



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Aug 29, 2017 – 10:48 AM EDT

PDB ID : 5NVU  
EMDB ID: : EMD-3705  
Title : Full length human cytoplasmic dynein-1 in the phi-particle conformation  
Authors : Zhang, K.; Foster, H.E.; Carter, A.P.  
Deposited on : unknown  
Resolution : 15.00 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

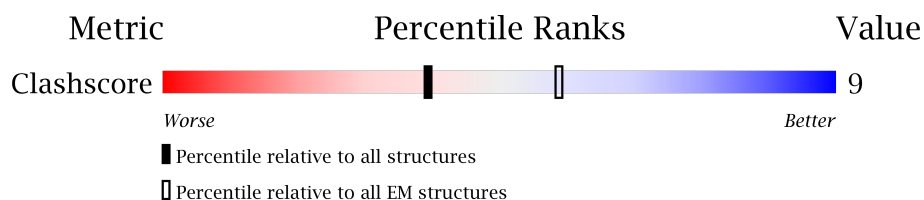
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

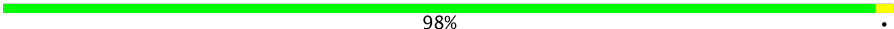
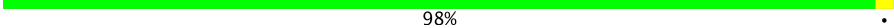


The reported resolution of this entry is 15.00 Å.

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)	EM structures (#Entries)
Clashscore	125131	1336

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

Mol	Chain	Length	Quality of chain
1	A	3169	 98% .
1	B	3169	 98% .
2	C	932	 80% 19% .
3	D	350	 96% .
3	E	350	 94% 6%
4	F	893	 83% 15% .
5	G	298	 99% .
6	H	295	 82% 17% .
7	I	125	 81% 19%
8	J	124	 88% 12%
9	K	85	 98% .

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Mol	Chain	Length	Quality of chain
9	L	85	 98% .
10	M	103	 92% 8%
11	N	104	 89% 11%
12	O	27	 100%
13	P	29	 100%
14	Q	120	 100%
14	R	120	 98% .

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51478 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Dynein motor domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	3169	Total	C	N	O	0	0
			15703	9365	3169	3169		
1	B	3169	Total	C	N	O	0	0
			15703	9365	3169	3169		

- Molecule 2 is a protein called Dynein tail heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	932	Total	C	N	O	0	0
			4654	2790	932	932		

- Molecule 3 is a protein called Dynein intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	350	Total	C	N	O	0	0
			1723	1023	350	350		
3	E	350	Total	C	N	O	0	0
			1723	1023	350	350		

- Molecule 4 is a protein called Dynein tail heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	893	Total	C	N	O	0	0
			4459	2673	893	893		

- Molecule 5 is a protein called Dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	298	Total	C	N	O	5	0
			1496	890	303	303		

- Molecule 6 is a protein called Dynein light intermediate chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	295	Total	C	N	O	0	0
			1459	869	295	295		

- Molecule 7 is a protein called N-terminal dimerization domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	125	Total	C	N	O	0	0
			625	375	125	125		

- Molecule 8 is a protein called N-terminal dimerization domain.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	124	Total	C	N	O	0	0
			620	372	124	124		

- Molecule 9 is a protein called LC8.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	85	Total	C	N	O	0	0
			421	251	85	85		
9	L	85	Total	C	N	O	0	0
			421	251	85	85		

- Molecule 10 is a protein called Tctex.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	103	Total	C	N	O	0	0
			507	301	103	103		

- Molecule 11 is a protein called Tctex.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	N	104	Total	C	N	O	0	0
			513	305	104	104		

- Molecule 12 is a protein called Intermediate chain N-terminus peptides.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	O	27	Total	C	N	O	0	0
			134	80	27	27		

- Molecule 13 is a protein called Intermediate chain N-terminus peptides.

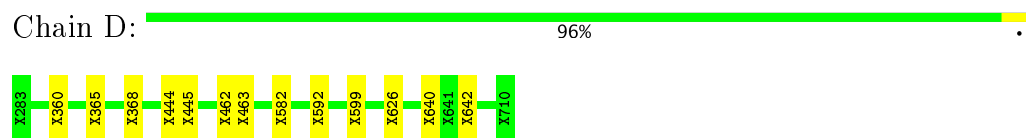
Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	29	Total	C	N	O	0	0
			143	85	29	29		

- Molecule 14 is a protein called Robl.

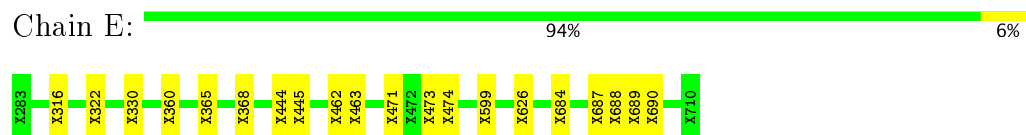
Mol	Chain	Residues	Atoms				AltConf	Trace
14	Q	120	Total	C	N	O	0	0
			587	347	120	120		
14	R	120	Total	C	N	O	0	0
			587	347	120	120		



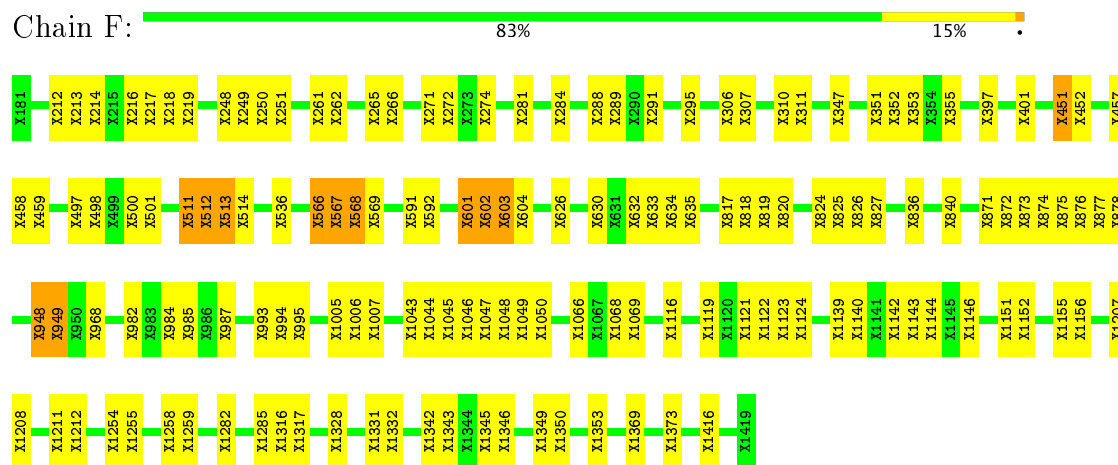
- Molecule 3: Dynein intermediate chain



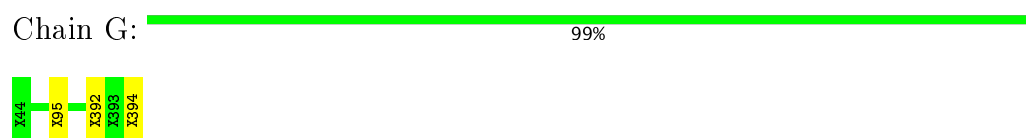
- Molecule 3: Dynein intermediate chain



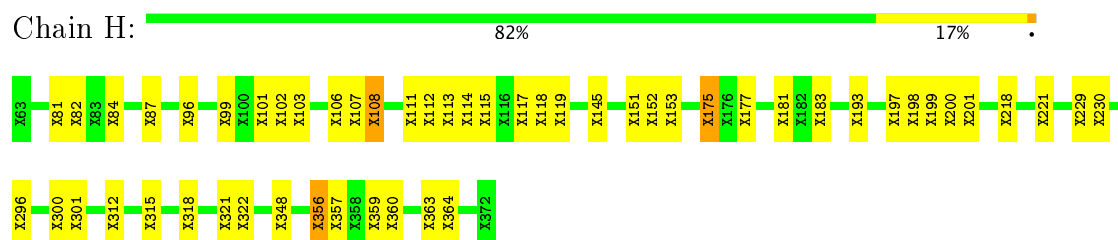
- Molecule 4: Dynein tail heavy chain



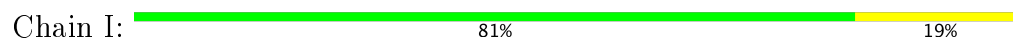
- Molecule 5: Dynein light intermediate chain



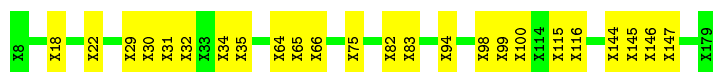
- Molecule 6: Dynein light intermediate chain



- Molecule 7: N-terminal dimerization domain

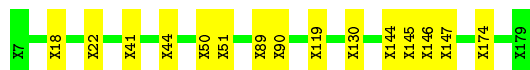






- Molecule 8: N-terminal dimerization domain

Chain J: 88% 12%



- Molecule 9: LC8

Chain K: 98% .



