



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:06 AM UTC

PDB ID : 9CZH / pdb_00009czh
EMDB ID : EMD-46416
Title : Ca²⁺ bound intermediate state of hSlo1 + beta2N-beta4 channel in detergent.
Authors : Agarwal, S.; Nimigean, C.
Deposited on : 2024-08-05
Resolution : 2.90 Å (reported)
Based on initial model : 6v35

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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

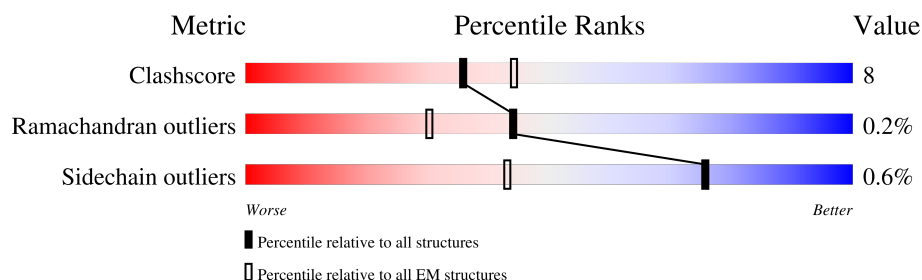
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1056	76% 8% 16%
1	B	1056	76% 8% 16%
1	C	1056	76% 8% 16%
1	D	1056	76% 8% 16%
2	E	239	72% 9% • 18%
2	F	239	72% 9% • 18%
2	G	239	73% 8% • 18%
2	H	239	72% 9% • 18%

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
5	POV	A	1108	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 35014 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 Isoform 5 of Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	891	Total	C	N	O	S	0	0
			7105	4616	1157	1284	48		
1	B	891	Total	C	N	O	S	0	0
			7105	4616	1157	1284	48		
1	C	891	Total	C	N	O	S	0	0
			7105	4616	1157	1284	48		
1	D	891	Total	C	N	O	S	0	0
			7105	4616	1157	1284	48		

- Molecule 2 is a protein called Large-conductance Ca²⁺-activated K⁺ channel beta2 subunit, Calcium-activated potassium channel subunit beta-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	197	Total	C	N	O	S	0	0
			1558	997	262	286	13		
2	F	197	Total	C	N	O	S	0	0
			1558	997	262	286	13		
2	G	197	Total	C	N	O	S	0	0
			1558	997	262	286	13		
2	H	197	Total	C	N	O	S	0	0
			1558	997	262	286	13		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	
3	B	2	Total	Ca	0
			2	2	
3	C	2	Total	Ca	0
			2	2	

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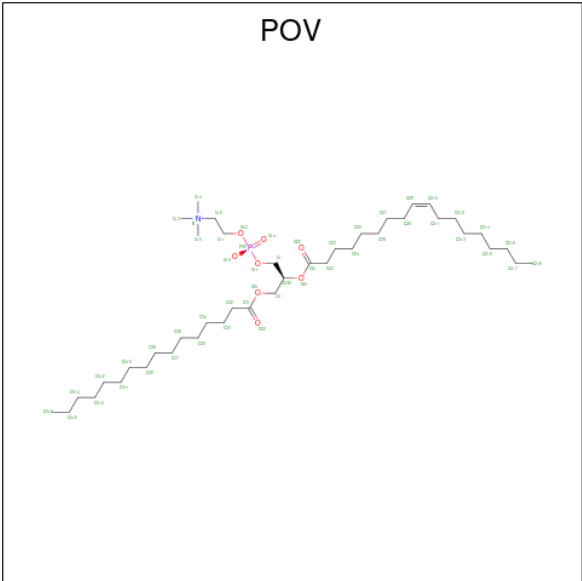
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Mol	Chain	Residues	Atoms		AltConf
3	D	2	Total	Ca	0
			2	2	

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	4	Total	K	0
			4	4	

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
5	A	1	Total	C	O			0
			42	37	5			
5	A	1	Total	C	O	P		0
			15	8	6	1		
5	B	1	Total	C	O	P		0
			33	24	8	1		
5	B	1	Total	C	O	P		0
			46	37	8	1		
5	C	1	Total	C	N	O	P	0
			38	28	1	8	1	

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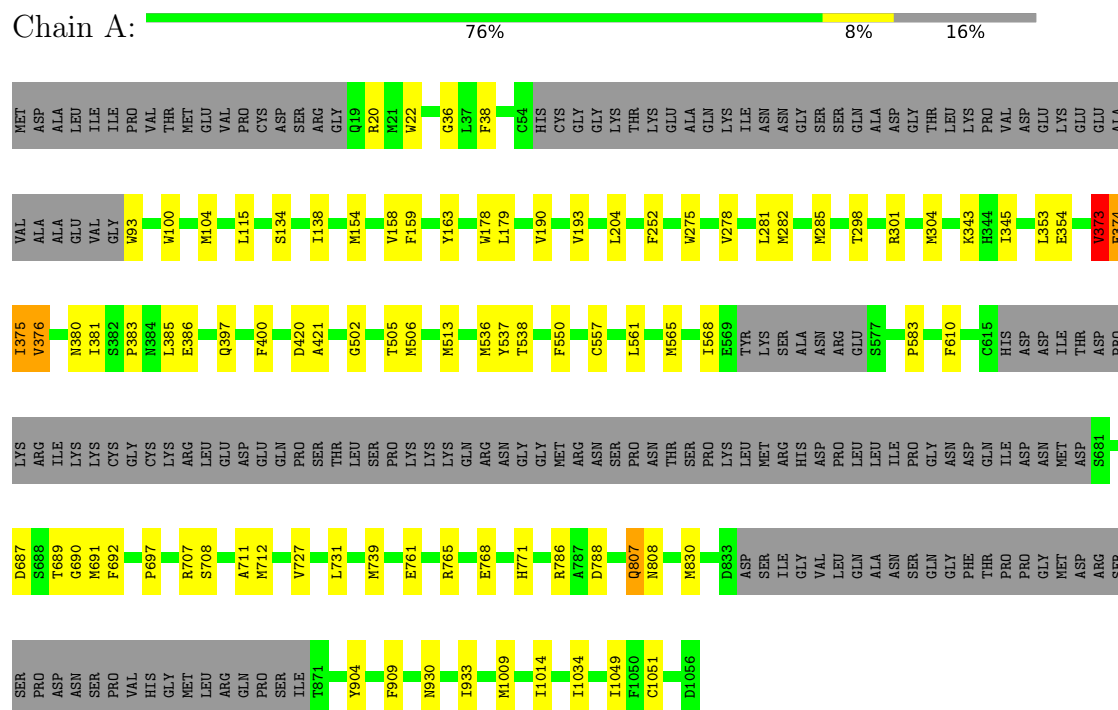
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	O	P	0
			46	37	8	1	
5	D	1	Total	C	O	P	0
			15	8	6	1	
5	D	1	Total	C	O	P	0
			33	24	8	1	
5	D	1	Total	C	O	P	0
			46	37	8	1	

