



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:50 AM UTC

PDB ID : 6TJV / pdb_00006tjv
EMDB ID : EMD-10513
Title : Structure of the NDH-1MS complex from *Thermosynechococcus elongatus*
Authors : Schuller, J.M.; Saura, P.; Thiemann, J.; Schuller, S.K.; Gamiz-Hernandez, A.P.; Kurisu, G.; Nowaczyk, M.M.; Kaila, V.R.I.
Deposited on : 2019-11-27
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

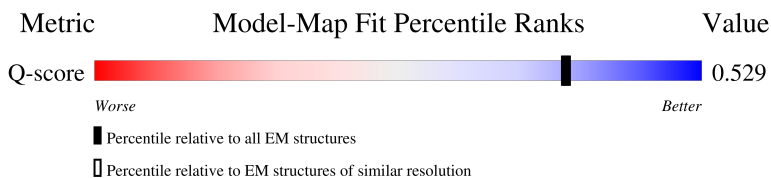
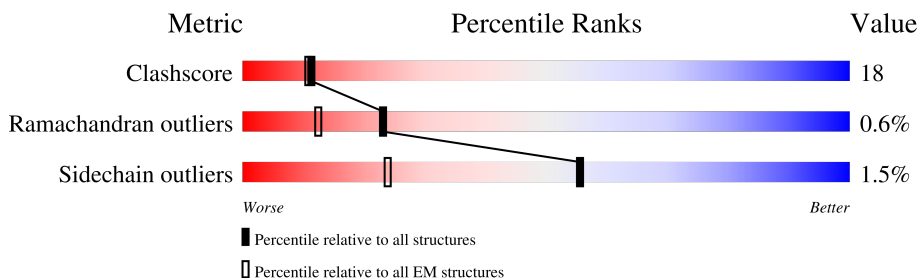
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



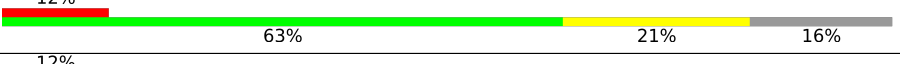
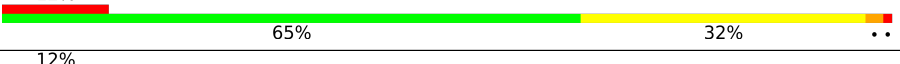
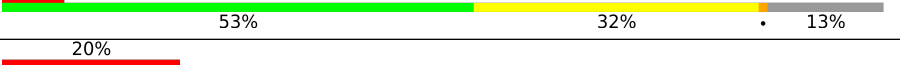
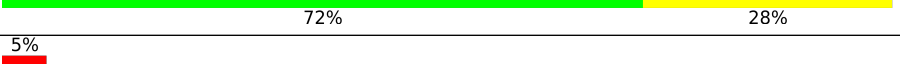
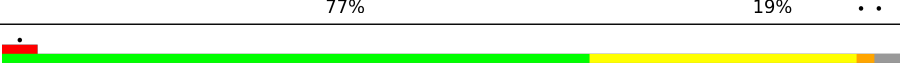
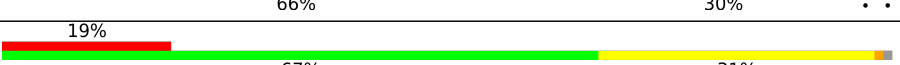
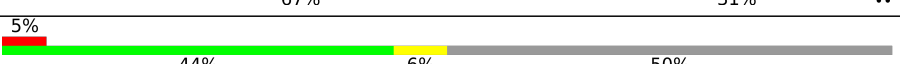
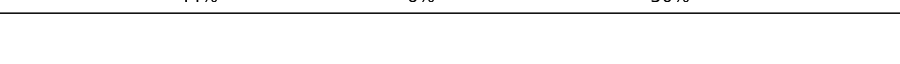
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	372	12% 60% 33% ...
2	B	515	10% 68% 24% 8%
3	C	132	11% 62% 20% .. 14%
4	D	501	8% 63% 31% .. 5%

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Mol	Chain	Length	Quality of chain
5	E	101	
6	F	611	
7	G	200	
8	H	394	
9	I	196	
10	J	168	
11	K	237	
12	L	76	
13	M	111	
14	N	150	
15	O	70	
16	P	437	
17	Q	149	
18	S	110	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	DGD	A	501	-	-	X	-
19	DGD	L	401	-	-	X	-
21	SQD	F	701	-	-	X	-
21	SQD	F	703	-	-	X	-
21	SQD	K	502	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 33838 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 NAD(P)H-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total	C	N	O	S	0	0
			2780	1871	431	468	10		

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	475	Total	C	N	O	S	0	0
			3541	2360	548	617	16		

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	114	Total	C	N	O	S	0	0
			914	629	138	143	4		

- Molecule 4 is a protein called NADH dehydrogenase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	478	Total	C	N	O	S	0	0
			3615	2423	573	605	14		

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	100	Total	C	N	O	S	0	0
			769	506	126	133	4		

- Molecule 6 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	600	Total	C	N	O	S	0	0
			4587	3070	718	776	23		

- Molecule 7 is a protein called NADH dehydrogenase subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	168	Total	C	N	O	S	0	0
			1262	844	196	218	4		

- Molecule 8 is a protein called NAD(P)H-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	393	Total	C	N	O	S	0	0
			3153	2035	540	559	19		

- Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	193	Total	C	N	O	S	0	0
			1520	970	260	277	13		

- Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	156	Total	C	N	O	S	0	0
			1278	817	218	238	5		

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1594	1024	276	281	13		

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	76	Total	C	N	O	S	0	0
			609	417	93	97	2		

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	110	Total	C	N	O	S	0	0
			879	548	160	169	2		

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	147	Total	C	N	O	S	0	0
			1160	755	200	204	1		

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	68	Total	C	N	O	0	0
			538	349	91	98		

- Molecule 16 is a protein called Tlr0906 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	426	Total	C	N	O	S	0	0
			3496	2294	583	599	20		

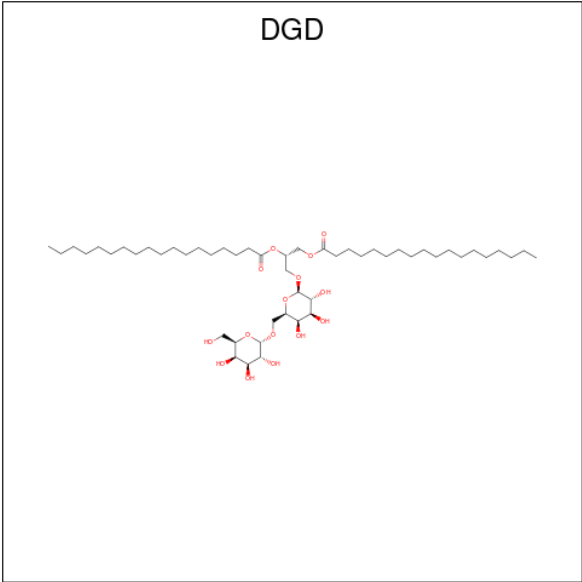
- Molecule 17 is a protein called Tll0220 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	148	Total	C	N	O	S	0	0
			1095	703	179	211	2		

- Molecule 18 is a protein called Tlr0636 protein.

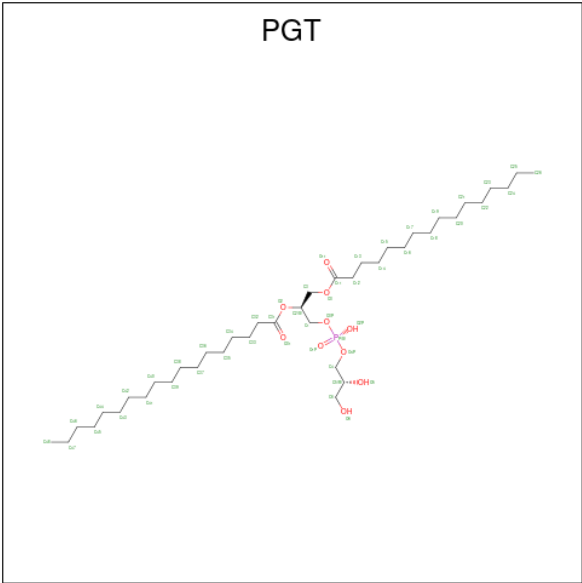
Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	55	Total	C	N	O	S	0	0
			432	280	69	82	1		

- Molecule 19 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			66	51	15	
19	L	1	Total	C	O	0
			66	51	15	

- Molecule 20 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSP HORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



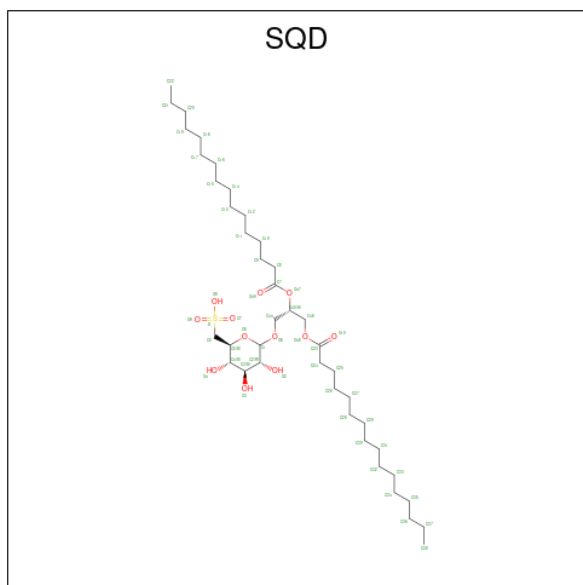
Mol	Chain	Residues	Atoms				AltConf
20	C	1	Total	C	O	P	0
			51	40	10	1	

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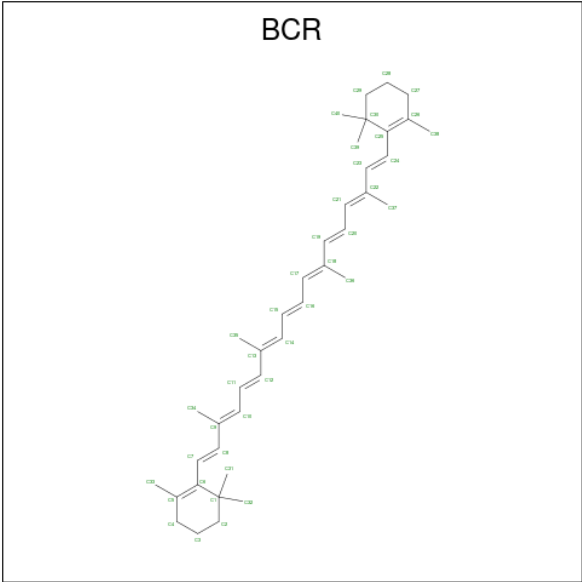
Mol	Chain	Residues	Atoms				AltConf
20	D	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



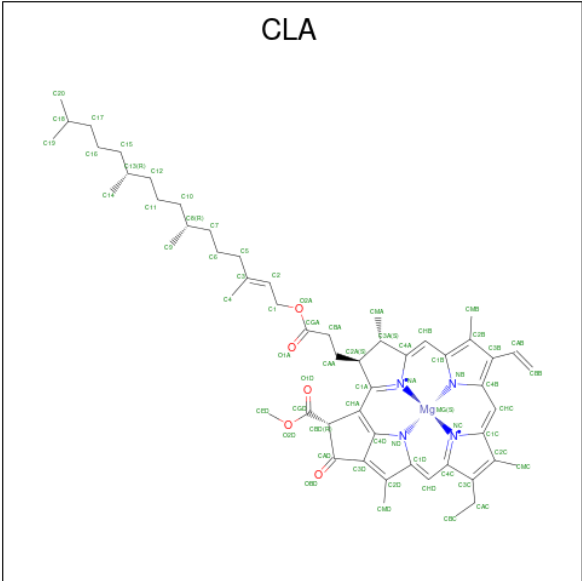
Mol	Chain	Residues	Atoms				AltConf
21	D	1	Total	C	O	S	0
			54	41	12	1	
21	F	1	Total	C	O	S	0
			54	41	12	1	
21	F	1	Total	C	O	S	0
			54	41	12	1	
21	K	1	Total	C	O	S	0
			54	41	12	1	
21	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



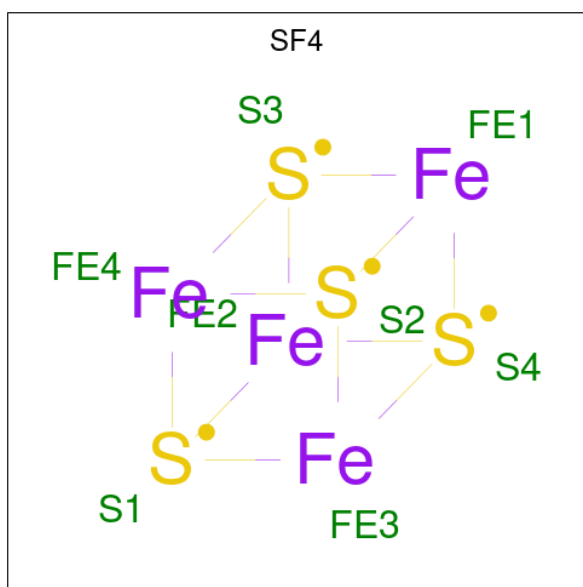
Mol	Chain	Residues	Atoms				AltConf
22	F	1	Total	C			0
			40	40			

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	F	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



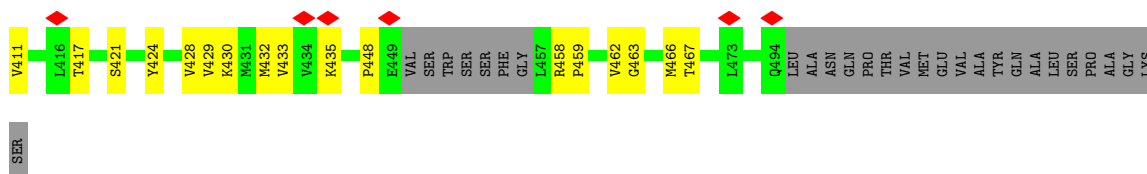
Mol	Chain	Residues	Atoms			AltConf
24	I	1	Total	Fe	S	0
			8	4	4	
24	I	1	Total	Fe	S	0
			8	4	4	
24	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
25	P	1	Total	Zn	0
			1	1	

- Molecule 26 is water.

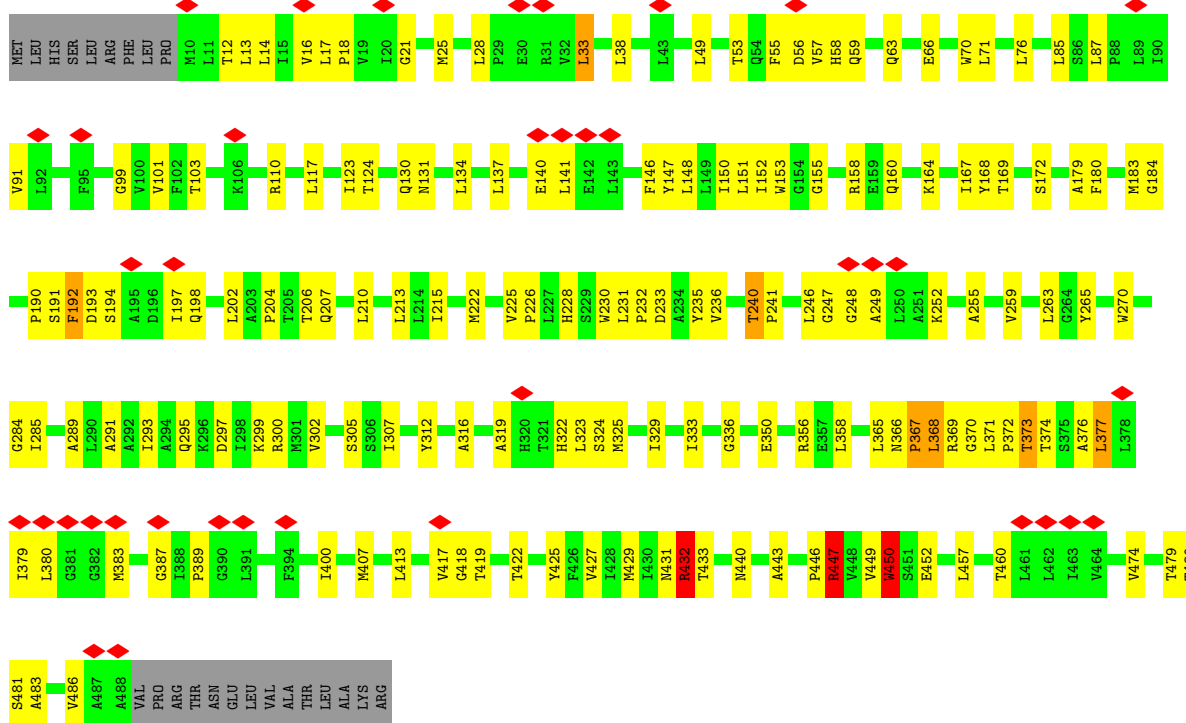
Mol	Chain	Residues	Atoms		AltConf
26	P	1	Total	O	0
			1	1	



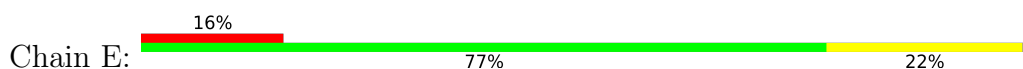
• Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3



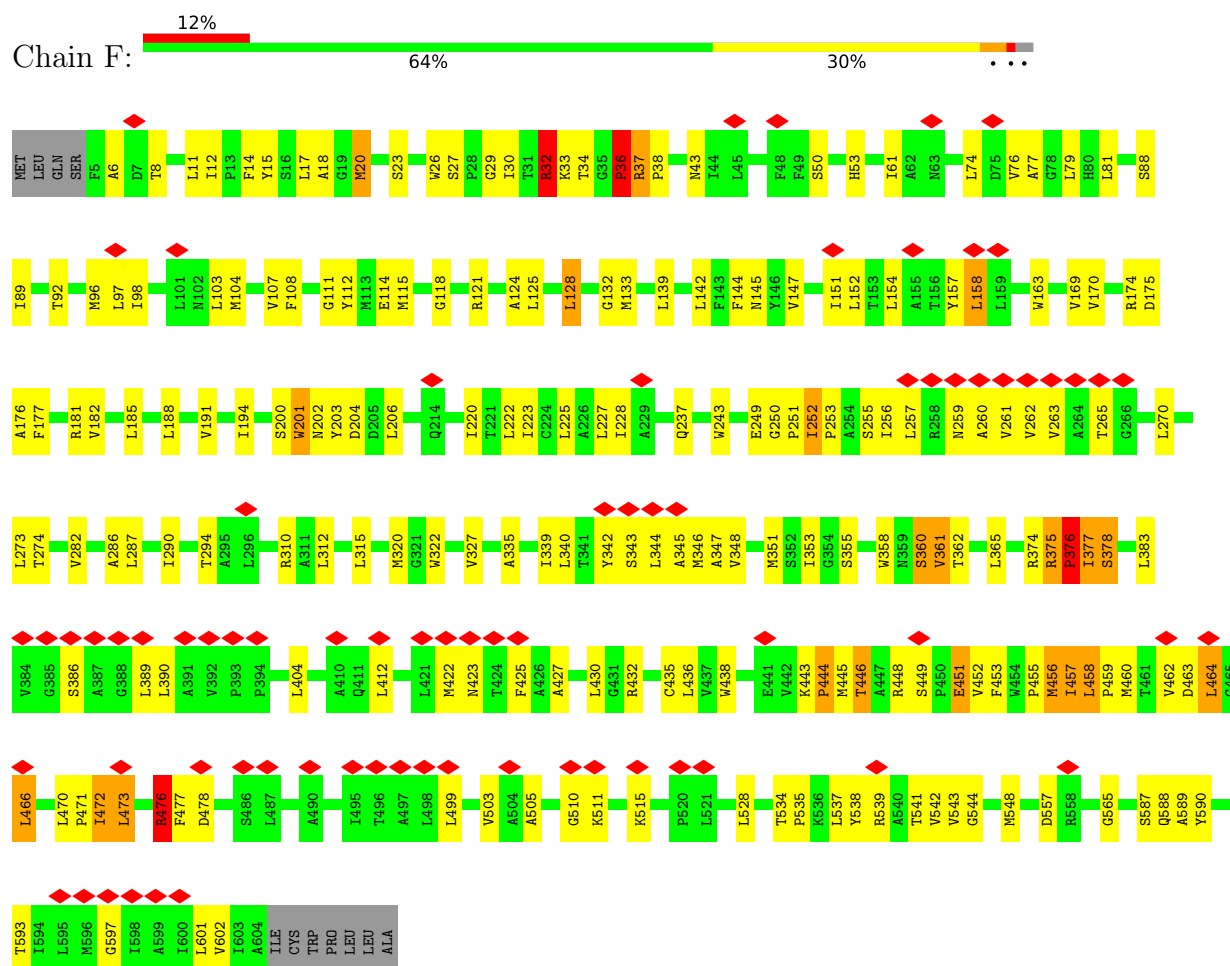
• Molecule 4: NADH dehydrogenase subunit 4



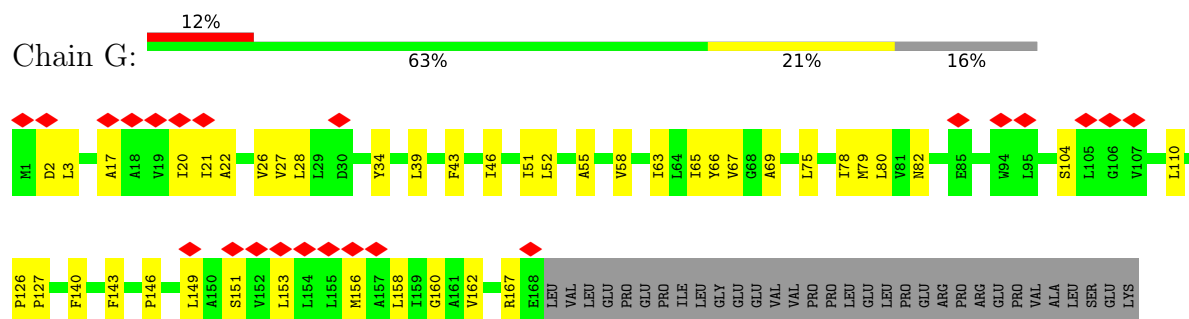
• Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L



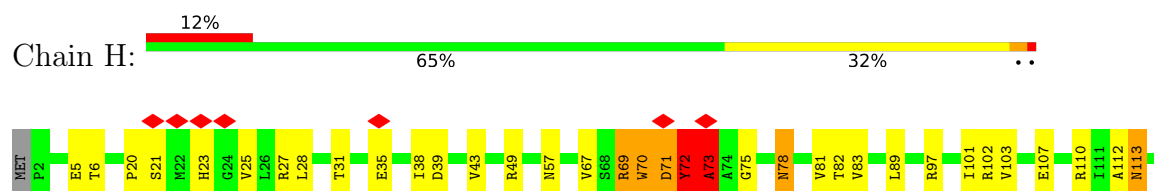
• Molecule 6: NADH dehydrogenase subunit 5

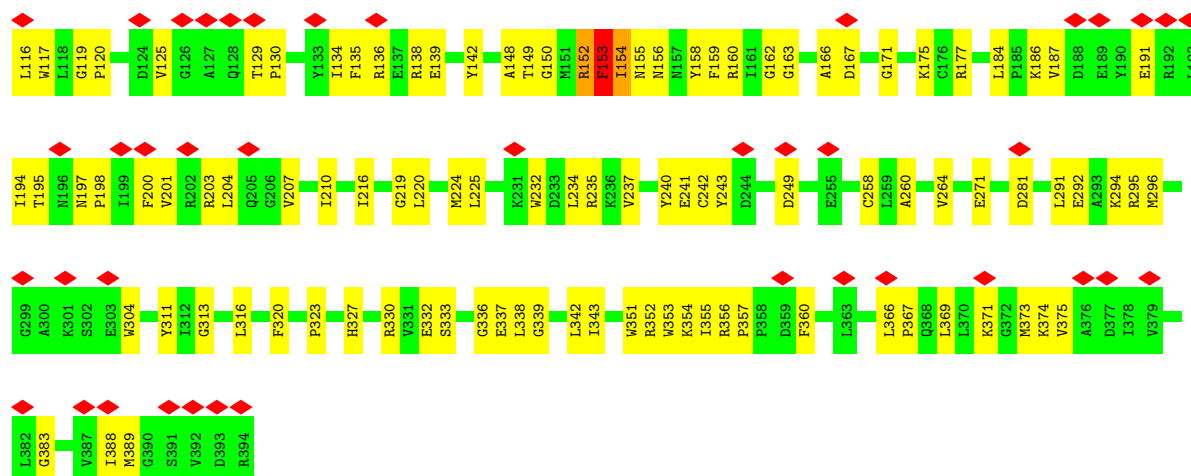


• Molecule 7: NADH dehydrogenase subunit 6

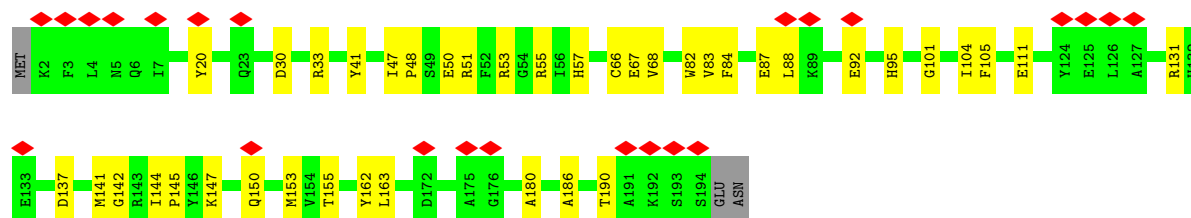
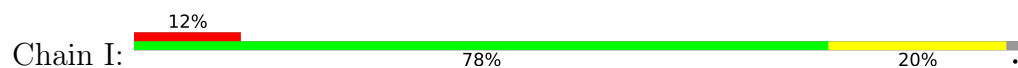


• Molecule 8: NAD(P)H-quinone oxidoreductase subunit H

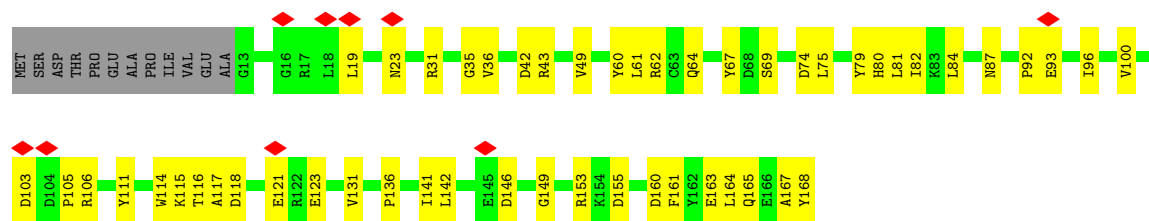




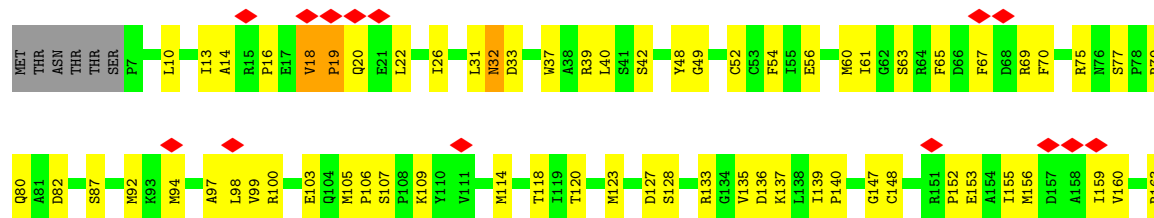
• Molecule 9: NAD(P)H-quinone oxidoreductase subunit I



• Molecule 10: NAD(P)H-quinone oxidoreductase subunit J



• Molecule 11: NAD(P)H-quinone oxidoreductase subunit K

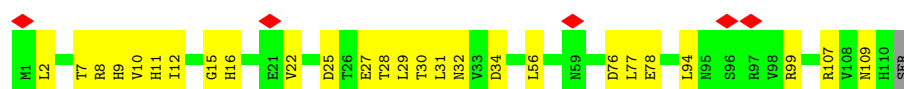
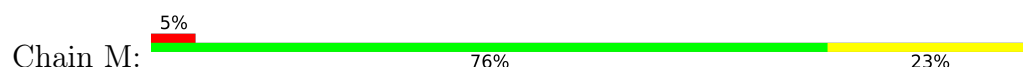




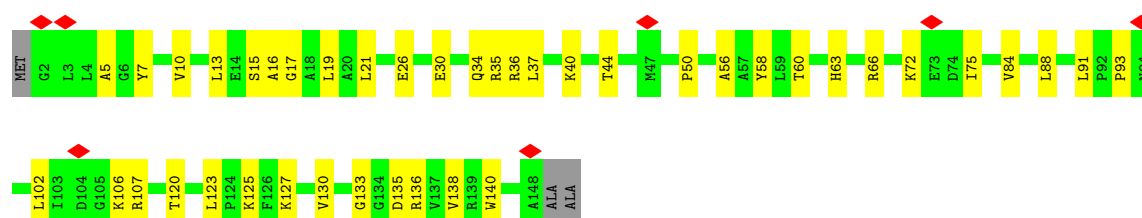
- Molecule 12: NAD(P)H-quinone oxidoreductase subunit L



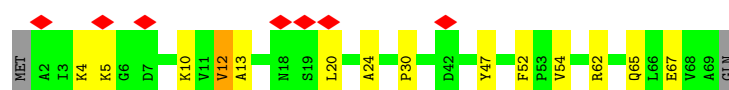
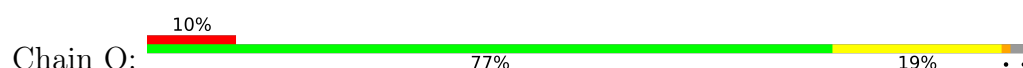
- Molecule 13: NAD(P)H-quinone oxidoreductase subunit M