- Molecule 9: LC8

Chain L: 98% .



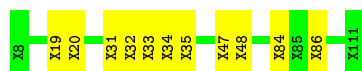
- Molecule 10: Tctex

Chain M: 92% 8%



- Molecule 11: Tctex

Chain N: 89% 11%



- Molecule 12: Intermediate chain N-terminus peptides

Chain O: 100%

There are no outlier residues recorded for this chain.

- Molecule 13: Intermediate chain N-terminus peptides

Chain P: 100%

There are no outlier residues recorded for this chain.

- Molecule 14: Robl

Chain Q: 100%

There are no outlier residues recorded for this chain.

- Molecule 14: Robl

Chain R:  98%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	28736	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.6	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
2	C	0	11
4	F	0	13
6	H	0	8
All	All	0	48

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2170	UNK	Peptide
1	A	2570	UNK	Peptide
1	A	2964	UNK	Peptide
1	A	3069	UNK	Peptide
1	A	3084	UNK	Peptide
1	A	3834	UNK	Peptide
1	A	3898	UNK	Peptide
1	A	4441	UNK	Peptide
1	B	2170	UNK	Peptide
1	B	2570	UNK	Peptide
1	B	2964	UNK	Peptide
1	B	3069	UNK	Peptide
1	B	3084	UNK	Peptide

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Mol	Chain	Res	Type	Group
1	B	3834	UNK	Peptide
1	B	3898	UNK	Peptide
1	B	4441	UNK	Peptide
2	C	477	UNK	Mainchain
2	C	566	UNK	Mainchain
2	C	567	UNK	Mainchain
2	C	568	UNK	Mainchain
2	C	601	UNK	Mainchain
2	C	602	UNK	Mainchain
2	C	603	UNK	Mainchain
2	C	641	UNK	Mainchain
2	C	642	UNK	Mainchain
2	C	643	UNK	Mainchain
2	C	994	UNK	Peptide
4	F	451	UNK	Mainchain
4	F	511	UNK	Mainchain
4	F	512	UNK	Mainchain
4	F	513	UNK	Mainchain
4	F	566	UNK	Mainchain
4	F	567	UNK	Mainchain
4	F	568	UNK	Mainchain
4	F	601	UNK	Mainchain
4	F	602	UNK	Mainchain
4	F	603	UNK	Mainchain
4	F	948	UNK	Mainchain
4	F	949	UNK	Mainchain
4	F	968	UNK	Peptide
6	H	108	UNK	Mainchain,Peptide
6	H	175	UNK	Mainchain
6	H	218	UNK	Mainchain
6	H	312	UNK	Mainchain
6	H	356	UNK	Mainchain
6	H	84	UNK	Mainchain
6	H	96	UNK	Mainchain

## 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	15703	0	3145	36	0
1	B	15703	0	3143	43	0
2	C	4654	0	984	212	0
3	D	1723	0	360	9	0
3	E	1723	0	358	48	0
4	F	4459	0	955	152	0
5	G	1496	0	301	2	0
6	H	1459	0	295	48	0
7	I	625	0	146	19	0
8	J	620	0	142	15	0
9	K	421	0	94	1	0
9	L	421	0	95	1	0
10	M	507	0	108	6	0
11	N	513	0	112	7	0
12	O	134	0	30	0	0
13	P	143	0	31	0	0
14	Q	587	0	113	0	0
14	R	587	0	114	2	0
All	All	51478	0	10526	554	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 9.

