.35	0.41
2:I:38:TYR:CD1	2:I:69:GLY:HA3	2.55	0.41
2:I:107:THR:OG1	2:I:111:ASP:OD2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:46:PHE:CZ	2:M:50:THR:HG22	2.56	0.41
1:A:96:VAL:CG1	1:A:285:LEU:HD22	2.51	0.40
1:B:362:THR:HG22	1:B:363:GLU:HG2	2.03	0.40
2:M:109:ILE:O	2:M:110:GLY:C	2.64	0.40
1:B:87:THR:HG23	1:B:274:SER:HB3	2.04	0.40
1:C:250:GLN:HA	1:C:250:GLN:HE21	1.85	0.40
2:L:19:GLN:HE22	2:L:162:PHE:HA	1.85	0.40
2:M:172:LEU:HA	2:M:172:LEU:HD23	1.84	0.40
2:N:172:LEU:CB	2:N:173:PRO:CD	2.99	0.40
1:B:265:LYS:O	1:B:266:GLY:C	2.64	0.40
1:B:443:ILE:CD1	2:H:72:LEU:HD11	2.51	0.40
2:H:105:ILE:HG13	2:H:121:LEU:HD13	2.02	0.40
2:M:118:ASP:O	2:M:119:GLN:HB2	2.21	0.40
2:N:115:PRO:HG3	2:N:121:LEU:HG	2.03	0.40
1:B:271:ALA:C	1:B:273:VAL:N	2.79	0.40
1:B:299:LYS:HE3	1:B:299:LYS:HB2	1.95	0.40
2:G:59:LEU:HA	2:G:59:LEU:HD12	1.82	0.40
2:H:13:VAL:HG12	2:H:14:VAL:N	2.36	0.40
2:H:137:LEU:HD13	2:N:136:ALA:HB1	2.02	0.40
1:A:10:VAL:HG12	1:A:14:ASP:OD2	2.21	0.40
1:B:49:THR:HB	1:B:50:PRO:HD2	2.03	0.40
1:C:5:THR:OG1	1:C:8:GLU:HG3	2.21	0.40
2:G:103:SER:O	2:G:115:PRO:HD3	2.22	0.40
2:G:107:THR:OG1	2:G:111:ASP:OD2	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	307/310 (99%)	277 (90%)	19 (6%)	11 (4%)	2 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	307/310 (99%)	283 (92%)	16 (5%)	8 (3%)	4	7
1	C	307/310 (99%)	281 (92%)	18 (6%)	8 (3%)	4	7
2	G	172/174 (99%)	153 (89%)	15 (9%)	4 (2%)	5	8
2	H	172/174 (99%)	157 (91%)	12 (7%)	3 (2%)	7	13
2	I	172/174 (99%)	158 (92%)	13 (8%)	1 (1%)	21	38
2	L	172/174 (99%)	144 (84%)	21 (12%)	7 (4%)	2	3
2	M	172/174 (99%)	149 (87%)	15 (9%)	8 (5%)	2	2
2	N	172/174 (99%)	144 (84%)	20 (12%)	8 (5%)	2	2
All	All	1953/1974 (99%)	1746 (89%)	149 (8%)	58 (3%)	3	5

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	VAL
1	A	434	VAL
1	A	437	GLU
1	A	439	LEU
1	B	267	GLU
1	C	269	SER
2	G	115	PRO
2	H	89	ARG
2	L	112	VAL
2	M	111	ASP
1	A	244	ALA
1	A	431	GLY
1	B	265	LYS
1	B	438	ASP
1	C	265	LYS
1	C	266	GLY
1	C	431	GLY
1	C	432	GLU
1	C	434	VAL
2	G	87	ALA
2	G	117	GLU
2	H	87	ALA
2	L	69	GLY
2	L	110	GLY
2	L	111	ASP
2	M	69	GLY