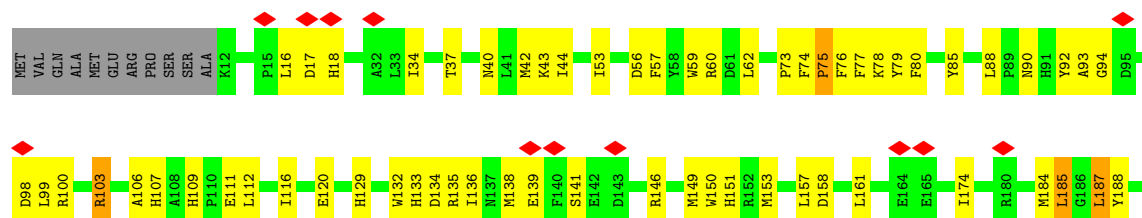
- Molecule 14: NAD(P)H-quinone oxidoreductase subunit N

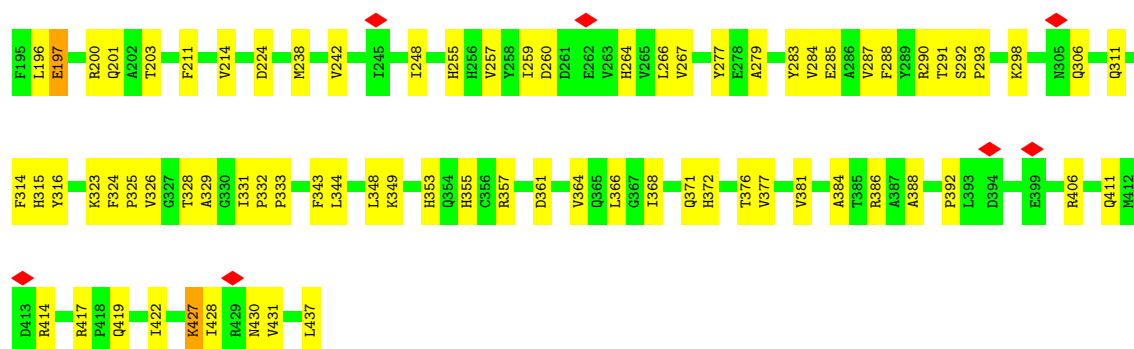


- Molecule 15: NAD(P)H-quinone oxidoreductase subunit O

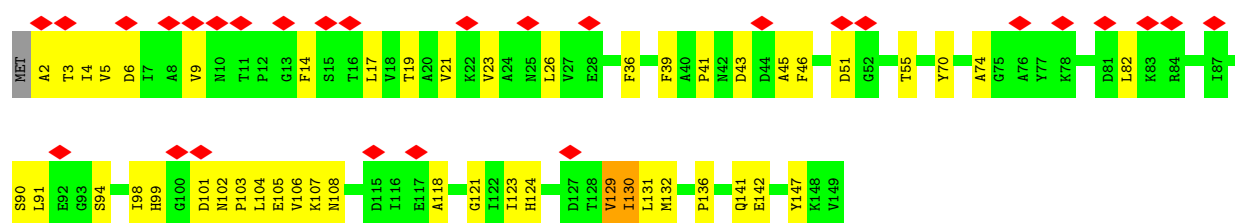


- Molecule 16: Thr0906 protein

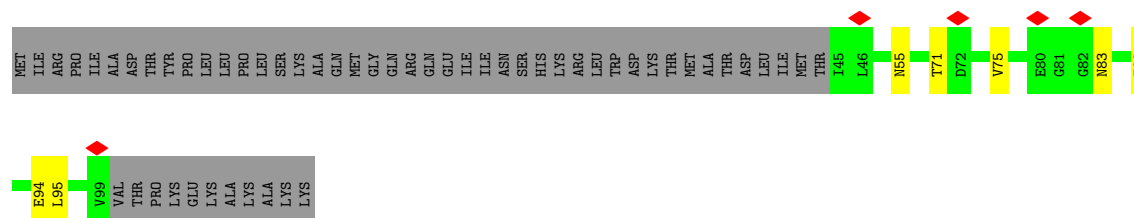
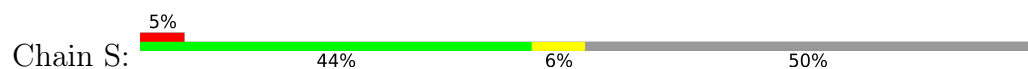




• Molecule 17: Tll0220 protein



• Molecule 18: Tlr0636 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	170151	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 ($e^-/\text{\AA}^2$)	40.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.267	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	378.0, 378.0, 378.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGT, DGD, SQD, CLA, SF4, ZN, BCR

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	0.36	1/2851 (0.0%)	0.67	12/3900 (0.3%)
2	B	0.29	0/3623	0.44	0/4947
3	C	0.45	1/942 (0.1%)	0.77	5/1285 (0.4%)
4	D	0.68	11/3703 (0.3%)	0.78	9/5065 (0.2%)
5	E	0.28	0/777	0.40	0/1054
6	F	0.63	11/4715 (0.2%)	0.81	18/6472 (0.3%)
7	G	0.26	0/1288	0.38	0/1765
8	H	0.32	1/3236 (0.0%)	0.61	3/4389 (0.1%)
9	I	0.28	0/1558	0.46	0/2116
10	J	0.27	0/1314	0.48	0/1789
11	K	0.31	0/1636	0.53	0/2228
12	L	0.21	0/629	0.50	0/860
13	M	0.28	0/895	0.49	0/1214
14	N	0.25	0/1192	0.48	0/1621
15	O	0.25	0/550	0.49	0/748
16	P	0.37	0/3615	0.61	1/4915 (0.0%)
17	Q	0.20	0/1117	0.54	0/1533
18	S	0.23	0/441	0.37	0/601
All	All	0.42	25/34082 (0.1%)	0.62	48/46502 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
4	D	0	3
6	F	1	4
8	H	0	2
11	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	P	0	1
All	All	1	13

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	376	PRO	N-CA	17.70	1.70	1.47
6	F	444	PRO	N-CA	17.52	1.69	1.47
4	D	367	PRO	N-CA	14.70	1.66	1.47
4	D	371	LEU	C-O	-12.99	1.17	1.23
4	D	446	PRO	C-O	-9.99	1.11	1.23
3	C	21	TYR	C-O	-9.92	1.11	1.24
4	D	450	TRP	C-O	-9.06	1.13	1.24
4	D	377	LEU	C-O	-8.93	1.13	1.24
6	F	124	ALA	C-O	-8.52	1.13	1.24
4	D	367	PRO	C-O	-8.07	1.13	1.24
4	D	372	PRO	C-O	-7.79	1.14	1.24
4	D	371	LEU	N-CA	7.78	1.51	1.46
6	F	121	ARG	C-O	-7.74	1.14	1.24
4	D	457	LEU	C-O	-7.61	1.14	1.24
8	H	73	ALA	C-N	-7.43	1.23	1.33
6	F	27	SER	C-N	6.97	1.50	1.33
1	A	300	PRO	C-O	-6.68	1.16	1.24
6	F	27	SER	C-O	-6.57	1.15	1.24
6	F	128	LEU	C-O	-6.50	1.15	1.24
4	D	374	THR	C-O	-6.40	1.15	1.24
6	F	125	LEU	C-O	-5.83	1.16	1.24
4	D	376	ALA	C-O	-5.68	1.17	1.24
6	F	158	LEU	C-O	-5.24	1.17	1.24
6	F	20	MET	C-O	-5.19	1.17	1.24
6	F	443	LYS	C-N	5.12	1.45	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	73	ALA	CA-C-N	-15.93	91.11	121.54
8	H	73	ALA	C-N-CA	-15.93	91.11	121.54
4	D	366	ASN	CA-C-N	15.28	138.94	119.84
4	D	366	ASN	C-N-CA	15.28	138.94	119.84
6	F	375	ARG	CA-C-N	15.20	138.85	119.84
6	F	375	ARG	C-N-CA	15.20	138.85	119.84
6	F	443	LYS	CA-C-N	14.09	137.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	443	LYS	C-N-CA	14.09	137.45	119.84
6	F	444	PRO	CA-N-CD	-11.71	95.60	112.00
4	D	372	PRO	N-CA-C	10.61	127.62	114.35
6	F	27	SER	CA-C-N	10.40	132.84	119.84
6	F	27	SER	C-N-CA	10.40	132.84	119.84
3	C	20	GLU	CB-CA-C	-8.80	92.91	110.42
4	D	372	PRO	CB-CA-C	-8.38	99.07	110.88
6	F	376	PRO	CA-N-CD	-7.95	100.87	112.00
4	D	373	THR	CB-CA-C	-7.91	95.89	109.65
4	D	367	PRO	CA-N-CD	-7.58	101.39	112.00
1	A	286	LEU	CA-C-N	7.42	135.72	121.54
1	A	286	LEU	C-N-CA	7.42	135.72	121.54
6	F	443	LYS	O-C-N	-7.40	114.39	121.57
4	D	374	THR	CA-CB-OG1	-7.29	98.67	109.60
3	C	21	TYR	CA-C-O	-7.12	112.34	120.24
1	A	288	THR	N-CA-C	-6.97	104.70	112.57
1	A	295	VAL	CA-C-O	-6.92	116.61	122.63
4	D	374	THR	N-CA-C	-6.84	104.75	113.23
6	F	29	GLY	CA-C-N	-6.83	116.19	123.08
6	F	29	GLY	C-N-CA	-6.83	116.19	123.08
6	F	36	PRO	N-CA-C	6.52	125.91	112.47
6	F	36	PRO	CB-CA-C	6.49	122.27	111.56
1	A	290	ALA	N-CA-C	-6.24	105.71	113.38
16	P	75	PRO	N-CA-C	-6.08	103.50	112.26
1	A	300	PRO	N-CA-C	-5.97	105.40	113.40
6	F	32	ARG	CG-CD-NE	-5.87	99.09	112.00
6	F	27	SER	CA-C-O	-5.79	113.99	120.25
6	F	36	PRO	CA-N-CD	-5.79	103.89	112.00
1	A	299	ASN	CA-CB-CG	-5.68	106.92	112.60
4	D	446	PRO	CB-CA-C	-5.52	103.72	110.95
1	A	298	THR	CA-C-N	-5.46	113.36	120.67
1	A	298	THR	C-N-CA	-5.46	113.36	120.67
1	A	301	PHE	CA-C-N	-5.40	111.23	121.54
1	A	301	PHE	C-N-CA	-5.40	111.23	121.54
8	H	73	ALA	O-C-N	-5.38	115.44	122.59
6	F	282	VAL	N-CA-C	-5.37	107.61	112.12
1	A	295	VAL	O-C-N	5.35	126.45	121.96
3	C	19	TYR	CB-CA-C	5.20	118.31	109.53
6	F	194	ILE	N-CA-C	-5.10	107.87	113.43
3	C	19	TYR	CA-C-N	5.04	131.17	121.54
3	C	19	TYR	C-N-CA	5.04	131.17	121.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	F	36	PRO	CA

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	387	PRO	Peptide
4	D	370	GLY	Mainchain
4	D	432	ARG	Sidechain
4	D	447	ARG	Sidechain
6	F	252	ILE	Peptide
6	F	32	ARG	Sidechain
6	F	360	SER	Peptide
6	F	476	ARG	Sidechain
8	H	153	PHE	Peptide
8	H	73	ALA	Mainchain
11	K	148	CYS	Peptide
11	K	18	VAL	Peptide
16	P	357	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2780	0	2901	168	0
2	B	3541	0	3650	100	0
3	C	914	0	945	37	0
4	D	3615	0	3819	151	0
5	E	769	0	827	25	0
6	F	4587	0	4763	243	0
7	G	1262	0	1334	42	0
8	H	3153	0	3116	109	0
9	I	1520	0	1474	34	0
10	J	1278	0	1233	44	0
11	K	1594	0	1629	100	0
12	L	609	0	625	39	0
13	M	879	0	860	23	0
14	N	1160	0	1171	33	0
15	O	538	0	549	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	3496	0	3375	113	0
17	Q	1095	0	1109	35	0
18	S	432	0	430	5	0
19	A	66	0	96	66	0
19	L	66	0	93	57	0
20	C	51	0	78	12	0
20	D	51	0	78	13	0
21	D	54	0	77	14	0
21	F	108	0	156	56	0
21	K	54	0	78	46	0
21	L	54	0	78	17	0
22	F	40	0	56	10	0
23	F	46	0	33	18	0
24	I	16	0	0	1	0
24	K	8	0	0	1	0
25	P	1	0	0	0	0
26	P	1	0	0	0	0
All	All	33838	0	34633	1234	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 18.