All (554) 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)
6:H:81:UNK:C	6:H:87:UNK:CB	1.85	1.53
2:C:1161:UNK:CB	2:C:1318:UNK:N	1.74	1.50
2:C:497:UNK:O	2:C:501:UNK:CB	1.66	1.43
2:C:817:UNK:O	2:C:819:UNK:N	1.58	1.37
4:F:817:UNK:O	4:F:819:UNK:N	1.58	1.36
7:I:31:UNK:CB	7:I:34:UNK:CB	2.01	1.35
2:C:1161:UNK:CB	2:C:1318:UNK:CA	2.09	1.31
2:C:689:UNK:O	2:C:693:UNK:CB	1.79	1.30
8:J:18:UNK:O	8:J:22:UNK:CB	1.82	1.27
2:C:522:UNK:CB	3:E:330:UNK:CB	2.12	1.26
1:A:3263:UNK:O	1:A:3266:UNK:CB	1.81	1.26
1:B:3263:UNK:O	1:B:3266:UNK:CB	1.81	1.26
7:I:31:UNK:O	7:I:34:UNK:N	1.67	1.26
2:C:536:UNK:O	2:C:540:UNK:CB	1.87	1.22
2:C:498:UNK:O	2:C:502:UNK:CB	1.88	1.22
2:C:522:UNK:HA	3:E:330:UNK:CB	1.70	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:82:UNK:N	6:H:87:UNK:CB	2.03	1.21
6:H:81:UNK:O	6:H:87:UNK:CB	1.83	1.21
4:F:1285:UNK:CB	4:F:1316:UNK:HA	1.68	1.21
4:F:1282:UNK:O	4:F:1316:UNK:CB	1.88	1.21
2:C:457:UNK:CB	2:C:459:UNK:N	2.04	1.21
2:C:1023:UNK:CB	2:C:1108:UNK:CB	2.19	1.20
8:J:18:UNK:O	8:J:22:UNK:N	1.74	1.19
4:F:457:UNK:CB	4:F:459:UNK:N	2.04	1.19
2:C:584:UNK:CA	3:E:689:UNK:C	1.76	1.18
2:C:1161:UNK:CB	2:C:1317:UNK:C	2.20	1.18
2:C:522:UNK:CA	3:E:330:UNK:CB	2.20	1.17
2:C:457:UNK:HA	2:C:458:UNK:CB	1.72	1.16
4:F:497:UNK:O	4:F:500:UNK:CB	1.93	1.16
4:F:1285:UNK:CB	4:F:1316:UNK:CA	2.22	1.15
6:H:101:UNK:O	6:H:119:UNK:O	1.64	1.15
2:C:319:UNK:CB	2:C:371:UNK:CB	2.24	1.15
4:F:457:UNK:HA	4:F:458:UNK:CB	1.71	1.14
2:C:584:UNK:CA	3:E:690:UNK:N	2.12	1.13
2:C:319:UNK:CB	2:C:371:UNK:CA	2.27	1.12
6:H:145:UNK:CB	6:H:301:UNK:CB	2.28	1.12
4:F:872:UNK:O	4:F:876:UNK:CB	1.99	1.10
2:C:872:UNK:O	2:C:876:UNK:CB	1.99	1.10
2:C:1161:UNK:CB	2:C:1318:UNK:HA	1.81	1.08
2:C:872:UNK:O	2:C:876:UNK:N	1.88	1.06
4:F:872:UNK:O	4:F:876:UNK:N	1.88	1.06
2:C:248:UNK:N	2:C:357:UNK:HA	1.71	1.06
4:F:512:UNK:HA	4:F:536:UNK:CB	1.85	1.05
6:H:359:UNK:O	6:H:360:UNK:O	1.75	1.05
6:H:82:UNK:CA	6:H:87:UNK:CB	2.35	1.04
2:C:698:UNK:CB	3:E:471:UNK:CB	2.35	1.04
2:C:537:UNK:O	2:C:541:UNK:N	1.89	1.04
6:H:107:UNK:HA	6:H:112:UNK:O	1.58	1.04
4:F:873:UNK:O	4:F:877:UNK:N	1.93	1.02
2:C:873:UNK:O	2:C:877:UNK:N	1.93	1.01
2:C:580:UNK:CB	3:E:684:UNK:CB	2.38	1.01
6:H:152:UNK:C	6:H:153:UNK:H2	1.74	1.00
4:F:1046:UNK:O	4:F:1050:UNK:CB	2.10	1.00
6:H:82:UNK:HA	6:H:87:UNK:CB	1.89	1.00
2:C:692:UNK:C	3:E:473:UNK:C	2.41	0.99
4:F:311:UNK:CB	4:F:347:UNK:C	2.40	0.99
2:C:1047:UNK:O	2:C:1051:UNK:CB	2.12	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:271:UNK:O	4:F:274:UNK:N	1.97	0.97
1:B:1389:UNK:O	4:F:1353:UNK:C	2.10	0.96
2:C:271:UNK:O	2:C:274:UNK:N	1.97	0.96
4:F:311:UNK:CB	4:F:347:UNK:O	2.12	0.96
2:C:695:UNK:C	3:E:474:UNK:CB	2.18	0.96
8:J:18:UNK:O	8:J:22:UNK:CA	2.12	0.96
6:H:315:UNK:CB	6:H:322:UNK:O	2.13	0.96
4:F:512:UNK:CA	4:F:536:UNK:CB	2.42	0.96
6:H:193:UNK:O	6:H:221:UNK:O	1.82	0.96
2:C:281:UNK:O	2:C:284:UNK:CA	2.16	0.93
2:C:537:UNK:O	2:C:541:UNK:CB	2.17	0.93
4:F:632:UNK:O	4:F:635:UNK:N	2.01	0.93
2:C:1350:UNK:CB	2:C:1418:UNK:CB	2.46	0.93
4:F:281:UNK:O	4:F:284:UNK:CA	2.16	0.92
2:C:585:UNK:C	3:E:689:UNK:CB	2.43	0.92
4:F:1350:UNK:CB	4:F:1416:UNK:CB	2.46	0.92
2:C:319:UNK:CB	2:C:371:UNK:C	2.48	0.91
4:F:497:UNK:O	4:F:500:UNK:CA	2.19	0.91
6:H:106:UNK:O	6:H:113:UNK:HA	1.69	0.90
4:F:632:UNK:O	4:F:634:UNK:N	2.04	0.90
1:A:3083:UNK:HA	1:A:3084:UNK:C	2.02	0.90
2:C:319:UNK:CB	2:C:371:UNK:HA	2.01	0.90
7:I:31:UNK:O	7:I:34:UNK:CA	2.19	0.90
1:B:3083:UNK:HA	1:B:3084:UNK:C	2.02	0.89
1:B:3263:UNK:O	1:B:3266:UNK:CA	2.19	0.89
2:C:584:UNK:N	3:E:687:UNK:C	2.36	0.88
2:C:431:UNK:O	2:C:433:UNK:N	2.06	0.88
3:E:365:UNK:HA	3:E:444:UNK:CB	2.03	0.88
8:J:144:UNK:O	8:J:146:UNK:N	2.06	0.88
2:C:431:UNK:O	2:C:434:UNK:N	2.06	0.88
1:A:3263:UNK:O	1:A:3266:UNK:CA	2.20	0.88
3:E:445:UNK:CB	3:E:463:UNK:CB	2.52	0.88
1:B:3263:UNK:C	1:B:3266:UNK:CB	2.52	0.88
4:F:1285:UNK:CB	4:F:1316:UNK:N	2.36	0.88
4:F:311:UNK:CB	4:F:347:UNK:CB	2.50	0.87
3:D:445:UNK:CB	3:D:463:UNK:CB	2.52	0.87
1:A:3263:UNK:C	1:A:3266:UNK:CB	2.52	0.87
2:C:281:UNK:O	2:C:284:UNK:N	2.08	0.87
8:J:144:UNK:O	8:J:145:UNK:C	2.21	0.87
2:C:536:UNK:O	2:C:540:UNK:N	2.08	0.87
3:D:365:UNK:HA	3:D:444:UNK:CB	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:199:UNK:O	6:H:200:UNK:CB	2.23	0.87
2:C:583:UNK:N	3:E:688:UNK:N	2.22	0.87
4:F:281:UNK:O	4:F:284:UNK:N	2.07	0.85
8:J:18:UNK:C	8:J:22:UNK:CB	2.55	0.85
2:C:534:UNK:O	2:C:536:UNK:N	2.10	0.83
4:F:281:UNK:O	4:F:284:UNK:CB	2.26	0.83
2:C:281:UNK:O	2:C:284:UNK:CB	2.26	0.83
4:F:457:UNK:CB	4:F:459:UNK:CB	2.56	0.83
2:C:1342:UNK:O	2:C:1345:UNK:CB	2.26	0.83
2:C:457:UNK:CB	2:C:459:UNK:CB	2.56	0.83
4:F:1044:UNK:O	4:F:1048:UNK:N	2.11	0.83
6:H:102:UNK:O	6:H:118:UNK:HA	1.79	0.83
4:F:1342:UNK:O	4:F:1345:UNK:CB	2.26	0.82
2:C:248:UNK:O	2:C:251:UNK:N	2.13	0.82
2:C:584:UNK:N	3:E:688:UNK:N	2.21	0.82
7:I:31:UNK:O	7:I:34:UNK:CB	2.28	0.82
4:F:248:UNK:O	4:F:251:UNK:N	2.13	0.81
2:C:817:UNK:O	2:C:818:UNK:C	2.29	0.81
2:C:612:UNK:H	2:C:613:UNK:C	1.94	0.81
2:C:817:UNK:C	2:C:819:UNK:N	2.43	0.81
4:F:817:UNK:O	4:F:818:UNK:C	2.29	0.81
4:F:512:UNK:CB	4:F:536:UNK:HA	2.11	0.80
2:C:476:UNK:O	2:C:478:UNK:N	2.15	0.80
2:C:586:UNK:N	3:E:689:UNK:CB	2.45	0.80
2:C:319:UNK:CB	2:C:371:UNK:O	2.29	0.80
4:F:982:UNK:CB	5:G:95:UNK:CB	2.60	0.80
4:F:836:UNK:O	4:F:840:UNK:CB	2.30	0.80
4:F:497:UNK:O	4:F:500:UNK:N	2.14	0.80
4:F:512:UNK:CB	4:F:536:UNK:CA	2.59	0.79
2:C:836:UNK:O	2:C:840:UNK:CB	2.31	0.79
8:J:50:UNK:O	8:J:51:UNK:O	2.01	0.78
4:F:824:UNK:O	4:F:827:UNK:N	2.16	0.78
7:I:115:UNK:CB	8:J:119:UNK:CB	2.61	0.78
1:B:1392:UNK:N	4:F:1353:UNK:O	2.17	0.78
4:F:497:UNK:C	4:F:500:UNK:CB	2.61	0.78
4:F:497:UNK:HA	4:F:500:UNK:CB	2.14	0.78
2:C:1209:UNK:O	2:C:1213:UNK:N	2.16	0.78
2:C:824:UNK:O	2:C:827:UNK:N	2.16	0.78
4:F:632:UNK:O	4:F:633:UNK:C	2.32	0.77
4:F:817:UNK:C	4:F:819:UNK:N	2.43	0.77
2:C:248:UNK:H2	2:C:357:UNK:HA	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1005:UNK:O	4:F:1007:UNK:CB	2.33	0.77
2:C:551:UNK:O	2:C:555:UNK:N	2.17	0.77
1:A:3263:UNK:O	1:A:3267:UNK:N	2.18	0.76
3:E:365:UNK:CA	3:E:444:UNK:CB	2.63	0.76