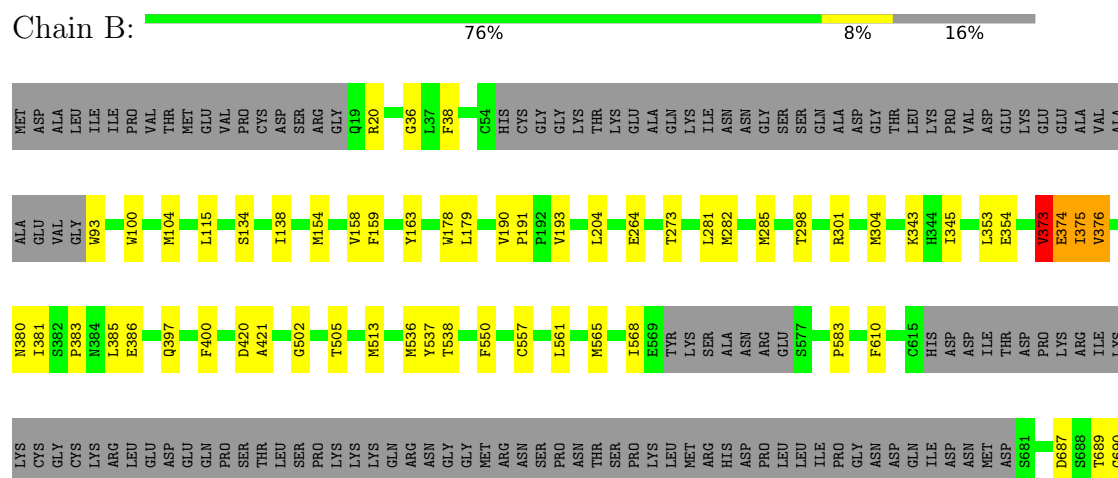
3 Residue-property plots

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

- Molecule 1: Isoform 5 of Calcium-activated potassium channel subunit alpha-1



- Molecule 1: Isoform 5 of Calcium-activated potassium channel subunit alpha-1





ASN	ASN	G690	LYS	V376	GLU	MET
SER	SER	M691	LYS	N380	VAL	ASP
PRO	PRO	F692	CYS	I381	GLY	ALA
HIS	HIS	F697	CYS	S382	W93	ILE
GLY	GLY		LYS	P383	W100	ILE
MET	MET	R707	ARG	N384	M104	PRO
VAL	VAL	S708	LEU	L385		VAL
ARG	ARG	A711	GLU	E386	L115	THR
GLN	GLN	M712	ASP	Q397		MET
PRO	PRO		GLU		S134	GLU
SER	SER	V727	GLN	F400		VAL
ILE	ILE		PRO		I138	PRO
T871	T871	L731	SER	D420		CYS
Y904	Y904	M739	THR		M154	SER
F309	F309	E761	SER	G502		ARG
N930	N930	R765	PRO	T505	V168	ARG
I933	I933		LYS	M513	F169	GLY
M1009	M1009	E768	LYS		Y163	Q19
I1014	I1014	H771	LYS	M536	W178	W22
		R786	GLN	Y537	L179	G36
I1034	I1034	A787	ARG	T538		
I1049	I1049		ASN	C557	V190	C544
F1050	F1050	Q807	GLY	F550	P191	HIS
C1051	C1051	N808	MET		P192	CYS
		M830	ARG		V193	GLY
D1056	D1056		ASN	L561	L204	LYS
			THR	M565	F266	THR
			SER			GLU
			PRO	1568	T273	ALA
		P833	LYS	E569	Y274	GLN
		ASP	LEU	TTR	W275	LYS
		ILE	MET	LYS		ILE
		VAL	ARG	SER	Y279	ASN
		VAL	HIS	ALA	L280	ASN
		GLN	ASP	ASN	L281	GLY
		LEU	PRO	ARG	W282	SER
		GLN	LEU	GLU		GLN
		ALA	LEU	S577	M285	ALA
		ASN	ILE		R301	ASP
		SER	PRO	P583	L302	GLY
		GLN	GLY		F303	THR
		PHE	ASN	F610	M304	LEU
		THR	ASP			LYS
		PRO	GLN	C615		PRO
		PRO	ILE		K343	VAL
		PRO	ASN	ASP	H344	ASP
		GLY	ASN	ASP	I345	GLU
		MET	MET	ILE		LYS
		ASP	THR		L353	GLU
		ARG	ASP		E354	ALA
		SER	S681	PRO		VAL
		SER	D687	LYS	V373	VAL
		PRO	E688	ARG	E374	ALA
		ASN	T589	ILE	T276	ALA

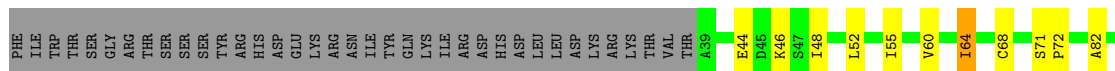
- Molecule 1: Isoform 5 of Calcium-activated potassium channel subunit alpha-1

M691	M692	P697	R707	S708	A711	M712	V727	L731	M739	E761	R765	E768	H771	R786	D788	Q807	M808	M830	D843	ASP	SER	ILE	GLY	VAL	LEU	GLN	ALA	LEU	ILE	ASN	SER	GLY	PHE	THR	PRO	PRO	GLY	MET	ASP	ARG	SER	PRO	ASN											
LYS	GLY	CYS	ARG	LEU	GLU	ASP	GLN	SER	THR	LYS	LYS	GLN	ASN	GLY	MET	ASN	PRO	ASN	THR	SER	LYS	LEU	MET	ARG	PRO	LEU	ALA	LEU	ILE	ASN	SER	GLY	ASP	THR	GLN	ILE	ASP	ASN	GLY	THR	PRO	PRO	GLY	MET	ASP	ARG	SER	PRO	ASN					
N380	L381	S382	P383	N384	L385	E386		Q397	F400	D420	A421	G502	T505	M513	M536	Y537	T538	F550	I568	E569	TYR	LYS	SER	ALA	ASN	ARG	GLU	S577	P583	F610	C615	HTS	ASP	ASP	ILE	ASN	THR	ASP	ASP	THR	PRO	ARG	LYS	ILE	S585									
ALA	GLU	VAL	GLY	W93		W100		M104	L115	S134		I138	M154	V158	Y163	L178	L179		V190	P191	P192	V193	L204	T273	E276	L281	M282	M285	R301	M304	V305	F306	K343	H344	I345	L353	E364	V373	E374	I375	V376													
MET	ASP	ALA	LEU	ILE	PRO	VAL	THR	MET	GLU	VAL	PRO	ASP	ARG	GLY	Q19	R20	G36	L37	F38	C54	HTS	CYS	GLY	GLY	LYS	THR	LYS	GLU	ALA	GLN	LYS	ILE	ASN	ASN	GLY	SER	SER	GLM	ALA	ASP	GLY	THR	LEU	LYS	PRO	PRO	VAL	ASP	GLU	LYS	GLU	ALA	VAL	ALA



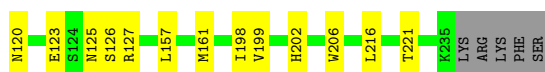
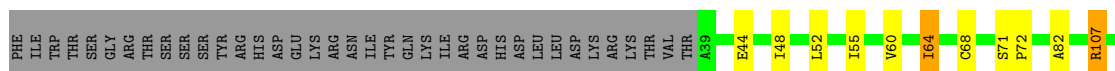
- Molecule 2: Large-conductance Ca^{2+} -activated K^{+} channel beta2 subunit, Calcium-activated potassium channel subunit beta-4

Chain E: 72% 9% 18%



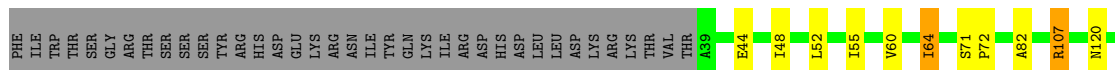
- Molecule 2: Large-conductance Ca^{2+} -activated K^{+} channel beta2 subunit, Calcium-activated potassium channel subunit beta-4

Chain F: 72% 9% 18%



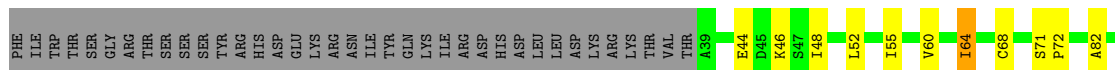
- Molecule 2: Large-conductance Ca^{2+} -activated K^{+} channel beta2 subunit, Calcium-activated potassium channel subunit beta-4

Chain G: 73% 8% 18%



- Molecule 2: Large-conductance Ca^{2+} -activated K^{+} channel beta2 subunit, Calcium-activated potassium channel subunit beta-4

Chain H: 72% 9% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	46625	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, POV, CA

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	0.28	0/7270	0.56	1/9869 (0.0%)
1	B	0.28	0/7270	0.56	1/9869 (0.0%)
1	C	0.28	0/7270	0.56	1/9869 (0.0%)
1	D	0.28	0/7270	0.56	1/9869 (0.0%)
2	E	0.36	0/1594	0.61	0/2168
2	F	0.36	0/1594	0.61	0/2168
2	G	0.36	0/1594	0.61	0/2168
2	H	0.36	0/1594	0.61	0/2168
All	All	0.30	0/35456	0.57	4/48148 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	VAL	N-CA-C	9.59	122.52	107.28
1	A	376	VAL	N-CA-C	9.58	122.51	107.28
1	C	376	VAL	N-CA-C	9.57	122.50	107.28
1	D	376	VAL	N-CA-C	9.56	122.48	107.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7105	0	7099	109	0
1	B	7105	0	7099	94	0
1	C	7105	0	7099	92	0
1	D	7105	0	7099	93	0
2	E	1558	0	1535	37	0
2	F	1558	0	1535	35	0
2	G	1558	0	1535	31	0
2	H	1558	0	1535	35	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	4	0	0	0	0
5	A	93	0	125	38	0
5	B	79	0	105	13	0
5	C	84	0	113	22	0
5	D	94	0	116	12	0
All	All	35014	0	34995	544	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 8.