All (1234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:CE	19:A:501:DGD:HA31	1.19	1.64
1:A:35:LEU:HD11	19:A:501:DGD:C6A	1.17	1.61
12:L:19:LEU:CD2	19:L:401:DGD:HBS2	1.30	1.59
19:A:501:DGD:CEB	19:L:401:DGD:HAV2	1.28	1.59
11:K:171:ILE:HD11	21:K:502:SQD:C9	1.36	1.56
19:A:501:DGD:HBFB	19:L:401:DGD:CHA	1.41	1.48
19:A:501:DGD:CEB	19:L:401:DGD:CHA	1.92	1.46
11:K:171:ILE:HD11	21:K:502:SQD:C10	1.47	1.45
6:F:444:PRO:N	6:F:444:PRO:CA	1.69	1.41
12:L:19:LEU:CD2	19:L:401:DGD:CGB	1.97	1.41
6:F:376:PRO:CA	6:F:376:PRO:N	1.70	1.40
11:K:171:ILE:CD1	21:K:502:SQD:C10	1.99	1.38
4:D:168:TYR:CE1	20:D:602:PGT:H362	1.60	1.35
11:K:171:ILE:HD11	21:K:502:SQD:C8	1.55	1.34
6:F:472:ILE:HD12	23:F:704:CLA:CAC	1.57	1.33
11:K:171:ILE:CD1	21:K:502:SQD:H82	1.55	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:CD1	19:A:501:DGD:HA61	1.58	1.33
11:K:171:ILE:CD1	21:K:502:SQD:H101	1.56	1.32
4:D:417:VAL:CG1	21:F:701:SQD:H371	1.63	1.28
6:F:499:LEU:CD1	21:F:703:SQD:H362	1.61	1.27
1:A:36:MET:CE	19:A:501:DGD:C3A	2.13	1.27
6:F:472:ILE:HD12	23:F:704:CLA:C3C	1.64	1.27
1:A:35:LEU:CD1	19:A:501:DGD:C6A	2.09	1.25
6:F:453:PHE:CE1	6:F:455:PRO:HG2	1.73	1.23
6:F:453:PHE:CE1	6:F:455:PRO:CG	2.25	1.20
19:A:501:DGD:CCB	19:L:401:DGD:HAS1	1.70	1.19
19:A:501:DGD:HBW2	19:L:401:DGD:CGA	1.71	1.19
4:D:417:VAL:HG22	21:F:701:SQD:C37	1.71	1.18
6:F:448:ARG:NH1	16:P:158:ASP:OD1	1.76	1.18
12:L:66:ASN:OD1	21:L:402:SQD:C3	1.91	1.16
4:D:417:VAL:HG13	21:F:701:SQD:C37	1.75	1.15
19:A:501:DGD:HBF1	19:L:401:DGD:HAV2	1.18	1.14
12:L:66:ASN:OD1	21:L:402:SQD:H3	0.99	1.13
4:D:168:TYR:HE1	20:D:602:PGT:C36	1.61	1.12
11:K:171:ILE:HD12	21:K:502:SQD:H101	1.13	1.10
1:A:35:LEU:HD11	19:A:501:DGD:HA62	1.27	1.10
6:F:472:ILE:HG21	23:F:704:CLA:CAC	1.80	1.10
12:L:19:LEU:HD22	19:L:401:DGD:HBS2	1.29	1.10
4:D:417:VAL:CG2	21:F:701:SQD:H372	1.81	1.08
12:L:56:PRO:HG3	19:L:401:DGD:CIA	1.73	1.07
6:F:453:PHE:CD1	6:F:455:PRO:HD3	1.91	1.05
11:K:171:ILE:CD1	21:K:502:SQD:C11	2.34	1.05
11:K:171:ILE:HD13	21:K:502:SQD:H82	1.30	1.05
12:L:19:LEU:HD23	19:L:401:DGD:HBS2	1.07	1.05
1:A:36:MET:HE3	19:A:501:DGD:C3A	1.77	1.04
1:A:36:MET:HE1	19:A:501:DGD:HA31	1.38	1.03
11:K:171:ILE:CD1	21:K:502:SQD:C8	2.22	1.03
6:F:472:ILE:CG2	23:F:704:CLA:HAC1	1.87	1.03
19:A:501:DGD:O4D	19:L:401:DGD:O2D	1.67	1.02
6:F:378:SER:OG	6:F:438:TRP:CH2	2.11	1.02
6:F:499:LEU:HD11	21:F:703:SQD:H362	1.03	1.01
6:F:472:ILE:CD1	23:F:704:CLA:CAC	2.39	1.00
6:F:362:THR:CG2	6:F:445:MET:SD	2.50	1.00
6:F:453:PHE:CD1	6:F:455:PRO:CD	2.44	1.00
4:D:417:VAL:HG22	21:F:701:SQD:H372	1.01	1.00
19:A:501:DGD:HBF2	19:L:401:DGD:HAV1	1.40	1.00
6:F:472:ILE:CG1	23:F:704:CLA:HAC2	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:499:LEU:HD21	21:F:703:SQD:C35	1.90	0.99
4:D:358:LEU:O	4:D:432:ARG:HD3	1.60	0.99
4:D:358:LEU:O	4:D:432:ARG:CD	2.11	0.99
1:A:299:ASN:OD1	1:A:300:PRO:HD2	1.61	0.98
11:K:171:ILE:CD1	21:K:502:SQD:H112	1.94	0.98
6:F:472:ILE:HD12	23:F:704:CLA:HAC2	1.42	0.97
12:L:19:LEU:HD21	19:L:401:DGD:CGB	1.89	0.96
6:F:453:PHE:CE1	6:F:455:PRO:CD	2.48	0.96
6:F:499:LEU:CD2	21:F:703:SQD:H342	1.95	0.96
6:F:499:LEU:HD21	21:F:703:SQD:H351	1.45	0.96
6:F:453:PHE:CZ	6:F:455:PRO:HG2	2.00	0.95
6:F:472:ILE:CD1	23:F:704:CLA:HAC2	1.95	0.95
12:L:19:LEU:HD22	19:L:401:DGD:CGB	1.83	0.95
6:F:111:GLY:C	6:F:456:MET:CE	2.40	0.95
4:D:168:TYR:HE1	20:D:602:PGT:H362	0.79	0.94
1:A:36:MET:HE2	19:A:501:DGD:HA51	1.49	0.94
6:F:112:TYR:N	6:F:456:MET:HE2	1.81	0.94
6:F:472:ILE:HG21	23:F:704:CLA:HAC1	0.97	0.94
6:F:499:LEU:HD11	21:F:703:SQD:C36	1.97	0.94
11:K:171:ILE:CD1	21:K:502:SQD:C9	2.32	0.94
19:A:501:DGD:CEB	19:L:401:DGD:HAV1	1.89	0.93
21:K:502:SQD:C19	21:L:402:SQD:H291	1.99	0.93
11:K:171:ILE:HD13	21:K:502:SQD:H112	1.51	0.92
6:F:472:ILE:CB	23:F:704:CLA:HAC2	1.99	0.92
19:A:501:DGD:CDB	19:L:401:DGD:HAV1	2.00	0.92
1:A:36:MET:HE2	19:A:501:DGD:HA31	1.52	0.91
1:A:299:ASN:OD1	1:A:300:PRO:CD	2.21	0.88
18:S:75:VAL:HG21	18:S:95:LEU:HD11	1.54	0.88
6:F:499:LEU:HD22	21:F:703:SQD:H342	1.53	0.88
6:F:111:GLY:HA2	6:F:453:PHE:HZ	1.37	0.88
19:A:501:DGD:CDB	19:L:401:DGD:CHA	2.51	0.88
1:A:27:LEU:HD12	20:C:201:PGT:H142	1.53	0.87
4:D:417:VAL:CG2	21:F:701:SQD:C37	2.47	0.87
1:A:35:LEU:CD1	19:A:501:DGD:HA62	1.89	0.87
6:F:378:SER:OG	6:F:438:TRP:HH2	1.48	0.86
1:A:36:MET:HE3	19:A:501:DGD:HA31	0.87	0.86
1:A:122:ASN:O	19:A:501:DGD:HD5	1.74	0.86
4:D:25:MET:SD	4:D:33:LEU:CD2	2.64	0.85
12:L:19:LEU:HD21	19:L:401:DGD:CHB	2.06	0.85
16:P:194:LEU:HD12	16:P:194:LEU:O	1.76	0.85
6:F:348:VAL:HG23	6:F:463:ASP:OD2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:348:VAL:CG2	6:F:463:ASP:OD2	2.26	0.84
1:A:122:ASN:O	19:A:501:DGD:C5D	2.24	0.84
3:C:46:LYS:NZ	21:K:502:SQD:H62	1.92	0.84
4:D:450:TRP:H	4:D:450:TRP:CD1	1.89	0.83
6:F:351:MET:HE3	6:F:460:MET:HA	1.60	0.83
6:F:362:THR:HG21	6:F:445:MET:SD	2.18	0.83
21:K:502:SQD:O49	21:K:502:SQD:H252	1.79	0.83
21:K:502:SQD:H191	21:L:402:SQD:H291	1.60	0.82
12:L:56:PRO:HG3	19:L:401:DGD:HAG3	1.61	0.82
3:C:46:LYS:HZ1	21:K:502:SQD:H62	1.43	0.81
1:A:123:LEU:O	19:A:501:DGD:HB21	1.80	0.81
19:A:501:DGD:HBF2	19:L:401:DGD:HAV2	0.93	0.81
1:A:32:LEU:HD12	19:A:501:DGD:HA21	1.62	0.81
21:D:601:SQD:H372	21:D:601:SQD:H181	1.62	0.81
4:D:160:GLN:HG3	20:D:602:PGT:H42	1.62	0.81
1:A:36:MET:HE2	19:A:501:DGD:C5A	2.11	0.80
1:A:29:TRP:HZ2	19:A:501:DGD:HO2D	1.27	0.80
6:F:472:ILE:CG2	23:F:704:CLA:CAC	2.53	0.80
19:A:501:DGD:HBH1	19:L:401:DGD:HAV1	1.63	0.80
6:F:425:PHE:HE1	21:F:703:SQD:H291	1.46	0.79
6:F:445:MET:O	16:P:150:TRP:NE1	2.15	0.79
3:C:70:PHE:HD2	7:G:80:LEU:HD12	1.46	0.79
1:A:280:TRP:CD1	19:L:401:DGD:HO4E	2.00	0.79
1:A:36:MET:CE	19:A:501:DGD:C5A	2.61	0.79
6:F:499:LEU:CD1	21:F:703:SQD:C36	2.54	0.79
6:F:128:LEU:HD23	6:F:128:LEU:O	1.82	0.79
5:E:32:MET:HG2	7:G:39:LEU:HD22	1.65	0.79
6:F:111:GLY:C	6:F:456:MET:HE2	2.07	0.78
6:F:378:SER:OG	6:F:438:TRP:CZ3	2.36	0.78
4:D:131:ASN:HA	4:D:193:ASP:HA	1.65	0.77
4:D:417:VAL:CG1	21:F:701:SQD:C37	2.49	0.77
12:L:19:LEU:CD2	19:L:401:DGD:HBS1	2.08	0.77
12:L:19:LEU:CD2	19:L:401:DGD:CHB	2.63	0.77
6:F:182:VAL:HG22	21:F:701:SQD:H342	1.65	0.76
21:K:502:SQD:H192	21:L:402:SQD:H291	1.65	0.76
11:K:171:ILE:HD12	21:K:502:SQD:C10	1.86	0.76
12:L:19:LEU:HD22	19:L:401:DGD:HBS1	1.66	0.76
12:L:56:PRO:CG	19:L:401:DGD:CIA	2.57	0.75
16:P:196:LEU:O	16:P:196:LEU:HD23	1.85	0.75
6:F:452:VAL:HG23	6:F:457:ILE:CG2	2.17	0.75
1:A:301:PHE:HE1	12:L:9:VAL:HG12	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:358:TRP:CE3	6:F:452:VAL:HG12	2.22	0.75
22:F:702:BCR:H383	22:F:702:BCR:H23C	1.69	0.75
8:H:152:ARG:O	8:H:156:ASN:ND2	2.20	0.75
6:F:111:GLY:CA	6:F:453:PHE:HZ	1.99	0.74
1:A:124:LEU:O	19:A:501:DGD:HE4	1.86	0.74
16:P:388:ALA:HB1	17:Q:131:LEU:HD12	1.70	0.74
16:P:16:LEU:HG	16:P:17:ASP:H	1.52	0.74
6:F:472:ILE:CB	23:F:704:CLA:CAC	2.66	0.74
19:A:501:DGD:HG32	19:A:501:DGD:O2D	1.84	0.74
4:D:358:LEU:O	4:D:432:ARG:HD2	1.87	0.74
6:F:425:PHE:CE1	21:F:703:SQD:H291	2.22	0.74
1:A:126:SER:HB3	3:C:21:TYR:CD2	2.22	0.74
6:F:362:THR:HG23	6:F:445:MET:SD	2.27	0.74
6:F:377:ILE:HD13	6:F:377:ILE:N	2.02	0.74
6:F:602:VAL:HG11	7:G:110:LEU:HD21	1.70	0.74
4:D:417:VAL:HG13	21:F:701:SQD:H371	0.81	0.73
11:K:171:ILE:HD11	21:K:502:SQD:H91	1.62	0.73
16:P:77:PHE:HB3	16:P:80:PHE:HD2	1.51	0.73
4:D:417:VAL:CB	21:F:701:SQD:H371	2.18	0.73
6:F:111:GLY:C	6:F:456:MET:HE1	2.13	0.73
4:D:417:VAL:CB	21:F:701:SQD:C37	2.66	0.73
2:B:137:VAL:HG12	7:G:149:LEU:HD23	1.70	0.73
16:P:285:GLU:OE2	16:P:414:ARG:NH2	2.23	0.72
4:D:365:LEU:HD12	4:D:365:LEU:O	1.90	0.72
1:A:32:LEU:HD12	19:A:501:DGD:C2A	2.18	0.72
7:G:153:LEU:HA	7:G:156:MET:HE3	1.70	0.72
16:P:138:MET:HE3	16:P:141:SER:OG	1.89	0.72
4:D:25:MET:SD	4:D:33:LEU:HD21	2.28	0.72
4:D:168:TYR:CE1	20:D:602:PGT:C36	2.50	0.72
6:F:104:MET:SD	6:F:463:ASP:HB2	2.29	0.72
20:D:602:PGT:O2P	20:D:602:PGT:O5	2.05	0.72
6:F:374:ARG:HD3	16:P:197:GLU:OE1	1.88	0.72
8:H:119:GLY:HA3	8:H:134:ILE:HD13	1.72	0.71
19:A:501:DGD:HBW2	19:L:401:DGD:HAS1	0.83	0.71
6:F:499:LEU:CD2	21:F:703:SQD:C34	2.66	0.71
16:P:194:LEU:HD12	16:P:194:LEU:C	2.14	0.71
17:Q:82:LEU:HB3	17:Q:98:ILE:HD12	1.72	0.71
2:B:126:ILE:HD11	2:B:258:LEU:HD22	1.72	0.71
6:F:228:ILE:HD12	6:F:287:LEU:HD13	1.73	0.71
6:F:473:LEU:HD23	6:F:473:LEU:C	2.15	0.71
2:B:290:ASN:HD22	2:B:417:THR:HB	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:98:ILE:HD13	6:F:133:MET:HB3	1.71	0.71
15:O:52:PHE:O	15:O:54:VAL:N	2.23	0.71
6:F:17:LEU:HD13	6:F:20:MET:HE3	1.72	0.71
6:F:358:TRP:HE3	6:F:452:VAL:HG12	1.56	0.71
10:J:123:GLU:HB2	10:J:141:ILE:HD11	1.72	0.71
6:F:374:ARG:HD2	6:F:449:SER:OG	1.91	0.71
4:D:417:VAL:HG22	21:F:701:SQD:C38	2.20	0.70
6:F:458:LEU:HB3	6:F:459:PRO:HD3	1.72	0.70
1:A:29:TRP:HZ3	19:A:501:DGD:HE62	1.56	0.70
1:A:121:GLN:H	19:L:401:DGD:HE61	1.56	0.70
19:L:401:DGD:HE2	19:L:401:DGD:O5E	1.92	0.70
6:F:543:VAL:HG21	21:F:701:SQD:O49	1.92	0.70
6:F:253:PRO:O	6:F:257:LEU:N	2.18	0.70
6:F:464:LEU:HD12	6:F:464:LEU:O	1.92	0.70
6:F:472:ILE:HB	23:F:704:CLA:HAC2	1.74	0.70
3:C:54:THR:O	11:K:79:ARG:NH2	2.25	0.69
6:F:175:ASP:OD1	21:F:701:SQD:H101	1.92	0.69
4:D:168:TYR:CE1	20:D:602:PGT:H381	2.27	0.69
8:H:27:ARG:HB3	8:H:43:VAL:HB	1.73	0.69
16:P:138:MET:CE	16:P:141:SER:OG	2.40	0.69
1:A:286:LEU:HG	1:A:286:LEU:O	1.93	0.69
8:H:75:GLY:HA3	8:H:154:ILE:HG22	1.75	0.69
6:F:132:GLY:HA3	6:F:152:LEU:HD11	1.74	0.69
8:H:110:ARG:NH2	8:H:332:GLU:O	2.21	0.69
6:F:499:LEU:HD21	21:F:703:SQD:C34	2.22	0.69
1:A:27:LEU:HD12	20:C:201:PGT:C14	2.22	0.69
1:A:35:LEU:HD11	19:A:501:DGD:HA61	0.69	0.69
4:D:28:LEU:O	4:D:110:ARG:NH1	2.26	0.69
1:A:36:MET:HE1	19:A:501:DGD:C3A	2.03	0.69
20:C:201:PGT:O2P	20:C:201:PGT:O5	2.10	0.69
21:L:402:SQD:O4	21:L:402:SQD:O2	2.09	0.68
1:A:55:ILE:HD12	1:A:326:ILE:HD11	1.74	0.68
6:F:499:LEU:HD13	21:F:703:SQD:H362	1.70	0.68
8:H:154:ILE:HD11	11:K:52:CYS:HB3	1.76	0.68
12:L:19:LEU:HD21	19:L:401:DGD:HBV1	1.76	0.68
8:H:210:ILE:HG12	8:H:369:LEU:HD21	1.76	0.67
1:A:196:VAL:HG11	1:A:280:TRP:CZ3	2.29	0.67
6:F:174:ARG:NH1	21:F:701:SQD:O7	2.28	0.67
6:F:26:TRP:HB3	6:F:36:PRO:HD3	1.77	0.67
16:P:161:LEU:O	16:P:200:ARG:NH1	2.27	0.67
2:B:430:LYS:HG3	4:D:151:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:501:DGD:HB1	19:L:401:DGD:CHA	1.92	0.67
2:B:335:VAL:HG12	2:B:339:MET:HE2	1.77	0.67
6:F:287:LEU:HD21	6:F:327:VAL:HG13	1.77	0.67
16:P:103:ARG:HH22	16:P:224:ASP:HB3	1.58	0.67
17:Q:39:PHE:HB3	17:Q:124:HIS:HB2	1.77	0.67
8:H:21:SER:HG	8:H:23:HIS:HD1	1.41	0.67
16:P:355:HIS:CE1	16:P:437:LEU:HG	2.30	0.67
16:P:411:GLN:NE2	17:Q:142:GLU:O	2.27	0.67
4:D:25:MET:SD	4:D:33:LEU:HD23	2.34	0.67
11:K:20:GLN:HB2	11:K:22:LEU:HD23	1.76	0.67
6:F:499:LEU:CD2	21:F:703:SQD:C35	2.70	0.66
8:H:102:ARG:NH2	8:H:163:GLY:O	2.28	0.66
6:F:249:GLU:OE2	6:F:310:ARG:NH2	2.28	0.66
4:D:380:LEU:HD23	4:D:460:THR:HG23	1.76	0.66
6:F:34:THR:HB	16:P:134:ASP:H	1.60	0.66
6:F:176:ALA:HA	6:F:243:TRP:HB2	1.77	0.66
14:N:5:ALA:HB3	14:N:36:ARG:HH12	1.61	0.66
1:A:29:TRP:CZ3	19:A:501:DGD:HE62	2.30	0.66
21:K:502:SQD:H192	21:L:402:SQD:H302	1.78	0.66
6:F:342:TYR:HD1	6:F:389:LEU:HD11	1.60	0.66
8:H:155:ASN:O	9:I:53:ARG:NH2	2.29	0.66
6:F:457:ILE:O	6:F:457:ILE:HD12	1.96	0.65
9:I:131:ARG:NH1	10:J:167:ALA:O	2.30	0.65
17:Q:106:VAL:HG12	17:Q:107:LYS:H	1.61	0.65
21:K:502:SQD:H192	21:L:402:SQD:C30	2.27	0.65
8:H:219:GLY:HA2	10:J:60:TYR:HE1	1.61	0.65
10:J:136:PRO:HB2	11:K:207:ARG:HD2	1.79	0.65
21:K:502:SQD:C19	21:L:402:SQD:C29	2.75	0.65
2:B:97:MET:HE2	2:B:348:ILE:HD12	1.79	0.65
4:D:417:VAL:HA	21:F:701:SQD:C37	2.25	0.65
6:F:541:THR:HG21	21:F:701:SQD:H211	1.79	0.65
1:A:308:VAL:HG13	19:L:401:DGD:HBH2	1.77	0.65
16:P:34:ILE:HD11	16:P:44:ILE:HD11	1.78	0.65
2:B:387:PRO:HB3	4:D:137:LEU:HD12	1.78	0.65
4:D:377:LEU:HD22	4:D:460:THR:OG1	1.96	0.65
6:F:111:GLY:HA2	6:F:453:PHE:CZ	2.28	0.65
8:H:330:ARG:HD3	10:J:62:ARG:HH22	1.61	0.65
11:K:128:SER:O	11:K:133:ARG:NH2	2.29	0.65
1:A:121:GLN:HB3	19:L:401:DGD:C6E	2.27	0.65
6:F:541:THR:HG23	6:F:542:VAL:HG23	1.79	0.65
1:A:65:PRO:HA	11:K:69:ARG:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PHE:HZ	12:L:8:LEU:HD22	1.62	0.64
1:A:98:LEU:HB2	1:A:152:ALA:HB2	1.79	0.64
2:B:165:LYS:HG3	6:F:587:SER:HB3	1.78	0.64
21:D:601:SQD:H1	21:D:601:SQD:H462	1.80	0.64
6:F:79:LEU:HD13	6:F:81:LEU:HG	1.78	0.64
16:P:151:HIS:HB3	16:P:153:MET:HG3	1.80	0.64
1:A:113:SER:HB2	1:A:267:LEU:HD11	1.80	0.64
1:A:289:ILE:HG22	1:A:289:ILE:O	1.98	0.64
8:H:112:ALA:O	8:H:138:ARG:NH1	2.31	0.64
16:P:53:ILE:HD12	16:P:343:PHE:HB3	1.80	0.63
2:B:310:GLN:OE1	2:B:332:TYR:OH	2.13	0.63
4:D:417:VAL:CB	21:F:701:SQD:H372	2.29	0.63
14:N:19:LEU:HD12	14:N:140:TRP:HB2	1.80	0.63
6:F:111:GLY:CA	6:F:453:PHE:CZ	2.81	0.63
6:F:237:GLN:NE2	6:F:294:THR:HG21	2.13	0.63
13:M:11:HIS:HB2	13:M:32:ASN:HB3	1.80	0.63
17:Q:41:PRO:HB3	17:Q:45:ALA:HB3	1.80	0.63
3:C:82:VAL:HG22	7:G:69:ALA:HB1	1.80	0.63
6:F:432:ARG:NH2	21:F:703:SQD:O8	2.29	0.63
15:O:10:LYS:NZ	15:O:67:GLU:OE2	2.29	0.63
8:H:69:ARG:HH22	8:H:155:ASN:HB2	1.63	0.63
8:H:138:ARG:NE	8:H:142:TYR:OH	2.23	0.63
11:K:163:ARG:NH1	14:N:26:GLU:O	2.31	0.63
16:P:428:ILE:HA	16:P:431:VAL:HG12	1.80	0.63
1:A:301:PHE:CE1	12:L:9:VAL:HG12	2.33	0.63
4:D:236:VAL:HG21	4:D:300:ARG:HG2	1.79	0.63
21:K:502:SQD:H192	21:L:402:SQD:C29	2.29	0.63
6:F:104:MET:HE1	6:F:466:LEU:CD2	2.29	0.63
4:D:231:LEU:HD23	4:D:307:ILE:HG13	1.81	0.62
6:F:104:MET:HE1	6:F:466:LEU:HD22	1.80	0.62
6:F:262:VAL:HG12	6:F:320:MET:HE3	1.79	0.62
8:H:194:ILE:HG22	8:H:195:THR:H	1.63	0.62
16:P:135:ARG:NH1	16:P:139:GLU:OE1	2.33	0.62
1:A:289:ILE:HG23	1:A:292:LEU:HG	1.80	0.62
6:F:453:PHE:HE1	6:F:455:PRO:CG	2.03	0.62
6:F:473:LEU:HD23	6:F:473:LEU:O	1.99	0.62
12:L:19:LEU:HD23	19:L:401:DGD:CGB	1.95	0.62
1:A:306:PHE:HB3	19:L:401:DGD:HE3	1.80	0.62
6:F:452:VAL:CG2	6:F:457:ILE:CG2	2.77	0.62
1:A:291:ASN:N	1:A:291:ASN:OD1	2.32	0.62
4:D:57:VAL:HG22	4:D:58:HIS:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:601:SQD:H101	21:D:601:SQD:O49	1.97	0.62
6:F:74:LEU:HD13	6:F:76:VAL:HG23	1.80	0.62
8:H:70:TRP:O	8:H:78:ASN:ND2	2.32	0.62
17:Q:17:LEU:HD12	17:Q:41:PRO:HD2	1.82	0.62
6:F:261:VAL:O	6:F:265:THR:OG1	2.08	0.61
6:F:348:VAL:HG22	6:F:463:ASP:OD2	2.00	0.61
11:K:182:ARG:NH1	13:M:34:ASP:O	2.33	0.61
4:D:58:HIS:HA	4:D:479:THR:HG21	1.82	0.61
10:J:75:LEU:HD11	10:J:153:ARG:HH12	1.65	0.61
2:B:421:SER:HA	2:B:424:TYR:CE2	2.35	0.61
4:D:225:VAL:O	4:D:228:HIS:ND1	2.33	0.61
4:D:447:ARG:HB3	4:D:447:ARG:NH1	2.16	0.61
9:I:144:ILE:HG13	18:S:71:THR:HG22	1.83	0.61
6:F:228:ILE:HD13	6:F:270:LEU:HD11	1.81	0.61
6:F:472:ILE:CD1	23:F:704:CLA:C3C	2.59	0.61
7:G:27:VAL:HG23	7:G:28:LEU:HD12	1.83	0.61
3:C:52:ARG:NH2	11:K:107:SER:OG	2.33	0.61
6:F:378:SER:HG	6:F:438:TRP:HH2	0.70	0.61
5:E:61:VAL:HG11	7:G:143:PHE:HD2	1.65	0.61
10:J:160:ASP:HB2	15:O:30:PRO:HB3	1.82	0.61
4:D:12:THR:OG1	4:D:66:GLU:OE1	2.19	0.61
11:K:105:MET:HG2	11:K:109:LYS:HD3	1.83	0.61
16:P:238:MET:O	16:P:242:VAL:HG23	2.01	0.61
2:B:226:VAL:HG12	2:B:229:HIS:CG	2.36	0.60
4:D:164:LYS:NZ	4:D:233:ASP:OD2	2.28	0.60
23:F:704:CLA:HBB1	23:F:704:CLA:CHC	2.31	0.60
8:H:333:SER:N	8:H:336:GLY:O	2.34	0.60
2:B:141:THR:HG23	7:G:156:MET:HE1	1.81	0.60
8:H:204:LEU:HB2	8:H:258:CYS:HB2	1.83	0.60
16:P:149:MET:HE1	16:P:201:GLN:HA	1.81	0.60
8:H:35:GLU:HG3	8:H:375:VAL:HG12	1.82	0.60
16:P:92:TYR:HB2	16:P:100:ARG:H	1.67	0.60
11:K:127:ASP:OD1	14:N:72:LYS:NZ	2.33	0.60
1:A:118:PRO:HA	1:A:124:LEU:HB3	1.84	0.60
2:B:220:SER:HB3	2:B:225:ALA:HB3	1.82	0.60
6:F:470:LEU:HB3	6:F:471:PRO:HD3	1.84	0.60
9:I:131:ARG:NH2	10:J:168:TYR:O	2.31	0.60
20:C:201:PGT:H341	20:C:201:PGT:O31	2.02	0.60
6:F:112:TYR:N	6:F:456:MET:CE	2.55	0.60
8:H:220:LEU:O	8:H:225:LEU:HB2	2.01	0.60
6:F:37:ARG:H	6:F:38:PRO:HD2	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:220:ILE:HA	6:F:223:ILE:HG12	1.83	0.60
10:J:141:ILE:HG13	10:J:142:LEU:H	1.67	0.60
1:A:36:MET:HE1	19:A:501:DGD:C5A	2.30	0.60
2:B:188:SER:HB2	2:B:200:ALA:HB3	1.84	0.60
9:I:55:ARG:NH1	9:I:141:MET:O	2.32	0.59
12:L:9:VAL:HA	12:L:12:VAL:HG12	1.82	0.59
1:A:36:MET:CE	19:A:501:DGD:C4A	2.80	0.59
11:K:13:ILE:HG22	11:K:14:ALA:H	1.67	0.59
2:B:459:PRO:HA	2:B:462:VAL:HG12	1.84	0.59
4:D:33:LEU:HD11	4:D:110:ARG:HB2	1.84	0.59
16:P:259:ILE:HG22	16:P:260:ASP:H	1.66	0.59
3:C:74:TYR:CE1	7:G:79:MET:HE1	2.37	0.59
6:F:351:MET:CE	6:F:460:MET:HA	2.31	0.59
8:H:39:ASP:OD2	11:K:201:TYR:N	2.32	0.59
9:I:150:GLN:HA	12:L:74:LEU:HD11	1.84	0.59
21:K:502:SQD:C7	21:K:502:SQD:C23	2.79	0.59
14:N:56:ALA:O	14:N:60:THR:OG1	2.19	0.59
17:Q:5:VAL:O	17:Q:9:VAL:HG23	2.03	0.59
4:D:169:THR:O	4:D:172:SER:HB3	2.01	0.59
4:D:231:LEU:HD11	4:D:235:TYR:CZ	2.38	0.59
12:L:68:ARG:NH1	14:N:136:ARG:O	2.35	0.59
1:A:60:GLN:OE1	1:A:62:ARG:NH1	2.35	0.59
3:C:86:VAL:HG11	5:E:68:THR:HG23	1.85	0.59
4:D:33:LEU:HD11	4:D:110:ARG:CB	2.33	0.59
17:Q:82:LEU:HB2	17:Q:104:LEU:HD21	1.85	0.59
4:D:422:THR:HA	4:D:425:TYR:CE2	2.37	0.59
6:F:76:VAL:HG12	6:F:77:ALA:H	1.68	0.59
8:H:134:ILE:O	8:H:138:ARG:N	2.31	0.59
11:K:75:ARG:HG2	11:K:80:GLN:HB2	1.84	0.59
6:F:26:TRP:HB3	6:F:36:PRO:CD	2.33	0.59
8:H:373:MET:O	8:H:374:LYS:HG2	2.03	0.59
1:A:298:THR:HG22	1:A:298:THR:O	2.03	0.58
4:D:191:SER:OG	4:D:193:ASP:OD2	2.19	0.58
9:I:87:GLU:HG3	9:I:88:LEU:H	1.68	0.58
16:P:283:TYR:CZ	16:P:287:VAL:HG21	2.38	0.58
16:P:174:ILE:HG21	16:P:188:TYR:CD2	2.38	0.58
1:A:15:LEU:HG	1:A:20:LEU:HD23	1.86	0.58
1:A:280:TRP:HD1	19:L:401:DGD:HO4E	1.49	0.58
2:B:268:PRO:HB2	2:B:270:VAL:HG12	1.83	0.58
16:P:135:ARG:HG2	16:P:136:ILE:H	1.69	0.58
14:N:7:TYR:HE1	14:N:36:ARG:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:111:GLY:O	6:F:456:MET:HE1	2.04	0.58
4:D:123:ILE:HG13	4:D:249:ALA:HB1	1.86	0.58
4:D:368:LEU:N	4:D:368:LEU:HD13	2.19	0.58
11:K:107:SER:HB3	11:K:177:LEU:HD21	1.85	0.58
14:N:10:VAL:HG11	14:N:40:LYS:HG3	1.85	0.58
9:I:95:HIS:NE2	9:I:137:ASP:OD1	2.37	0.58
4:D:168:TYR:CD1	20:D:602:PGT:H362	2.30	0.58
1:A:33:PRO:HB3	19:A:501:DGD:HG31	1.85	0.57
1:A:86:LYS:HZ2	11:K:106:PRO:HB2	1.69	0.57
4:D:431:ASN:ND2	6:F:170:VAL:O	2.37	0.57
4:D:293:ILE:HG12	4:D:425:TYR:HB3	1.85	0.57
2:B:109:LEU:HD11	2:B:113:MET:HE3	1.86	0.57
16:P:77:PHE:O	16:P:79:TYR:N	2.36	0.57
1:A:121:GLN:HB3	19:L:401:DGD:HE61	1.85	0.57
1:A:295:VAL:HG22	1:A:295:VAL:O	2.04	0.57
19:A:501:DGD:CEB	19:L:401:DGD:CGA	2.80	0.57
2:B:388:PRO:HD2	4:D:141:LEU:HD12	1.85	0.57
4:D:431:ASN:OD1	6:F:157:TYR:OH	2.20	0.57
16:P:153:MET:HE1	16:P:285:GLU:HG2	1.85	0.57
3:C:61:GLU:OE2	11:K:100:ARG:NH2	2.38	0.57
6:F:8:THR:HB	6:F:11:LEU:HD12	1.85	0.57
13:M:56:LEU:HD21	13:M:76:ASP:HB2	1.85	0.57
1:A:35:LEU:CG	19:A:501:DGD:HA61	2.31	0.57
4:D:14:LEU:HB3	4:D:124:THR:HG21	1.86	0.57
6:F:259:ASN:HD22	6:F:346:MET:HB3	1.69	0.57
2:B:236:TYR:O	2:B:300:LYS:HE2	2.04	0.57
2:B:148:LEU:HD13	7:G:160:GLY:HA3	1.87	0.57
2:B:288:LEU:O	2:B:292:VAL:HG12	2.05	0.57
6:F:377:ILE:HD13	6:F:377:ILE:H	1.70	0.57