4:F:216:UNK:O	4:F:219:UNK:N	2.18	0.76
4:F:497:UNK:O	4:F:501:UNK:N	2.18	0.76
2:C:873:UNK:O	2:C:877:UNK:CB	2.34	0.76
1:B:3263:UNK:O	1:B:3267:UNK:N	2.18	0.76
2:C:216:UNK:O	2:C:219:UNK:N	2.18	0.76
2:C:319:UNK:N	2:C:371:UNK:CB	2.49	0.76
2:C:587:UNK:CB	3:E:689:UNK:O	2.33	0.76
3:D:365:UNK:CA	3:D:444:UNK:CB	2.63	0.76
4:F:1316:UNK:O	4:F:1317:UNK:N	2.19	0.76
2:C:431:UNK:O	2:C:432:UNK:C	2.33	0.76
2:C:457:UNK:CA	2:C:458:UNK:CB	2.57	0.75
4:F:271:UNK:O	4:F:274:UNK:CA	2.35	0.75
4:F:873:UNK:O	4:F:877:UNK:CB	2.34	0.75
2:C:696:UNK:N	3:E:474:UNK:CB	2.50	0.75
2:C:534:UNK:C	2:C:536:UNK:N	2.50	0.75
2:C:271:UNK:O	2:C:274:UNK:CA	2.35	0.75
4:F:872:UNK:O	4:F:876:UNK:CA	2.34	0.75
7:I:65:UNK:CB	7:I:75:UNK:CB	2.65	0.75
2:C:872:UNK:O	2:C:876:UNK:CA	2.35	0.74
6:H:103:UNK:CB	6:H:117:UNK:O	2.35	0.74
2:C:248:UNK:CB	2:C:361:UNK:N	2.48	0.74
1:B:1392:UNK:CA	4:F:1353:UNK:O	2.35	0.74
2:C:248:UNK:CA	2:C:357:UNK:HA	2.18	0.73
6:H:81:UNK:O	6:H:87:UNK:CA	2.36	0.73
2:C:531:UNK:HA	2:C:532:UNK:CB	2.18	0.73
6:H:107:UNK:HA	6:H:112:UNK:C	2.18	0.73
7:I:144:UNK:O	7:I:145:UNK:C	2.33	0.73
4:F:1044:UNK:O	4:F:1048:UNK:CB	2.37	0.72
2:C:583:UNK:O	3:E:689:UNK:CB	2.37	0.72
1:A:3433:UNK:O	1:A:3437:UNK:N	2.23	0.72
1:B:3433:UNK:O	1:B:3437:UNK:N	2.23	0.72
4:F:512:UNK:CB	4:F:536:UNK:CB	2.68	0.72
4:F:291:UNK:O	4:F:295:UNK:N	2.24	0.71
1:A:3263:UNK:HA	1:A:3266:UNK:CB	2.21	0.71
1:B:3263:UNK:HA	1:B:3266:UNK:CB	2.21	0.71
2:C:695:UNK:HA	3:E:471:UNK:CB	2.21	0.70
2:C:529:UNK:O	2:C:532:UNK:HA	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:UNK:O	2:C:295:UNK:N	2.24	0.70
6:H:152:UNK:C	6:H:153:UNK:N	2.53	0.70
2:C:580:UNK:CB	3:E:684:UNK:O	2.40	0.70
2:C:1121:UNK:O	2:C:1124:UNK:N	2.25	0.69
2:C:271:UNK:O	2:C:274:UNK:HA	1.92	0.69
2:C:536:UNK:O	2:C:540:UNK:CA	2.39	0.69
2:C:616:UNK:O	2:C:619:UNK:N	2.26	0.69
4:F:1121:UNK:O	4:F:1124:UNK:N	2.25	0.69
6:H:107:UNK:CB	6:H:111:UNK:HA	2.22	0.69
2:C:1210:UNK:O	2:C:1214:UNK:CB	2.42	0.68
6:H:106:UNK:O	6:H:114:UNK:N	2.27	0.68
2:C:689:UNK:O	2:C:693:UNK:N	2.26	0.68
4:F:1255:UNK:O	4:F:1259:UNK:N	2.27	0.68
2:C:1391:UNK:O	2:C:1395:UNK:N	2.27	0.68
2:C:306:UNK:O	2:C:310:UNK:N	2.27	0.68
4:F:1207:UNK:O	4:F:1211:UNK:N	2.27	0.68
6:H:107:UNK:CB	6:H:111:UNK:C	2.72	0.68
2:C:497:UNK:C	2:C:501:UNK:CB	2.67	0.67
2:C:583:UNK:N	3:E:687:UNK:C	2.56	0.67
4:F:213:UNK:N	4:F:214:UNK:CB	2.28	0.67
4:F:271:UNK:O	4:F:274:UNK:HA	1.92	0.67
4:F:306:UNK:O	4:F:310:UNK:N	2.27	0.67
2:C:694:UNK:C	3:E:471:UNK:C	2.73	0.67
4:F:1285:UNK:CB	4:F:1316:UNK:H2	2.08	0.67
2:C:580:UNK:HA	3:E:684:UNK:O	1.93	0.67
4:F:497:UNK:C	4:F:500:UNK:N	2.57	0.67
3:D:445:UNK:O	3:D:462:UNK:CB	2.42	0.67
4:F:1285:UNK:CB	4:F:1316:UNK:CB	2.72	0.67
2:C:281:UNK:O	2:C:284:UNK:C	2.42	0.67
3:E:445:UNK:O	3:E:462:UNK:CB	2.43	0.67
2:C:1255:UNK:O	2:C:1259:UNK:N	2.27	0.67
4:F:281:UNK:O	4:F:284:UNK:C	2.42	0.66
1:B:3419:UNK:O	1:B:3423:UNK:CB	2.43	0.66
1:A:3419:UNK:O	1:A:3423:UNK:CB	2.43	0.66
1:A:3402:UNK:O	1:A:3406:UNK:N	2.28	0.66
1:B:3402:UNK:O	1:B:3406:UNK:N	2.29	0.66
4:F:948:UNK:O	4:F:949:UNK:CB	2.40	0.66
4:F:212:UNK:C	4:F:214:UNK:CB	2.74	0.66
2:C:583:UNK:C	3:E:687:UNK:C	2.74	0.66
6:H:107:UNK:CA	6:H:112:UNK:O	2.41	0.66
2:C:497:UNK:O	2:C:501:UNK:CA	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1161:UNK:HA	2:C:1317:UNK:CB	2.26	0.65
1:B:3260:UNK:CB	1:B:3430:UNK:CB	2.74	0.65
4:F:632:UNK:C	4:F:634:UNK:N	2.59	0.65
4:F:1005:UNK:O	4:F:1006:UNK:C	2.43	0.65
2:C:1049:UNK:O	2:C:1052:UNK:N	2.29	0.65
1:A:3260:UNK:CB	1:A:3430:UNK:CB	2.74	0.65
2:C:476:UNK:C	2:C:478:UNK:N	2.57	0.65
4:F:351:UNK:C	4:F:353:UNK:N	2.58	0.65
8:J:144:UNK:C	8:J:146:UNK:N	2.52	0.65
2:C:817:UNK:O	2:C:820:UNK:N	2.30	0.64
4:F:351:UNK:O	4:F:352:UNK:C	2.45	0.64
4:F:817:UNK:O	4:F:820:UNK:N	2.30	0.64
2:C:351:UNK:C	2:C:353:UNK:N	2.58	0.64
2:C:583:UNK:N	3:E:687:UNK:CA	2.32	0.64
2:C:692:UNK:C	3:E:473:UNK:O	2.34	0.64
6:H:101:UNK:O	6:H:119:UNK:C	2.45	0.64
2:C:351:UNK:O	2:C:352:UNK:C	2.45	0.64
1:A:3432:UNK:O	1:A:3436:UNK:N	2.31	0.64
4:F:1152:UNK:O	4:F:1156:UNK:CB	2.45	0.64
1:B:3432:UNK:O	1:B:3436:UNK:N	2.31	0.63
2:C:1152:UNK:O	2:C:1156:UNK:CB	2.45	0.63
6:H:200:UNK:C	6:H:201:UNK:N	2.61	0.63
2:C:537:UNK:O	2:C:541:UNK:CA	2.46	0.63
1:A:3263:UNK:CA	1:A:3266:UNK:CB	2.77	0.63
2:C:1062:UNK:O	2:C:1065:UNK:N	2.32	0.63
4:F:817:UNK:O	4:F:819:UNK:CA	2.45	0.63
1:B:3263:UNK:O	1:B:3266:UNK:C	2.47	0.63
1:B:3420:UNK:O	1:B:3424:UNK:N	2.32	0.63
2:C:817:UNK:O	2:C:819:UNK:CA	2.45	0.62
1:A:3420:UNK:O	1:A:3424:UNK:N	2.32	0.62
2:C:616:UNK:O	2:C:617:UNK:C	2.48	0.62
1:A:3250:UNK:O	1:A:3253:UNK:CB	2.48	0.62
2:C:431:UNK:C	2:C:433:UNK:N	2.62	0.62
6:H:107:UNK:CB	6:H:111:UNK:CA	2.78	0.62
2:C:690:UNK:O	3:E:473:UNK:HA	1.99	0.62
2:C:1342:UNK:O	2:C:1346:UNK:N	2.33	0.62
4:F:1116:UNK:O	4:F:1119:UNK:N	2.32	0.62
4:F:457:UNK:CA	4:F:458:UNK:CB	2.56	0.62
1:A:3263:UNK:O	1:A:3266:UNK:C	2.47	0.62
1:B:3250:UNK:O	1:B:3253:UNK:CB	2.48	0.62
10:M:54:UNK:C	10:M:56:UNK:H2	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1342:UNK:O	4:F:1346:UNK:N	2.33	0.62
4:F:457:UNK:CB	4:F:459:UNK:CA	2.78	0.62
2:C:457:UNK:CB	2:C:459:UNK:CA	2.78	0.61
4:F:262:UNK:O	4:F:266:UNK:N	2.33	0.61
4:F:1285:UNK:HA	4:F:1316:UNK:CB	2.30	0.61
2:C:689:UNK:O	2:C:693:UNK:CA	2.47	0.61
2:C:692:UNK:O	3:E:473:UNK:C	2.48	0.61
1:B:3263:UNK:CA	1:B:3266:UNK:CB	2.77	0.61
2:C:262:UNK:O	2:C:266:UNK:N	2.33	0.61
2:C:1116:UNK:O	2:C:1119:UNK:N	2.32	0.61
4:F:1285:UNK:CA	4:F:1316:UNK:CB	2.79	0.61
4:F:1254:UNK:O	4:F:1258:UNK:CB	2.49	0.61
2:C:1254:UNK:O	2:C:1258:UNK:CB	2.49	0.61
4:F:497:UNK:CA	4:F:500:UNK:CB	2.79	0.61
4:F:1151:UNK:O	4:F:1155:UNK:N	2.34	0.60
2:C:1151:UNK:O	2:C:1155:UNK:N	2.34	0.60
2:C:1350:UNK:CB	2:C:1418:UNK:C	2.79	0.60
2:C:694:UNK:O	3:E:471:UNK:CB	2.50	0.60
2:C:1140:UNK:O	2:C:1144:UNK:N	2.35	0.60
4:F:1350:UNK:CB	4:F:1416:UNK:C	2.79	0.60
4:F:248:UNK:O	4:F:249:UNK:C	2.48	0.60
6:H:106:UNK:O	6:H:113:UNK:CA	2.46	0.60
2:C:1121:UNK:O	2:C:1122:UNK:C	2.50	0.60
2:C:1350:UNK:CB	2:C:1418:UNK:CA	2.80	0.60
4:F:626:UNK:O	4:F:630:UNK:N	2.34	0.60