All (544) 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:22:TRP:HZ2	5:A:1108:POV:H27	1.09	1.14
1:A:22:TRP:HE1	5:A:1108:POV:H24A	1.01	1.08
2:G:120:ASN:HA	2:G:127:ARG:HH12	1.22	1.03
2:F:120:ASN:HA	2:F:127:ARG:HH12	1.22	1.02
1:B:345:ILE:HB	1:B:374:GLU:HA	1.42	1.01
2:H:120:ASN:HA	2:H:127:ARG:HH12	1.21	1.01
2:E:120:ASN:HA	2:E:127:ARG:HH12	1.22	1.00
1:A:345:ILE:HB	1:A:374:GLU:HA	1.43	1.00
1:C:345:ILE:HB	1:C:374:GLU:HA	1.42	0.99
1:D:345:ILE:HB	1:D:374:GLU:HA	1.43	0.97
2:F:107:ARG:H	2:F:107:ARG:HD2	1.31	0.96
1:A:22:TRP:CZ2	5:A:1108:POV:H27	1.99	0.96
2:E:107:ARG:H	2:E:107:ARG:HD2	1.31	0.95
2:G:107:ARG:H	2:G:107:ARG:HD2	1.31	0.93
2:H:107:ARG:H	2:H:107:ARG:HD2	1.31	0.93
1:D:285:MET:HG3	5:D:1101:POV:H25	1.51	0.93
1:A:22:TRP:NE1	5:A:1108:POV:H24A	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:52:LEU:HA	2:G:55:ILE:HD12	1.52	0.92
1:D:20:ARG:NH1	5:D:1105:POV:H3A	1.86	0.91
1:A:22:TRP:HZ2	5:A:1108:POV:C27	1.84	0.91
2:E:52:LEU:HA	2:E:55:ILE:HD12	1.52	0.91
2:F:107:ARG:HD2	2:F:107:ARG:N	1.85	0.90
2:F:52:LEU:HA	2:F:55:ILE:HD12	1.52	0.90
1:A:380:ASN:OD1	1:A:381:ILE:HG13	1.72	0.89
2:H:52:LEU:HA	2:H:55:ILE:HD12	1.52	0.89
1:D:380:ASN:OD1	1:D:381:ILE:HG13	1.72	0.89
1:C:380:ASN:OD1	1:C:381:ILE:HG13	1.72	0.88
1:B:380:ASN:OD1	1:B:381:ILE:HG13	1.72	0.88
2:G:107:ARG:HD2	2:G:107:ARG:N	1.85	0.86
2:E:107:ARG:HD2	2:E:107:ARG:N	1.85	0.85
1:C:557:CYS:HA	1:C:561:LEU:HD21	1.58	0.84
1:A:557:CYS:HA	1:A:561:LEU:HD21	1.58	0.84
1:D:557:CYS:HA	1:D:561:LEU:HD21	1.59	0.84
1:A:22:TRP:HH2	5:A:1108:POV:H29	1.43	0.83
2:H:107:ARG:HD2	2:H:107:ARG:N	1.85	0.83
1:B:557:CYS:HA	1:B:561:LEU:HD21	1.58	0.83
1:D:557:CYS:HA	1:D:561:LEU:CD2	2.09	0.83
2:G:120:ASN:HA	2:G:127:ARG:NH1	1.95	0.82
1:C:557:CYS:HA	1:C:561:LEU:CD2	2.09	0.82
2:H:120:ASN:HA	2:H:127:ARG:NH1	1.95	0.82
2:E:120:ASN:HA	2:E:127:ARG:NH1	1.95	0.82
1:A:22:TRP:HE1	5:A:1108:POV:C24	1.91	0.81
1:A:557:CYS:HA	1:A:561:LEU:CD2	2.09	0.81
2:F:120:ASN:HA	2:F:127:ARG:NH1	1.95	0.81
1:B:557:CYS:HA	1:B:561:LEU:CD2	2.09	0.81
1:D:115:LEU:HB3	1:D:163:TYR:HE1	1.47	0.80
5:A:1107:POV:H35	1:D:301:ARG:HB3	1.65	0.79
1:A:115:LEU:HB3	1:A:163:TYR:HE1	1.46	0.79
1:C:115:LEU:HB3	1:C:163:TYR:HE1	1.47	0.79
1:B:115:LEU:HB3	1:B:163:TYR:HE1	1.46	0.77
1:C:707:ARG:HD3	1:C:788:ASP:OD1	1.85	0.77
1:A:707:ARG:HD3	1:A:788:ASP:OD1	1.85	0.77
1:B:707:ARG:HD3	1:B:788:ASP:OD1	1.85	0.77
5:C:1103:POV:H22A	2:F:68:CYS:HB3	1.67	0.77
2:H:48:ILE:CD1	2:H:221:THR:HG21	2.15	0.76
2:F:48:ILE:CD1	2:F:221:THR:HG21	2.15	0.76
2:E:48:ILE:CD1	2:E:221:THR:HG21	2.15	0.76
1:B:282:MET:HA	1:B:282:MET:HE2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:MET:HE2	1:A:282:MET:HA	1.67	0.76
1:C:282:MET:HE2	1:C:282:MET:HA	1.67	0.76
1:D:282:MET:HA	1:D:282:MET:HE2	1.67	0.76
1:A:22:TRP:CH2	5:A:1108:POV:H29	2.19	0.76
2:G:48:ILE:CD1	2:G:221:THR:HG21	2.15	0.76
1:B:115:LEU:HB3	1:B:163:TYR:CE1	2.21	0.76
1:D:115:LEU:HB3	1:D:163:TYR:CE1	2.21	0.75
1:D:707:ARG:HD3	1:D:788:ASP:OD1	1.85	0.75
1:C:115:LEU:HB3	1:C:163:TYR:CE1	2.21	0.75
1:A:115:LEU:HB3	1:A:163:TYR:CE1	2.21	0.75
2:E:157:LEU:O	2:E:161:MET:HE2	1.87	0.74
2:F:157:LEU:O	2:F:161:MET:HE2	1.87	0.74
2:G:157:LEU:O	2:G:161:MET:HE2	1.87	0.74
2:H:157:LEU:O	2:H:161:MET:HE2	1.87	0.73
1:A:301:ARG:HB3	5:B:1103:POV:H33	1.69	0.73
1:B:727:VAL:HG12	1:B:761:GLU:HB3	1.71	0.73
1:A:727:VAL:HG12	1:A:761:GLU:HB3	1.71	0.72
1:D:727:VAL:HG12	1:D:761:GLU:HB3	1.71	0.72
1:A:692:PHE:CE1	1:A:739:MET:HG2	2.25	0.72
1:B:692:PHE:CE1	1:B:739:MET:HG2	2.25	0.72
1:C:692:PHE:CE1	1:C:739:MET:HG2	2.24	0.72
1:D:692:PHE:CE1	1:D:739:MET:HG2	2.24	0.72
1:A:38:PHE:CZ	2:E:216:LEU:HD22	2.25	0.71
1:C:727:VAL:HG12	1:C:761:GLU:HB3	1.71	0.71
1:C:711:ALA:HB3	1:C:712:MET:HE2	1.73	0.70
1:A:711:ALA:HB3	1:A:712:MET:HE2	1.73	0.70
1:D:20:ARG:HH12	5:D:1105:POV:H3A	1.56	0.70
1:B:273:THR:HG21	5:B:1103:POV:C1	2.21	0.70
1:B:354:GLU:OE1	1:B:354:GLU:N	2.20	0.69
1:D:711:ALA:HB3	1:D:712:MET:HE2	1.73	0.69
5:A:1107:POV:H13A	5:A:1107:POV:P	2.32	0.69
5:B:1104:POV:H22	2:F:199:VAL:HG22	1.73	0.69
1:B:20:ARG:HB2	5:B:1104:POV:O32	1.92	0.69
1:D:354:GLU:OE1	1:D:354:GLU:N	2.20	0.69
1:B:711:ALA:HB3	1:B:712:MET:HE2	1.73	0.68
1:B:301:ARG:HB3	5:C:1103:POV:H33	1.74	0.68
1:C:273:THR:HG21	5:C:1103:POV:H1	1.76	0.67
2:E:216:LEU:C	2:E:216:LEU:HD23	2.21	0.66
2:F:216:LEU:HD23	2:F:216:LEU:C	2.21	0.66
1:A:768:GLU:HA	1:A:771:HIS:ND1	2.11	0.66
1:C:768:GLU:HA	1:C:771:HIS:ND1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:216:LEU:C	2:G:216:LEU:HD23	2.21	0.65
1:B:768:GLU:HA	1:B:771:HIS:ND1	2.11	0.65
1:A:38:PHE:CZ	2:E:216:LEU:CD2	2.78	0.65
5:A:1107:POV:H22A	2:H:68:CYS:HB3	1.77	0.65
2:H:216:LEU:HD23	2:H:216:LEU:C	2.21	0.65
1:D:768:GLU:HA	1:D:771:HIS:ND1	2.11	0.64
1:B:273:THR:HG21	5:B:1103:POV:H1A	1.80	0.64
1:B:375:ILE:HG12	1:B:397:GLN:C	2.23	0.64
1:A:1014:ILE:CD1	1:A:1034:ILE:HB	2.28	0.64
1:C:1014:ILE:CD1	1:C:1034:ILE:HB	2.28	0.64
1:D:100:TRP:O	1:D:104:MET:HG2	1.98	0.64