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Mol	Chain	Res	Type
2	M	117	GLU
2	N	68	GLN
2	N	69	GLY
2	N	115	PRO
1	B	89	VAL
2	H	115	PRO
2	L	9	ASN
2	L	68	GLN
2	M	101	LYS
2	M	110	GLY
2	N	70	HIS
2	N	111	ASP
1	A	42	GLU
1	A	268	TYR
1	B	43	PRO
1	B	269	SER
2	G	86	ARG
2	M	172	LEU
2	N	172	LEU
1	B	437	GLU
1	C	43	PRO
2	N	173	PRO
1	A	43	PRO
2	L	109	ILE
2	M	68	GLN
1	A	90	GLY
2	M	109	ILE
1	B	42	GLU
2	N	110	GLY
1	A	92	VAL
1	C	42	GLU
2	I	115	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	255/256 (100%)	237 (93%)	18 (7%)	13	29
1	B	255/256 (100%)	237 (93%)	18 (7%)	13	29
1	C	255/256 (100%)	235 (92%)	20 (8%)	11	24
2	G	139/140 (99%)	128 (92%)	11 (8%)	11	24
2	H	139/140 (99%)	129 (93%)	10 (7%)	13	28
2	I	139/140 (99%)	123 (88%)	16 (12%)	5	11
2	L	139/140 (99%)	137 (99%)	2 (1%)	59	81
2	M	139/140 (99%)	136 (98%)	3 (2%)	45	73
2	N	139/140 (99%)	134 (96%)	5 (4%)	31	58
All	All	1599/1608 (99%)	1496 (94%)	103 (6%)	16	33

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	39	GLN
1	A	48	VAL
1	A	82	GLU
1	A	264	LYS
1	A	267	GLU
1	A	291	VAL
1	A	298	VAL
1	A	345	LEU
1	A	359	LEU
1	A	362	THR
1	A	367	ILE
1	A	372	ASP
1	A	379	GLU
1	A	384	VAL
1	A	394	ARG
1	A	420	ASN
1	A	428	ASP
1	B	7	ARG
1	B	20	GLN
1	B	34	ARG
1	B	39	GLN
1	B	46	HIS
1	B	48	VAL
1	B	82	GLU
1	B	291	VAL

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Mol	Chain	Res	Type
1	B	298	VAL
1	B	336	LEU
1	B	345	LEU
1	B	359	LEU
1	B	362	THR
1	B	367	ILE
1	B	394	ARG
1	B	418	THR
1	B	428	ASP
1	B	441	ARG
1	C	7	ARG
1	C	20	GLN
1	C	34	ARG
1	C	38	MET
1	C	39	GLN
1	C	42	GLU
1	C	48	VAL
1	C	75	ASN
1	C	82	GLU
1	C	268	TYR
1	C	298	VAL
1	C	331	VAL
1	C	332	GLU
1	C	336	LEU
1	C	345	LEU
1	C	359	LEU
1	C	418	THR
1	C	428	ASP
1	C	432	GLU
1	C	437	GLU
2	G	55	THR
2	G	56	LEU
2	G	59	LEU
2	G	71	LEU
2	G	72	LEU
2	G	86	ARG
2	G	104	LEU
2	G	105	ILE
2	G	137	LEU
2	G	141	THR
2	G	164	ASN
2	H	21	SER

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Mol	Chain	Res	Type
2	H	55	THR
2	H	56	LEU
2	H	72	LEU
2	H	91	LEU
2	H	112	VAL
2	H	135	ARG
2	H	137	LEU
2	H	141	THR
2	H	164	ASN
2	I	22	LEU
2	I	41	LYS
2	I	55	THR
2	I	56	LEU
2	I	72	LEU
2	I	76	VAL
2	I	84	THR
2	I	86	ARG
2	I	90	LYS
2	I	91	LEU
2	I	101	LYS
2	I	104	LEU
2	I	107	THR
2	I	111	ASP
2	I	137	LEU
2	I	164	ASN
2	L	43	LEU
2	L	91	LEU
2	M	43	LEU
2	M	73	LYS
2	M	117	GLU
2	N	25	THR
2	N	73	LYS
2	N	80	LYS
2	N	117	GLU
2	N	137	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	39	GLN
1	A	41	GLN

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Mol	Chain	Res	Type
1	A	250	GLN
1	A	295	HIS
1	A	302	HIS
1	A	324	GLN
1	A	436	ASN
1	B	20	GLN
1	B	39	GLN
1	B	41	GLN
1	B	250	GLN
1	B	295	HIS
1	B	312	GLN
1	B	324	GLN
1	B	417	GLN
1	C	20	GLN
1	C	39	GLN
1	C	41	GLN
1	C	52	ASN
1	C	75	ASN
1	C	250	GLN
1	C	295	HIS
2	G	19	GLN
2	G	24	ASN
2	G	119	GLN
2	G	128	ASN
2	G	164	ASN
2	H	19	GLN
2	H	24	ASN
2	H	119	GLN
2	H	164	ASN
2	I	11	GLN
2	I	19	GLN
2	I	24	ASN
2	I	140	ASN
2	I	164	ASN
2	L	11	GLN
2	L	19	GLN
2	L	30	ASN
2	L	39	ASN
2	L	128	ASN
2	L	166	ASN
2	M	19	GLN
2	M	39	ASN