4:F:1282:UNK:C	4:F:1316:UNK:CB	2.79	0.60
2:C:319:UNK:CA	2:C:371:UNK:CB	2.79	0.59
2:C:583:UNK:CA	3:E:687:UNK:C	2.42	0.59
3:D:599:UNK:HA	3:D:626:UNK:O	2.02	0.59
2:C:248:UNK:O	2:C:249:UNK:C	2.48	0.59
4:F:1121:UNK:O	4:F:1122:UNK:C	2.50	0.59
8:J:144:UNK:O	8:J:147:UNK:N	2.35	0.59
4:F:1282:UNK:O	4:F:1316:UNK:N	2.36	0.59
1:A:3419:UNK:O	1:A:3423:UNK:N	2.36	0.59
2:C:1161:UNK:CB	2:C:1318:UNK:CB	2.81	0.59
4:F:1350:UNK:CB	4:F:1416:UNK:CA	2.80	0.59
1:B:3419:UNK:O	1:B:3423:UNK:N	2.36	0.59
4:F:397:UNK:O	4:F:401:UNK:N	2.35	0.59
4:F:874:UNK:O	4:F:878:UNK:N	2.35	0.59
2:C:248:UNK:HA	2:C:357:UNK:HA	1.84	0.59
4:F:1140:UNK:O	4:F:1144:UNK:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:599:UNK:HA	3:E:626:UNK:O	2.02	0.59
2:C:580:UNK:CA	3:E:684:UNK:O	2.51	0.59
4:F:824:UNK:O	4:F:825:UNK:C	2.50	0.59
2:C:307:UNK:O	2:C:311:UNK:N	2.36	0.58
4:F:1152:UNK:O	4:F:1156:UNK:N	2.36	0.58
4:F:1255:UNK:O	4:F:1259:UNK:CB	2.52	0.58
2:C:1391:UNK:O	2:C:1395:UNK:CB	2.52	0.58
8:J:130:UNK:CB	8:J:174:UNK:CB	2.81	0.58
2:C:874:UNK:O	2:C:878:UNK:N	2.35	0.58
2:C:824:UNK:O	2:C:825:UNK:C	2.50	0.58
4:F:568:UNK:O	4:F:569:UNK:C	2.51	0.58
4:F:307:UNK:O	4:F:311:UNK:N	2.37	0.58
2:C:1152:UNK:O	2:C:1156:UNK:N	2.36	0.58
2:C:641:UNK:O	2:C:642:UNK:C	2.51	0.58
2:C:1201:UNK:O	2:C:1205:UNK:N	2.37	0.58
2:C:583:UNK:C	3:E:689:UNK:CB	2.80	0.57
4:F:216:UNK:O	4:F:217:UNK:C	2.52	0.57
4:F:281:UNK:O	4:F:284:UNK:O	2.22	0.57
1:A:3370:UNK:O	1:A:3374:UNK:N	2.38	0.57
2:C:281:UNK:O	2:C:284:UNK:O	2.22	0.57
6:H:82:UNK:HA	6:H:87:UNK:C	2.33	0.57
2:C:1255:UNK:O	2:C:1259:UNK:CB	2.51	0.57
2:C:566:UNK:O	2:C:567:UNK:C	2.51	0.57
2:C:643:UNK:O	2:C:644:UNK:C	2.52	0.57
4:F:603:UNK:O	4:F:604:UNK:C	2.51	0.57
2:C:1202:UNK:O	2:C:1206:UNK:CB	2.52	0.57
8:J:41:UNK:O	8:J:44:UNK:CB	2.53	0.57
1:B:3370:UNK:O	1:B:3374:UNK:N	2.38	0.57
2:C:216:UNK:O	2:C:217:UNK:C	2.52	0.57
2:C:601:UNK:O	2:C:602:UNK:C	2.52	0.57
4:F:351:UNK:O	4:F:353:UNK:N	2.38	0.57
2:C:251:UNK:CB	2:C:357:UNK:CB	2.82	0.57
4:F:451:UNK:O	4:F:452:UNK:C	2.51	0.57
4:F:1068:UNK:HA	4:F:1069:UNK:C	2.34	0.57
2:C:1139:UNK:O	2:C:1143:UNK:N	2.38	0.56
4:F:1139:UNK:O	4:F:1143:UNK:N	2.38	0.56
4:F:567:UNK:O	4:F:568:UNK:C	2.51	0.56
4:F:511:UNK:O	4:F:512:UNK:C	2.51	0.56
4:F:1043:UNK:O	4:F:1047:UNK:CB	2.53	0.56
7:I:144:UNK:O	7:I:146:UNK:N	2.38	0.56
2:C:351:UNK:O	2:C:353:UNK:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:512:UNK:O	4:F:513:UNK:C	2.51	0.56
2:C:603:UNK:O	2:C:604:UNK:C	2.51	0.56
1:A:3482:UNK:O	1:A:3486:UNK:N	2.39	0.56
2:C:1023:UNK:CA	2:C:1108:UNK:CB	2.83	0.56
2:C:567:UNK:O	2:C:568:UNK:C	2.51	0.56
4:F:1369:UNK:O	4:F:1373:UNK:CB	2.54	0.56
4:F:602:UNK:O	4:F:603:UNK:C	2.51	0.56
6:H:181:UNK:O	6:H:183:UNK:N	2.39	0.56
2:C:871:UNK:O	2:C:875:UNK:N	2.39	0.56
4:F:871:UNK:O	4:F:875:UNK:N	2.39	0.56
1:B:3482:UNK:O	1:B:3486:UNK:N	2.39	0.55
4:F:498:UNK:C	4:F:500:UNK:N	2.58	0.55
2:C:1370:UNK:O	2:C:1374:UNK:CB	2.54	0.55
4:F:513:UNK:O	4:F:514:UNK:C	2.52	0.55
2:C:587:UNK:N	3:E:689:UNK:CB	2.70	0.55
2:C:602:UNK:O	2:C:603:UNK:C	2.52	0.55
2:C:552:UNK:O	2:C:556:UNK:N	2.39	0.55
7:I:29:UNK:O	7:I:30:UNK:C	2.53	0.55
1:A:3886:UNK:C	1:A:3887:UNK:N	2.70	0.55
2:C:288:UNK:O	2:C:289:UNK:C	2.53	0.55
2:C:568:UNK:O	2:C:569:UNK:C	2.52	0.55
4:F:1282:UNK:O	4:F:1316:UNK:CA	2.55	0.55
2:C:873:UNK:O	2:C:877:UNK:CA	2.55	0.54
6:H:103:UNK:CA	6:H:117:UNK:O	2.54	0.54
4:F:288:UNK:O	4:F:289:UNK:C	2.53	0.54
4:F:566:UNK:O	4:F:567:UNK:C	2.52	0.54
6:H:151:UNK:O	6:H:153:UNK:N	2.40	0.54
7:I:18:UNK:O	7:I:22:UNK:N	2.41	0.54
4:F:873:UNK:O	4:F:877:UNK:CA	2.55	0.54
2:C:612:UNK:CB	2:C:613:UNK:CB	2.85	0.54
4:F:1045:UNK:O	4:F:1049:UNK:CB	2.56	0.54
1:B:3886:UNK:C	1:B:3887:UNK:N	2.70	0.54
2:C:642:UNK:O	2:C:643:UNK:C	2.52	0.54
4:F:281:UNK:C	4:F:284:UNK:N	2.71	0.54
2:C:531:UNK:CA	2:C:532:UNK:CB	2.86	0.54
4:F:311:UNK:CB	4:F:347:UNK:CA	2.86	0.54
2:C:281:UNK:C	2:C:284:UNK:N	2.71	0.53
4:F:601:UNK:O	4:F:602:UNK:C	2.52	0.53
2:C:1153:UNK:CB	2:C:1278:UNK:CB	2.86	0.53
2:C:1350:UNK:CB	2:C:1418:UNK:O	2.57	0.53
2:C:993:UNK:O	2:C:994:UNK:C	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1316:UNK:C	4:F:1317:UNK:N	2.70	0.53
1:B:2145:UNK:O	1:B:2148:UNK:N	2.42	0.53
2:C:551:UNK:O	2:C:555:UNK:CB	2.57	0.53
4:F:1350:UNK:CB	4:F:1416:UNK:O	2.57	0.53
1:A:2145:UNK:O	1:A:2148:UNK:N	2.42	0.53
4:F:1044:UNK:O	4:F:1048:UNK:CA	2.57	0.53
2:C:1202:UNK:O	2:C:1206:UNK:N	2.42	0.52
3:D:365:UNK:CB	3:D:444:UNK:CB	2.87	0.52
3:E:365:UNK:CB	3:E:444:UNK:CB	2.87	0.52
2:C:998:UNK:C	2:C:1000:UNK:N	2.71	0.52
6:H:363:UNK:O	6:H:364:UNK:CB	2.58	0.52
4:F:457:UNK:CA	4:F:459:UNK:N	2.72	0.52
4:F:497:UNK:O	4:F:500:UNK:C	2.57	0.52
4:F:984:UNK:O	4:F:985:UNK:C	2.58	0.52
2:C:612:UNK:N	2:C:613:UNK:CB	2.73	0.51
2:C:616:UNK:O	2:C:618:UNK:N	2.42	0.51
2:C:742:UNK:HA	2:C:806:UNK:CB	2.40	0.51
6:H:114:UNK:O	6:H:115:UNK:CB	2.58	0.51
1:B:1389:UNK:O	4:F:1353:UNK:O	2.27	0.51
2:C:986:UNK:CB	6:H:102:UNK:CB	2.88	0.51
6:H:102:UNK:O	6:H:118:UNK:CA	2.55	0.51
7:I:98:UNK:O	7:I:116:UNK:CB	2.59	0.51
2:C:612:UNK:CA	2:C:613:UNK:CB	2.89	0.51
6:H:229:UNK:O	6:H:230:UNK:CB	2.58	0.51
6:H:200:UNK:C	6:H:201:UNK:H2	2.24	0.51
1:B:3495:UNK:O	1:B:3499:UNK:N	2.44	0.51
6:H:348:UNK:CB	6:H:364:UNK:O	2.59	0.51
7:I:64:UNK:HA	7:I:75:UNK:O	2.11	0.51
1:A:3495:UNK:O	1:A:3499:UNK:N	2.44	0.50
1:B:4292:UNK:O	1:B:4293:UNK:C	2.59	0.50
1:A:3263:UNK:O	1:A:3266:UNK:N	2.45	0.50
1:A:3883:UNK:O	1:A:3887:UNK:N	2.45	0.50
1:B:3263:UNK:O	1:B:3266:UNK:N	2.45	0.50
6:H:108:UNK:N	6:H:112:UNK:O	2.45	0.50
6:H:152:UNK:CA	6:H:153:UNK:H2	2.25	0.50
1:A:4292:UNK:O	1:A:4293:UNK:C	2.58	0.50
7:I:99:UNK:O	7:I:100:UNK:CB	2.60	0.50
2:C:1049:UNK:O	2:C:1050:UNK:C	2.60	0.49
2:C:457:UNK:CA	2:C:459:UNK:N	2.72	0.49
1:B:3883:UNK:O	1:B:3887:UNK:N	2.45	0.49
2:C:536:UNK:C	2:C:540:UNK:CB	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:31:UNK:O	7:I:35:UNK:N	2.45	0.49
1:A:3373:UNK:O	1:A:3377:UNK:N	2.46	0.49
2:C:871:UNK:O	2:C:875:UNK:CB	2.60	0.49
4:F:1328:UNK:O	4:F:1331:UNK:CB	2.61	0.49
4:F:984:UNK:O	4:F:987:UNK:N	2.45	0.49
6:H:103:UNK:HA	6:H:117:UNK:O	2.12	0.49