1:C:375:ILE:HG12	1:C:397:GLN:C	2.23	0.64
1:A:100:TRP:O	1:A:104:MET:HG2	1.98	0.64
1:A:375:ILE:HG12	1:A:397:GLN:C	2.23	0.64
2:F:157:LEU:C	2:F:161:MET:HE2	2.23	0.63
1:B:100:TRP:O	1:B:104:MET:HG2	1.98	0.63
1:C:354:GLU:OE1	1:C:354:GLU:N	2.20	0.63
1:C:100:TRP:O	1:C:104:MET:HG2	1.98	0.63
1:D:375:ILE:HG12	1:D:397:GLN:C	2.23	0.63
1:D:1014:ILE:CD1	1:D:1034:ILE:HB	2.28	0.63
2:H:157:LEU:C	2:H:161:MET:HE2	2.23	0.63
1:B:1014:ILE:CD1	1:B:1034:ILE:HB	2.28	0.63
2:E:157:LEU:C	2:E:161:MET:HE2	2.23	0.62
2:F:48:ILE:HD11	2:F:221:THR:HG21	1.81	0.62
1:C:375:ILE:HG12	1:C:397:GLN:CA	2.30	0.62
2:G:157:LEU:C	2:G:161:MET:HE2	2.23	0.62
1:D:375:ILE:HG12	1:D:397:GLN:CA	2.30	0.62
1:A:375:ILE:HG12	1:A:397:GLN:CA	2.30	0.62
1:B:375:ILE:HG12	1:B:397:GLN:CA	2.30	0.62
2:G:48:ILE:HD11	2:G:221:THR:HG21	1.81	0.62
1:A:354:GLU:OE1	1:A:354:GLU:N	2.20	0.62
5:C:1103:POV:H13A	5:C:1103:POV:O11	1.99	0.62
2:E:202:HIS:CE1	2:E:206:TRP:HE1	2.18	0.62
1:D:190:VAL:O	1:D:193:VAL:HG12	2.00	0.62
2:E:48:ILE:HD11	2:E:221:THR:HG21	1.81	0.62
1:B:190:VAL:O	1:B:193:VAL:HG12	2.00	0.61
1:A:190:VAL:O	1:A:193:VAL:HG12	2.00	0.61
1:C:190:VAL:O	1:C:193:VAL:HG12	2.00	0.61
1:C:138:ILE:HG13	1:C:138:ILE:O	2.01	0.61
1:D:375:ILE:HG12	1:D:397:GLN:HA	1.83	0.61
1:D:343:LYS:HB3	1:D:373:VAL:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:ILE:HD11	2:H:221:THR:HG21	1.81	0.61
1:C:375:ILE:HG12	1:C:397:GLN:HA	1.83	0.61
2:F:202:HIS:CE1	2:F:206:TRP:HE1	2.18	0.61
1:A:1014:ILE:HD12	1:A:1034:ILE:HB	1.82	0.61
1:C:343:LYS:HB3	1:C:373:VAL:HG12	1.83	0.61
1:B:138:ILE:HG13	1:B:138:ILE:O	2.01	0.60
1:D:1014:ILE:HD12	1:D:1034:ILE:HB	1.82	0.60
1:A:343:LYS:HB3	1:A:373:VAL:HG12	1.83	0.60
1:A:708:SER:O	1:A:712:MET:HG2	2.01	0.60
1:B:375:ILE:HG12	1:B:397:GLN:HA	1.83	0.60
2:G:202:HIS:CE1	2:G:206:TRP:HE1	2.18	0.60
2:H:202:HIS:CE1	2:H:206:TRP:HE1	2.18	0.60
1:B:1014:ILE:HD12	1:B:1034:ILE:HB	1.82	0.60
1:C:708:SER:O	1:C:712:MET:HG2	2.01	0.60
1:C:786:ARG:HD3	1:C:830:MET:HE2	1.83	0.60
1:C:1014:ILE:HD12	1:C:1034:ILE:HB	1.82	0.60
2:G:52:LEU:CA	2:G:55:ILE:HD12	2.29	0.60
1:B:786:ARG:HD3	1:B:830:MET:HE2	1.84	0.60
1:A:375:ILE:HG12	1:A:397:GLN:HA	1.83	0.60
1:B:708:SER:O	1:B:712:MET:HG2	2.01	0.60
1:A:278:VAL:HG11	5:A:1107:POV:H31A	1.82	0.60
1:A:786:ARG:HD3	1:A:830:MET:HE2	1.84	0.60
1:D:708:SER:O	1:D:712:MET:HG2	2.01	0.60
2:E:52:LEU:CA	2:E:55:ILE:HD12	2.29	0.60
1:A:138:ILE:HG13	1:A:138:ILE:O	2.01	0.60
1:B:343:LYS:HB3	1:B:373:VAL:HG12	1.83	0.60
1:D:138:ILE:HG13	1:D:138:ILE:O	2.01	0.60
2:H:52:LEU:CA	2:H:55:ILE:HD12	2.29	0.60
5:C:1103:POV:O11	5:C:1103:POV:H15B	2.01	0.59
1:D:708:SER:O	1:D:712:MET:HE2	2.03	0.59
5:B:1103:POV:H23A	2:E:68:CYS:HB3	1.83	0.59
5:C:1103:POV:H3	5:C:1103:POV:O13	2.02	0.59
5:A:1108:POV:C3	5:A:1108:POV:H22	2.33	0.59
1:C:154:MET:O	1:C:158:VAL:HG13	2.03	0.59
1:D:786:ARG:HD3	1:D:830:MET:HE2	1.83	0.59
1:C:708:SER:O	1:C:712:MET:HE2	2.03	0.59
1:B:273:THR:HG21	5:B:1103:POV:H1	1.84	0.59
1:A:708:SER:O	1:A:712:MET:HE2	2.03	0.58
1:A:697:PRO:CB	1:A:771:HIS:HD2	2.17	0.58
1:B:708:SER:O	1:B:712:MET:HE2	2.03	0.58
1:D:276:GLU:HG3	5:D:1104:POV:H3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:PRO:CB	1:B:771:HIS:HD2	2.17	0.58
2:F:52:LEU:CA	2:F:55:ILE:HD12	2.29	0.58
1:B:353:LEU:HD22	1:B:386:GLU:HG3	1.86	0.58
1:B:154:MET:O	1:B:158:VAL:HG13	2.03	0.58
1:B:345:ILE:O	1:B:376:VAL:HB	2.04	0.58
1:C:692:PHE:CE1	1:C:739:MET:CG	2.87	0.58
1:C:697:PRO:CB	1:C:771:HIS:HD2	2.17	0.58
1:A:154:MET:O	1:A:158:VAL:HG13	2.03	0.58
1:A:345:ILE:O	1:A:376:VAL:HB	2.04	0.57
1:D:345:ILE:O	1:D:376:VAL:HB	2.04	0.57
1:C:345:ILE:O	1:C:376:VAL:HB	2.04	0.57
5:A:1108:POV:O31	5:A:1108:POV:H34A	2.02	0.57
1:B:692:PHE:CE1	1:B:739:MET:CG	2.87	0.57
1:D:697:PRO:CB	1:D:771:HIS:HD2	2.17	0.57
1:D:154:MET:O	1:D:158:VAL:HG13	2.03	0.57
1:D:692:PHE:CE1	1:D:739:MET:CG	2.87	0.57
1:C:275:TRP:CD2	5:C:1103:POV:H25A	2.39	0.57
1:C:610:PHE:O	1:C:610:PHE:CD1	2.58	0.57
1:D:38:PHE:CZ	2:H:216:LEU:HD22	2.39	0.57
1:D:610:PHE:O	1:D:610:PHE:CD1	2.58	0.57
1:C:557:CYS:HA	1:C:561:LEU:HD23	1.87	0.57
1:A:692:PHE:CE1	1:A:739:MET:CG	2.87	0.57
1:B:610:PHE:O	1:B:610:PHE:CD1	2.58	0.57
1:A:1009:MET:HE1	1:A:1051:CYS:SG	2.45	0.56
1:C:353:LEU:HD22	1:C:386:GLU:HG3	1.86	0.56
1:D:353:LEU:HD22	1:D:386:GLU:HG3	1.86	0.56
5:A:1107:POV:H13A	5:A:1107:POV:O11	2.05	0.56
1:C:807:GLN:OE1	1:C:808:ASN:HB3	2.05	0.56
1:C:1009:MET:HE1	1:C:1051:CYS:SG	2.45	0.56
1:C:273:THR:HG21	5:C:1103:POV:C1	2.35	0.56
1:B:807:GLN:OE1	1:B:808:ASN:HB3	2.05	0.56
1:D:557:CYS:HA	1:D:561:LEU:HD23	1.87	0.56
1:D:807:GLN:OE1	1:D:808:ASN:HB3	2.05	0.56
1:A:610:PHE:CD1	1:A:610:PHE:O	2.58	0.56
1:A:343:LYS:CB	1:A:373:VAL:HG12	2.36	0.56
1:A:353:LEU:HD22	1:A:386:GLU:HG3	1.86	0.56
1:A:278:VAL:HG11	5:A:1107:POV:C310	2.36	0.56
1:A:354:GLU:H	1:A:354:GLU:CD	2.13	0.56
1:C:343:LYS:CB	1:C:373:VAL:HG12	2.36	0.56
1:D:179:LEU:CD1	2:H:46:LYS:HD3	2.35	0.56
1:A:375:ILE:HG22	1:A:375:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LYS:CB	1:B:373:VAL:HG12	2.36	0.56