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Mol	Chain	Res	Type
2	N	19	GLN
2	N	67	HIS
2	N	70	HIS
2	N	140	ASN
2	N	166	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	ADP	B	450	4	28,29,29	2.55	10 (35%)	43,45,45	1.67	8 (18%)
5	PO4	C	452	4	4,4,4	1.34	0	6,6,6	0.50	0
5	PO4	A	452	4	4,4,4	1.44	0	6,6,6	0.47	0
3	ADP	C	450	4	28,29,29	2.61	11 (39%)	43,45,45	1.66	8 (18%)
3	ADP	A	450	4	28,29,29	2.64	10 (35%)	43,45,45	1.62	8 (18%)
5	PO4	B	452	4	4,4,4	1.49	0	6,6,6	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	450	4	-	2/16/32/32	0/3/3/3
3	ADP	B	450	4	-	2/16/32/32	0/3/3/3
3	ADP	C	450	4	-	2/16/32/32	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	450	ADP	C2-N1	6.30	1.45	1.33
3	A	450	ADP	PA-O3A	6.29	1.66	1.59
3	C	450	ADP	PA-O3A	6.23	1.66	1.59
3	B	450	ADP	PA-O3A	6.09	1.66	1.59
3	B	450	ADP	C2-N1	5.87	1.44	1.33
3	C	450	ADP	C2-N1	5.83	1.44	1.33
3	C	450	ADP	PB-O1B	5.15	1.66	1.50
3	A	450	ADP	PB-O1B	4.83	1.65	1.50
3	B	450	ADP	PB-O1B	4.65	1.64	1.50
3	A	450	ADP	C4-N3	4.60	1.43	1.34
3	B	450	ADP	C4-N3	4.44	1.42	1.34
3	C	450	ADP	C4-N3	4.43	1.42	1.34
3	B	450	ADP	PB-O2B	3.58	1.68	1.54
3	A	450	ADP	C8-N9	3.42	1.43	1.37
3	B	450	ADP	C8-N9	3.37	1.43	1.37
3	C	450	ADP	C8-N9	3.28	1.43	1.37
3	C	450	ADP	PB-O2B	3.18	1.66	1.54
3	A	450	ADP	PB-O2B	3.18	1.66	1.54
3	C	450	ADP	PA-O2A	2.90	1.68	1.55
3	A	450	ADP	PA-O2A	2.85	1.68	1.55
3	B	450	ADP	PA-O2A	2.80	1.68	1.55
3	A	450	ADP	PA-O1A	2.73	1.60	1.50
3	C	450	ADP	C6-N6	2.73	1.41	1.34
3	B	450	ADP	PA-O1A	2.59	1.59	1.50
3	A	450	ADP	C6-N6	2.43	1.40	1.34
3	B	450	ADP	C6-N6	2.40	1.40	1.34
3	C	450	ADP	PA-O1A	2.30	1.58	1.50
3	C	450	ADP	C5-C4	-2.18	1.35	1.39
3	A	450	ADP	C5-C6	2.17	1.47	1.41
3	C	450	ADP	C5-C6	2.14	1.46	1.41
3	B	450	ADP	C5-C6	2.11	1.46	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	450	ADP	N3-C2-N1	-5.58	120.14	128.58
3	B	450	ADP	N3-C2-N1	-5.44	120.35	128.58
3	A	450	ADP	N3-C2-N1	-5.39	120.42	128.58
3	B	450	ADP	C5-C4-N3	-3.50	121.90	126.72
3	A	450	ADP	C5-C4-N3	-3.48	121.93	126.72
3	C	450	ADP	C5-C4-N3	-3.31	122.16	126.72
3	B	450	ADP	O2A-PA-O3A	2.94	115.22	107.27
3	C	450	ADP	C2-N3-C4	2.91	118.94	111.83
3	B	450	ADP	C2-N3-C4	2.82	118.72	111.83
3	A	450	ADP	C2-N3-C4	2.74	118.52	111.83
3	B	450	ADP	O2B-PB-O3A	2.66	113.56	104.64
3	B	450	ADP	N3-C4-N9	2.65	131.67	127.17
3	A	450	ADP	N3-C4-N9	2.61	131.60	127.17
3	A	450	ADP	O2B-PB-O3A	2.54	113.15	104.64
3	C	450	ADP	C2-N1-C6	2.53	122.88	118.73
3	A	450	ADP	C2-N1-C6	2.51	122.85	118.73
3	B	450	ADP	C2-N1-C6	2.46	122.77	118.73
3	C	450	ADP	N3-C4-N9	2.43	131.31	127.17
3	C	450	ADP	O2A-PA-O3A	2.38	113.69	107.27
3	C	450	ADP	O2B-PB-O3A	2.29	112.32	104.64
3	C	450	ADP	O5'-PA-O1A	-2.22	100.15	108.94
3	A	450	ADP	O2A-PA-O3A	2.17	113.13	107.27
3	B	450	ADP	O3A-PA-O1A	-2.10	104.40	110.70
3	A	450	ADP	O3A-PA-O1A	-2.01	104.67	110.70