1:B:1389:UNK:N	4:F:1349:UNK:O	2.46	0.49
6:H:359:UNK:C	6:H:360:UNK:O	2.58	0.48
1:B:3373:UNK:O	1:B:3377:UNK:N	2.46	0.48
4:F:1066:UNK:C	4:F:1068:UNK:H	2.26	0.48
4:F:871:UNK:O	4:F:875:UNK:CB	2.61	0.48
14:R:73:UNK:C	14:R:75:UNK:N	2.75	0.48
2:C:616:UNK:C	2:C:618:UNK:N	2.76	0.48
2:C:1328:UNK:O	2:C:1331:UNK:CB	2.61	0.48
4:F:281:UNK:HA	4:F:284:UNK:CB	2.43	0.48
1:A:2147:UNK:O	1:A:2363:UNK:N	2.46	0.48
2:C:1268:UNK:O	2:C:1272:UNK:N	2.46	0.48
11:N:33:UNK:C	11:N:35:UNK:N	2.73	0.48
4:F:272:UNK:C	4:F:274:UNK:N	2.73	0.48
4:F:512:UNK:N	4:F:536:UNK:CB	2.76	0.48
2:C:248:UNK:C	2:C:250:UNK:N	2.76	0.48
1:B:2147:UNK:O	1:B:2363:UNK:N	2.47	0.47
2:C:281:UNK:HA	2:C:284:UNK:CB	2.44	0.47
2:C:1342:UNK:O	2:C:1345:UNK:CA	2.62	0.47
6:H:175:UNK:C	6:H:177:UNK:N	2.75	0.47
1:B:3823:UNK:O	1:B:3824:UNK:CB	2.61	0.47
2:C:272:UNK:C	2:C:274:UNK:N	2.73	0.47
3:E:360:UNK:HA	3:E:368:UNK:O	2.15	0.47
4:F:248:UNK:C	4:F:250:UNK:N	2.76	0.47
2:C:261:UNK:O	2:C:265:UNK:N	2.48	0.47
10:M:55:UNK:O	10:M:57:UNK:N	2.48	0.47
2:C:579:UNK:O	3:E:687:UNK:CA	2.63	0.47
4:F:261:UNK:O	4:F:265:UNK:N	2.48	0.47
9:K:13:UNK:O	9:K:14:UNK:C	2.63	0.47
10:M:33:UNK:O	10:M:34:UNK:C	2.61	0.47
2:C:1204:UNK:O	2:C:1205:UNK:C	2.63	0.47
1:A:3823:UNK:O	1:A:3824:UNK:CB	2.61	0.47
2:C:585:UNK:N	3:E:689:UNK:N	2.19	0.47
3:D:360:UNK:HA	3:D:368:UNK:O	2.15	0.46
4:F:1342:UNK:O	4:F:1345:UNK:CA	2.62	0.46
2:C:352:UNK:O	2:C:355:UNK:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:993:UNK:O	4:F:994:UNK:C	2.61	0.46
2:C:693:UNK:N	3:E:473:UNK:C	2.79	0.46
4:F:352:UNK:O	4:F:355:UNK:N	2.49	0.46
7:I:31:UNK:O	7:I:32:UNK:C	2.63	0.46
7:I:82:UNK:O	7:I:83:UNK:CB	2.62	0.46
1:A:2951:UNK:O	1:A:2955:UNK:N	2.49	0.46
2:C:824:UNK:O	2:C:826:UNK:N	2.49	0.46
4:F:591:UNK:O	4:F:592:UNK:C	2.64	0.46
1:B:2169:UNK:HA	1:B:2170:UNK:CB	2.45	0.46
1:B:2951:UNK:O	1:B:2955:UNK:N	2.49	0.46
2:C:587:UNK:CB	3:E:689:UNK:C	2.93	0.46
2:C:530:UNK:C	2:C:532:UNK:HA	2.46	0.45
1:A:3250:UNK:O	1:A:3253:UNK:N	2.50	0.45
4:F:824:UNK:O	4:F:826:UNK:N	2.49	0.45
1:A:2169:UNK:HA	1:A:2170:UNK:CB	2.46	0.45
4:F:216:UNK:C	4:F:218:UNK:N	2.79	0.45
6:H:356:UNK:N	6:H:357:UNK:CA	2.79	0.45
2:C:1161:UNK:CA	2:C:1317:UNK:CB	2.93	0.45
2:C:824:UNK:C	2:C:826:UNK:N	2.80	0.45
11:N:33:UNK:O	11:N:34:UNK:C	2.64	0.45
1:B:3250:UNK:O	1:B:3253:UNK:N	2.49	0.45
6:H:197:UNK:O	6:H:198:UNK:CB	2.64	0.45
2:C:521:UNK:O	2:C:525:UNK:N	2.50	0.44
1:B:2197:UNK:HA	1:B:2198:UNK:CB	2.48	0.44
2:C:1209:UNK:O	2:C:1213:UNK:CB	2.66	0.44
1:A:2230:UNK:O	1:A:2231:UNK:C	2.66	0.44
1:B:2230:UNK:O	1:B:2231:UNK:C	2.66	0.44
4:F:824:UNK:C	4:F:826:UNK:N	2.79	0.43
2:C:702:UNK:O	2:C:706:UNK:N	2.51	0.43
2:C:522:UNK:HA	3:E:330:UNK:CA	2.44	0.43
6:H:99:UNK:CB	6:H:103:UNK:O	2.66	0.43
9:L:52:UNK:HA	9:L:53:UNK:HA	1.76	0.43
2:C:534:UNK:O	2:C:535:UNK:CB	2.61	0.43
7:I:146:UNK:HA	7:I:147:UNK:HA	1.80	0.43
14:R:73:UNK:O	14:R:75:UNK:N	2.51	0.43
8:J:89:UNK:C	8:J:90:UNK:O	2.67	0.43
1:A:2328:UNK:O	1:A:2329:UNK:C	2.67	0.43
11:N:31:UNK:O	11:N:32:UNK:C	2.67	0.43
2:C:1142:UNK:O	2:C:1146:UNK:N	2.52	0.42
2:C:612:UNK:N	2:C:613:UNK:C	2.72	0.42
4:F:1142:UNK:O	4:F:1146:UNK:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3410:UNK:O	1:A:3411:UNK:C	2.67	0.42
1:B:3410:UNK:O	1:B:3411:UNK:C	2.67	0.42
1:A:2197:UNK:HA	1:A:2198:UNK:CB	2.48	0.42
2:C:289:UNK:C	2:C:291:UNK:N	2.81	0.42
2:C:692:UNK:O	3:E:474:UNK:N	2.52	0.42
1:B:2328:UNK:O	1:B:2329:UNK:C	2.67	0.42
1:A:3420:UNK:O	1:A:3424:UNK:CB	2.67	0.42
2:C:216:UNK:C	2:C:218:UNK:N	2.79	0.42
11:N:33:UNK:O	11:N:35:UNK:N	2.52	0.42
1:B:3420:UNK:O	1:B:3424:UNK:CB	2.67	0.42
2:C:612:UNK:N	2:C:613:UNK:CA	2.83	0.42
2:C:1121:UNK:C	2:C:1123:UNK:N	2.81	0.42
2:C:1328:UNK:O	2:C:1332:UNK:N	2.53	0.42
2:C:583:UNK:CA	3:E:688:UNK:N	2.74	0.42
2:C:497:UNK:O	2:C:501:UNK:N	2.53	0.41
10:M:54:UNK:O	10:M:56:UNK:N	2.35	0.41
4:F:1208:UNK:O	4:F:1212:UNK:CB	2.68	0.41
4:F:1328:UNK:O	4:F:1332:UNK:N	2.53	0.41
11:N:19:UNK:O	11:N:20:UNK:C	2.69	0.41
2:C:388:UNK:O	2:C:391:UNK:CB	2.68	0.41
4:F:289:UNK:C	4:F:291:UNK:N	2.81	0.41
10:M:55:UNK:O	10:M:56:UNK:C	2.69	0.41
4:F:1121:UNK:C	4:F:1123:UNK:N	2.81	0.41
1:B:3264:UNK:C	1:B:3266:UNK:N	2.78	0.41
1:A:2807:UNK:O	1:A:2811:UNK:N	2.54	0.41
4:F:1343:UNK:HA	4:F:1346:UNK:CB	2.51	0.41
5:G:392:UNK:C	5:G:394:UNK:N	2.84	0.41
8:J:89:UNK:O	8:J:90:UNK:O	2.38	0.41
1:B:2807:UNK:O	1:B:2811:UNK:N	2.54	0.41
6:H:318:UNK:O	6:H:321:UNK:N	2.53	0.41
7:I:144:UNK:C	7:I:146:UNK:N	2.81	0.41
10:M:58:UNK:O	10:M:111:UNK:O	2.38	0.41
11:N:84:UNK:C	11:N:86:UNK:N	2.83	0.41
2:C:1343:UNK:HA	2:C:1346:UNK:CB	2.51	0.40
2:C:248:UNK:H2	2:C:357:UNK:CA	2.25	0.40
3:D:640:UNK:C	3:D:642:UNK:N	2.84	0.40
7:I:66:UNK:O	7:I:94:UNK:HA	2.21	0.40
8:J:50:UNK:O	8:J:51:UNK:C	2.67	0.40
2:C:1368:UNK:O	2:C:1371:UNK:N	2.54	0.40
3:D:582:UNK:HA	3:D:592:UNK:O	2.21	0.40
11:N:47:UNK:O	11:N:48:UNK:C	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:296:UNK:O	6:H:300:UNK:N	2.54	0.40
1:B:3214:UNK:O	1:B:3218:UNK:N	2.55	0.40
3:E:316:UNK:O	3:E:322:UNK:HA	2.21	0.40
3:E:599:UNK:CA	3:E:626:UNK:O	2.70	0.40
4:F:994:UNK:HA	4:F:995:UNK:HA	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	F	29
2	C	27
1	B	14
1	A	14
8	J	7
7	I	7
5	G	3
3	D	3
3	E	3
6	H	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	1161:UNK	C	1190:UNK	N	65.65
1	F	1161:UNK	C	1190:UNK	N	65.10
1	C	1354:UNK	C	1356:UNK	N	52.82
1	F	1354:UNK	C	1356:UNK	N	52.47
1	C	1389:UNK	C	1391:UNK	N	50.97
1	F	1388:UNK	C	1390:UNK	N	50.26
1	C	1070:UNK	C	1103:UNK	N	45.07
1	F	1009:UNK	C	1039:UNK	N	43.38
1	F	1223:UNK	C	1254:UNK	N	41.42
1	C	1223:UNK	C	1254:UNK	N	40.65
1	F	950:UNK	C	968:UNK	N	39.06
1	F	1070:UNK	C	1103:UNK	N	35.87
1	C	950:UNK	C	968:UNK	N	34.77
1	F	311:UNK	C	328:UNK	N	33.44
1	C	1010:UNK	C	1012:UNK	N	32.93
1	G	73:UNK	C	89:UNK	N	29.12
1	F	474:UNK	C	484:UNK	N	28.56
1	C	1025:UNK	C	1033:UNK	N	25.99
1	F	514:UNK	C	519:UNK	N	21.59
1	F	718:UNK	C	728:UNK	N	21.33
1	C	514:UNK	C	519:UNK	N	20.21
1	I	51:UNK	C	61:UNK	N	19.81
1	J	78:UNK	C	82:UNK	N	19.13
1	J	51:UNK	C	61:UNK	N	18.63
1	C	767:UNK	C	773:UNK	N	18.57
1	F	644:UNK	C	679:UNK	N	18.32