1:A:807:GLN:OE1	1:A:808:ASN:HB3	2.05	0.55
1:B:1009:MET:HE1	1:B:1051:CYS:SG	2.45	0.55
1:D:1009:MET:HE1	1:D:1051:CYS:SG	2.45	0.55
1:B:557:CYS:HA	1:B:561:LEU:HD23	1.87	0.55
1:D:343:LYS:CB	1:D:373:VAL:HG12	2.36	0.55
1:A:22:TRP:CZ2	5:A:1108:POV:C27	2.76	0.55
1:C:375:ILE:HG22	1:C:375:ILE:O	2.06	0.55
5:C:1103:POV:H15B	5:C:1103:POV:P	2.47	0.55
1:A:22:TRP:CZ2	5:A:1108:POV:C28	2.89	0.54
1:A:557:CYS:HA	1:A:561:LEU:HD23	1.87	0.54
1:D:375:ILE:HG22	1:D:375:ILE:O	2.06	0.54
1:B:375:ILE:HG22	1:B:375:ILE:O	2.06	0.54
1:B:343:LYS:CB	1:B:373:VAL:CG1	2.86	0.54
1:D:354:GLU:H	1:D:354:GLU:CD	2.13	0.54
1:C:697:PRO:CB	1:C:771:HIS:CD2	2.91	0.54
1:A:22:TRP:CH2	5:A:1108:POV:C29	2.89	0.54
1:A:697:PRO:CB	1:A:771:HIS:CD2	2.91	0.54
1:D:343:LYS:CB	1:D:373:VAL:CG1	2.86	0.54
2:H:157:LEU:CA	2:H:161:MET:HE2	2.38	0.54
5:A:1107:POV:O12	5:A:1107:POV:H15B	2.07	0.54
2:E:157:LEU:CA	2:E:161:MET:HE2	2.38	0.54
1:A:343:LYS:CB	1:A:373:VAL:CG1	2.86	0.53
1:B:301:ARG:CB	5:C:1103:POV:H33	2.36	0.53
1:B:697:PRO:CB	1:B:771:HIS:CD2	2.91	0.53
1:D:179:LEU:HD11	2:H:46:LYS:HD3	1.89	0.53
1:D:697:PRO:CB	1:D:771:HIS:CD2	2.91	0.53
5:A:1107:POV:O11	5:A:1107:POV:H15B	2.08	0.53
1:C:343:LYS:CB	1:C:373:VAL:CG1	2.86	0.53
2:F:157:LEU:CA	2:F:161:MET:HE2	2.38	0.53
2:H:126:SER:N	2:H:127:ARG:NH2	2.57	0.53
5:A:1107:POV:H35	1:D:301:ARG:CB	2.37	0.53
2:E:126:SER:N	2:E:127:ARG:NH2	2.57	0.53
2:G:157:LEU:CA	2:G:161:MET:HE2	2.38	0.53
1:B:38:PHE:CZ	2:F:216:LEU:HD22	2.44	0.53
1:A:22:TRP:HZ2	5:A:1108:POV:C28	2.21	0.53
5:D:1104:POV:H28A	2:G:64:ILE:HG12	1.89	0.52
1:A:689:THR:HG22	1:A:691:MET:HG2	1.92	0.52
1:A:281:LEU:O	1:A:285:MET:HG2	2.10	0.52
5:A:1108:POV:H22	5:A:1108:POV:H3A	1.90	0.52
2:E:157:LEU:HA	2:E:161:MET:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:126:SER:N	2:G:127:ARG:NH2	2.57	0.52
1:B:689:THR:HG22	1:B:691:MET:HG2	1.92	0.52
2:H:157:LEU:HA	2:H:161:MET:HE2	1.92	0.52
1:C:343:LYS:HB3	1:C:373:VAL:CG1	2.40	0.52
1:C:689:THR:HG22	1:C:691:MET:HG2	1.92	0.52
1:C:354:GLU:H	1:C:354:GLU:CD	2.13	0.52
1:D:343:LYS:HB3	1:D:373:VAL:CG1	2.40	0.52
2:F:126:SER:N	2:F:127:ARG:NH2	2.57	0.52
1:D:689:THR:HG22	1:D:691:MET:HG2	1.92	0.52
1:B:281:LEU:O	1:B:285:MET:HG2	2.10	0.51
1:B:343:LYS:HB3	1:B:373:VAL:CG1	2.40	0.51
5:C:1103:POV:H12	5:C:1103:POV:O14	2.10	0.51
2:G:82:ALA:HB2	2:G:123:GLU:HG2	1.92	0.51
1:A:301:ARG:CB	5:B:1103:POV:H33	2.40	0.51
5:A:1108:POV:H27A	2:E:202:HIS:ND1	2.26	0.51
2:F:82:ALA:HB2	2:F:123:GLU:HG2	1.92	0.51
2:G:157:LEU:HA	2:G:161:MET:HE2	1.92	0.51
2:E:127:ARG:N	2:E:127:ARG:NE	2.59	0.51
1:C:281:LEU:O	1:C:285:MET:HG2	2.10	0.51
1:D:281:LEU:O	1:D:285:MET:HG2	2.10	0.51
2:F:126:SER:C	2:F:127:ARG:CZ	2.84	0.51
1:C:376:VAL:HG12	1:C:376:VAL:O	2.11	0.51
2:E:126:SER:C	2:E:127:ARG:CZ	2.84	0.51
1:A:343:LYS:HB3	1:A:373:VAL:CG1	2.40	0.51
2:G:126:SER:CA	2:G:127:ARG:NH2	2.74	0.51
2:F:157:LEU:HA	2:F:161:MET:HE2	1.91	0.50
2:H:127:ARG:N	2:H:127:ARG:NE	2.59	0.50
2:G:127:ARG:N	2:G:127:ARG:NE	2.59	0.50
2:E:125:ASN:C	2:E:127:ARG:HH21	2.20	0.50
2:E:126:SER:CA	2:E:127:ARG:NH2	2.74	0.50
1:A:689:THR:HG22	1:A:689:THR:O	2.11	0.50
1:D:38:PHE:CZ	2:H:216:LEU:CD2	2.95	0.50
1:D:375:ILE:CG1	1:D:397:GLN:O	2.60	0.50
2:E:82:ALA:HB2	2:E:123:GLU:HG2	1.92	0.50
2:F:127:ARG:N	2:F:127:ARG:NE	2.59	0.50
2:G:125:ASN:C	2:G:127:ARG:HH21	2.20	0.50
2:G:126:SER:C	2:G:127:ARG:CZ	2.84	0.50
2:H:82:ALA:HB2	2:H:123:GLU:HG2	1.92	0.50
2:H:125:ASN:C	2:H:127:ARG:HH21	2.20	0.50
2:H:126:SER:C	2:H:127:ARG:CZ	2.84	0.50
2:F:126:SER:CA	2:F:127:ARG:NH2	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LYS:HE2	1:B:420:ASP:HB2	1.94	0.50
2:F:125:ASN:C	2:F:127:ARG:HH21	2.20	0.50
1:B:376:VAL:O	1:B:376:VAL:HG12	2.11	0.49
1:D:343:LYS:HB2	1:D:373:VAL:CG1	2.42	0.49
1:D:376:VAL:HG12	1:D:376:VAL:O	2.11	0.49
1:D:689:THR:HG22	1:D:689:THR:O	2.11	0.49
1:A:376:VAL:O	1:A:376:VAL:HG12	2.11	0.49
1:A:343:LYS:HB2	1:A:373:VAL:CG1	2.42	0.49
1:C:343:LYS:HB2	1:C:373:VAL:CG1	2.42	0.49
2:H:126:SER:CA	2:H:127:ARG:NH2	2.74	0.49
1:C:375:ILE:CG1	1:C:397:GLN:O	2.60	0.49
1:C:689:THR:HG22	1:C:689:THR:O	2.11	0.49
1:A:375:ILE:CG1	1:A:397:GLN:O	2.60	0.49
1:B:375:ILE:CG1	1:B:397:GLN:O	2.60	0.49
1:C:343:LYS:HE2	1:C:420:ASP:HB2	1.94	0.49
1:C:134:SER:HA	1:C:204:LEU:HD21	1.95	0.49
2:G:52:LEU:HA	2:G:55:ILE:CD1	2.35	0.49
2:H:82:ALA:CB	2:H:123:GLU:HG2	2.43	0.49
1:B:689:THR:HG22	1:B:689:THR:O	2.11	0.49
1:B:343:LYS:HB2	1:B:373:VAL:CG1	2.42	0.49
1:C:550:PHE:CZ	1:C:583:PRO:HD2	2.48	0.49
1:A:343:LYS:HE2	1:A:420:ASP:HB2	1.94	0.48
2:G:82:ALA:CB	2:G:123:GLU:HG2	2.43	0.48
2:F:82:ALA:CB	2:F:123:GLU:HG2	2.43	0.48
1:B:38:PHE:CZ	2:F:216:LEU:CD2	2.97	0.48
1:B:550:PHE:CZ	1:B:583:PRO:HD2	2.48	0.48
1:D:134:SER:HA	1:D:204:LEU:HD21	1.95	0.48
1:A:550:PHE:CZ	1:A:583:PRO:HD2	2.48	0.48
5:A:1108:POV:H21A	5:A:1108:POV:H21D	1.53	0.48
2:E:82:ALA:CB	2:E:123:GLU:HG2	2.43	0.48
2:H:48:ILE:HD11	2:H:221:THR:CG2	2.43	0.48