16:P:255:HIS:HB2	16:P:267:VAL:HG12	1.86	0.57
5:E:86:ARG:HG3	7:G:167:ARG:HH12	1.70	0.57
6:F:139:LEU:HD23	6:F:144:PHE:HB3	1.86	0.57
12:L:66:ASN:OD1	21:L:402:SQD:C4	2.53	0.56
16:P:157:LEU:O	16:P:161:LEU:N	2.38	0.56
8:H:216:ILE:HG23	10:J:84:LEU:HD23	1.86	0.56
21:L:402:SQD:O3	21:L:402:SQD:H61	2.05	0.56
1:A:122:ASN:HB3	19:A:501:DGD:HD5	1.87	0.56
11:K:26:ILE:H	11:K:26:ILE:HD12	1.71	0.56
21:K:502:SQD:H81	21:K:502:SQD:H272	1.85	0.56
2:B:140:GLU:OE2	5:E:69:VAL:HG21	2.05	0.56
4:D:373:THR:HG22	4:D:373:THR:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:65:PHE:CE1	11:K:152:PRO:HB2	2.39	0.56
21:K:502:SQD:C20	21:L:402:SQD:H302	2.36	0.56
16:P:187:LEU:O	16:P:187:LEU:HD12	2.05	0.56
16:P:290:ARG:HA	16:P:314:PHE:O	2.06	0.56
1:A:187:SER:HB3	1:A:195:ILE:HA	1.88	0.56
2:B:53:GLY:O	2:B:57:THR:OG1	2.23	0.56
19:L:401:DGD:HGB2	19:L:401:DGD:HBF1	1.88	0.56
14:N:50:PRO:HG3	14:N:107:ARG:HB2	1.86	0.56
6:F:365:LEU:HB3	6:F:436:LEU:HD13	1.88	0.56
11:K:39:ARG:NH2	11:K:169:GLU:OE1	2.39	0.56
17:Q:90:SER:N	17:Q:94:SER:OG	2.38	0.56
1:A:168:GLN:HG3	1:A:340:LEU:HD21	1.87	0.56
10:J:31:ARG:NH1	10:J:35:GLY:O	2.38	0.56
19:L:401:DGD:HE1	19:L:401:DGD:O4D	2.05	0.56
6:F:355:SER:O	6:F:375:ARG:NH2	2.39	0.56
6:F:528:LEU:CD1	21:F:703:SQD:O10	2.54	0.56
11:K:65:PHE:HE1	11:K:152:PRO:HB2	1.70	0.56
16:P:417:ARG:O	16:P:422:ILE:HB	2.05	0.56
21:D:601:SQD:H172	21:D:601:SQD:H382	1.88	0.55
21:K:502:SQD:C30	21:K:502:SQD:C26	2.85	0.55
1:A:188:ASN:HA	3:C:99:HIS:HE1	1.71	0.55
4:D:71:LEU:HD12	4:D:76:LEU:HD23	1.86	0.55
4:D:248:GLY:O	4:D:252:LYS:HD3	2.05	0.55
17:Q:4:ILE:HG23	17:Q:123:ILE:HD11	1.87	0.55
17:Q:101:ASP:OD1	17:Q:101:ASP:N	2.38	0.55
1:A:56:SER:OG	1:A:330:TRP:NE1	2.40	0.55
21:D:601:SQD:C25	21:D:601:SQD:C29	2.84	0.55
6:F:541:THR:HG21	21:F:701:SQD:C21	2.37	0.55
8:H:57:ASN:ND2	11:K:127:ASP:OD2	2.25	0.55
21:F:703:SQD:H461	21:F:703:SQD:H82	1.88	0.55
8:H:69:ARG:HD2	8:H:69:ARG:N	2.22	0.55
8:H:241:GLU:HG3	8:H:242:CYS:H	1.72	0.55
5:E:28:VAL:HG21	7:G:78:ILE:HG12	1.88	0.55
22:F:702:BCR:H393	16:P:73:PRO:HB3	1.89	0.55
8:H:134:ILE:HG13	8:H:135:PHE:N	2.21	0.55
16:P:92:TYR:OH	16:P:214:VAL:HG13	2.07	0.55
1:A:268:SER:O	1:A:272:VAL:HG23	2.07	0.55
19:A:501:DGD:HE2	19:A:501:DGD:O5E	2.06	0.55
2:B:226:VAL:CG2	2:B:284:LEU:HB3	2.37	0.55
9:I:186:ALA:O	9:I:190:THR:HG23	2.07	0.55
11:K:20:GLN:HG2	11:K:22:LEU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:136:ARG:HH12	8:H:186:LYS:NZ	2.04	0.55
8:H:220:LEU:HD13	8:H:224:MET:HE2	1.88	0.55
21:K:502:SQD:C19	21:L:402:SQD:H302	2.37	0.55
4:D:240:THR:HG23	4:D:241:PRO:HD3	1.87	0.55
6:F:163:TRP:CZ2	6:F:250:GLY:HA2	2.42	0.55
6:F:312:LEU:HD11	6:F:353:ILE:HG13	1.88	0.55
6:F:499:LEU:HD21	21:F:703:SQD:C36	2.37	0.55
9:I:95:HIS:ND1	14:N:66:ARG:HD2	2.23	0.55
14:N:84:VAL:HG11	14:N:123:LEU:HD21	1.87	0.55
2:B:46:PHE:HA	2:B:49:VAL:HB	1.88	0.54
2:B:306:SER:O	2:B:310:GLN:HG2	2.07	0.54
6:F:425:PHE:CD1	21:F:703:SQD:H292	2.42	0.54
14:N:17:GLY:HA2	14:N:127:LYS:HD2	1.88	0.54
12:L:25:PRO:HB3	12:L:58:LEU:HD12	1.89	0.54
8:H:159:PHE:O	8:H:160:ARG:NH1	2.37	0.54
8:H:219:GLY:HA2	10:J:60:TYR:CE1	2.42	0.54
4:D:168:TYR:CD2	4:D:230:TRP:HB3	2.42	0.54
6:F:452:VAL:HG23	6:F:457:ILE:HG23	1.90	0.54
6:F:251:PRO:O	6:F:252:ILE:HG12	2.08	0.54
6:F:453:PHE:CD1	6:F:455:PRO:HD2	2.38	0.54
6:F:499:LEU:CD2	21:F:703:SQD:C36	2.85	0.54
14:N:7:TYR:CE1	14:N:36:ARG:HG3	2.43	0.54
1:A:15:LEU:HD21	1:A:28:LEU:HD23	1.88	0.54
19:A:501:DGD:HBF1	19:L:401:DGD:CGA	2.38	0.54
8:H:357:PRO:HG2	8:H:360:PHE:HB2	1.89	0.54
12:L:32:LEU:HG	12:L:47:MET:HE3	1.89	0.54
2:B:137:VAL:HA	2:B:140:GLU:OE2	2.07	0.54
14:N:10:VAL:HG22	14:N:37:LEU:HD23	1.89	0.54
17:Q:36:PHE:HA	17:Q:74:ALA:HA	1.90	0.54
1:A:301:PHE:CD1	1:A:301:PHE:N	2.73	0.54
2:B:27:VAL:HG21	2:B:50:GLY:HA3	1.88	0.54
8:H:89:LEU:HG	8:H:327:HIS:CE1	2.43	0.54
11:K:140:PRO:HA	13:M:8:ARG:HH12	1.73	0.54
1:A:29:TRP:HZ2	19:A:501:DGD:O2D	1.90	0.54
6:F:23:SER:HB3	6:F:43:ASN:HD21	1.72	0.54
6:F:259:ASN:ND2	6:F:343:SER:O	2.31	0.54
13:M:12:ILE:HD11	13:M:77:LEU:HD12	1.89	0.54
1:A:284:ILE:O	1:A:286:LEU:N	2.41	0.54
4:D:225:VAL:HB	4:D:226:PRO:HD3	1.88	0.54
2:B:169:ILE:HD11	6:F:590:TYR:HD2	1.73	0.53
8:H:110:ARG:HE	8:H:235:ARG:HH21	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:343:ILE:HD12	8:H:352:ARG:HB3	1.88	0.53
3:C:26:LEU:HD11	20:C:201:PGT:C46	2.38	0.53
8:H:198:PRO:HA	8:H:201:VAL:HG12	1.91	0.53
8:H:260:ALA:O	8:H:264:VAL:HG23	2.08	0.53
8:H:343:ILE:HB	8:H:351:TRP:O	2.09	0.53
1:A:301:PHE:O	1:A:304:ILE:N	2.41	0.53
6:F:589:ALA:O	6:F:593:THR:HG23	2.08	0.53
8:H:191:GLU:HG2	8:H:195:THR:HG21	1.90	0.53
2:B:20:ILE:HD11	2:B:61:LEU:HD21	1.90	0.53
2:B:301:ARG:HH22	5:E:99:LEU:HD21	1.73	0.53
7:G:17:ALA:O	7:G:21:ILE:HG12	2.09	0.53
11:K:61:ILE:HG12	11:K:67:PHE:CZ	2.44	0.53
1:A:47:VAL:HG11	12:L:52:THR:HG23	1.89	0.53
16:P:74:PHE:HB3	16:P:76:PHE:CE1	2.44	0.53
4:D:325:MET:O	4:D:329:ILE:HG12	2.09	0.53
16:P:284:VAL:O	16:P:288:PHE:HB2	2.09	0.53
7:G:43:PHE:CD2	7:G:66:TYR:HB3	2.44	0.53
13:M:15:GLY:O	13:M:30:THR:OG1	2.23	0.53
1:A:307:ALA:HB2	19:L:401:DGD:HG32	1.89	0.53
4:D:190:PRO:HD2	4:D:197:ILE:HD13	1.90	0.53
1:A:40:VAL:CG1	19:A:501:DGD:HB91	2.39	0.53
19:L:401:DGD:O5E	19:L:401:DGD:O4E	2.24	0.53
13:M:2:LEU:HD11	13:M:22:VAL:HG21	1.89	0.53
16:P:60:ARG:NH1	16:P:107:HIS:O	2.42	0.53
16:P:242:VAL:HG13	16:P:384:ALA:HB2	1.91	0.53
16:P:406:ARG:NH2	17:Q:147:TYR:O	2.27	0.53
6:F:472:ILE:HD12	23:F:704:CLA:HAC1	1.78	0.53
9:I:67:GLU:OE2	9:I:82:TRP:NE1	2.40	0.53
11:K:60:MET:HE2	11:K:67:PHE:HB3	1.91	0.53
6:F:374:ARG:CD	6:F:449:SER:OG	2.57	0.52
2:B:21:LEU:HD11	2:B:124:MET:HB2	1.91	0.52
4:D:417:VAL:CA	21:F:701:SQD:C37	2.87	0.52
4:D:447:ARG:NH1	4:D:447:ARG:CB	2.73	0.52
6:F:97:LEU:HD13	6:F:340:LEU:HD12	1.92	0.52
6:F:528:LEU:HD12	21:F:703:SQD:O10	2.09	0.52
1:A:146:LEU:HD13	1:A:165:ALA:HB1	1.90	0.52
2:B:367:GLN:NE2	2:B:435:LYS:O	2.34	0.52
4:D:369:ARG:NE	16:P:361:ASP:OD2	2.42	0.52
1:A:37:MET:HA	1:A:40:VAL:HG22	1.92	0.52
14:N:30:GLU:OE1	14:N:30:GLU:N	2.42	0.52
1:A:36:MET:HE1	19:A:501:DGD:C4A	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:ILE:HD12	8:H:6:THR:HG22	1.90	0.52
1:A:364:LEU:HD11	3:C:103:LEU:HD13	1.92	0.52
5:E:31:LEU:HD13	5:E:78:LEU:HD22	1.91	0.52
6:F:452:VAL:CG2	6:F:457:ILE:HG22	2.40	0.52
21:F:703:SQD:O8	21:F:703:SQD:O5	2.17	0.52
8:H:148:ALA:O	9:I:51:ARG:NH1	2.38	0.52
8:H:158:TYR:OH	8:H:166:ALA:O	2.20	0.52
12:L:13:TYR:HA	12:L:16:LEU:HB2	1.92	0.52
16:P:371:GLN:HE22	16:P:427:LYS:HG3	1.74	0.52
1:A:212:GLN:OE1	1:A:359:THR:OG1	2.21	0.52
2:B:76:SER:O	2:B:76:SER:OG	2.27	0.52
2:B:365:LEU:HD21	2:B:372:LEU:HD22	1.92	0.52
4:D:474:VAL:HG11	6:F:76:VAL:HG22	1.90	0.52
10:J:69:SER:OG	10:J:74:ASP:OD1	2.25	0.52
10:J:79:TYR:HB2	10:J:96:ILE:HG12	1.91	0.52
14:N:13:LEU:HD12	14:N:19:LEU:HD23	1.91	0.52
16:P:100:ARG:HE	16:P:103:ARG:HA	1.75	0.52
2:B:293:ALA:HB2	2:B:305:TYR:HB3	1.92	0.52
7:G:2:ASP:OD1	7:G:3:LEU:N	2.38	0.52
8:H:197:ASN:HB2	8:H:200:PHE:HB3	1.92	0.52
1:A:121:GLN:CB	19:L:401:DGD:HE61	2.39	0.52
2:B:429:VAL:O	2:B:433:VAL:HG22	2.09	0.52
3:C:89:VAL:HG21	7:G:65:ILE:HD11	1.92	0.52
4:D:447:ARG:CB	4:D:447:ARG:HH11	2.22	0.52
9:I:104:ILE:HG22	24:I:201:SF4:S2	2.50	0.52
1:A:273:SER:O	1:A:278:GLY:N	2.28	0.52
2:B:212:LEU:O	2:B:216:ILE:HG12	2.10	0.52
4:D:259:VAL:O	4:D:263:LEU:HB2	2.10	0.52
6:F:375:ARG:N	6:F:376:PRO:HD3	2.25	0.52
12:L:17:ALA:HA	19:L:401:DGD:HA71	1.92	0.52
2:B:430:LYS:NZ	20:D:602:PGT:O6	2.43	0.51
3:C:84:PHE:O	3:C:88:THR:HG23	2.10	0.51
6:F:15:TYR:HD2	6:F:50:SER:HB3	1.74	0.51
6:F:425:PHE:CE1	21:F:703:SQD:C29	2.93	0.51
11:K:77:SER:OG	11:K:80:GLN:OE1	2.28	0.51
11:K:183:LEU:HA	13:M:31:LEU:O	2.10	0.51
2:B:341:LEU:O	2:B:345:THR:OG1	2.26	0.51
3:C:26:LEU:HD11	20:C:201:PGT:H461	1.93	0.51
6:F:188:LEU:HA	6:F:191:VAL:HG12	1.93	0.51
10:J:61:LEU:HD12	10:J:80:HIS:O	2.09	0.51
11:K:171:ILE:HD12	21:K:502:SQD:C11	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:90:SER:OG	17:Q:91:LEU:N	2.40	0.51
1:A:21:SER:O	1:A:24:LEU:N	2.32	0.51
1:A:122:ASN:O	19:A:501:DGD:O6D	2.27	0.51
1:A:157:TYR:OH	1:A:242:VAL:N	2.32	0.51
4:D:155:GLY:O	4:D:158:ARG:HG3	2.11	0.51
8:H:72:TYR:O	8:H:73:ALA:C	2.54	0.51
14:N:34:GLN:HG3	14:N:44:THR:HG21	1.93	0.51
21:D:601:SQD:O49	21:D:601:SQD:H461	2.09	0.51
21:D:601:SQD:H292	21:D:601:SQD:H252	1.93	0.51
8:H:171:GLY:HA3	9:I:180:ALA:HB3	1.93	0.51
10:J:146:ASP:OD1	10:J:146:ASP:N	2.40	0.51
17:Q:51:ASP:O	17:Q:55:THR:HG23	2.11	0.51
2:B:258:LEU:O	2:B:262:PHE:HB2	2.11	0.51
21:D:601:SQD:C8	21:D:601:SQD:H441	2.39	0.51
11:K:33:ASP:OD1	14:N:35:ARG:NH2	2.42	0.51
1:A:46:LEU:HD22	1:A:76:PRO:HB2	1.93	0.51
1:A:53:ARG:NH1	1:A:79:ASP:OD2	2.39	0.51
1:A:242:VAL:HG22	8:H:20:PRO:HG3	1.91	0.51
10:J:118:ASP:OD2	11:K:207:ARG:NH1	2.34	0.51
4:D:49:LEU:O	4:D:53:THR:HG23	2.10	0.51
6:F:169:VAL:HG22	6:F:249:GLU:HB3	1.93	0.51
6:F:361:VAL:HG11	16:P:293:PRO:HD2	1.93	0.51
8:H:67:VAL:HG11	8:H:82:THR:HG21	1.93	0.51
16:P:99:LEU:HD13	16:P:248:ILE:HD13	1.92	0.51
16:P:371:GLN:HE22	16:P:427:LYS:CG	2.24	0.51
1:A:247:THR:HG23	1:A:248:GLU:HG2	1.93	0.51
8:H:339:GLY:O	8:H:356:ARG:N	2.35	0.51
15:O:12:VAL:HG23	15:O:13:ALA:H	1.76	0.51
16:P:57:PHE:CD1	16:P:136:ILE:HG21	2.46	0.51
1:A:282:PHE:O	1:A:284:ILE:N	2.44	0.50
1:A:301:PHE:CZ	12:L:8:LEU:HD22	2.43	0.50
6:F:458:LEU:CB	6:F:459:PRO:HD3	2.40	0.50
6:F:499:LEU:O	6:F:503:VAL:HG23	2.11	0.50
7:G:82:ASN:HB3	8:H:5:GLU:HA	1.93	0.50
16:P:77:PHE:C	16:P:79:TYR:H	2.19	0.50
1:A:36:MET:HE1	19:A:501:DGD:HA52	1.91	0.50
1:A:126:SER:HB3	3:C:21:TYR:CG	2.46	0.50
14:N:5:ALA:O	14:N:36:ARG:NH2	2.45	0.50
16:P:109:HIS:HD2	16:P:111:GLU:H	1.59	0.50
16:P:377:VAL:O	16:P:381:VAL:HG23	2.11	0.50
21:D:601:SQD:H1	21:D:601:SQD:C46	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:292:GLU:O	8:H:296:MET:HG2	2.11	0.50
8:H:371:LYS:HD3	11:K:202:LEU:HD13	1.92	0.50
6:F:390:LEU:HD22	6:F:427:ALA:HB2	1.94	0.50
8:H:117:TRP:NE1	8:H:383:GLY:O	2.43	0.50
2:B:150:THR:HG23	2:B:239:ALA:HB2	1.93	0.50
22:F:702:BCR:H383	22:F:702:BCR:C23	2.41	0.50
13:M:9:HIS:O	13:M:10:VAL:HG23	2.11	0.50
16:P:344:LEU:HD11	16:P:366:LEU:HD12	1.92	0.50
1:A:159:LEU:HD23	3:C:68:ILE:HD11	1.93	0.50
5:E:31:LEU:O	5:E:35:GLU:HG2	2.11	0.50
6:F:377:ILE:N	6:F:377:ILE:CD1	2.73	0.50
11:K:16:PRO:HD3	13:M:94:LEU:HD23	1.94	0.50
1:A:183:VAL:O	1:A:187:SER:OG	2.26	0.50
5:E:18:ILE:HG13	5:E:37:LEU:HD21	1.93	0.50
10:J:75:LEU:HD11	10:J:153:ARG:NH1	2.27	0.50
21:K:502:SQD:C30	21:K:502:SQD:H262	2.42	0.50
4:D:204:PRO:C	4:D:206:THR:H	2.19	0.50
6:F:147:VAL:O	6:F:151:ILE:HG13	2.12	0.50
6:F:390:LEU:HB3	6:F:423:ASN:OD1	2.11	0.50
7:G:63:ILE:HA	7:G:67:VAL:HG12	1.94	0.50
8:H:234:LEU:HA	8:H:237:VAL:HG22	1.93	0.50
8:H:352:ARG:HG2	10:J:67:TYR:CB	2.41	0.50
11:K:10:LEU:HB2	13:M:107:ARG:HG3	1.93	0.50
11:K:19:PRO:HB2	11:K:20:GLN:OE1	2.12	0.50
21:L:402:SQD:O8	14:N:138:VAL:HG23	2.12	0.50
1:A:157:TYR:CZ	1:A:241:LEU:HD22	2.47	0.49
2:B:14:THR:O	2:B:17:PRO:HD2	2.12	0.49
4:D:55:PHE:CG	4:D:55:PHE:O	2.65	0.49
4:D:417:VAL:CA	21:F:701:SQD:H372	2.42	0.49
6:F:386:SER:OG	6:F:430:LEU:HD23	2.12	0.49
8:H:110:ARG:HH21	8:H:235:ARG:HH21	1.60	0.49
14:N:75:ILE:HD12	14:N:75:ILE:H	1.77	0.49
2:B:30:LEU:HD22	2:B:46:PHE:CD2	2.47	0.49
6:F:252:ILE:HA	6:F:255:SER:H	1.77	0.49
8:H:139:GLU:OE1	8:H:152:ARG:NH2	2.45	0.49
8:H:175:LYS:NZ	9:I:163:LEU:O	2.29	0.49
15:O:62:ARG:HG2	15:O:65:GLN:NE2	2.27	0.49
6:F:259:ASN:ND2	6:F:346:MET:HB3	2.27	0.49
6:F:425:PHE:HD1	21:F:703:SQD:H292	1.76	0.49
10:J:155:ASP:N	10:J:155:ASP:OD1	2.44	0.49
11:K:171:ILE:HD11	21:K:502:SQD:C11	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:102:ASN:HB3	17:Q:103:PRO:HD3	1.94	0.49
6:F:499:LEU:CD2	21:F:703:SQD:H362	2.42	0.49
12:L:66:ASN:HD21	21:L:402:SQD:H4	1.77	0.49
4:D:319:ALA:HB1	4:D:407:MET:HG3	1.95	0.49
8:H:330:ARG:CD	10:J:62:ARG:HH22	2.25	0.49
4:D:179:ALA:HB2	4:D:213:LEU:HB3	1.93	0.49
8:H:31:THR:HG22	8:H:39:ASP:O	2.13	0.49
1:A:229:ARG:HB3	1:A:231:PRO:HD2	1.95	0.49
2:B:428:VAL:O	2:B:432:MET:HG3	2.13	0.49
9:I:105:PHE:HD2	11:K:147:GLY:HA2	1.77	0.49
2:B:16:LEU:O	2:B:19:THR:HG22	2.12	0.49
2:B:363:ALA:HB1	2:B:435:LYS:HG3	1.95	0.49
3:C:106:PHE:O	3:C:110:LEU:HB2	2.13	0.49
4:D:131:ASN:HB3	4:D:134:LEU:HB3	1.95	0.49
4:D:413:LEU:O	4:D:417:VAL:HG23	2.12	0.49
6:F:92:THR:O	6:F:96:MET:HG3	2.13	0.49
6:F:378:SER:O	6:F:438:TRP:CH2	2.66	0.49
9:I:30:ASP:O	9:I:33:ARG:HG2	2.13	0.49
16:P:75:PRO:O	16:P:78:LYS:HB2	2.13	0.49
17:Q:136:PRO:O	17:Q:141:GLN:OE1	2.30	0.49
3:C:46:LYS:HZ2	21:K:502:SQD:H62	1.75	0.49
6:F:237:GLN:HE22	6:F:294:THR:HG21	1.78	0.49
6:F:538:TYR:CE1	21:F:701:SQD:H201	2.47	0.49
8:H:240:TYR:HB3	8:H:243:TYR:CD2	2.48	0.49
9:I:101:GLY:O	11:K:120:THR:OG1	2.31	0.49
4:D:152:ILE:HB	4:D:153:TRP:CE3	2.48	0.48
6:F:185:LEU:HD23	21:F:701:SQD:H361	1.94	0.48
8:H:103:VAL:O	8:H:107:GLU:HG2	2.13	0.48
11:K:188:HIS:CD2	13:M:27:GLU:HA	2.47	0.48
16:P:325:PRO:O	16:P:331:ILE:HD13	2.12	0.48
1:A:117:VAL:HG11	1:A:270:LEU:HD13	1.94	0.48
6:F:253:PRO:HA	6:F:256:ILE:HG22	1.94	0.48
8:H:78:ASN:HA	8:H:81:VAL:HG12	1.96	0.48
2:B:95:ILE:HG23	2:B:113:MET:HE2	1.95	0.48
14:N:50:PRO:HG2	14:N:107:ARG:HH11	1.79	0.48
2:B:316:ILE:HA	2:B:319:VAL:HG12	1.94	0.48
3:C:22:PHE:O	3:C:26:LEU:HB2	2.14	0.48
20:C:201:PGT:H361	7:G:52:LEU:CD1	2.43	0.48
6:F:200:SER:OG	6:F:201:TRP:N	2.47	0.48
6:F:472:ILE:HB	23:F:704:CLA:CAC	2.39	0.48
6:F:537:LEU:O	6:F:541:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:417:ARG:HB2	16:P:419:GLN:HE22	1.79	0.48
4:D:160:GLN:HG3	20:D:602:PGT:C4	2.39	0.48
17:Q:21:VAL:HG13	17:Q:26:LEU:HB2	1.95	0.48
1:A:199:GLN:HG2	1:A:207:TRP:HA	1.96	0.48
19:A:501:DGD:CCB	19:L:401:DGD:CGA	2.56	0.48
6:F:202:ASN:C	6:F:204:ASP:H	2.22	0.48
6:F:378:SER:C	6:F:438:TRP:CH2	2.92	0.48
21:K:502:SQD:H332	21:K:502:SQD:C29	2.43	0.48
16:P:92:TYR:HB3	16:P:98:ASP:H	1.78	0.48
1:A:230:LEU:HA	1:A:233:ASP:OD2	2.12	0.48
10:J:164:LEU:HA	11:K:133:ARG:HD3	1.95	0.48
16:P:99:LEU:HD23	16:P:99:LEU:O	2.14	0.48
16:P:428:ILE:C	16:P:430:ASN:H	2.20	0.48
1:A:232:PHE:HB3	1:A:340:LEU:HD11	1.96	0.48
20:C:201:PGT:H372	7:G:52:LEU:HD13	1.96	0.48
8:H:78:ASN:OD1	8:H:78:ASN:N	2.47	0.48
8:H:224:MET:HE2	8:H:224:MET:HB3	1.77	0.48
1:A:43:VAL:HG21	19:L:401:DGD:HAG3	1.28	0.48
4:D:235:TYR:OH	4:D:247:GLY:HA2	2.14	0.48
4:D:449:VAL:HG23	4:D:452:GLU:HB2	1.96	0.48
10:J:69:SER:OG	10:J:74:ASP:O	2.32	0.48
16:P:298:LYS:HE3	16:P:306:GLN:HG2	1.96	0.48
4:D:225:VAL:HG13	4:D:284:GLY:HA2	1.95	0.47
4:D:228:HIS:NE2	6:F:557:ASP:OD2	2.36	0.47
4:D:379:ILE:O	4:D:383:MET:HG2	2.13	0.47
11:K:19:PRO:HG3	14:N:93:PRO:HB2	1.95	0.47
1:A:160:LEU:HD21	3:C:68:ILE:HG23	1.95	0.47
2:B:137:VAL:O	2:B:140:GLU:HG2	2.15	0.47
2:B:137:VAL:HG21	7:G:146:PRO:HB3	1.96	0.47
2:B:220:SER:HA	2:B:223:ILE:HG12	1.96	0.47
4:D:183:MET:HB3	4:D:210:LEU:HD13	1.96	0.47
5:E:39:ASN:HB3	7:G:46:ILE:HD13	1.96	0.47
8:H:352:ARG:HG2	10:J:67:TYR:HB2	1.97	0.47
10:J:106:ARG:HB2	10:J:131:VAL:O	2.14	0.47
12:L:19:LEU:CD2	19:L:401:DGD:HBV1	2.36	0.47
4:D:380:LEU:CD2	4:D:460:THR:HG23	2.43	0.47
6:F:453:PHE:CE2	6:F:456:MET:HE3	2.50	0.47
1:A:188:ASN:HA	3:C:99:HIS:CE1	2.49	0.47
1:A:270:LEU:O	1:A:274:VAL:HG13	2.14	0.47
2:B:22:ILE:HA	2:B:25:LEU:HB2	1.97	0.47
6:F:145:ASN:ND2	6:F:203:TYR:OH	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:89:LEU:HB3	8:H:323:PRO:HG2	1.96	0.47
21:K:502:SQD:H301	21:K:502:SQD:H261	1.95	0.47
1:A:5:ILE:HD11	1:A:300:PRO:O	2.15	0.47
1:A:236:GLU:HG2	1:A:236:GLU:O	2.15	0.47
16:P:150:TRP:O	16:P:311:GLN:NE2	2.46	0.47
16:P:427:LYS:O	16:P:430:ASN:HB3	2.14	0.47
4:D:368:LEU:HD23	16:P:326:VAL:O	2.15	0.47
6:F:133:MET:HE1	6:F:265:THR:OG1	2.14	0.47
16:P:277:TYR:HE2	17:Q:132:MET:HE2	1.79	0.47
1:A:319:TYR:CE2	12:L:49:PHE:HB2	2.50	0.47
2:B:93:GLY:HA3	2:B:341:LEU:HD13	1.96	0.47
2:B:237:GLU:CD	2:B:301:ARG:HE	2.22	0.47
4:D:38:LEU:HD22	4:D:101:VAL:HG12	1.96	0.47
4:D:329:ILE:O	4:D:333:ILE:HG12	2.15	0.47
4:D:417:VAL:HA	21:F:701:SQD:H372	1.96	0.47
6:F:111:GLY:O	6:F:114:GLU:HG2	2.15	0.47
8:H:197:ASN:OD1	9:I:20:TYR:HB3	2.15	0.47
11:K:31:LEU:HD23	21:K:502:SQD:H291	1.96	0.47
13:M:27:GLU:HG2	13:M:27:GLU:O	2.15	0.47
15:O:4:LYS:HD3	15:O:5:LYS:HG2	1.97	0.47
16:P:355:HIS:HE1	16:P:437:LEU:HG	1.78	0.47
1:A:292:LEU:N	1:A:292:LEU:HD23	2.29	0.47
2:B:387:PRO:HG2	4:D:140:GLU:C	2.40	0.47
2:B:462:VAL:O	2:B:466:MET:HG3	2.15	0.47
4:D:427:VAL:HG21	6:F:177:PHE:CD2	2.49	0.47
16:P:185:LEU:HD13	16:P:185:LEU:HA	1.72	0.47
1:A:82:LYS:HD3	11:K:42:SER:OG	2.15	0.47
1:A:151:TYR:CE2	7:G:75:LEU:HD12	2.49	0.47
6:F:362:THR:CG2	6:F:445:MET:CE	2.92	0.47
6:F:227:LEU:HD12	6:F:273:LEU:HG	1.95	0.47
6:F:457:ILE:HG12	22:F:702:BCR:H271	1.96	0.47
11:K:48:TYR:OH	11:K:98:LEU:HD12	2.15	0.47
14:N:102:LEU:HD12	14:N:130:VAL:HG22	1.97	0.47
16:P:386:ARG:NH1	16:P:392:PRO:HA	2.30	0.47
1:A:33:PRO:HB2	1:A:125:ILE:HG12	1.96	0.46
1:A:126:SER:O	1:A:126:SER:OG	2.31	0.46
1:A:183:VAL:HG11	1:A:275:LEU:HD22	1.97	0.46
1:A:230:LEU:HA	1:A:233:ASP:CG	2.41	0.46
6:F:259:ASN:OD1	6:F:347:ALA:HB2	2.15	0.46
6:F:374:ARG:CD	16:P:197:GLU:OE1	2.60	0.46
6:F:457:ILE:HG12	22:F:702:BCR:C27	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:99:VAL:O	11:K:103:GLU:HG2	2.15	0.46
4:D:146:PHE:O	4:D:150:ILE:HG12	2.15	0.46
4:D:180:PHE:O	4:D:184:GLY:N	2.48	0.46
4:D:194:SER:HG	4:D:265:TYR:HH	1.57	0.46
6:F:451:GLU:OE1	22:F:702:BCR:H282	2.15	0.46
4:D:202:LEU:O	4:D:207:GLN:NE2	2.48	0.46
10:J:80:HIS:O	10:J:81:LEU:HD12	2.14	0.46
11:K:92:MET:HE2	11:K:92:MET:HB3	1.69	0.46
16:P:257:VAL:HG13	16:P:264:HIS:HB2	1.97	0.46
18:S:55:ASN:ND2	18:S:94:GLU:OE2	2.48	0.46
1:A:186:MET:HE2	1:A:370:PHE:CE2	2.51	0.46
6:F:263:VAL:HG12	6:F:342:TYR:HE2	1.80	0.46
11:K:37:TRP:HA	11:K:40:LEU:HD22	1.97	0.46
1:A:45:VAL:O	1:A:49:VAL:HG23	2.15	0.46
1:A:313:MET:HG3	1:A:317:LYS:NZ	2.30	0.46
4:D:387:GLY:O	6:F:181:ARG:NH2	2.49	0.46
5:E:30:VAL:O	5:E:34:ILE:HG13	2.16	0.46
8:H:294:LYS:HE3	8:H:304:TRP:CE2	2.50	0.46
9:I:83:VAL:HG12	9:I:92:GLU:HB3	1.98	0.46
16:P:16:LEU:HG	16:P:17:ASP:N	2.27	0.46
16:P:85:TYR:CD1	16:P:88:LEU:HD12	2.51	0.46
16:P:324:PHE:HE1	16:P:368:ILE:HD11	1.80	0.46
17:Q:2:ALA:O	17:Q:6:ASP:N	2.30	0.46
2:B:351:SER:HA	2:B:356:THR:H	1.80	0.46
7:G:158:LEU:O	7:G:162:VAL:HG23	2.16	0.46
10:J:82:ILE:HG13	10:J:93:GLU:HB3	1.98	0.46
16:P:16:LEU:H	16:P:16:LEU:HD23	1.81	0.46
16:P:328:THR:HG23	16:P:331:ILE:HD12	1.98	0.46
17:Q:107:LYS:NZ	17:Q:131:LEU:O	2.41	0.46
17:Q:118:ALA:HB3	17:Q:121:GLY:O	2.14	0.46
1:A:158:SER:HB2	1:A:245:TYR:HA	1.98	0.46
2:B:351:SER:O	2:B:356:THR:HG22	2.15	0.46
20:D:602:PGT:H372	20:D:602:PGT:H181	1.98	0.46
6:F:383:LEU:HD23	6:F:383:LEU:HA	1.79	0.46
8:H:107:GLU:CD	8:H:235:ARG:HH22	2.23	0.46
8:H:149:THR:OG1	8:H:150:GLY:N	2.49	0.46
8:H:366:LEU:HB3	8:H:367:PRO:HD3	1.98	0.46
13:M:7:THR:OG1	13:M:78:GLU:OE2	2.28	0.46
16:P:211:PHE:HB2	16:P:279:ALA:HB1	1.98	0.46
1:A:62:ARG:HG3	11:K:63:SER:HA	1.98	0.46