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	417:UNK	C	419:UNK	N	18.30
1	F	569:UNK	C	576:UNK	N	17.15
1	C	787:UNK	C	804:UNK	N	17.11
1	C	718:UNK	C	728:UNK	N	16.76
1	F	742:UNK	C	753:UNK	N	16.70
1	A	2389:UNK	C	2408:UNK	N	16.60
1	B	2389:UNK	C	2408:UNK	N	16.60
1	F	417:UNK	C	423:UNK	N	16.51
1	C	374:UNK	C	381:UNK	N	16.27
1	A	4361:UNK	C	4379:UNK	N	16.15
1	B	4361:UNK	C	4379:UNK	N	16.15
1	F	530:UNK	C	534:UNK	N	15.31
1	G	201:UNK	C	211:UNK	N	15.26
1	F	373:UNK	C	381:UNK	N	15.18
1	D	383:UNK	C	441:UNK	N	14.69
1	E	383:UNK	C	441:UNK	N	14.69
1	A	4595:UNK	C	4603:UNK	N	14.62
1	B	4595:UNK	C	4603:UNK	N	14.62
1	C	604:UNK	C	612:UNK	N	14.39
1	C	237:UNK	C	248:UNK	N	14.35
1	F	237:UNK	C	248:UNK	N	14.35
1	F	604:UNK	C	611:UNK	N	13.86
1	I	119:UNK	C	125:UNK	N	13.52
1	A	1987:UNK	C	1996:UNK	N	13.18
1	B	1987:UNK	C	1996:UNK	N	13.18
1	C	569:UNK	C	576:UNK	N	13.17
1	C	887:UNK	C	915:UNK	N	13.07
1	F	887:UNK	C	915:UNK	N	13.07
1	J	90:UNK	C	94:UNK	N	12.85
1	C	1285:UNK	C	1316:UNK	N	12.77
1	C	478:UNK	C	488:UNK	N	12.61
1	A	4498:UNK	C	4502:UNK	N	12.60
1	B	4498:UNK	C	4502:UNK	N	12.60
1	C	532:UNK	C	534:UNK	N	12.54
1	C	853:UNK	C	862:UNK	N	12.53
1	F	853:UNK	C	862:UNK	N	12.53
1	F	787:UNK	C	804:UNK	N	12.30
1	A	4545:UNK	C	4557:UNK	N	12.27
1	B	4545:UNK	C	4557:UNK	N	12.27
1	F	767:UNK	C	773:UNK	N	12.24
1	F	453:UNK	C	456:UNK	N	12.10
1	J	119:UNK	C	125:UNK	N	11.74