1:D:550:PHE:CZ	1:D:583:PRO:HD2	2.48	0.48
2:E:48:ILE:HD12	2:E:221:THR:HG21	1.95	0.48
1:B:354:GLU:H	1:B:354:GLU:CD	2.13	0.48
1:D:343:LYS:HE2	1:D:420:ASP:HB2	1.94	0.48
1:C:93:TRP:CD1	1:C:93:TRP:C	2.91	0.48
1:C:159:PHE:CD1	1:C:159:PHE:C	2.92	0.48
1:A:134:SER:HA	1:A:204:LEU:HD21	1.95	0.48
1:B:134:SER:HA	1:B:204:LEU:HD21	1.95	0.48
1:B:380:ASN:OD1	1:B:380:ASN:C	2.57	0.48
2:F:48:ILE:HD12	2:F:221:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1107:POV:H13A	5:A:1107:POV:O13	2.14	0.48
1:D:380:ASN:OD1	1:D:380:ASN:C	2.57	0.47
1:A:93:TRP:CD1	1:A:93:TRP:C	2.91	0.47
1:B:386:GLU:OE1	1:B:386:GLU:O	2.32	0.47
1:C:380:ASN:OD1	1:C:380:ASN:C	2.57	0.47
2:E:48:ILE:HD11	2:E:221:THR:CG2	2.43	0.47
1:C:386:GLU:O	1:C:386:GLU:OE1	2.32	0.47
1:D:93:TRP:CD1	1:D:93:TRP:C	2.91	0.47
1:D:386:GLU:OE1	1:D:386:GLU:O	2.32	0.47
1:A:179:LEU:CD1	2:E:46:LYS:HD3	2.44	0.47
1:A:386:GLU:O	1:A:386:GLU:OE1	2.32	0.47
1:A:380:ASN:OD1	1:A:380:ASN:C	2.57	0.47
1:A:550:PHE:CE2	1:A:565:MET:CE	2.98	0.47
1:B:285:MET:HE3	1:B:285:MET:HA	1.97	0.47
1:D:159:PHE:CD1	1:D:159:PHE:C	2.92	0.47
1:D:306:PHE:CZ	5:D:1101:POV:O14	2.67	0.47
1:D:550:PHE:CE2	1:D:565:MET:CE	2.98	0.47
1:B:159:PHE:CD1	1:B:159:PHE:C	2.92	0.47
1:A:20:ARG:NH1	5:A:1108:POV:O11	2.48	0.47
1:B:550:PHE:CE2	1:B:565:MET:CE	2.98	0.47
1:C:550:PHE:CE2	1:C:565:MET:CE	2.98	0.47
1:D:285:MET:HE3	1:D:285:MET:HA	1.97	0.47
2:G:48:ILE:HD11	2:G:221:THR:CG2	2.43	0.47
1:A:275:TRP:HB2	5:A:1107:POV:C32	2.45	0.47
5:A:1108:POV:H36A	5:A:1108:POV:H33	1.37	0.47
2:F:48:ILE:HD11	2:F:221:THR:CG2	2.43	0.47
1:C:536:MET:HG2	1:C:933:ILE:HD12	1.97	0.46
5:C:1104:POV:H36	5:C:1104:POV:H39	1.46	0.46
1:A:159:PHE:CD1	1:A:159:PHE:C	2.92	0.46
1:B:93:TRP:CD1	1:B:93:TRP:C	2.91	0.46
1:B:565:MET:HE3	1:B:568:ILE:HG23	1.98	0.46
1:A:565:MET:HE3	1:A:568:ILE:HG23	1.98	0.46
2:H:52:LEU:HA	2:H:55:ILE:CD1	2.35	0.46
1:D:536:MET:HG2	1:D:933:ILE:HD12	1.97	0.46
1:D:565:MET:HE3	1:D:568:ILE:HG23	1.97	0.46
2:F:125:ASN:C	2:F:127:ARG:NH2	2.74	0.46
2:G:125:ASN:C	2:G:127:ARG:NH2	2.74	0.46
2:E:52:LEU:HA	2:E:55:ILE:CD1	2.35	0.46
1:A:536:MET:HG2	1:A:933:ILE:HD12	1.97	0.46
1:A:697:PRO:HB3	1:A:771:HIS:CD2	2.51	0.46
1:C:285:MET:HE3	1:C:285:MET:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:HD23	5:D:1104:POV:H36	1.97	0.46
1:D:285:MET:CG	5:D:1101:POV:H25	2.36	0.46
1:C:565:MET:HE3	1:C:568:ILE:HG23	1.98	0.46
1:D:697:PRO:HB3	1:D:771:HIS:CD2	2.51	0.46
2:H:125:ASN:C	2:H:127:ARG:NH2	2.74	0.46
1:A:285:MET:HE3	1:A:285:MET:HA	1.97	0.46
5:A:1108:POV:H38	5:A:1108:POV:H31B	1.44	0.46
1:B:697:PRO:HB3	1:B:771:HIS:CD2	2.51	0.46
1:C:279:TYR:HB2	5:C:1103:POV:H35	1.98	0.46
1:C:1009:MET:HB3	1:C:1009:MET:HE3	1.42	0.46
2:F:52:LEU:HA	2:F:55:ILE:CD1	2.35	0.46
2:H:71:SER:HB3	2:H:72:PRO:HD3	1.98	0.46
2:E:125:ASN:C	2:E:127:ARG:NH2	2.74	0.45
1:A:252:PHE:CE2	5:A:1109:POV:C26	2.99	0.45
5:B:1104:POV:H22	2:F:199:VAL:CG2	2.41	0.45
1:C:711:ALA:HB3	1:C:712:MET:CE	2.43	0.45
2:E:44:GLU:OE2	2:E:221:THR:HG23	2.17	0.45
2:G:71:SER:HB3	2:G:72:PRO:HD3	1.98	0.45
5:B:1104:POV:H21A	5:B:1104:POV:H214	1.46	0.45
1:C:697:PRO:HB3	1:C:771:HIS:CD2	2.51	0.45
1:D:711:ALA:HB3	1:D:712:MET:CE	2.43	0.45
1:B:36:GLY:HA3	1:B:178:TRP:CZ2	2.52	0.45
1:C:36:GLY:HA3	1:C:178:TRP:CZ2	2.52	0.45
2:H:44:GLU:OE2	2:H:221:THR:HG23	2.17	0.45
1:B:536:MET:HG2	1:B:933:ILE:HD12	1.97	0.45
1:D:1009:MET:HE3	1:D:1009:MET:HB3	1.42	0.45
1:A:38:PHE:CZ	2:E:216:LEU:HD21	2.51	0.45
1:B:298:THR:HG21	5:C:1103:POV:H22	1.98	0.45
1:B:264:GLU:OE2	5:C:1103:POV:H11	2.17	0.45
2:E:71:SER:HB3	2:E:72:PRO:HD3	1.98	0.45
1:A:711:ALA:HB3	1:A:712:MET:CE	2.43	0.44
1:A:383:PRO:HD3	1:A:400:PHE:CE1	2.53	0.44
1:C:383:PRO:HD3	1:C:400:PHE:CE1	2.53	0.44
1:C:373:VAL:HB	1:C:374:GLU:H	1.59	0.44
5:C:1104:POV:H28	5:C:1104:POV:H25A	1.52	0.44
1:D:304:MET:HE3	1:D:304:MET:HA	2.00	0.44
1:D:383:PRO:HD3	1:D:400:PHE:CE1	2.53	0.44
2:F:44:GLU:OE2	2:F:221:THR:HG23	2.17	0.44
2:F:71:SER:HB3	2:F:72:PRO:HD3	1.98	0.44
2:G:44:GLU:OE2	2:G:221:THR:HG23	2.17	0.44
1:C:1014:ILE:HD11	1:C:1034:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLY:HA3	1:A:178:TRP:CZ2	2.52	0.44
1:A:304:MET:HE3	1:A:304:MET:HA	2.00	0.44
1:B:1014:ILE:HD11	1:B:1034:ILE:HB	2.00	0.44
1:C:304:MET:HE3	1:C:304:MET:HA	2.00	0.44
1:D:36:GLY:HA3	1:D:178:TRP:CZ2	2.52	0.44
1:B:304:MET:HE3	1:B:304:MET:HA	2.00	0.44
1:B:561:LEU:HD23	1:B:561:LEU:N	2.33	0.44
1:A:1009:MET:HB3	1:A:1009:MET:HE3	1.42	0.44
1:B:383:PRO:HD3	1:B:400:PHE:CE1	2.53	0.44
1:D:1014:ILE:HD11	1:D:1034:ILE:HB	2.00	0.44
1:A:1014:ILE:HG22	1:A:1049:ILE:HD13	2.01	0.43
1:D:273:THR:HG21	5:D:1104:POV:C1	2.48	0.43
5:D:1101:POV:H25	5:D:1101:POV:H22	1.78	0.43
2:E:161:MET:SD	2:E:161:MET:N	2.91	0.43
2:G:48:ILE:HD12	2:G:221:THR:HG21	1.95	0.43
1:A:561:LEU:HD23	1:A:561:LEU:N	2.33	0.43
1:B:179:LEU:HD12	1:B:179:LEU:O	2.19	0.43
1:B:538:THR:HG22	1:B:930:ASN:HD21	1.83	0.43
1:B:731:LEU:HD13	1:B:765:ARG:NH1	2.33	0.43
1:C:561:LEU:HD23	1:C:561:LEU:N	2.33	0.43