1:A:71:LEU:HD13	12:L:32:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PHE:CE1	1:A:272:VAL:HG22	2.51	0.46
2:B:243:VAL:O	2:B:247:LEU:HB2	2.16	0.46
4:D:33:LEU:HD11	4:D:110:ARG:HA	1.98	0.46
6:F:33:LYS:HD3	16:P:120:GLU:HG2	1.98	0.46
8:H:371:LYS:HD2	8:H:371:LYS:HA	1.72	0.46
11:K:155:ILE:O	11:K:159:ILE:HG12	2.16	0.46
12:L:17:ALA:O	12:L:21:LEU:HG	2.16	0.46
16:P:149:MET:CE	16:P:201:GLN:HA	2.46	0.46
20:C:201:PGT:H5	20:C:201:PGT:O3P	2.16	0.46
4:D:148:LEU:O	4:D:152:ILE:HG12	2.16	0.46
6:F:6:ALA:HB1	6:F:61:ILE:HD11	1.98	0.46
6:F:446:THR:O	6:F:446:THR:OG1	2.12	0.46
6:F:543:VAL:CG2	21:F:701:SQD:O49	2.61	0.46
9:I:57:HIS:CD2	9:I:142:GLY:HA2	2.50	0.46
4:D:389:PRO:HG2	6:F:147:VAL:HA	1.97	0.46
8:H:49:ARG:O	11:K:128:SER:OG	2.34	0.46
16:P:43:LYS:HA	16:P:348:LEU:HD21	1.97	0.46
6:F:34:THR:O	6:F:34:THR:OG1	2.33	0.45
6:F:142:LEU:HB3	6:F:201:TRP:HB2	1.97	0.45
8:H:367:PRO:HG2	11:K:201:TYR:CE2	2.51	0.45
10:J:36:VAL:HG13	10:J:93:GLU:O	2.15	0.45
10:J:161:PHE:O	10:J:165:GLN:HG2	2.16	0.45
16:P:349:LYS:O	16:P:353:HIS:ND1	2.47	0.45
16:P:427:LYS:HD3	16:P:427:LYS:HA	1.63	0.45
4:D:99:GLY:O	4:D:103:THR:HG22	2.16	0.45
4:D:316:ALA:HB1	4:D:324:SER:O	2.16	0.45
4:D:481:SER:O	4:D:486:VAL:HG22	2.15	0.45
7:G:126:PRO:HA	7:G:127:PRO:HD3	1.88	0.45
8:H:71:ASP:CG	8:H:71:ASP:O	2.58	0.45
8:H:354:LYS:HG2	8:H:355:ILE:N	2.30	0.45
16:P:149:MET:C	16:P:151:HIS:H	2.23	0.45
2:B:403:TRP:CD1	2:B:411:VAL:HG11	2.51	0.45
6:F:444:PRO:N	6:F:444:PRO:C	2.64	0.45
6:F:476:ARG:HE	6:F:476:ARG:HB3	1.46	0.45
8:H:116:LEU:HB2	8:H:138:ARG:NH1	2.31	0.45
8:H:152:ARG:NH1	11:K:56:GLU:OE2	2.49	0.45
8:H:204:LEU:HA	8:H:207:VAL:HG22	1.98	0.45
11:K:188:HIS:CE1	11:K:190:MET:HB2	2.52	0.45
1:A:363:LYS:HD3	3:C:98:PHE:HD2	1.81	0.45
2:B:314:VAL:HG13	2:B:329:MET:HG3	1.98	0.45
4:D:191:SER:O	4:D:193:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:425:PHE:CD1	21:F:703:SQD:C29	2.99	0.45
6:F:435:CYS:SG	6:F:505:ALA:HA	2.57	0.45
8:H:31:THR:HG23	8:H:38:ILE:HB	1.98	0.45
8:H:177:ARG:NH1	8:H:281:ASP:OD1	2.50	0.45
9:I:153:MET:HE1	14:N:135:ASP:HA	1.98	0.45
10:J:149:GLY:HA2	15:O:24:ALA:O	2.16	0.45
4:D:167:ILE:HD12	20:D:602:PGT:C33	2.46	0.45
10:J:61:LEU:HD22	10:J:114:TRP:HE1	1.81	0.45
14:N:88:LEU:HD11	14:N:125:LYS:O	2.17	0.45
2:B:237:GLU:OE2	2:B:301:ARG:NE	2.45	0.45
4:D:222:MET:HE2	4:D:255:ALA:HA	1.97	0.45
2:B:319:VAL:HG13	2:B:320:VAL:HG13	1.98	0.45
6:F:543:VAL:HG22	21:F:701:SQD:H272	1.98	0.45
16:P:37:THR:OG1	16:P:40:ASN:HB2	2.17	0.45
2:B:20:ILE:HD11	2:B:61:LEU:HD11	1.97	0.45
2:B:297:THR:O	2:B:358:GLN:HB2	2.17	0.45
3:C:70:PHE:CD2	7:G:80:LEU:HD12	2.38	0.45
11:K:128:SER:HB3	11:K:133:ARG:HH21	1.82	0.45
13:M:9:HIS:HA	13:M:34:ASP:HA	1.98	0.45
2:B:463:GLY:O	2:B:467:THR:HG23	2.16	0.45
4:D:322:HIS:CE1	4:D:483:ALA:HB2	2.52	0.45
8:H:113:ASN:C	8:H:113:ASN:HD22	2.25	0.45
16:P:255:HIS:HB3	16:P:266:LEU:HB3	1.99	0.45
2:B:20:ILE:HG21	2:B:58:MET:HE2	1.99	0.45
4:D:429:MET:O	4:D:433:THR:HB	2.17	0.45
1:A:54:LYS:HD3	1:A:65:PRO:HD2	1.99	0.44
2:B:299:MET:HE2	2:B:359:ILE:HG12	1.98	0.44
6:F:510:GLY:O	6:F:511:LYS:HG2	2.17	0.44
16:P:291:THR:O	16:P:316:TYR:HB2	2.17	0.44
1:A:50:TRP:CE3	1:A:51:LEU:HD23	2.53	0.44
3:C:83:ILE:HG13	7:G:158:LEU:HD13	2.00	0.44
4:D:407:MET:HE3	4:D:407:MET:HB3	1.80	0.44
16:P:188:TYR:CD1	16:P:188:TYR:C	2.95	0.44
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.82	0.44
1:A:315:LEU:HD11	19:A:501:DGD:HBT1	1.99	0.44
4:D:59:GLN:HG2	4:D:63:GLN:HE21	1.82	0.44
6:F:345:ALA:HB3	6:F:389:LEU:HD13	1.99	0.44
10:J:19:LEU:HD13	10:J:49:VAL:HG13	2.00	0.44
2:B:83:PHE:O	2:B:87:ILE:HG13	2.17	0.44
3:C:43:LEU:O	3:C:43:LEU:HD12	2.18	0.44
4:D:231:LEU:HB3	4:D:232:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:702:BCR:H20C	22:F:702:BCR:H361	1.87	0.44
8:H:97:ARG:O	8:H:101:ILE:HG13	2.18	0.44
8:H:330:ARG:HA	8:H:338:LEU:O	2.18	0.44
8:H:337:GLU:CD	10:J:62:ARG:HH21	2.25	0.44
9:I:147:LYS:HB2	18:S:89:THR:OG1	2.17	0.44
16:P:133:HIS:O	16:P:135:ARG:HB2	2.17	0.44
2:B:30:LEU:HD22	2:B:46:PHE:CE2	2.52	0.44
2:B:301:ARG:HH22	5:E:99:LEU:CD2	2.31	0.44
6:F:174:ARG:NE	21:F:701:SQD:H81	2.32	0.44
6:F:543:VAL:HG13	21:F:701:SQD:H461	1.98	0.44
11:K:60:MET:HE3	11:K:156:MET:HG2	1.99	0.44
1:A:67:TYR:HD2	11:K:70:PHE:HD2	1.64	0.44
3:C:112:PHE:CD1	7:G:151:SER:HB3	2.53	0.44
4:D:168:TYR:CD1	20:D:602:PGT:H381	2.52	0.44
4:D:440:ASN:OD1	4:D:440:ASN:N	2.51	0.44
6:F:250:GLY:O	6:F:253:PRO:HD2	2.18	0.44
9:I:105:PHE:CD2	11:K:147:GLY:HA2	2.51	0.44
2:B:194:LEU:HD22	2:B:266:ALA:HB2	1.98	0.44
5:E:86:ARG:HG3	7:G:167:ARG:HH22	1.83	0.44
10:J:61:LEU:HD13	10:J:114:TRP:NE1	2.33	0.44
19:L:401:DGD:C6E	19:L:401:DGD:C2E	2.93	0.44
16:P:112:LEU:O	16:P:116:ILE:HG12	2.17	0.44
16:P:277:TYR:CE2	17:Q:132:MET:HE2	2.53	0.44
1:A:29:TRP:CZ2	19:A:501:DGD:O2D	2.64	0.44
1:A:280:TRP:HD1	19:L:401:DGD:O4E	2.01	0.44
19:A:501:DGD:O3D	19:A:501:DGD:C6D	2.66	0.44
4:D:285:ILE:HG22	4:D:418:GLY:HA3	1.98	0.44
4:D:297:ASP:HB3	4:D:300:ARG:HG3	2.00	0.44
8:H:184:LEU:O	8:H:187:VAL:HG12	2.17	0.44
9:I:41:TYR:CD1	11:K:153:GLU:HB2	2.53	0.44
10:J:42:ASP:OD1	10:J:43:ARG:N	2.50	0.44
11:K:123:MET:HE3	24:K:501:SF4:S2	2.58	0.44
1:A:286:LEU:HD12	1:A:286:LEU:C	2.42	0.44
2:B:140:GLU:OE1	5:E:69:VAL:HG11	2.18	0.44
8:H:116:LEU:O	8:H:120:PRO:HD2	2.18	0.44
10:J:163:GLU:HA	11:K:137:LYS:HD3	1.99	0.44
11:K:87:SER:HB3	11:K:114:MET:SD	2.58	0.44
1:A:40:VAL:HG11	19:A:501:DGD:HB91	2.00	0.43
1:A:196:VAL:HG11	1:A:280:TRP:CH2	2.53	0.43
2:B:140:GLU:HG3	7:G:153:LEU:HD11	1.99	0.43
6:F:473:LEU:C	6:F:473:LEU:CD2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:67:VAL:C	8:H:69:ARG:H	2.26	0.43
8:H:110:ARG:HE	8:H:235:ARG:NH2	2.16	0.43
21:K:502:SQD:C26	21:K:502:SQD:H301	2.47	0.43
19:L:401:DGD:HE2	19:L:401:DGD:C6E	2.48	0.43
14:N:135:ASP:OD1	14:N:136:ARG:N	2.51	0.43
1:A:7:LEU:HD13	19:L:401:DGD:O1B	2.17	0.43
1:A:181:LEU:HD21	3:C:92:TYR:HA	2.00	0.43
2:B:458:ARG:N	2:B:459:PRO:HD2	2.33	0.43
4:D:130:GLN:O	4:D:194:SER:N	2.49	0.43
6:F:544:GLY:O	6:F:548:MET:HB2	2.18	0.43
8:H:249:ASP:HB2	8:H:271:GLU:CD	2.43	0.43
17:Q:19:THR:O	17:Q:23:VAL:HG23	2.18	0.43
4:D:379:ILE:O	4:D:379:ILE:HG22	2.16	0.43
6:F:360:SER:O	6:F:362:THR:N	2.51	0.43
21:K:502:SQD:C19	21:L:402:SQD:C30	2.96	0.43
2:B:215:VAL:O	2:B:219:ILE:HG12	2.18	0.43
11:K:13:ILE:HG22	11:K:14:ALA:N	2.31	0.43
16:P:44:ILE:HD13	16:P:376:THR:HG21	2.01	0.43
1:A:7:LEU:CD1	19:L:401:DGD:O1B	2.66	0.43
4:D:85:LEU:H	4:D:480:THR:HG21	1.83	0.43
4:D:184:GLY:HA3	4:D:192:PHE:CE1	2.53	0.43
21:D:601:SQD:H461	21:D:601:SQD:H241	1.80	0.43
9:I:41:TYR:H	11:K:69:ARG:NH1	2.16	0.43
9:I:66:CYS:SG	9:I:68:VAL:HG23	2.59	0.43
14:N:88:LEU:HD13	14:N:91:LEU:HD11	2.01	0.43
16:P:187:LEU:HD12	16:P:187:LEU:C	2.44	0.43
17:Q:104:LEU:HD12	17:Q:104:LEU:HA	1.85	0.43
1:A:95:ASP:OD2	7:G:34:TYR:OH	2.25	0.43
1:A:248:GLU:HA	11:K:79:ARG:HG3	2.00	0.43
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.83	0.43
8:H:129:THR:N	8:H:130:PRO:HD2	2.33	0.43
8:H:162:GLY:O	8:H:313:GLY:N	2.45	0.43
12:L:50:LEU:HA	12:L:50:LEU:HD23	1.86	0.43
1:A:38:LEU:HD11	3:C:28:ILE:HG22	2.00	0.43
1:A:79:ASP:OD1	11:K:42:SER:HB2	2.18	0.43
1:A:230:LEU:HD23	1:A:230:LEU:O	2.18	0.43
1:A:232:PHE:O	1:A:234:LEU:HD22	2.19	0.43
6:F:515:LYS:HD3	6:F:515:LYS:HA	1.84	0.43
6:F:597:GLY:O	6:F:601:LEU:HG	2.18	0.43
21:K:502:SQD:O10	21:K:502:SQD:H92	2.19	0.43
16:P:188:TYR:CD1	16:P:188:TYR:O	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.86	0.43
1:A:154:ASN:HB3	3:C:55:THR:HG21	2.00	0.43
4:D:252:LYS:HZ3	4:D:336:GLY:HA2	1.84	0.43
21:D:601:SQD:H181	21:D:601:SQD:C22	2.49	0.43
21:D:601:SQD:O49	21:D:601:SQD:C46	2.67	0.43
8:H:71:ASP:HA	8:H:388:ILE:HG21	1.99	0.43
8:H:167:ASP:OD1	8:H:311:TYR:HB3	2.18	0.43
11:K:49:GLY:HA3	11:K:54:PHE:CG	2.54	0.43
1:A:295:VAL:O	1:A:295:VAL:HG13	2.19	0.43
2:B:314:VAL:HG22	2:B:332:TYR:HD2	1.84	0.43
5:E:15:CYS:SG	7:G:104:SER:HB3	2.59	0.43
6:F:270:LEU:HD21	6:F:287:LEU:HD11	2.01	0.43
6:F:342:TYR:CD1	6:F:389:LEU:HD11	2.48	0.43
9:I:50:GLU:HG2	9:I:162:TYR:OH	2.18	0.43
11:K:185:THR:HG23	13:M:28:THR:HG22	2.01	0.43
1:A:54:LYS:HA	1:A:54:LYS:HD2	1.86	0.43
2:B:17:PRO:HB3	2:B:76:SER:HB2	2.00	0.43
8:H:357:PRO:HG2	8:H:360:PHE:CB	2.49	0.43
10:J:111:TYR:HA	10:J:117:ALA:HB3	2.01	0.43
11:K:118:THR:O	11:K:135:VAL:HG12	2.19	0.43
14:N:15:SER:OG	14:N:16:ALA:N	2.52	0.43
15:O:47:TYR:CD2	15:O:62:ARG:HB3	2.54	0.43
16:P:203:THR:HA	16:P:255:HIS:CE1	2.53	0.43
2:B:45:TYR:C	2:B:47:ALA:H	2.26	0.42
4:D:70:TRP:HB3	4:D:76:LEU:O	2.19	0.42
6:F:201:TRP:HA	6:F:206:LEU:HD13	2.01	0.42
6:F:322:TRP:CD1	6:F:422:MET:HE1	2.55	0.42
6:F:457:ILE:HD11	22:F:702:BCR:H23C	2.01	0.42
2:B:167:LEU:HD23	2:B:168:LEU:HD23	2.01	0.42
5:E:39:ASN:ND2	7:G:43:PHE:CE1	2.87	0.42
5:E:86:ARG:CG	7:G:167:ARG:HH12	2.32	0.42
6:F:361:VAL:HG21	16:P:292:SER:HB2	2.02	0.42
9:I:111:GLU:CD	18:S:83:ASN:HD21	2.27	0.42
11:K:10:LEU:HG	13:M:109:ASN:HB2	2.01	0.42
14:N:21:LEU:HD23	14:N:140:TRP:HB3	2.00	0.42
16:P:94:GLY:N	16:P:106:ALA:HB2	2.33	0.42
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.83	0.42
4:D:55:PHE:O	4:D:56:ASP:C	2.62	0.42
4:D:71:LEU:HA	4:D:71:LEU:HD23	1.69	0.42
4:D:350:GLU:OE2	4:D:356:ARG:HD3	2.20	0.42
4:D:380:LEU:HD23	4:D:460:THR:CG2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:153:MET:HE2	12:L:71:PRO:HB3	2.01	0.42
16:P:57:PHE:CE1	16:P:136:ILE:HG21	2.54	0.42
2:B:19:THR:HA	2:B:22:ILE:HG22	2.01	0.42
2:B:247:LEU:O	2:B:251:SER:HB3	2.19	0.42
2:B:410:LEU:HD23	2:B:410:LEU:HA	1.92	0.42
3:C:114:ALA:O	3:C:118:VAL:HG23	2.20	0.42
4:D:312:TYR:OH	4:D:419:THR:OG1	2.23	0.42
4:D:383:MET:HG3	6:F:154:LEU:HD13	2.01	0.42
6:F:108:PHE:CD2	6:F:252:ILE:HG21	2.54	0.42
22:F:702:BCR:H24C	22:F:702:BCR:H371	1.74	0.42
9:I:142:GLY:O	9:I:144:ILE:N	2.52	0.42
1:A:123:LEU:C	19:A:501:DGD:HB21	2.41	0.42
4:D:18:PRO:HB2	4:D:117:LEU:O	2.19	0.42
6:F:174:ARG:CD	21:F:701:SQD:H81	2.49	0.42
6:F:539:ARG:HA	6:F:543:VAL:HB	2.00	0.42
16:P:94:GLY:O	16:P:100:ARG:HD3	2.19	0.42
16:P:146:ARG:HA	16:P:149:MET:HG2	2.01	0.42
16:P:332:PRO:N	16:P:333:PRO:HD2	2.35	0.42
17:Q:70:TYR:HE1	17:Q:94:SER:HB2	1.85	0.42
2:B:354:THR:OG1	2:B:448:PRO:HD3	2.20	0.42
20:C:201:PGT:O5	20:C:201:PGT:P	2.78	0.42
4:D:302:VAL:O	4:D:305:SER:HB3	2.19	0.42
6:F:96:MET:HE2	6:F:96:MET:HB3	1.73	0.42
6:F:404:LEU:HD12	6:F:404:LEU:HA	1.86	0.42
23:F:704:CLA:HAA2	23:F:704:CLA:HBD	2.00	0.42
7:G:55:ALA:HB1	7:G:58:VAL:HG12	2.02	0.42
8:H:83:VAL:HG21	8:H:159:PHE:HB3	2.02	0.42
8:H:291:LEU:HD21	8:H:295:ARG:HH22	1.84	0.42
16:P:56:ASP:HA	16:P:59:TRP:CD1	2.55	0.42
1:A:32:LEU:CD1	19:A:501:DGD:HA42	2.49	0.42
1:A:121:GLN:N	19:L:401:DGD:HE61	2.28	0.42
21:D:601:SQD:H372	21:D:601:SQD:C22	2.49	0.42
6:F:88:SER:OG	6:F:89:ILE:N	2.51	0.42
9:I:82:TRP:HZ3	9:I:84:PHE:HB2	1.85	0.42
11:K:174:ARG:HH11	21:K:502:SQD:H441	1.84	0.42
16:P:74:PHE:HB3	16:P:76:PHE:CD1	2.54	0.42
16:P:238:MET:HE2	16:P:238:MET:HB3	1.82	0.42
1:A:187:SER:HA	1:A:198:GLN:HG3	2.02	0.42
1:A:342:ASP:O	1:A:346:LYS:HB2	2.19	0.42
2:B:140:GLU:CD	5:E:69:VAL:HG21	2.45	0.42
4:D:168:TYR:HD2	4:D:230:TRP:CD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:118:GLY:HA3	16:P:329:ALA:HB2	2.02	0.42
11:K:164:LYS:HB3	11:K:164:LYS:HE2	1.81	0.42
21:K:502:SQD:H252	21:K:502:SQD:C7	2.49	0.42
1:A:114:TYR:CE1	1:A:267:LEU:HD12	2.55	0.42
1:A:208:ASN:HB2	1:A:276:TYR:HA	2.01	0.42
5:E:35:GLU:OE2	5:E:74:ALA:HB2	2.19	0.42
6:F:103:LEU:O	6:F:107:VAL:HG23	2.20	0.42
6:F:115:MET:HE2	6:F:115:MET:HB2	1.96	0.42
16:P:132:TRP:O	16:P:133:HIS:C	2.62	0.42
17:Q:3:THR:OG1	17:Q:4:ILE:N	2.53	0.42
1:A:32:LEU:HD12	19:A:501:DGD:HA22	2.01	0.42
2:B:277:ILE:HG23	6:F:601:LEU:HD13	2.02	0.42
6:F:112:TYR:CA	6:F:456:MET:HE2	2.49	0.42
22:F:702:BCR:H11C	22:F:702:BCR:H341	1.84	0.42
10:J:64:GLN:CD	10:J:121:GLU:HG2	2.45	0.42
1:A:287:GLU:OE1	1:A:287:GLU:HA	2.20	0.41
2:B:158:ARG:O	2:B:161:GLU:HG3	2.20	0.41
2:B:178:LEU:HG	5:E:41:VAL:HG11	2.02	0.41
4:D:150:ILE:HD11	4:D:246:LEU:HD13	2.01	0.41
4:D:450:TRP:CD1	4:D:450:TRP:N	2.71	0.41
5:E:93:MET:SD	6:F:588:GLN:NE2	2.91	0.41
6:F:111:GLY:CA	6:F:456:MET:CE	2.98	0.41
10:J:100:VAL:HG23	10:J:105:PRO:HB2	2.02	0.41
10:J:103:ASP:HB3	15:O:20:LEU:HD21	2.02	0.41
1:A:39:ILE:O	1:A:43:VAL:HG23	2.19	0.41
2:B:178:LEU:HD12	2:B:178:LEU:HA	1.83	0.41
4:D:291:ALA:O	4:D:295:GLN:HG2	2.20	0.41
5:E:81:ILE:HA	5:E:84:ILE:HG22	2.02	0.41
6:F:312:LEU:HA	6:F:315:LEU:HD12	2.02	0.41
8:H:152:ARG:C	8:H:153:PHE:O	2.63	0.41
11:K:136:ASP:OD1	11:K:136:ASP:N	2.53	0.41
1:A:36:MET:CE	19:A:501:DGD:HA52	2.44	0.41
1:A:185:MET:HG2	3:C:95:ALA:HB1	2.01	0.41
1:A:278:GLY:C	1:A:280:TRP:H	2.28	0.41
4:D:87:LEU:O	4:D:91:VAL:HG23	2.20	0.41
6:F:412:LEU:HD12	6:F:412:LEU:HA	1.83	0.41
7:G:17:ALA:O	7:G:20:ILE:HG22	2.20	0.41
7:G:22:ALA:O	7:G:26:VAL:HG23	2.20	0.41
16:P:93:ALA:HB3	16:P:106:ALA:HA	2.01	0.41
17:Q:3:THR:OG1	17:Q:4:ILE:HD12	2.19	0.41
3:C:19:TYR:HE2	7:G:51:ILE:HD13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:316:ALA:HB2	4:D:400:ILE:HG12	2.02	0.41
6:F:477:PHE:CD1	6:F:477:PHE:N	2.89	0.41
12:L:53:PHE:CZ	19:L:401:DGD:HBH1	2.55	0.41
13:M:99:ARG:HE	13:M:99:ARG:HB2	1.68	0.41
16:P:62:LEU:HG	16:P:138:MET:HE1	2.01	0.41
17:Q:99:HIS:O	17:Q:105:GLU:N	2.45	0.41
1:A:30:LEU:N	1:A:31:PRO:HD2	2.36	0.41
2:B:313:PHE:O	2:B:316:ILE:HG12	2.20	0.41
4:D:57:VAL:HG22	4:D:58:HIS:N	2.33	0.41
4:D:215:ILE:HD11	4:D:270:TRP:HZ3	1.85	0.41
4:D:299:LYS:HG3	4:D:356:ARG:HD2	2.03	0.41
6:F:534:THR:N	6:F:535:PRO:HD2	2.35	0.41
10:J:43:ARG:NH1	10:J:105:PRO:HB3	2.35	0.41
11:K:188:HIS:NE2	13:M:27:GLU:HA	2.36	0.41
21:K:502:SQD:H81	21:K:502:SQD:C27	2.50	0.41
14:N:106:LYS:HG2	14:N:133:GLY:H	1.85	0.41
4:D:194:SER:OG	4:D:265:TYR:OH	2.29	0.41
6:F:225:LEU:HD23	6:F:225:LEU:HA	1.85	0.41
6:F:453:PHE:CE1	6:F:455:PRO:HD2	2.44	0.41
11:K:114:MET:HE3	11:K:114:MET:HB2	1.94	0.41
21:K:502:SQD:H211	21:K:502:SQD:H181	1.84	0.41
12:L:56:PRO:HD3	19:L:401:DGD:CHA	2.50	0.41
14:N:58:TYR:HA	14:N:63:HIS:CE1	2.56	0.41
1:A:50:TRP:HE3	1:A:51:LEU:HD23	1.85	0.41
1:A:234:LEU:HD11	1:A:336:ARG:O	2.20	0.41
2:B:165:LYS:HB2	2:B:165:LYS:HE3	1.76	0.41
2:B:201:LEU:HD13	2:B:208:LEU:HD22	2.03	0.41
21:D:601:SQD:C25	21:D:601:SQD:H292	2.50	0.41
6:F:20:MET:O	6:F:20:MET:SD	2.78	0.41
6:F:157:TYR:HB2	6:F:177:PHE:CD1	2.54	0.41
11:K:184:PHE:HD2	13:M:31:LEU:HD23	1.85	0.41
13:M:16:HIS:HB3	13:M:28:THR:HG21	2.03	0.41
17:Q:70:TYR:CG	17:Q:132:MET:HG3	2.56	0.41
19:A:501:DGD:O5E	19:A:501:DGD:C2E	2.69	0.41
6:F:12:ILE:HD11	6:F:53:HIS:CG	2.56	0.41
1:A:229:ARG:O	1:A:233:ASP:N	2.54	0.41
2:B:22:ILE:HA	2:B:22:ILE:HD12	1.94	0.41
2:B:201:LEU:HD12	2:B:201:LEU:O	2.21	0.41
4:D:13:LEU:HA	4:D:16:VAL:HG12	2.02	0.41
4:D:17:LEU:HD23	4:D:17:LEU:HA	1.84	0.41
4:D:147:TYR:CE2	4:D:151:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:235:TYR:HE1	4:D:246:LEU:HD22	1.85	0.41
6:F:163:TRP:HZ2	6:F:250:GLY:HA2	1.85	0.41
6:F:286:ALA:O	6:F:290:ILE:HG13	2.21	0.41
6:F:340:LEU:O	6:F:344:LEU:HD23	2.21	0.41
8:H:232:TRP:CD1	8:H:237:VAL:HG11	2.56	0.41
8:H:342:LEU:HD12	8:H:353:TRP:CZ3	2.56	0.41
9:I:155:THR:O	9:I:155:THR:OG1	2.33	0.41
16:P:315:HIS:CB	16:P:422:ILE:HG23	2.51	0.41
17:Q:41:PRO:HG2	17:Q:46:PHE:HE1	1.86	0.41
17:Q:106:VAL:O	17:Q:107:LYS:C	2.64	0.41
2:B:387:PRO:HG2	4:D:141:LEU:N	2.36	0.41
4:D:21:GLY:O	4:D:25:MET:HG2	2.21	0.41
4:D:168:TYR:HD2	4:D:230:TRP:HB3	1.86	0.41
4:D:168:TYR:OH	6:F:565:GLY:HA3	2.20	0.41
6:F:470:LEU:HD12	6:F:470:LEU:HA	1.80	0.41
7:G:21:ILE:HG13	7:G:22:ALA:N	2.36	0.41
8:H:28:LEU:HD11	8:H:366:LEU:HD21	2.03	0.41
10:J:92:PRO:O	10:J:93:GLU:HG2	2.21	0.41
11:K:82:ASP:OD1	11:K:82:ASP:N	2.54	0.41
14:N:17:GLY:C	14:N:120:THR:HG21	2.46	0.41
16:P:100:ARG:HA	16:P:100:ARG:HD2	1.84	0.41
1:A:27:LEU:CD1	20:C:201:PGT:H142	2.37	0.40
1:A:35:LEU:CD1	19:A:501:DGD:C5A	2.92	0.40
1:A:126:SER:CB	3:C:21:TYR:CD2	2.98	0.40
19:A:501:DGD:O1B	19:A:501:DGD:C3G	2.67	0.40
4:D:289:ALA:O	4:D:293:ILE:HG13	2.20	0.40
6:F:14:PHE:HA	6:F:17:LEU:HB2	2.02	0.40
6:F:335:ALA:O	6:F:339:ILE:HG12	2.21	0.40
8:H:125:VAL:HG13	8:H:203:ARG:HG2	2.03	0.40
8:H:352:ARG:HG2	10:J:67:TYR:HB3	2.03	0.40
9:I:47:ILE:HA	9:I:48:PRO:HD3	1.94	0.40
11:K:18:VAL:O	11:K:18:VAL:HG23	2.20	0.40
16:P:323:LYS:O	16:P:364:VAL:HG13	2.21	0.40
2:B:83:PHE:CG	2:B:257:ALA:HB2	2.56	0.40
2:B:178:LEU:HD21	5:E:66:VAL:HG22	2.03	0.40
20:C:201:PGT:C31	20:C:201:PGT:O3	2.70	0.40
4:D:358:LEU:HD23	4:D:358:LEU:HA	1.93	0.40
6:F:222:LEU:HD23	6:F:222:LEU:HA	1.89	0.40
8:H:316:LEU:HD13	8:H:320:PHE:CD1	2.56	0.40
11:K:32:ASN:HD22	11:K:32:ASN:HA	1.59	0.40
16:P:372:HIS:CE1	16:P:431:VAL:HG23	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:14:PHE:N	17:Q:43:ASP:OD2	2.54	0.40
1:A:287:GLU:OE1	1:A:287:GLU:CA	2.70	0.40
3:C:94:TRP:HB2	7:G:140:PHE:HZ	1.86	0.40
6:F:14:PHE:O	6:F:18:ALA:N	2.54	0.40
8:H:107:GLU:OE2	8:H:235:ARG:NH2	2.48	0.40
8:H:294:LYS:HE3	8:H:304:TRP:CZ2	2.57	0.40
11:K:156:MET:O	11:K:160:VAL:HG23	2.22	0.40
13:M:16:HIS:CE1	13:M:25:ASP:HB2	2.57	0.40
16:P:203:THR:HA	16:P:255:HIS:ND1	2.35	0.40
17:Q:129:VAL:O	17:Q:130:ILE:HB	2.20	0.40
1:A:349:LEU:HB3	1:A:350:PRO:HD3	2.04	0.40
2:B:314:VAL:CG1	2:B:329:MET:HG3	2.51	0.40
4:D:323:LEU:HD21	6:F:79:LEU:HD23	2.03	0.40
5:E:93:MET:HE2	5:E:93:MET:HB3	1.99	0.40
6:F:542:VAL:CG2	21:F:701:SQD:H202	2.51	0.40
7:G:143:PHE:C	7:G:146:PRO:HD2	2.46	0.40
10:J:115:LYS:O	10:J:116:THR:OG1	2.34	0.40
11:K:65:PHE:HB2	11:K:156:MET:HE1	2.03	0.40
11:K:98:LEU:HD21	11:K:139:ILE:HD13	2.03	0.40
11:K:174:ARG:HH11	21:K:502:SQD:C44	2.34	0.40
11:K:183:LEU:HD23	11:K:183:LEU:H	1.86	0.40
16:P:42:MET:HE2	16:P:42:MET:HB3	1.85	0.40
16:P:90:ASN:O	16:P:92:TYR:N	2.55	0.40
2:B:382:SER:O	2:B:391:GLY:HA3	2.21	0.40
6:F:256:ILE:O	6:F:260:ALA:N	2.47	0.40
8:H:25:VAL:O	8:H:389:MET:HE2	2.22	0.40
11:K:94:MET:HG2	11:K:97:ALA:HB3	2.03	0.40
11:K:188:HIS:HD2	13:M:29:LEU:HG	1.85	0.40
21:K:502:SQD:H81	21:K:502:SQD:C26	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	357/372 (96%)	314 (88%)	38 (11%)	5 (1%)	9	39
2	B	471/515 (92%)	428 (91%)	42 (9%)	1 (0%)	43	73
3	C	112/132 (85%)	101 (90%)	10 (9%)	1 (1%)	14	47
4	D	476/501 (95%)	428 (90%)	45 (10%)	3 (1%)	21	56
5	E	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
6	F	598/611 (98%)	539 (90%)	54 (9%)	5 (1%)	16	50
7	G	166/200 (83%)	155 (93%)	11 (7%)	0	100	100
8	H	391/394 (99%)	341 (87%)	45 (12%)	5 (1%)	9	40
9	I	191/196 (97%)	168 (88%)	22 (12%)	1 (0%)	24	59
10	J	154/168 (92%)	128 (83%)	26 (17%)	0	100	100
11	K	204/237 (86%)	174 (85%)	29 (14%)	1 (0%)	24	59
12	L	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
13	M	108/111 (97%)	86 (80%)	22 (20%)	0	100	100
14	N	145/150 (97%)	118 (81%)	27 (19%)	0	100	100
15	O	66/70 (94%)	52 (79%)	13 (20%)	1 (2%)	8	37
16	P	424/437 (97%)	367 (87%)	55 (13%)	2 (0%)	24	59
17	Q	146/149 (98%)	116 (80%)	28 (19%)	2 (1%)	9	39
18	S	53/110 (48%)	49 (92%)	4 (8%)	0	100	100
All	All	4234/4530 (94%)	3725 (88%)	482 (11%)	27 (1%)	23	56