*Continued on next page...*

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	319:UNK	C	328:UNK	N	11.38
1	I	78:UNK	C	82:UNK	N	11.27
1	A	2115:UNK	C	2128:UNK	N	10.73
1	B	2115:UNK	C	2128:UNK	N	10.73
1	C	644:UNK	C	679:UNK	N	9.60
1	C	742:UNK	C	753:UNK	N	9.45
1	A	1768:UNK	C	1775:UNK	N	8.82
1	B	1768:UNK	C	1775:UNK	N	8.82
1	J	147:UNK	C	157:UNK	N	8.69
1	I	90:UNK	C	94:UNK	N	8.37
1	H	179:UNK	C	181:UNK	N	7.77
1	A	3974:UNK	C	3978:UNK	N	7.61
1	B	3974:UNK	C	3978:UNK	N	7.61
1	G	345:UNK	C	375:UNK	N	7.49
1	I	148:UNK	C	157:UNK	N	7.15
1	I	66:UNK	C	73:UNK	N	7.13
1	C	454:UNK	C	456:UNK	N	6.88
1	D	566:UNK	C	573:UNK	N	6.80
1	E	566:UNK	C	573:UNK	N	6.80
1	D	605:UNK	C	621:UNK	N	6.16
1	E	605:UNK	C	621:UNK	N	6.16
1	J	66:UNK	C	73:UNK	N	6.08
1	A	4401:UNK	C	4403:UNK	N	5.96
1	B	4401:UNK	C	4403:UNK	N	5.96
1	J	99:UNK	C	114:UNK	N	5.31
1	I	100:UNK	C	114:UNK	N	5.09
1	F	1285:UNK	C	1316:UNK	N	4.77
1	A	3895:UNK	C	3897:UNK	N	3.73
1	B	3895:UNK	C	3897:UNK	N	3.73
1	A	3846:UNK	C	3849:UNK	N	3.32
1	B	3846:UNK	C	3849:UNK	N	3.32
1	F	543:UNK	C	545:UNK	N	3.27
1	B	4562:UNK	C	4563:UNK	N	3.05
1	A	4562:UNK	C	4563:UNK	N	3.04
1	A	3886:UNK	C	3887:UNK	N	2.70
1	B	3886:UNK	C	3887:UNK	N	2.70
1	F	1316:UNK	C	1317:UNK	N	2.70
1	H	200:UNK	C	201:UNK	N	2.61
1	H	152:UNK	C	153:UNK	N	2.53
1	F	213:UNK	C	214:UNK	N	2.10
1	C	804:UNK	C	805:UNK	N	1.05
1	F	804:UNK	C	805:UNK	N	1.05