1:C:1014:ILE:HG22	1:C:1049:ILE:HD13	2.00	0.43
1:B:1009:MET:HB3	1:B:1009:MET:HE3	1.42	0.43
1:C:179:LEU:O	1:C:179:LEU:HD12	2.18	0.43
1:D:179:LEU:HD12	1:D:179:LEU:O	2.19	0.43
1:D:561:LEU:HD23	1:D:561:LEU:N	2.33	0.43
1:A:731:LEU:HD13	1:A:765:ARG:NH1	2.33	0.43
1:A:1014:ILE:HD11	1:A:1034:ILE:HB	2.00	0.43
1:B:711:ALA:HB3	1:B:712:MET:CE	2.43	0.43
1:C:538:THR:HG22	1:C:930:ASN:HD21	1.83	0.43
1:B:373:VAL:HB	1:B:374:GLU:H	1.59	0.43
1:B:1014:ILE:HG22	1:B:1049:ILE:HD13	2.01	0.43
1:C:731:LEU:HD13	1:C:765:ARG:NH1	2.33	0.43
1:D:513:MET:HE1	1:D:537:TYR:OH	2.19	0.43
1:D:1014:ILE:HG22	1:D:1049:ILE:HD13	2.00	0.43
2:F:161:MET:SD	2:F:161:MET:N	2.91	0.43
2:H:48:ILE:HD12	2:H:221:THR:HG21	1.95	0.43
1:A:373:VAL:HB	1:A:374:GLU:H	1.59	0.43
1:A:538:THR:HG22	1:A:930:ASN:HD21	1.83	0.43
5:A:1107:POV:H36	5:A:1107:POV:H33	1.40	0.43
1:C:513:MET:HE1	1:C:537:TYR:OH	2.19	0.43
1:C:561:LEU:HD23	1:C:561:LEU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:60:VAL:HG12	2:E:64:ILE:HD12	2.01	0.43
2:F:60:VAL:HG12	2:F:64:ILE:HD12	2.01	0.43
5:A:1108:POV:H38A	5:A:1108:POV:H35	1.86	0.43
1:D:561:LEU:HD23	1:D:561:LEU:H	1.84	0.43
2:H:161:MET:N	2:H:161:MET:SD	2.91	0.43
1:A:513:MET:HE1	1:A:537:TYR:OH	2.19	0.43
2:G:161:MET:SD	2:G:161:MET:N	2.91	0.43
1:C:610:PHE:O	1:C:610:PHE:CG	2.72	0.42
1:D:538:THR:HG22	1:D:930:ASN:HD21	1.83	0.42
1:D:731:LEU:HD13	1:D:765:ARG:NH1	2.33	0.42
5:D:1104:POV:H2	5:D:1104:POV:H23A	2.01	0.42
2:E:198:ILE:O	2:E:202:HIS:HB2	2.19	0.42
1:A:610:PHE:O	1:A:610:PHE:CG	2.72	0.42
2:F:198:ILE:O	2:F:202:HIS:HB2	2.19	0.42
1:A:179:LEU:O	1:A:179:LEU:HD12	2.19	0.42
1:B:513:MET:HE1	1:B:537:TYR:OH	2.19	0.42
1:C:266:PHE:CE2	5:C:1104:POV:H3	2.54	0.42
1:D:610:PHE:O	1:D:610:PHE:CG	2.72	0.42
2:G:198:ILE:O	2:G:202:HIS:HB2	2.19	0.42
2:H:60:VAL:HG12	2:H:64:ILE:HD12	2.01	0.42
1:B:561:LEU:HD23	1:B:561:LEU:H	1.84	0.42
1:A:561:LEU:HD23	1:A:561:LEU:H	1.84	0.42
1:A:38:PHE:CE1	2:E:216:LEU:HD22	2.55	0.42
1:C:22:TRP:NE1	5:C:1104:POV:O21	2.49	0.42
1:B:768:GLU:O	1:B:771:HIS:CE1	2.73	0.42
1:A:298:THR:HG21	5:B:1103:POV:H23	2.02	0.42
5:A:1108:POV:H313	5:A:1108:POV:H31A	1.89	0.42
2:H:198:ILE:O	2:H:202:HIS:HB2	2.19	0.42
1:C:768:GLU:O	1:C:771:HIS:CE1	2.73	0.42
1:D:1014:ILE:HD12	1:D:1014:ILE:C	2.45	0.42
2:G:60:VAL:HG12	2:G:64:ILE:HD12	2.01	0.42
1:B:610:PHE:O	1:B:610:PHE:CG	2.72	0.41
5:B:1104:POV:H38A	5:B:1104:POV:H31B	1.56	0.41
1:C:190:VAL:HB	1:C:191:PRO:HD3	2.02	0.41
1:D:502:GLY:O	1:D:505:THR:HG22	2.20	0.41
1:A:1014:ILE:HD12	1:A:1014:ILE:C	2.45	0.41
1:B:1014:ILE:HD12	1:B:1014:ILE:C	2.45	0.41
5:C:1104:POV:H21B	5:C:1104:POV:C216	2.51	0.41
1:C:353:LEU:HD22	1:C:386:GLU:CG	2.51	0.41
1:D:550:PHE:CE2	1:D:565:MET:HE3	2.55	0.41
1:A:204:LEU:HD12	1:A:204:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLY:O	1:A:505:THR:HG22	2.20	0.41
1:A:768:GLU:O	1:A:771:HIS:CE1	2.73	0.41
1:B:502:GLY:O	1:B:505:THR:HG22	2.20	0.41
1:A:550:PHE:CE2	1:A:565:MET:HE3	2.55	0.41
1:A:904:TYR:HA	1:A:909:PHE:CD2	2.56	0.41
5:A:1108:POV:H21J	5:A:1108:POV:H215	1.81	0.41
1:B:190:VAL:HB	1:B:191:PRO:HD3	2.02	0.41
1:C:550:PHE:CE2	1:C:565:MET:HE3	2.55	0.41
5:C:1103:POV:H15B	5:C:1103:POV:O14	2.21	0.41
1:D:768:GLU:O	1:D:771:HIS:CE1	2.73	0.41
1:A:345:ILE:HD13	1:A:421:ALA:O	2.21	0.41
1:B:273:THR:CG2	5:B:1103:POV:H1	2.50	0.41
1:A:275:TRP:HB2	5:A:1107:POV:H32	2.03	0.41
1:A:353:LEU:HD22	1:A:386:GLU:CG	2.51	0.41
1:B:345:ILE:HD13	1:B:421:ALA:O	2.21	0.41
1:B:904:TYR:HA	1:B:909:PHE:CD2	2.56	0.41
1:C:502:GLY:O	1:C:505:THR:HG22	2.20	0.41
1:B:298:THR:CG2	5:C:1103:POV:H22	2.51	0.41
1:C:275:TRP:CD1	5:C:1103:POV:H23A	2.55	0.41
1:C:1014:ILE:HD12	1:C:1014:ILE:O	2.21	0.41
1:A:687:ASP:OD1	1:A:690:GLY:N	2.55	0.40
1:B:1014:ILE:HD12	1:B:1014:ILE:O	2.21	0.40
1:C:1014:ILE:HD12	1:C:1014:ILE:C	2.45	0.40
1:B:204:LEU:HD12	1:B:204:LEU:HA	1.90	0.40
1:D:190:VAL:HB	1:D:191:PRO:HD3	2.02	0.40
1:D:904:TYR:HA	1:D:909:PHE:CD2	2.56	0.40
5:A:1108:POV:H36	5:A:1108:POV:H39	1.96	0.40
1:C:687:ASP:OD1	1:C:690:GLY:N	2.55	0.40
1:B:687:ASP:OD1	1:B:690:GLY:N	2.55	0.40
1:C:301:ARG:HB3	5:D:1104:POV:H33A	2.04	0.40
1:C:687:ASP:OD1	1:C:687:ASP:C	2.65	0.40
1:C:904:TYR:HA	1:C:909:PHE:CD2	2.56	0.40
1:D:345:ILE:HD13	1:D:421:ALA:O	2.21	0.40
1:D:687:ASP:OD1	1:D:690:GLY:N	2.55	0.40
1:A:506:MET:HE3	1:A:506:MET:HB2	1.98	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	881/1056 (83%)	836 (95%)	43 (5%)	2 (0%)	43	72
1	B	881/1056 (83%)	836 (95%)	43 (5%)	2 (0%)	43	72
1	C	881/1056 (83%)	836 (95%)	43 (5%)	2 (0%)	43	72
1	D	881/1056 (83%)	836 (95%)	43 (5%)	2 (0%)	43	72
2	E	195/239 (82%)	186 (95%)	9 (5%)	0	100	100
2	F	195/239 (82%)	186 (95%)	9 (5%)	0	100	100
2	G	195/239 (82%)	186 (95%)	9 (5%)	0	100	100
2	H	195/239 (82%)	187 (96%)	8 (4%)	0	100	100
All	All	4304/5180 (83%)	4089 (95%)	207 (5%)	8 (0%)	44	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	ILE
1	B	375	ILE
1	C	375	ILE
1	D	375	ILE
1	A	373	VAL
1	B	373	VAL
1	C	373	VAL
1	D	373	VAL