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	GLU
1	A	302	LEU
6	F	36	PRO
6	F	478	ASP
8	H	73	ALA
8	H	153	PHE
8	H	154	ILE
16	P	427	LYS
1	A	233	ASP
3	C	20	GLU
8	H	72	TYR
1	A	297	GLU
1	A	336	ARG
4	D	192	PHE

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Mol	Chain	Res	Type
6	F	37	ARG
8	H	152	ARG
17	Q	129	VAL
17	Q	130	ILE
4	D	443	ALA
16	P	103	ARG
4	D	367	PRO
15	O	12	VAL
6	F	361	VAL
2	B	388	PRO
9	I	145	PRO
11	K	19	PRO
6	F	376	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 PDB entries followed by that with respect to all EM entries.

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	291/302 (96%)	285 (98%)	6 (2%)	47	71
2	B	367/413 (89%)	367 (100%)	0	100	100
3	C	93/109 (85%)	90 (97%)	3 (3%)	34	65
4	D	374/397 (94%)	367 (98%)	7 (2%)	50	73
5	E	81/82 (99%)	81 (100%)	0	100	100
6	F	481/492 (98%)	463 (96%)	18 (4%)	30	63
7	G	134/166 (81%)	134 (100%)	0	100	100
8	H	331/338 (98%)	325 (98%)	6 (2%)	51	74
9	I	162/172 (94%)	162 (100%)	0	100	100
10	J	138/148 (93%)	136 (99%)	2 (1%)	59	77
11	K	174/196 (89%)	173 (99%)	1 (1%)	78	84
12	L	63/63 (100%)	63 (100%)	0	100	100
13	M	95/96 (99%)	95 (100%)	0	100	100
14	N	119/120 (99%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	57/59 (97%)	57 (100%)	0	100	100
16	P	358/374 (96%)	351 (98%)	7 (2%)	48	72
17	Q	120/123 (98%)	119 (99%)	1 (1%)	73	82
18	S	48/97 (50%)	48 (100%)	0	100	100
All	All	3486/3747 (93%)	3435 (98%)	51 (2%)	55	76

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	LEU
1	A	287	GLU
1	A	289	ILE
1	A	291	ASN
1	A	293	LEU
1	A	295	VAL
3	C	20	GLU
3	C	43	LEU
3	C	46	LYS
4	D	33	LEU
4	D	198	GLN
4	D	240	THR
4	D	368	LEU
4	D	432	ARG
4	D	447	ARG
4	D	450	TRP
6	F	30	ILE
6	F	32	ARG
6	F	158	LEU
6	F	201	TRP
6	F	274	THR
6	F	377	ILE
6	F	378	SER
6	F	446	THR
6	F	451	GLU
6	F	456	MET
6	F	457	ILE
6	F	458	LEU
6	F	462	VAL
6	F	464	LEU
6	F	466	LEU
6	F	472	ILE

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Mol	Chain	Res	Type
6	F	473	LEU
6	F	476	ARG
8	H	69	ARG
8	H	70	TRP
8	H	71	ASP
8	H	72	TYR
8	H	78	ASN
8	H	113	ASN
10	J	23	ASN
10	J	87	ASN
11	K	32	ASN
16	P	18	HIS
16	P	129	HIS
16	P	184	MET
16	P	185	LEU
16	P	187	LEU
16	P	194	LEU
16	P	197	GLU
17	Q	108	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	208	ASN
2	B	130	GLN
2	B	229	HIS
2	B	483	ASN
4	D	63	GLN
4	D	359	ASN
4	D	484	GLN
6	F	43	ASN
6	F	64	GLN
6	F	165	ASN
7	G	117	GLN
8	H	19	HIS
8	H	290	ASN
9	I	40	GLN
11	K	104	GLN
13	M	9	HIS
13	M	23	HIS
13	M	42	ASN

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Mol	Chain	Res	Type
15	O	65	GLN
16	P	346	GLN
16	P	371	GLN
16	P	400	HIS
17	Q	59	GLN
17	Q	124	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	$\# Z > 2$
24	SF4	K	501	-	0,12,12	-	-	-		
21	SQD	L	402	-	52,54,54	1.36	9 (17%)	62,65,65	2.11	15 (24%)
24	SF4	I	201	-	0,12,12	-	-	-		
20	PGT	D	602	-	50,50,50	0.97	4 (8%)	53,56,56	1.64	6 (11%)
19	DGD	A	501	-	67,67,67	1.06	3 (4%)	81,81,81	2.43	24 (29%)
20	PGT	C	201	-	50,50,50	0.90	4 (8%)	53,56,56	1.66	6 (11%)
21	SQD	F	701	-	52,54,54	1.08	3 (5%)	62,65,65	1.43	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	SQD	D	601	-	52,54,54	1.61	12 (23%)	62,65,65	2.72	19 (30%)
21	SQD	F	703	-	52,54,54	1.10	4 (7%)	62,65,65	1.49	11 (17%)
22	BCR	F	702	-	41,41,41	0.90	2 (4%)	56,56,56	4.94	25 (44%)
23	CLA	F	704	-	50,54,73	2.47	19 (38%)	59,90,113	3.99	30 (50%)
21	SQD	K	502	-	52,54,54	1.38	10 (19%)	62,65,65	1.98	12 (19%)
24	SF4	I	202	-	0,12,12	-	-	-	-	-
19	DGD	L	401	-	67,67,67	0.86	2 (2%)	81,81,81	0.95	4 (4%)

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
24	SF4	K	501	-	-	-	0/6/5/5
21	SQD	L	402	-	-	26/49/69/69	0/1/1/1
24	SF4	I	201	-	-	-	0/6/5/5
20	PGT	D	602	-	-	26/55/55/55	-
19	DGD	A	501	-	-	25/55/95/95	0/2/2/2
20	PGT	C	201	-	-	24/55/55/55	-
21	SQD	F	701	-	-	20/49/69/69	0/1/1/1
21	SQD	D	601	-	-	25/49/69/69	0/1/1/1
21	SQD	F	703	-	-	26/49/69/69	0/1/1/1
22	BCR	F	702	-	-	4/29/63/63	0/2/2/2
23	CLA	F	704	-	-	0/17/93/115	-
21	SQD	K	502	-	-	23/49/69/69	0/1/1/1
24	SF4	I	202	-	-	-	0/6/5/5
19	DGD	L	401	-	-	30/55/95/95	0/2/2/2

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	704	CLA	C1D-ND	7.42	1.47	1.37
23	F	704	CLA	O2D-CGD	5.16	1.45	1.33
23	F	704	CLA	C3C-C2C	5.06	1.47	1.36
23	F	704	CLA	C3D-C4D	-4.61	1.33	1.44
23	F	704	CLA	CHC-C1C	4.36	1.47	1.38
19	L	401	DGD	O1G-C1A	4.29	1.45	1.33
23	F	704	CLA	O2A-CGA	4.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	F	703	SQD	O48-C23	4.11	1.45	1.33
19	L	401	DGD	O2G-C1B	4.07	1.45	1.34
21	F	703	SQD	O8-S	3.96	1.62	1.47
21	F	701	SQD	O48-C23	3.92	1.44	1.33
23	F	704	CLA	CHD-C1D	3.91	1.46	1.38
21	F	701	SQD	O47-C7	3.88	1.45	1.34
21	D	601	SQD	O9-S	-3.86	1.34	1.45
21	F	703	SQD	O47-C7	3.84	1.45	1.34
21	F	701	SQD	O8-S	3.83	1.61	1.47
23	F	704	CLA	OBD-CAD	3.79	1.29	1.22
21	D	601	SQD	O6-C44	-3.69	1.37	1.43
21	L	402	SQD	O48-C23	3.63	1.43	1.33
21	D	601	SQD	O47-C45	-3.61	1.38	1.46
23	F	704	CLA	CHD-C4C	3.59	1.47	1.39
21	K	502	SQD	O47-C7	3.54	1.44	1.34
21	L	402	SQD	O9-S	-3.47	1.35	1.45
19	A	501	DGD	O2G-C2G	-3.44	1.38	1.46
21	K	502	SQD	O47-C45	-3.36	1.38	1.46
20	C	201	PGT	O3-C11	3.30	1.43	1.33
21	D	601	SQD	O48-C23	3.25	1.42	1.33
21	D	601	SQD	O7-S	-3.24	1.36	1.45
21	K	502	SQD	O48-C23	3.19	1.42	1.33
20	C	201	PGT	O2-C31	3.07	1.42	1.34
23	F	704	CLA	CHC-C4B	3.05	1.46	1.39
22	F	702	BCR	C30-C25	-3.03	1.49	1.53
23	F	704	CLA	CHB-C1B	3.03	1.46	1.39
23	F	704	CLA	C1D-C2D	3.01	1.51	1.45
21	K	502	SQD	O9-S	-2.98	1.36	1.45
19	A	501	DGD	O2G-C1B	2.98	1.42	1.34
21	L	402	SQD	O47-C7	2.97	1.42	1.34
23	F	704	CLA	C3D-C2D	2.96	1.47	1.39
20	D	602	PGT	O2-C31	2.94	1.42	1.34
19	A	501	DGD	O1G-C1A	2.93	1.41	1.33
21	L	402	SQD	O6-C1	2.92	1.45	1.40
21	D	601	SQD	O48-C46	-2.92	1.38	1.45
20	D	602	PGT	O11-C11	-2.91	1.13	1.22
21	K	502	SQD	O6-C44	-2.90	1.38	1.43
21	K	502	SQD	O8-S	2.84	1.57	1.47
21	K	502	SQD	O5-C5	-2.84	1.37	1.44
21	L	402	SQD	C4-C5	-2.84	1.47	1.53
23	F	704	CLA	C1B-C2B	2.84	1.49	1.43
21	D	601	SQD	O2-C2	-2.81	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	601	SQD	O5-C5	-2.80	1.37	1.44
20	D	602	PGT	O3-C11	2.76	1.41	1.33
21	L	402	SQD	O7-S	-2.65	1.37	1.45
21	L	402	SQD	C3-C2	-2.62	1.45	1.52
23	F	704	CLA	C4C-C3C	2.58	1.49	1.45
21	D	601	SQD	C3-C2	-2.54	1.45	1.52
21	D	601	SQD	C1-C2	-2.53	1.45	1.52
23	F	704	CLA	C4B-NB	-2.51	1.34	1.37
21	D	601	SQD	O6-C1	-2.51	1.36	1.40
21	L	402	SQD	O47-C45	-2.47	1.40	1.46
21	D	601	SQD	O3-C3	-2.38	1.37	1.43
21	K	502	SQD	O7-S	-2.36	1.38	1.45
21	L	402	SQD	O49-C7	-2.36	1.15	1.22
22	F	702	BCR	C5-C6	-2.29	1.30	1.34
20	D	602	PGT	O2-C2	-2.28	1.41	1.46
20	C	201	PGT	O31-C31	-2.26	1.15	1.22
23	F	704	CLA	CHB-C4A	-2.22	1.32	1.37
20	C	201	PGT	O2-C2	-2.15	1.41	1.46
21	K	502	SQD	O48-C46	-2.14	1.40	1.45
23	F	704	CLA	C1C-C2C	2.12	1.48	1.44
21	K	502	SQD	C1-C2	-2.11	1.46	1.52
23	F	704	CLA	MG-NA	-2.05	2.01	2.06
21	F	703	SQD	O47-C45	-2.01	1.41	1.46

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	702	BCR	C2-C1-C6	-18.77	83.17	110.44
22	F	702	BCR	C31-C1-C6	-15.78	85.49	110.24
23	F	704	CLA	C1D-ND-C4D	-13.29	96.99	106.31
22	F	702	BCR	C32-C1-C6	12.20	129.38	110.24
21	D	601	SQD	O3-C3-C2	-12.03	82.01	110.38
22	F	702	BCR	C32-C1-C31	-11.24	76.44	108.63
23	F	704	CLA	C4B-CHC-C1C	-10.48	101.60	126.25
19	A	501	DGD	O6D-C1D-C2D	-10.39	89.03	110.37
19	A	501	DGD	O3G-C1D-C2D	8.96	121.88	108.27
22	F	702	BCR	C31-C1-C2	8.26	140.68	108.95
23	F	704	CLA	CMD-C2D-C1D	8.21	139.19	124.73
20	C	201	PGT	O2-C31-C32	7.82	128.40	111.48
23	F	704	CLA	C4D-CHA-C1A	-7.46	112.34	121.24
22	F	702	BCR	C1-C6-C5	-7.11	112.92	122.64
22	F	702	BCR	C32-C1-C2	-6.99	82.13	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	502	SQD	O9-S-C6	6.99	117.19	106.76
21	L	402	SQD	O9-S-C6	6.88	117.03	106.76
23	F	704	CLA	C2C-C1C-NC	6.88	117.21	109.98
23	F	704	CLA	C3D-C4D-ND	6.63	120.77	109.99
21	L	402	SQD	O47-C7-C8	6.58	125.71	111.48
23	F	704	CLA	CHD-C1D-ND	-6.28	115.96	124.80
19	A	501	DGD	C8B-C7B-C6B	-6.19	83.07	114.37
23	F	704	CLA	C2B-C1B-NB	6.12	116.67	110.33
20	D	602	PGT	O2-C31-C32	5.80	124.03	111.48
21	D	601	SQD	O8-S-O7	-5.76	96.98	111.40
22	F	702	BCR	C4-C5-C6	-5.76	114.92	122.70
21	K	502	SQD	C1-C2-C3	-5.61	98.21	110.01
20	D	602	PGT	O3-C11-C12	5.54	128.73	111.83
23	F	704	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
23	F	704	CLA	CHC-C4B-NB	-5.51	115.79	124.05
23	F	704	CLA	C3B-C4B-NB	5.50	115.44	110.53
22	F	702	BCR	C33-C5-C4	5.50	125.33	113.60
21	D	601	SQD	O8-S-C6	5.46	116.51	105.97
23	F	704	CLA	CHC-C1C-NC	-5.11	116.61	124.31
23	F	704	CLA	O2D-CGD-CBD	5.07	120.10	111.23
21	F	703	SQD	O47-C7-C8	5.06	122.43	111.48
21	D	601	SQD	C4-C3-C2	5.01	119.63	110.83
23	F	704	CLA	C1C-C2C-C3C	-4.96	101.76	106.98
21	L	402	SQD	C1-O5-C5	4.81	123.11	113.72
21	D	601	SQD	O3-C3-C4	-4.78	99.10	110.38
22	F	702	BCR	C24-C23-C22	-4.77	119.17	126.23
23	F	704	CLA	C1D-CHD-C4C	-4.74	115.95	126.02
19	A	501	DGD	O1G-C1A-C2A	4.70	126.16	111.83
22	F	702	BCR	C1-C6-C7	4.69	128.36	115.65
22	F	702	BCR	C15-C14-C13	-4.66	120.75	127.28
23	F	704	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
21	F	701	SQD	O47-C7-C8	4.61	121.46	111.48
19	A	501	DGD	C1D-O6D-C5D	4.58	122.66	113.72
22	F	702	BCR	C20-C21-C22	-4.52	120.94	127.28
21	D	601	SQD	O9-S-C6	4.52	113.51	106.76
21	L	402	SQD	O7-S-C6	4.52	113.50	106.76
21	K	502	SQD	O5-C1-C2	-4.49	101.14	110.37
23	F	704	CLA	C2D-C1D-ND	4.49	114.57	110.13
21	K	502	SQD	C44-O6-C1	-4.49	104.18	113.80
21	D	601	SQD	C44-O6-C1	-4.43	104.31	113.80
22	F	702	BCR	C33-C5-C6	-4.35	119.74	124.48
21	K	502	SQD	C1-O5-C5	-4.31	105.31	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	501	DGD	O2G-C1B-C2B	4.29	120.76	111.48
20	C	201	PGT	O2-C31-O31	-4.23	113.81	123.70
21	L	402	SQD	O48-C23-C24	4.19	124.60	111.83
21	D	601	SQD	O7-S-C6	4.13	112.93	106.76
21	F	701	SQD	O9-S-C6	4.10	112.88	106.76
19	A	501	DGD	C4E-C3E-C2E	-4.08	103.68	110.83
20	D	602	PGT	O2-C31-O31	-4.05	114.23	123.70
20	C	201	PGT	C36-C37-C38	4.03	134.76	114.37
19	L	401	DGD	O2G-C1B-C2B	4.01	120.16	111.48
21	L	402	SQD	O8-S-O9	-4.00	101.39	111.40
21	D	601	SQD	O6-C1-C2	-3.98	102.22	108.27
21	K	502	SQD	O48-C23-O10	-3.90	113.88	123.63
23	F	704	CLA	C3C-C4C-NC	3.88	115.40	110.43
22	F	702	BCR	C7-C8-C9	-3.80	120.61	126.23
21	F	703	SQD	O5-C1-C2	-3.77	102.62	110.37
21	L	402	SQD	O3-C3-C2	-3.74	101.57	110.38
19	A	501	DGD	C1E-O6E-C5E	3.72	120.98	113.72
21	D	601	SQD	C9-C8-C7	-3.68	100.20	113.69
21	F	703	SQD	C1-C2-C3	-3.67	102.29	110.01
21	D	601	SQD	O9-S-O7	-3.63	102.00	113.82
20	D	602	PGT	O3-C11-O11	-3.60	114.62	123.63
21	K	502	SQD	O8-S-O7	-3.60	102.39	111.40
22	F	702	BCR	C16-C17-C18	-3.60	122.24	127.28
22	F	702	BCR	C30-C25-C26	-3.58	117.75	122.64
19	A	501	DGD	O1G-C1A-O1A	-3.49	114.89	123.63
21	L	402	SQD	C4-C3-C2	-3.48	104.72	110.83
22	F	702	BCR	C11-C10-C9	-3.39	122.52	127.28
19	A	501	DGD	O5E-C6E-C5E	-3.36	99.89	111.33
23	F	704	CLA	CHB-C1B-NB	-3.32	119.07	124.05
22	F	702	BCR	C38-C26-C25	-3.30	120.88	124.48
21	L	402	SQD	O47-C7-O49	-3.29	116.01	123.70
22	F	702	BCR	C38-C26-C27	3.20	120.42	113.60
21	F	701	SQD	O48-C23-C24	3.19	121.55	111.83
21	D	601	SQD	C1-O5-C5	-3.18	107.51	113.72
19	A	501	DGD	C6D-C5D-C4D	3.07	118.51	112.07
21	D	601	SQD	O48-C23-C24	3.06	121.16	111.83
21	K	502	SQD	O48-C23-C24	3.04	121.10	111.83
20	C	201	PGT	C2-O2-C31	-3.02	110.56	117.80
21	F	703	SQD	O48-C23-C24	3.01	121.02	111.83
19	A	501	DGD	O3G-C3G-C2G	3.00	118.11	110.82
22	F	702	BCR	C27-C26-C25	-2.99	118.67	122.70
21	L	402	SQD	C46-O48-C23	2.93	127.84	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	502	SQD	O6-C44-C45	-2.92	103.70	110.82
21	F	703	SQD	O7-S-C6	2.87	111.04	106.76
21	D	601	SQD	O4-C4-C3	-2.87	103.62	110.38
23	F	704	CLA	C4A-NA-C1A	-2.86	105.37	106.68
22	F	702	BCR	C3-C4-C5	-2.85	108.98	114.06
21	L	402	SQD	O2-C2-C3	-2.84	103.69	110.38
19	A	501	DGD	C3D-C4D-C5D	-2.83	105.10	110.23
23	F	704	CLA	CHA-C1A-NA	-2.82	120.00	126.39
23	F	704	CLA	CMB-C2B-C1B	2.81	129.69	125.42
23	F	704	CLA	CMD-C2D-C3D	-2.79	121.29	127.69
21	F	703	SQD	O6-C1-C2	2.77	112.48	108.27
19	A	501	DGD	O6D-C5D-C4D	-2.75	104.75	109.70
19	L	401	DGD	O1G-C1A-C2A	2.73	120.15	111.83
21	F	701	SQD	O5-C1-C2	-2.72	104.78	110.37
23	F	704	CLA	CAC-C3C-C4C	2.72	128.33	124.79
22	F	702	BCR	C8-C7-C6	-2.64	119.95	127.00
21	F	701	SQD	O7-S-C6	2.63	110.69	106.76
19	L	401	DGD	O6D-C5D-C6D	2.61	111.88	106.69
21	L	402	SQD	O8-S-O7	-2.60	104.89	111.40
19	A	501	DGD	C2G-O2G-C1B	-2.59	111.59	117.80
21	F	703	SQD	O47-C7-O49	-2.59	117.65	123.70
23	F	704	CLA	CMC-C2C-C1C	2.59	129.08	125.03
23	F	704	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
21	D	601	SQD	O2-C2-C1	-2.56	103.97	110.08
20	D	602	PGT	C14-C13-C12	-2.53	103.81	113.13
19	A	501	DGD	O1G-C1G-C2G	-2.53	101.10	108.40
23	F	704	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
19	L	401	DGD	C2G-O2G-C1B	-2.50	111.80	117.80
21	D	601	SQD	O47-C7-C8	2.49	116.88	111.48
19	A	501	DGD	O3D-C3D-C2D	-2.40	104.71	110.38
21	L	402	SQD	O4-C4-C5	-2.40	103.41	109.32
23	F	704	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
21	D	601	SQD	C45-O47-C7	-2.37	112.13	117.80
19	A	501	DGD	O4E-C4E-C3E	-2.36	104.80	110.38
19	A	501	DGD	O3D-C3D-C4D	-2.32	104.92	110.38
21	F	701	SQD	C1-C2-C3	-2.31	105.15	110.01
21	L	402	SQD	O5-C1-C2	2.29	115.07	110.37
22	F	702	BCR	C10-C11-C12	-2.28	116.58	123.20
21	K	502	SQD	C25-C24-C23	-2.28	105.34	113.69
20	D	602	PGT	C13-C12-C11	-2.26	105.43	113.69
22	F	702	BCR	C15-C16-C17	-2.24	118.94	123.52
19	A	501	DGD	C4B-C3B-C2B	-2.24	104.91	113.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	201	PGT	O3-C11-C12	2.21	118.57	111.83
21	D	601	SQD	C11-C10-C9	-2.21	103.22	114.37
19	A	501	DGD	O1B-C1B-C2B	-2.20	115.20	123.78
21	F	703	SQD	C45-O47-C7	-2.19	112.56	117.80
21	K	502	SQD	O7-S-C6	2.18	110.00	106.76
19	A	501	DGD	O6E-C5E-C4E	2.17	113.62	109.70
21	L	402	SQD	O48-C23-O10	-2.17	118.20	123.63
21	D	601	SQD	O47-C7-O49	-2.15	118.67	123.70
21	F	703	SQD	C1-O5-C5	-2.13	109.57	113.72
21	F	703	SQD	C44-O6-C1	-2.11	109.26	113.80
23	F	704	CLA	O2A-CGA-CBA	2.11	120.10	112.14
19	A	501	DGD	O2D-C2D-C1D	2.10	115.08	110.08
19	A	501	DGD	C3B-C2B-C1B	-2.05	106.18	113.69
23	F	704	CLA	CHD-C4C-C3C	-2.04	121.80	124.77
20	C	201	PGT	C3-C2-C1	2.04	116.54	111.78
21	F	703	SQD	O9-S-C6	2.03	109.79	106.76
21	K	502	SQD	C28-C27-C26	-2.02	104.16	114.37

There are no chirality outliers.

All (229) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	501	DGD	C2D-C1D-O3G-C3G
19	L	401	DGD	C2B-C1B-O2G-C2G
19	L	401	DGD	O6E-C1E-O5D-C6D
20	C	201	PGT	C5-C4-O4P-P
20	C	201	PGT	O5-C5-C6-O6
20	D	602	PGT	C4-O4P-P-O3P
21	D	601	SQD	C8-C7-O47-C45
21	D	601	SQD	O10-C23-O48-C46
21	D	601	SQD	C24-C23-O48-C46
21	F	701	SQD	C8-C7-O47-C45
21	F	701	SQD	O10-C23-O48-C46
21	F	701	SQD	C24-C23-O48-C46
21	F	701	SQD	C5-C6-S-O7
21	F	701	SQD	C5-C6-S-O8
21	F	701	SQD	C5-C6-S-O9
21	F	703	SQD	C2-C1-O6-C44
21	F	703	SQD	O5-C1-O6-C44
21	F	703	SQD	C8-C7-O47-C45
21	F	703	SQD	O10-C23-O48-C46
21	F	703	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
21	F	703	SQD	O5-C5-C6-S
21	K	502	SQD	C5-C6-S-O7
21	K	502	SQD	C5-C6-S-O9
21	L	402	SQD	O5-C1-O6-C44
22	F	702	BCR	C1-C6-C7-C8
22	F	702	BCR	C5-C6-C7-C8
22	F	702	BCR	C23-C24-C25-C26
19	L	401	DGD	O6D-C5D-C6D-O5D
19	L	401	DGD	O1B-C1B-O2G-C2G
21	D	601	SQD	O49-C7-O47-C45
21	F	701	SQD	O49-C7-O47-C45
19	L	401	DGD	C4E-C5E-C6E-O5E
21	F	703	SQD	O49-C7-O47-C45
21	K	502	SQD	C34-C35-C36-C37
19	L	401	DGD	O6E-C5E-C6E-O5E
21	L	402	SQD	O10-C23-O48-C46
19	A	501	DGD	O6D-C1D-O3G-C3G
19	L	401	DGD	C4D-C5D-C6D-O5D
21	L	402	SQD	C24-C23-O48-C46
19	A	501	DGD	C4A-C5A-C6A-C7A
19	L	401	DGD	C2E-C1E-O5D-C6D
20	D	602	PGT	C31-C32-C33-C34
20	C	201	PGT	C32-C31-O2-C2
19	A	501	DGD	O2G-C2G-C3G-O3G
21	L	402	SQD	C7-C8-C9-C10
19	L	401	DGD	CCB-CDB-CEB-CFB
19	L	401	DGD	C1A-C2A-C3A-C4A
21	F	701	SQD	C7-C8-C9-C10
21	K	502	SQD	C11-C10-C9-C8
20	C	201	PGT	C11-C12-C13-C14
21	K	502	SQD	C23-C24-C25-C26
20	C	201	PGT	C43-C44-C45-C46
20	C	201	PGT	O31-C31-O2-C2
21	K	502	SQD	C30-C31-C32-C33
20	C	201	PGT	C4-C5-C6-O6
20	C	201	PGT	C12-C11-O3-C3
20	C	201	PGT	C41-C42-C43-C44
21	L	402	SQD	C33-C34-C35-C36
20	C	201	PGT	C40-C41-C42-C43
21	D	601	SQD	C12-C13-C14-C15
19	A	501	DGD	CBA-CCA-CDA-CEA
20	D	602	PGT	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	F	701	SQD	C34-C35-C36-C37
21	F	703	SQD	C14-C15-C16-C17
19	A	501	DGD	C2A-C3A-C4A-C5A
21	F	701	SQD	C28-C29-C30-C31
20	C	201	PGT	C36-C37-C38-C39
21	F	703	SQD	C11-C10-C9-C8
19	L	401	DGD	C3A-C4A-C5A-C6A
19	L	401	DGD	C8A-C9A-CAA-CBA
19	L	401	DGD	CDA-CEA-CFA-CGA
19	L	401	DGD	C7B-C8B-C9B-CAB
21	F	701	SQD	C26-C27-C28-C29
21	K	502	SQD	C14-C15-C16-C17
21	F	701	SQD	C25-C26-C27-C28
19	A	501	DGD	C7A-C8A-C9A-CAA
21	F	701	SQD	C14-C15-C16-C17
19	L	401	DGD	C1B-C2B-C3B-C4B
19	L	401	DGD	C5A-C6A-C7A-C8A
19	L	401	DGD	C6A-C7A-C8A-C9A
20	D	602	PGT	C44-C45-C46-C47
20	D	602	PGT	C42-C43-C44-C45
19	L	401	DGD	CCA-CDA-CEA-CFA
19	L	401	DGD	C4B-C5B-C6B-C7B
20	C	201	PGT	C39-C40-C41-C42
21	L	402	SQD	C11-C12-C13-C14
22	F	702	BCR	C23-C24-C25-C30
19	L	401	DGD	CBA-CCA-CDA-CEA
19	A	501	DGD	C7B-C8B-C9B-CAB
21	F	701	SQD	C24-C25-C26-C27
21	F	703	SQD	C29-C30-C31-C32
20	D	602	PGT	C38-C39-C40-C41
21	L	402	SQD	C10-C11-C12-C13
19	A	501	DGD	CCB-CDB-CEB-CFB
21	D	601	SQD	C34-C35-C36-C37
21	D	601	SQD	C18-C19-C20-C21
21	F	703	SQD	C17-C18-C19-C20
21	L	402	SQD	C2-C1-O6-C44
20	D	602	PGT	C32-C31-O2-C2
21	L	402	SQD	C8-C7-O47-C45
19	A	501	DGD	C1B-C2B-C3B-C4B
21	F	701	SQD	C33-C34-C35-C36
19	A	501	DGD	CCA-CDA-CEA-CFA
21	D	601	SQD	C45-C44-O6-C1

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Mol	Chain	Res	Type	Atoms
19	A	501	DGD	C9A-CAA-CBA-CCA
20	C	201	PGT	C16-C17-C18-C19
20	C	201	PGT	C38-C39-C40-C41
20	C	201	PGT	O11-C11-O3-C3
19	L	401	DGD	CAA-CBA-CCA-CDA
20	D	602	PGT	O31-C31-O2-C2
21	D	601	SQD	C31-C32-C33-C34
21	F	703	SQD	C12-C13-C14-C15
20	C	201	PGT	C13-C14-C15-C16
21	K	502	SQD	C16-C17-C18-C19
20	D	602	PGT	O2-C2-C3-O3
21	L	402	SQD	O6-C44-C45-O47
20	C	201	PGT	C33-C34-C35-C36
20	D	602	PGT	C33-C34-C35-C36
19	A	501	DGD	C9B-CAB-CBB-CCB
21	D	601	SQD	C33-C34-C35-C36
21	L	402	SQD	C32-C33-C34-C35
21	K	502	SQD	C17-C18-C19-C20
21	L	402	SQD	C12-C13-C14-C15
21	F	703	SQD	C15-C16-C17-C18
21	L	402	SQD	O49-C7-O47-C45
19	A	501	DGD	CAA-CBA-CCA-CDA
20	D	602	PGT	C36-C37-C38-C39
20	D	602	PGT	C11-C12-C13-C14
21	D	601	SQD	C29-C30-C31-C32
21	D	601	SQD	C15-C16-C17-C18
19	A	501	DGD	C1G-C2G-C3G-O3G
21	F	703	SQD	C26-C27-C28-C29
21	F	701	SQD	C10-C11-C12-C13
21	L	402	SQD	C11-C10-C9-C8
21	F	703	SQD	C34-C35-C36-C37
19	A	501	DGD	CDA-CEA-CFA-CGA
19	L	401	DGD	C4A-C5A-C6A-C7A
20	D	602	PGT	C41-C42-C43-C44
21	F	703	SQD	C24-C25-C26-C27
21	K	502	SQD	C18-C19-C20-C21
21	F	703	SQD	C9-C10-C11-C12
19	L	401	DGD	CFA-CGA-CHA-CIA
21	D	601	SQD	C32-C33-C34-C35
19	L	401	DGD	CFB-CGB-CHB-CIB
21	D	601	SQD	C24-C25-C26-C27
20	D	602	PGT	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
20	C	201	PGT	C34-C35-C36-C37
19	L	401	DGD	C2A-C3A-C4A-C5A
20	D	602	PGT	C19-C20-C21-C22
20	C	201	PGT	C15-C16-C17-C18
20	D	602	PGT	C17-C18-C19-C20
20	D	602	PGT	O3P-C1-C2-C3
20	D	602	PGT	C12-C13-C14-C15
19	A	501	DGD	C8A-C9A-CAA-CBA
21	D	601	SQD	C19-C20-C21-C22
20	D	602	PGT	C1-C2-C3-O3
21	D	601	SQD	O6-C44-C45-C46
21	L	402	SQD	O6-C44-C45-C46
21	L	402	SQD	C44-C45-C46-O48
21	F	703	SQD	C16-C17-C18-C19
20	D	602	PGT	C5-C4-O4P-P
21	F	703	SQD	C27-C28-C29-C30
21	K	502	SQD	C12-C13-C14-C15
21	D	601	SQD	O6-C44-C45-O47
21	F	703	SQD	C18-C19-C20-C21
21	D	601	SQD	C27-C28-C29-C30
21	F	703	SQD	C10-C11-C12-C13
21	F	701	SQD	C32-C33-C34-C35
21	K	502	SQD	C5-C6-S-O8
20	D	602	PGT	C18-C19-C20-C21
21	D	601	SQD	C16-C17-C18-C19
19	A	501	DGD	O1G-C1G-C2G-C3G
21	K	502	SQD	O6-C44-C45-C46
21	L	402	SQD	C35-C36-C37-C38
21	K	502	SQD	C28-C29-C30-C31
21	K	502	SQD	O6-C44-C45-O47
21	K	502	SQD	C27-C28-C29-C30
19	L	401	DGD	CEA-CFA-CGA-CHA
20	C	201	PGT	C14-C15-C16-C17
20	D	602	PGT	C39-C40-C41-C42
20	D	602	PGT	O3P-C1-C2-O2
19	A	501	DGD	C4B-C5B-C6B-C7B
21	L	402	SQD	C19-C20-C21-C22
21	L	402	SQD	O47-C45-C46-O48
19	L	401	DGD	C3B-C4B-C5B-C6B
19	A	501	DGD	C8B-C9B-CAB-CBB
20	D	602	PGT	C4-O4P-P-O1P
21	D	601	SQD	C25-C26-C27-C28