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	450	ADP	O4'-C4'-C5'-O5'
3	C	450	ADP	C3'-C4'-C5'-O5'
3	A	450	ADP	O4'-C4'-C5'-O5'
3	B	450	ADP	O4'-C4'-C5'-O5'
3	A	450	ADP	C3'-C4'-C5'-O5'
3	B	450	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 7 short contacts:

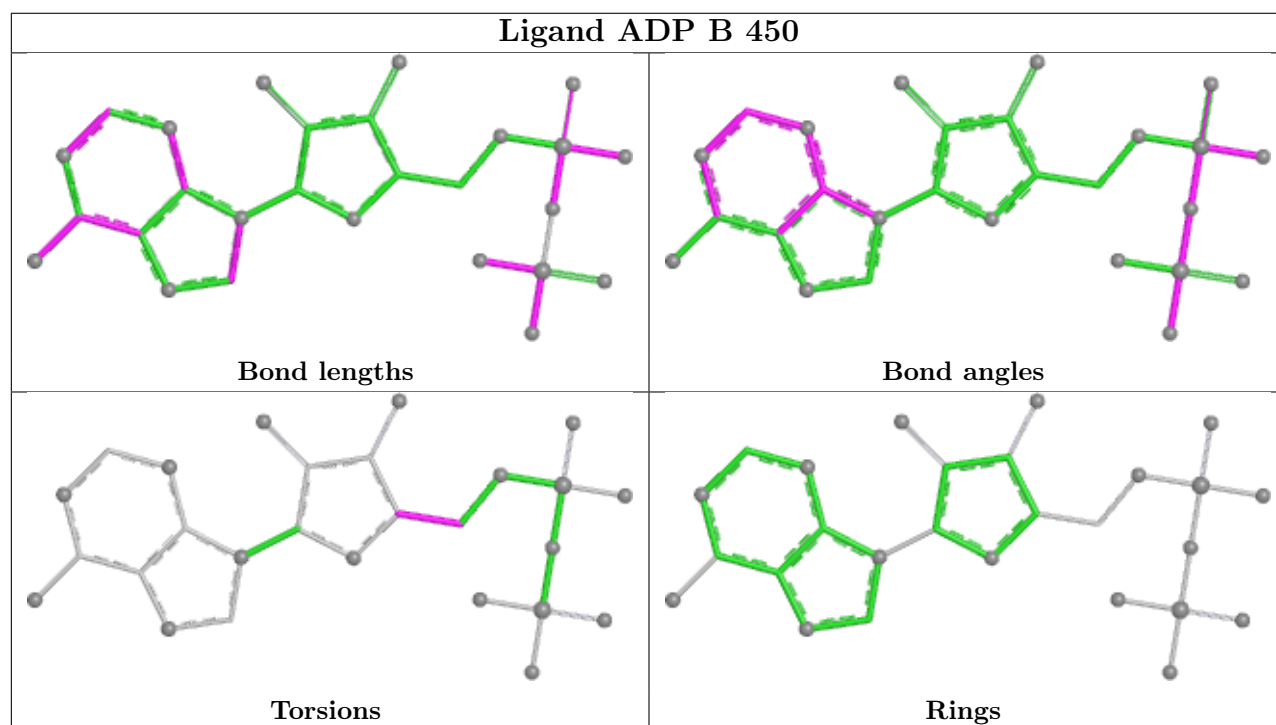
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	450	ADP	1	0