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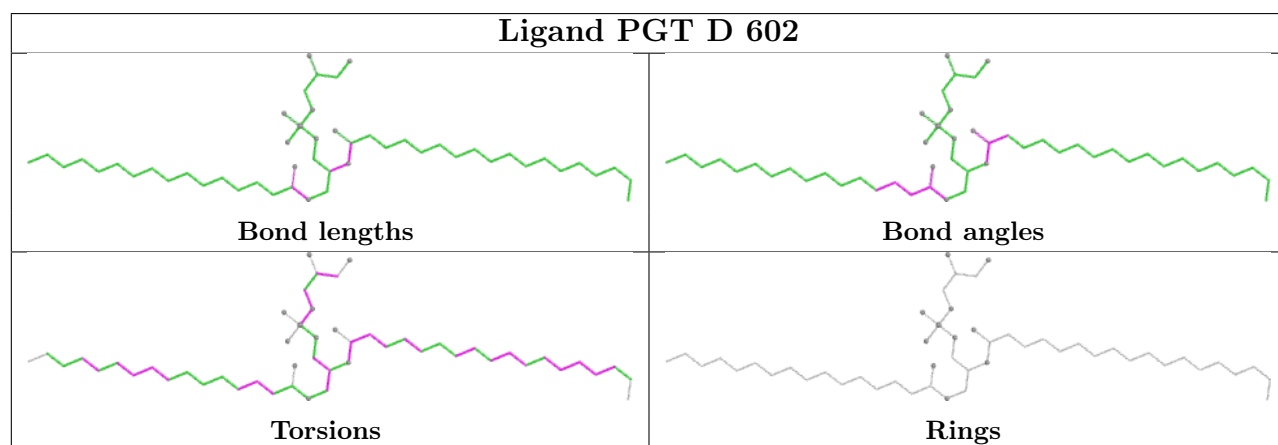
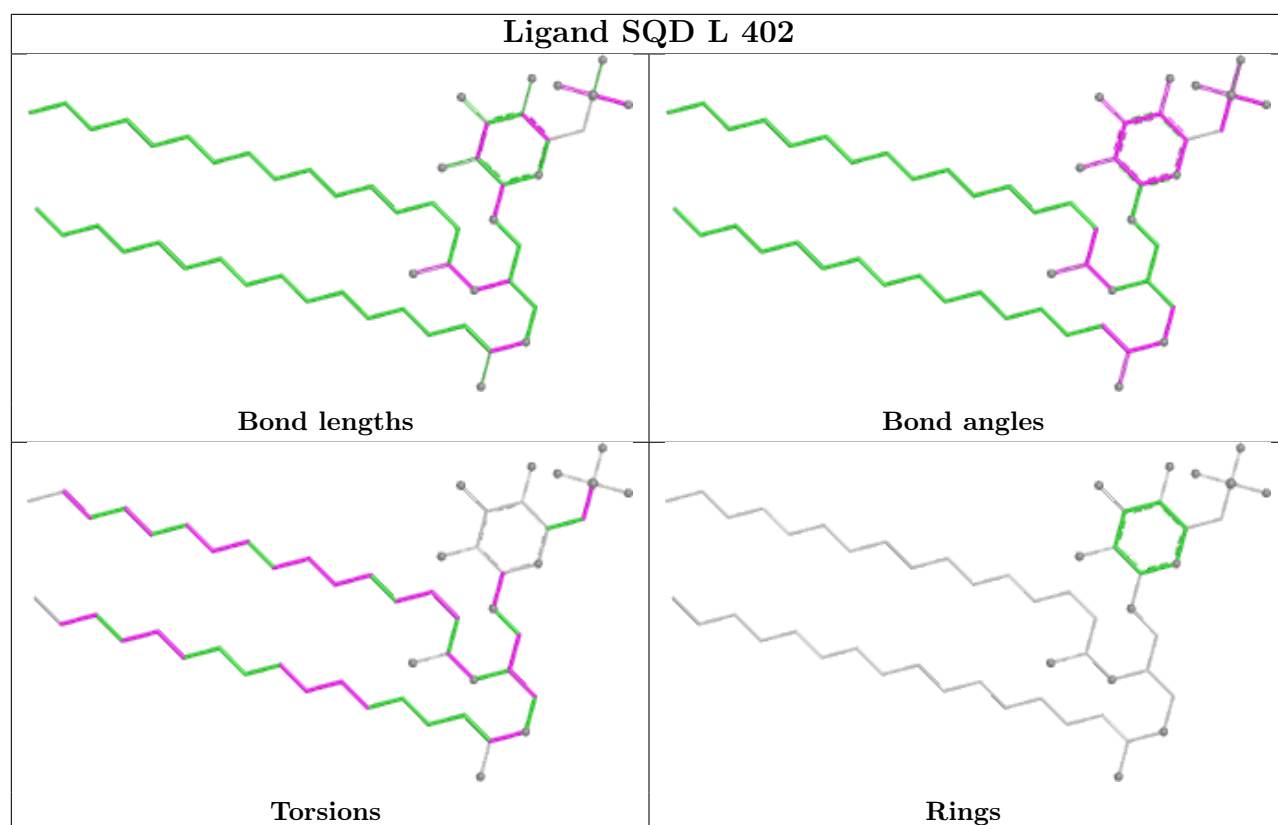
Mol	Chain	Res	Type	Atoms
21	D	601	SQD	C11-C12-C13-C14
19	L	401	DGD	O6D-C1D-O3G-C3G
19	A	501	DGD	O1G-C1G-C2G-O2G
21	F	701	SQD	C15-C16-C17-C18
21	K	502	SQD	C9-C10-C11-C12
21	K	502	SQD	C24-C25-C26-C27
21	F	703	SQD	C11-C12-C13-C14
21	K	502	SQD	C7-C8-C9-C10
21	L	402	SQD	C15-C16-C17-C18
21	K	502	SQD	C15-C16-C17-C18
21	L	402	SQD	C28-C29-C30-C31
21	L	402	SQD	C17-C18-C19-C20
21	D	601	SQD	C44-C45-O47-C7
21	F	703	SQD	C44-C45-O47-C7
19	A	501	DGD	C6B-C7B-C8B-C9B
21	F	703	SQD	C35-C36-C37-C38
21	L	402	SQD	C27-C28-C29-C30
21	K	502	SQD	O47-C7-C8-C9
21	D	601	SQD	C5-C6-S-O8
21	L	402	SQD	C26-C27-C28-C29
20	D	602	PGT	O2-C31-C32-C33
21	F	703	SQD	C46-C45-O47-C7
21	F	701	SQD	C11-C12-C13-C14
21	L	402	SQD	C14-C15-C16-C17
19	L	401	DGD	O2G-C2G-C3G-O3G
21	K	502	SQD	C13-C14-C15-C16
20	C	201	PGT	C19-C20-C21-C22
20	C	201	PGT	C23-C24-C25-C26
20	C	201	PGT	C45-C46-C47-C48
19	A	501	DGD	O2G-C1B-C2B-C3B
21	K	502	SQD	C26-C27-C28-C29
21	L	402	SQD	C5-C6-S-O7
21	D	601	SQD	C46-C45-O47-C7
19	L	401	DGD	C2B-C3B-C4B-C5B
20	D	602	PGT	C43-C44-C45-C46
19	A	501	DGD	O6E-C1E-O5D-C6D
21	D	601	SQD	O47-C7-C8-C9
20	C	201	PGT	O4P-C4-C5-C6
21	F	701	SQD	C31-C32-C33-C34
21	F	703	SQD	C28-C29-C30-C31
19	A	501	DGD	O1B-C1B-C2B-C3B

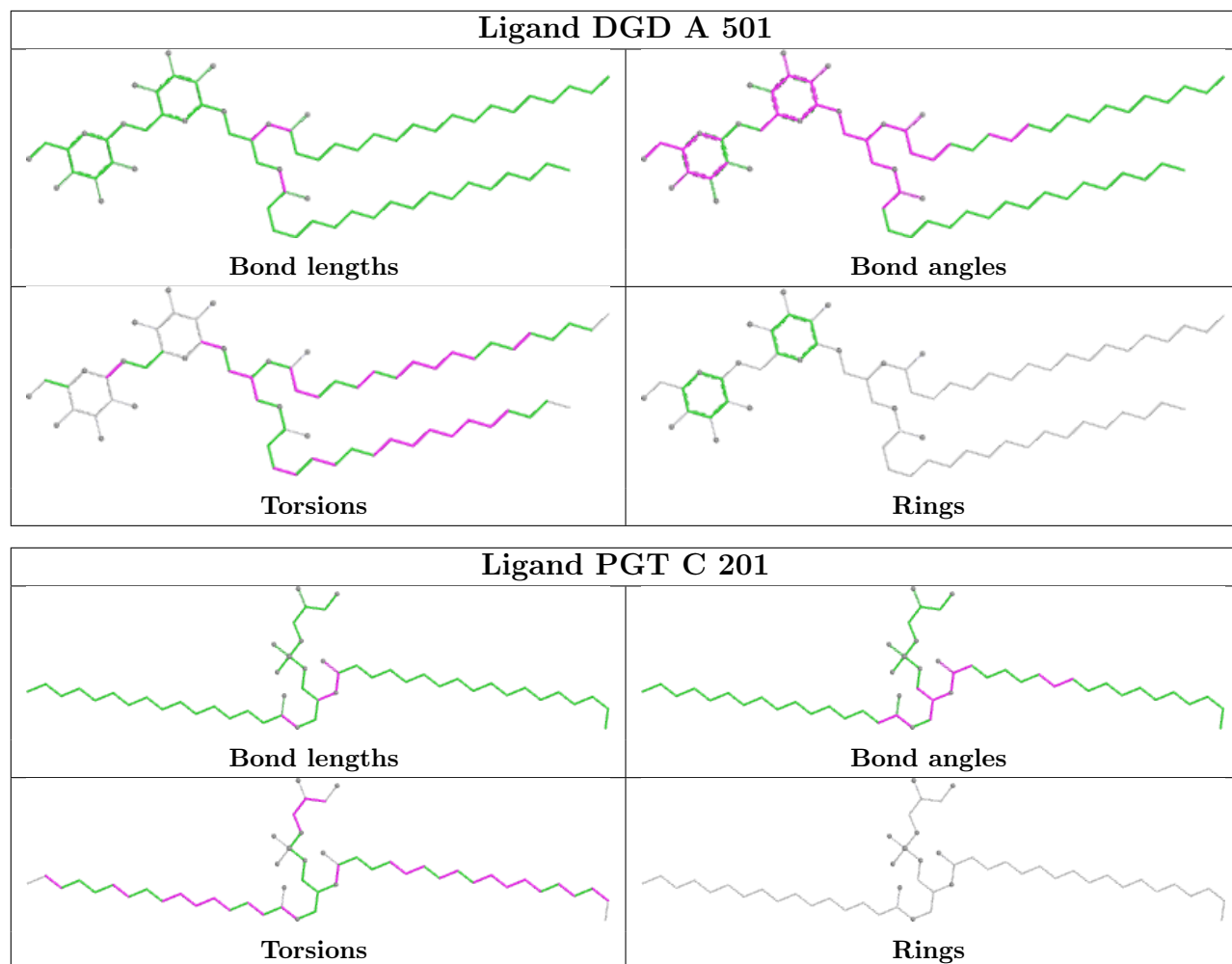
There are no ring outliers.

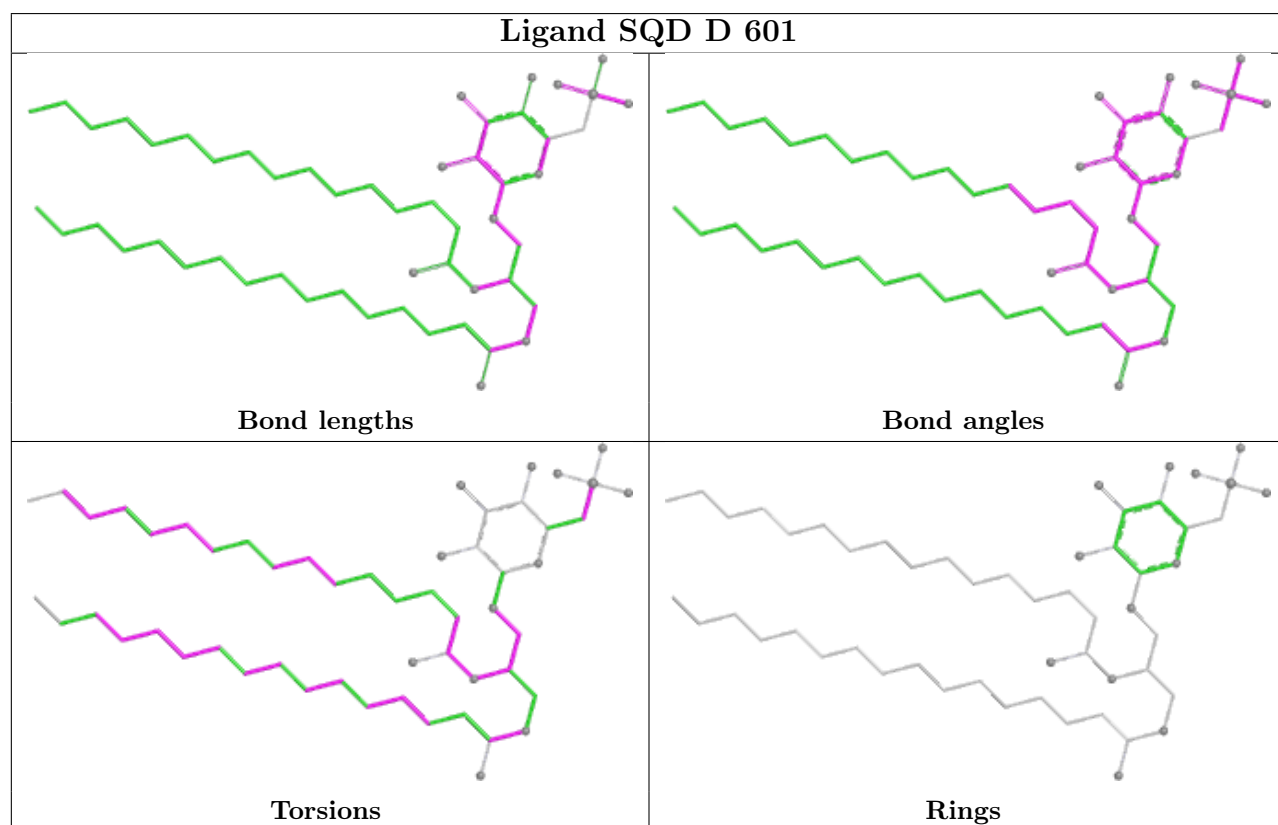
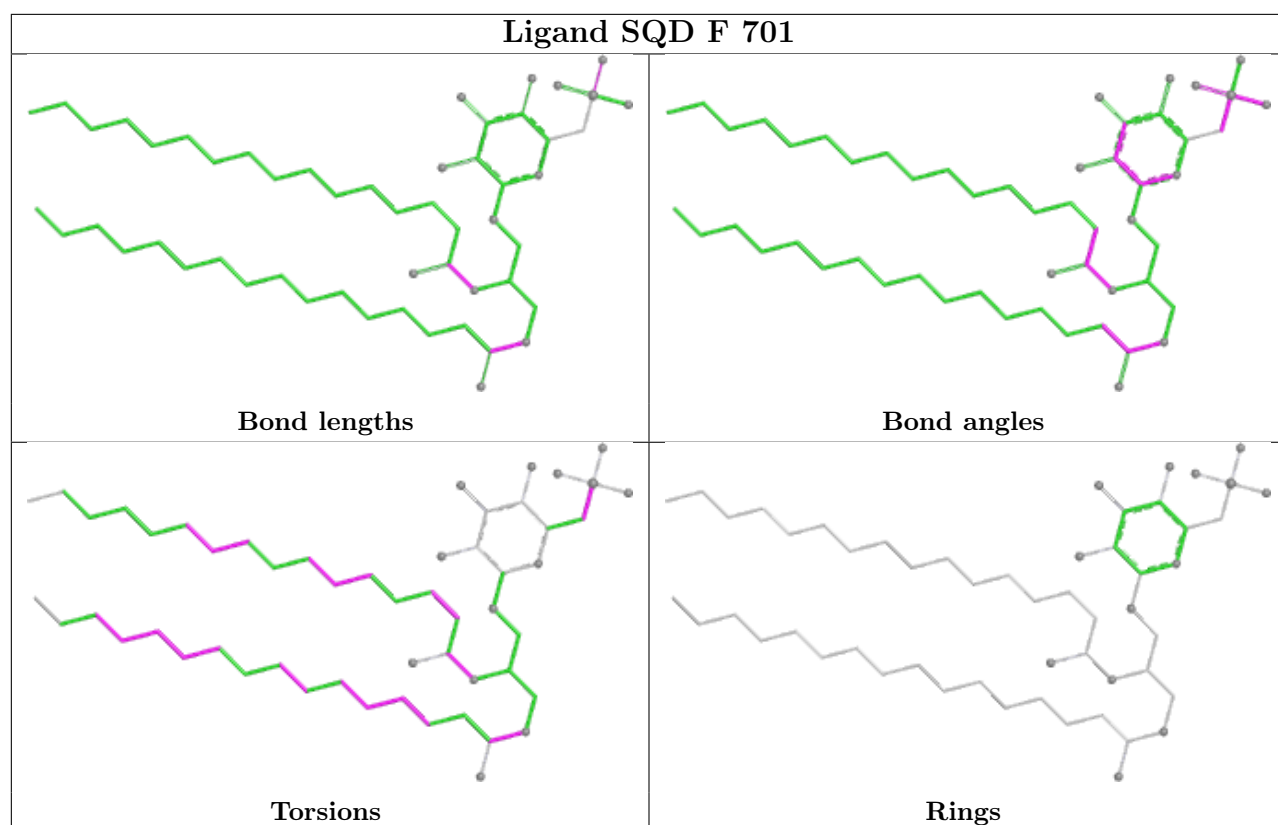
13 monomers are involved in 283 short contacts:

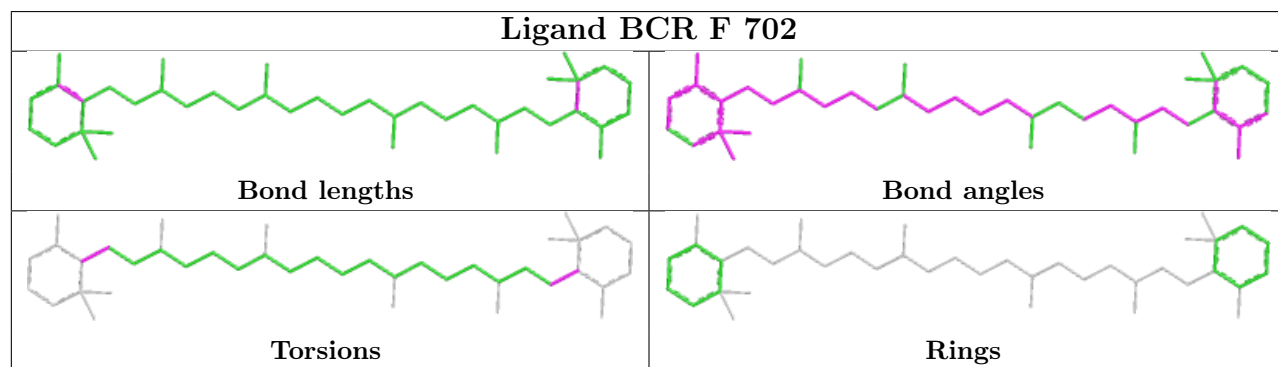
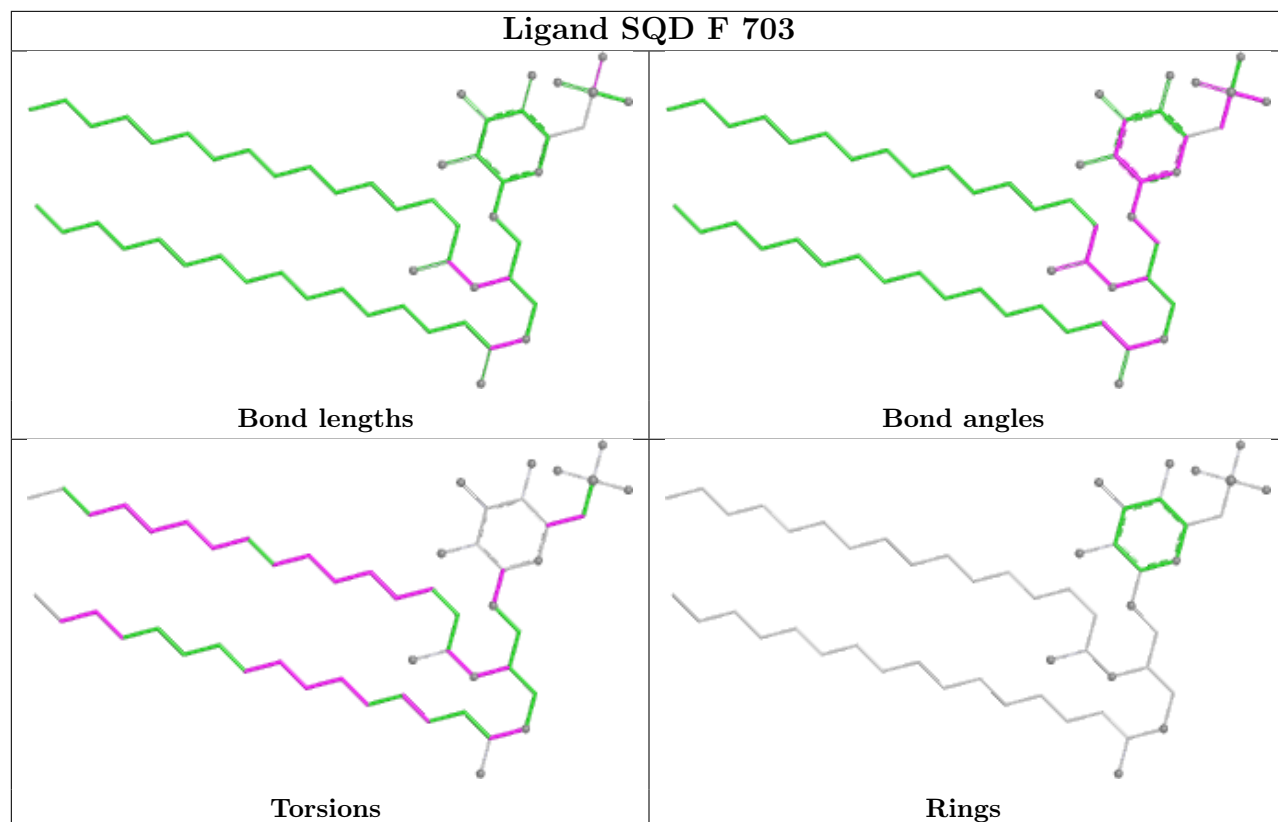
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	K	501	SF4	1	0
21	L	402	SQD	17	0
24	I	201	SF4	1	0
20	D	602	PGT	13	0
19	A	501	DGD	66	0
20	C	201	PGT	12	0
21	F	701	SQD	30	0
21	D	601	SQD	14	0
21	F	703	SQD	26	0
22	F	702	BCR	10	0
23	F	704	CLA	18	0
21	K	502	SQD	46	0
19	L	401	DGD	57	0

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.

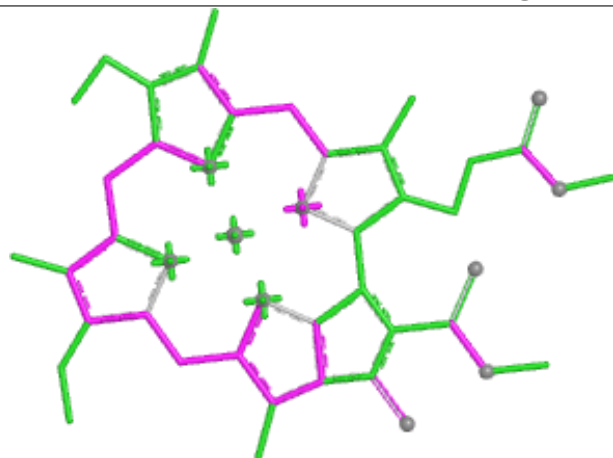




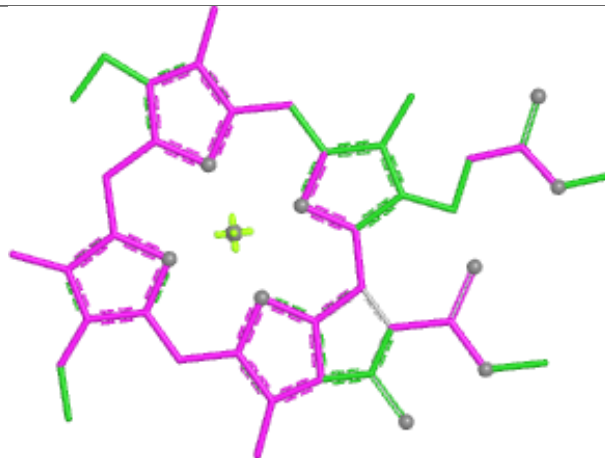




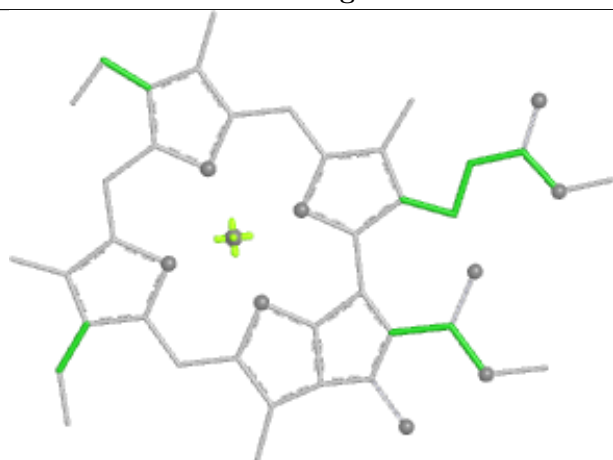
Ligand CLA F 704



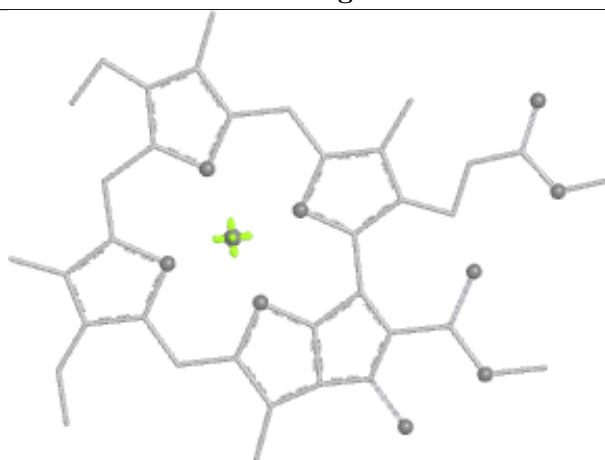
Bond lengths



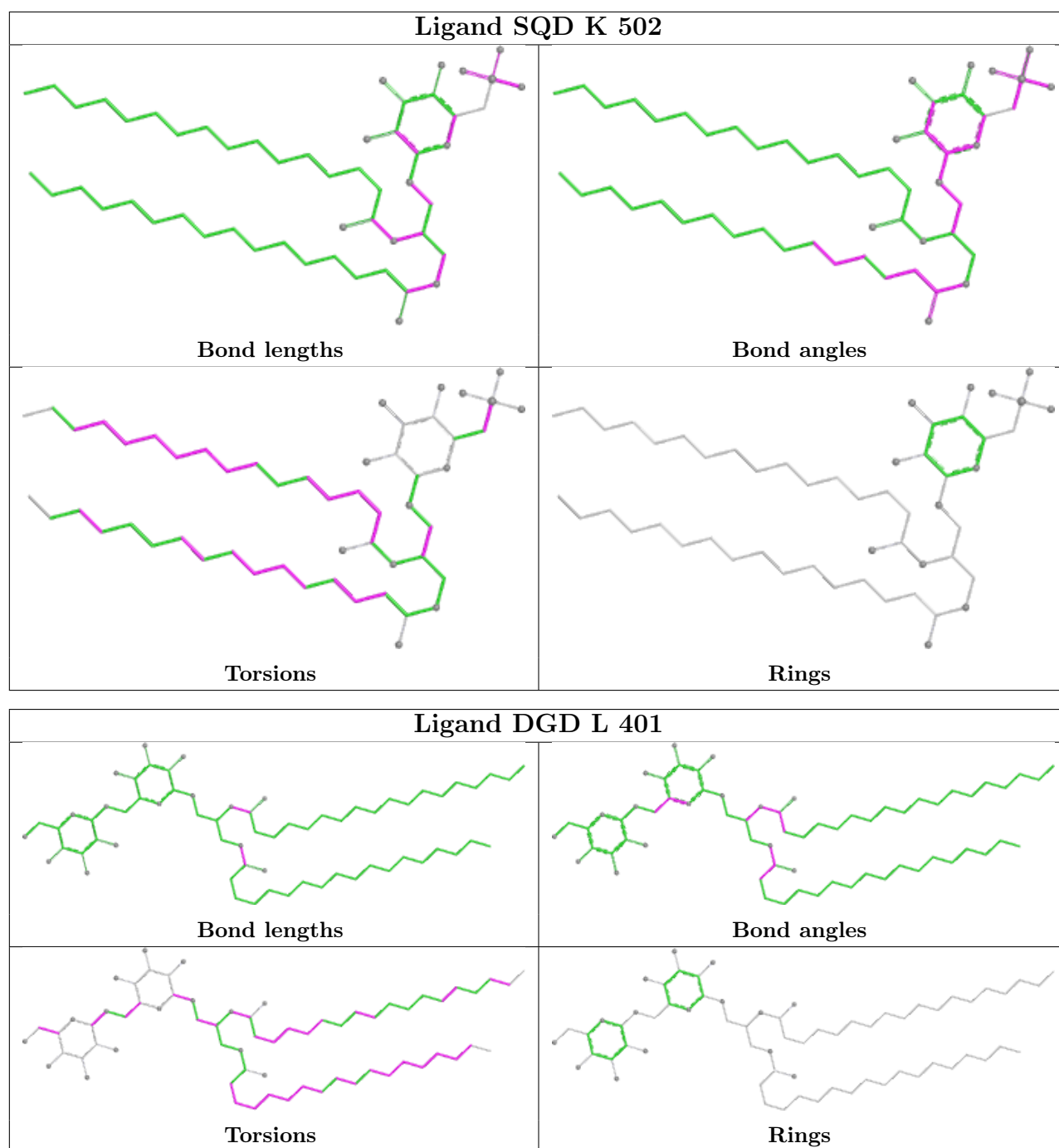
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

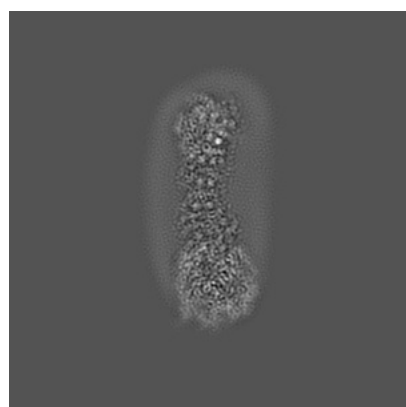
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10513. These allow visual inspection of the internal detail of the map and identification of artifacts.

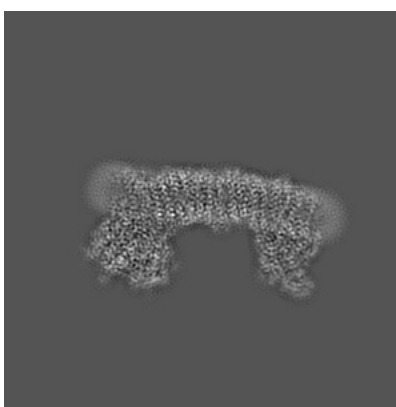
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

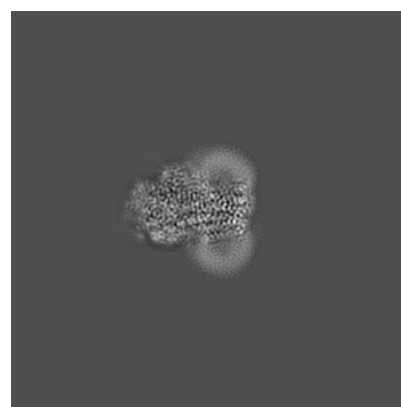
6.1.1 Primary map



X



Y

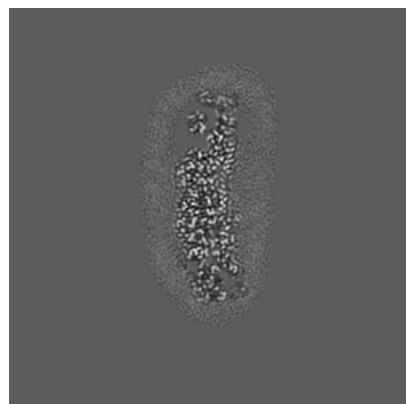


Z

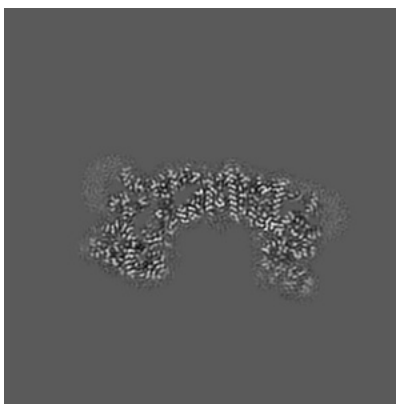
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 140



Y Index: 140

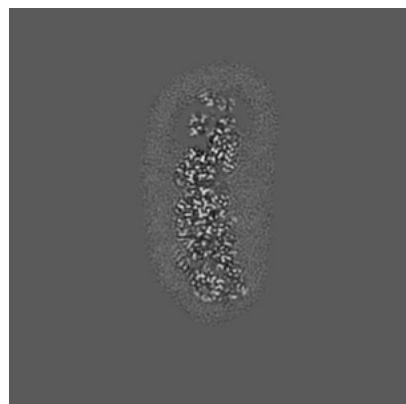


Z Index: 140

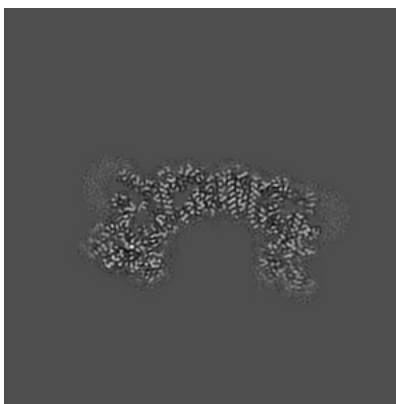
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

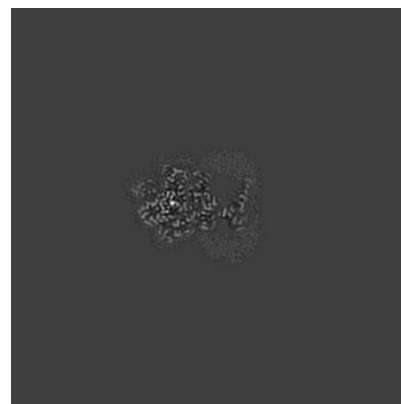
6.3.1 Primary map



X Index: 138



Y Index: 142

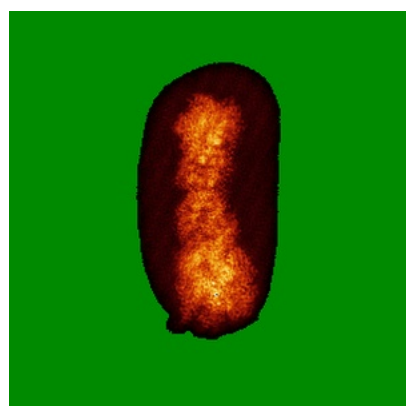


Z Index: 89

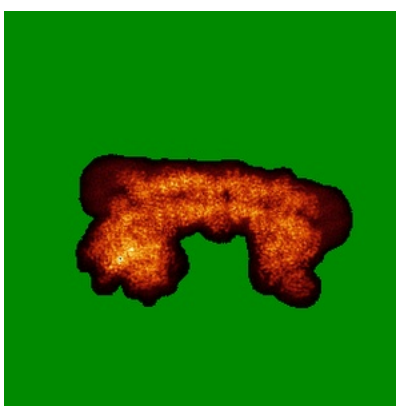
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

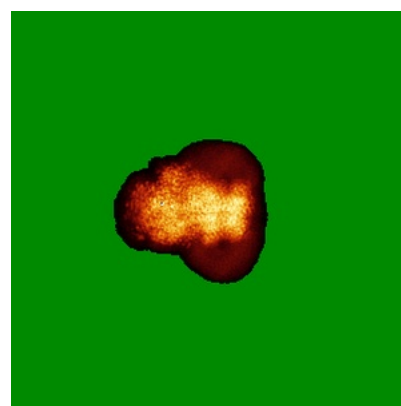
6.4.1 Primary map



X



Y

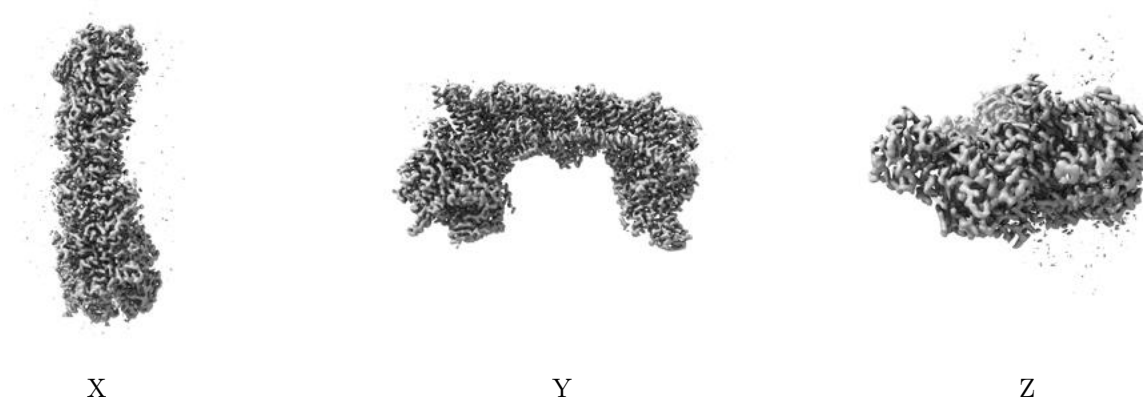


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

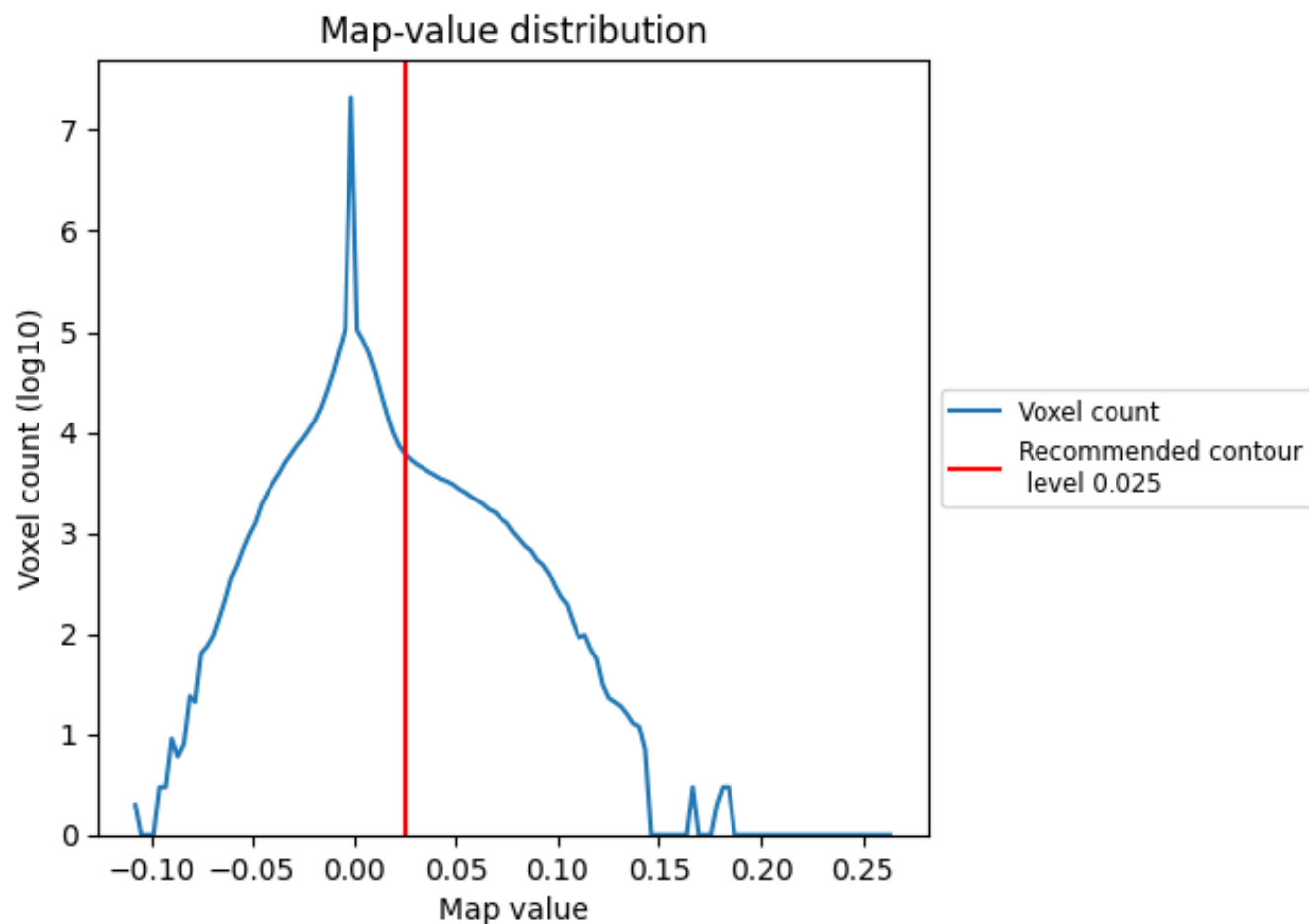
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

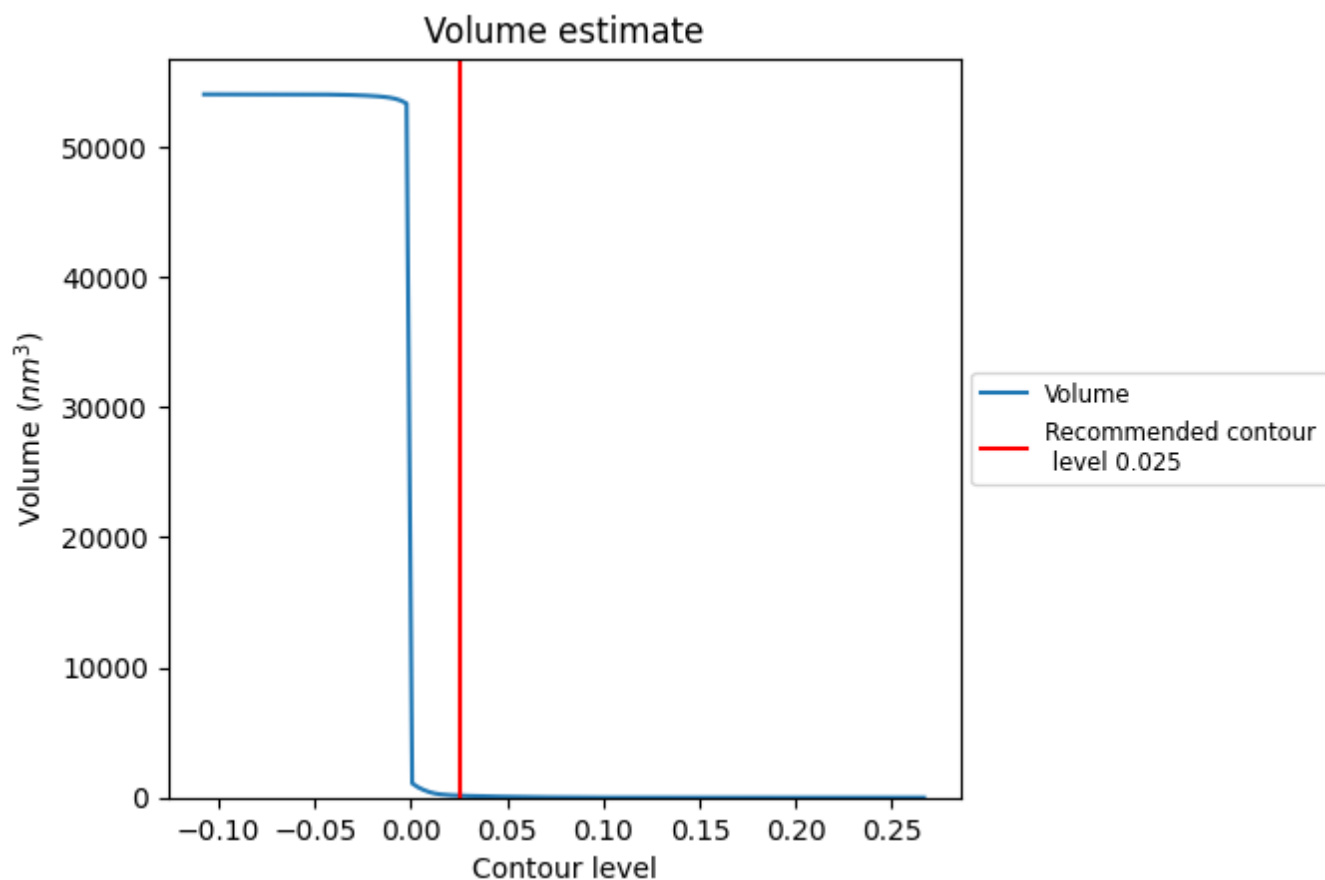
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

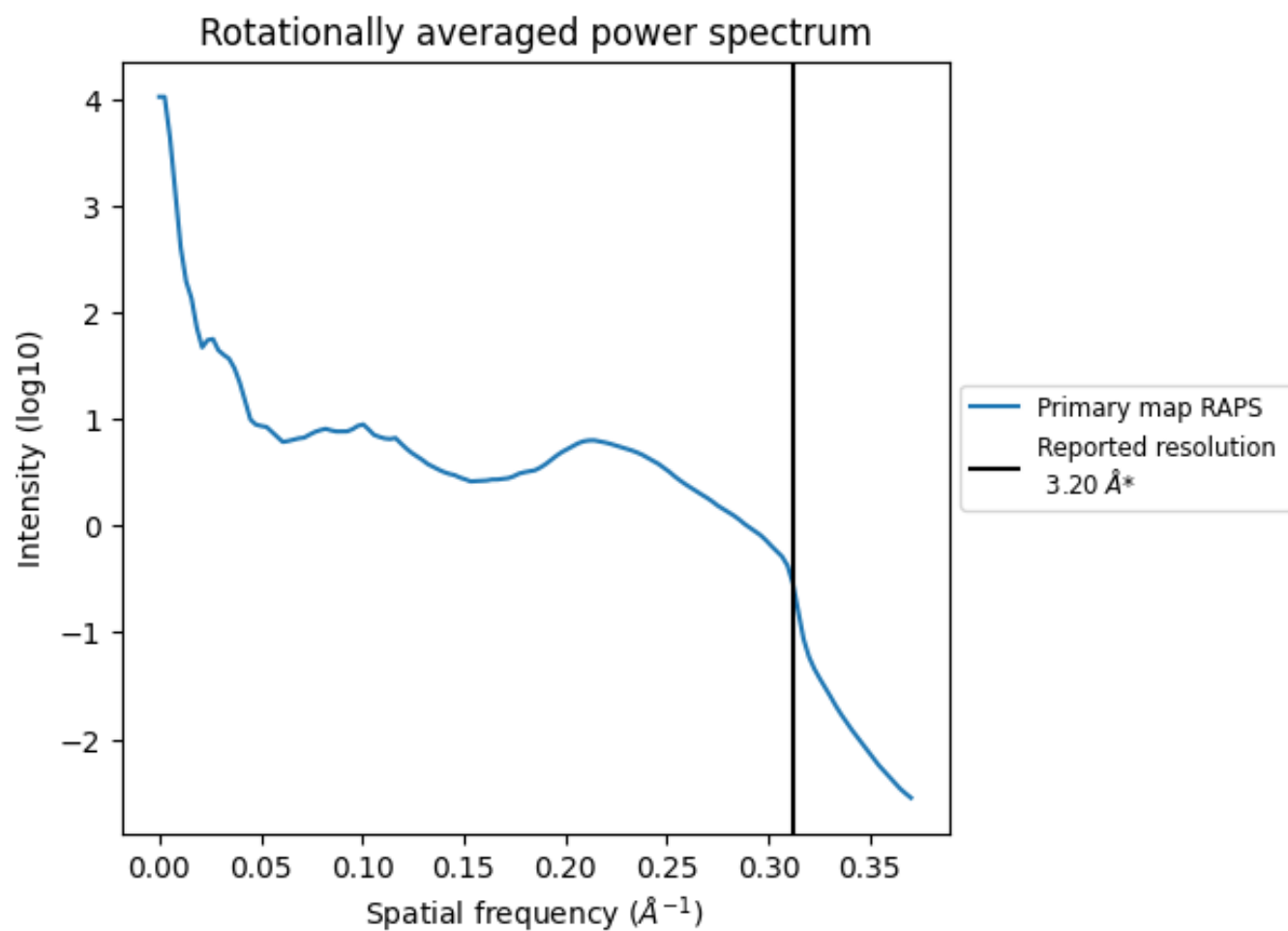
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm^3 ; this corresponds to an approximate mass of 138 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

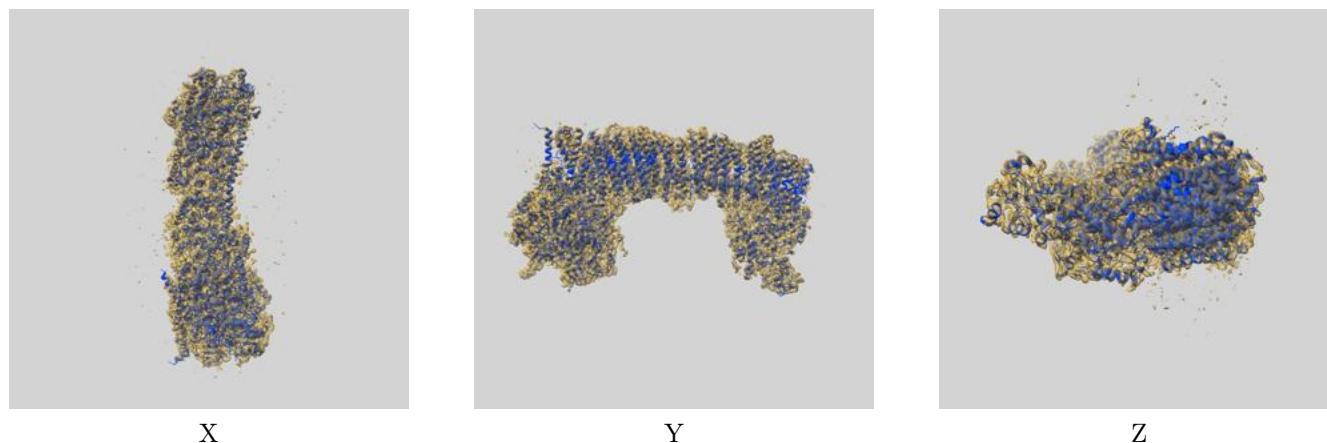
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

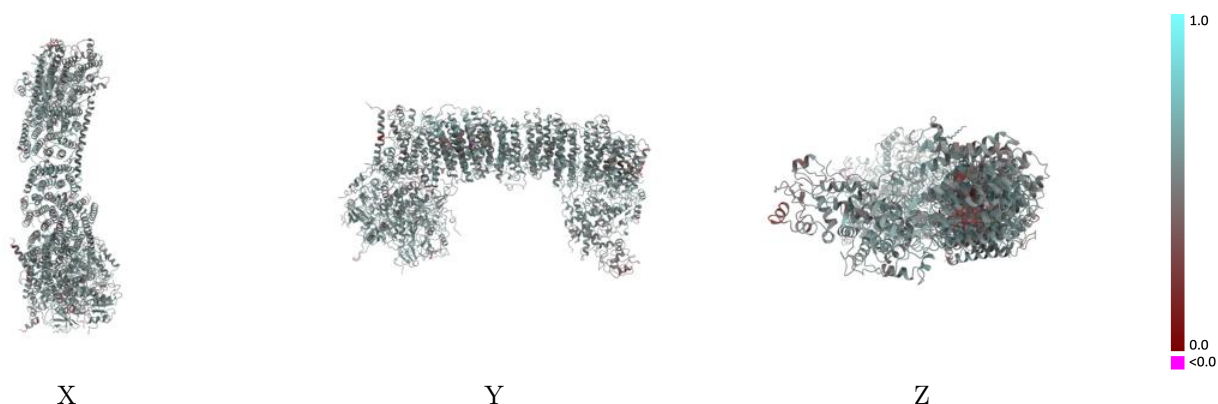
This section contains information regarding the fit between EMDB map EMD-10513 and PDB model 6TJV. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



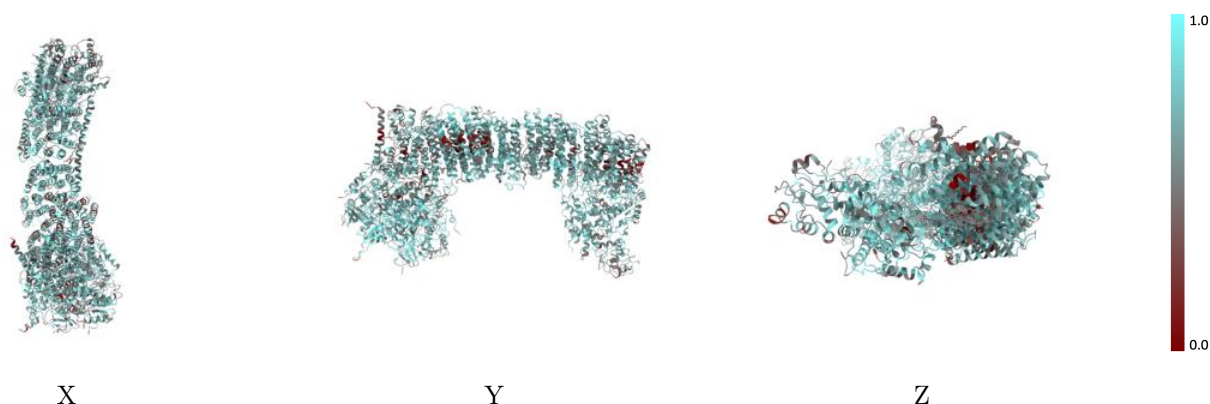
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



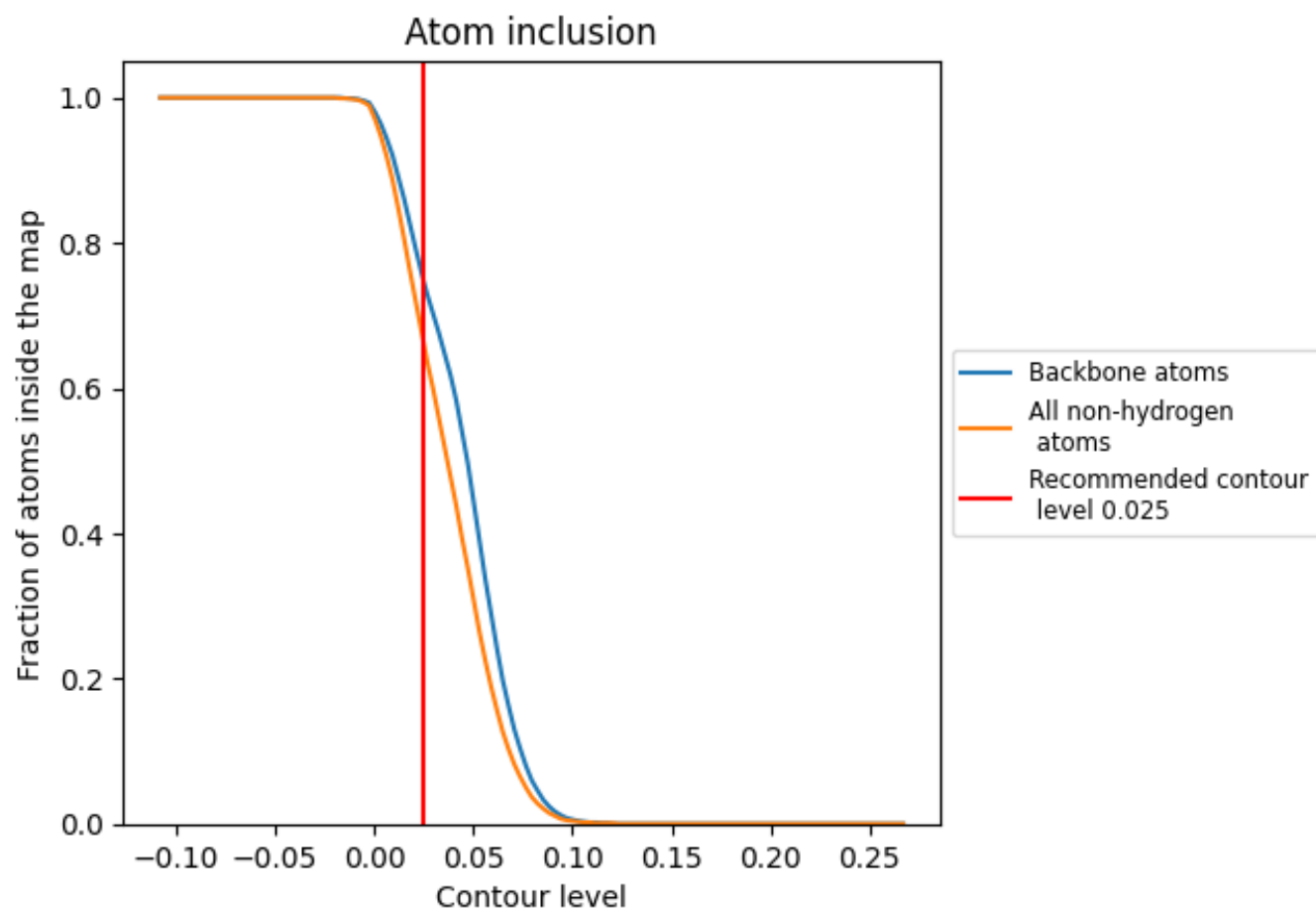
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6630	0.5290
A	0.6310	0.5260
B	0.6850	0.5340
C	0.6220	0.5210
D	0.6890	0.5430
E	0.6580	0.5340
F	0.6200	0.5220
G	0.6380	0.5280
H	0.6660	0.5310
I	0.6930	0.5310
J	0.6850	0.5240
K	0.6880	0.5460
L	0.5320	0.5080
M	0.7180	0.5320
N	0.6890	0.5360
O	0.6770	0.5070
P	0.7200	0.5390
Q	0.5670	0.4690
S	0.6490	0.5480

1.0

0.0

<0.0