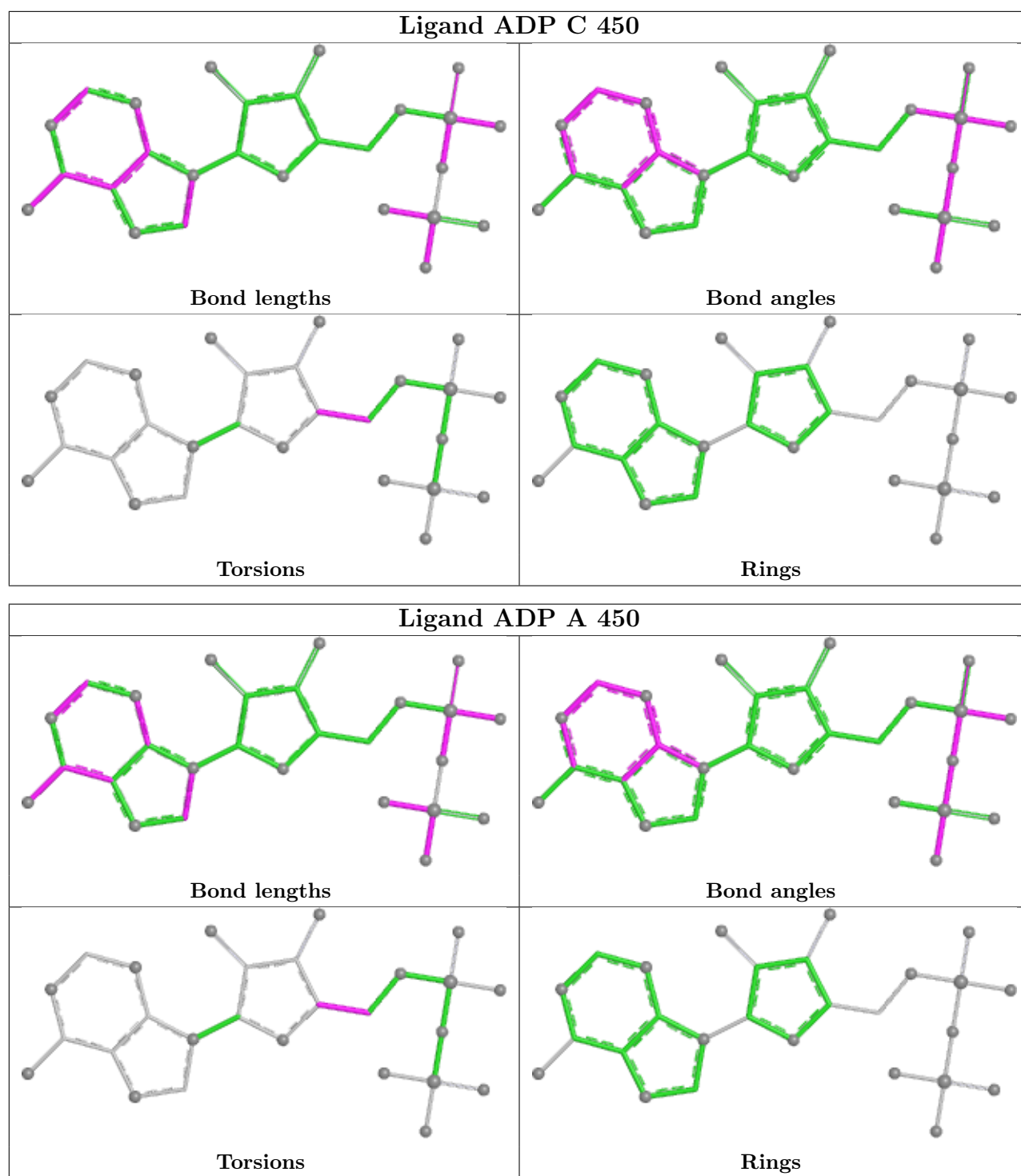
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	450	ADP	2	0
3	A	450	ADP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.