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	785/928 (85%)	781 (100%)	4 (0%)	81	93
1	B	785/928 (85%)	781 (100%)	4 (0%)	81	93
1	C	785/928 (85%)	781 (100%)	4 (0%)	81	93
1	D	785/928 (85%)	781 (100%)	4 (0%)	81	93
2	E	177/218 (81%)	175 (99%)	2 (1%)	65	88
2	F	177/218 (81%)	175 (99%)	2 (1%)	65	88
2	G	177/218 (81%)	175 (99%)	2 (1%)	65	88
2	H	177/218 (81%)	175 (99%)	2 (1%)	65	88
All	All	3848/4584 (84%)	3824 (99%)	24 (1%)	76	93

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	VAL
1	A	374	GLU
1	A	385	LEU
1	A	807	GLN
1	B	373	VAL
1	B	374	GLU
1	B	385	LEU
1	B	807	GLN
1	C	373	VAL
1	C	374	GLU
1	C	385	LEU
1	C	807	GLN
1	D	373	VAL
1	D	374	GLU
1	D	385	LEU
1	D	807	GLN
2	E	64	ILE
2	E	107	ARG
2	F	64	ILE
2	F	107	ARG
2	G	64	ILE
2	G	107	ARG
2	H	64	ILE
2	H	107	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	216	GLN
1	A	270	GLN
1	A	462	GLN
1	A	465	ASN
1	A	534	ASN
1	A	585	ASN
1	A	749	HIS
1	A	771	HIS
1	A	875	ASN
1	A	932	ASN
1	A	1008	ASN
1	A	1036	ASN
1	B	216	GLN
1	B	270	GLN
1	B	462	GLN
1	B	465	ASN
1	B	534	ASN
1	B	585	ASN
1	B	749	HIS
1	B	771	HIS
1	B	875	ASN
1	B	932	ASN
1	B	1008	ASN
1	B	1036	ASN
1	C	142	GLN
1	C	216	GLN
1	C	270	GLN
1	C	462	GLN
1	C	465	ASN
1	C	534	ASN
1	C	585	ASN
1	C	749	HIS
1	C	875	ASN
1	C	932	ASN
1	C	1008	ASN
1	C	1036	ASN
1	D	142	GLN
1	D	216	GLN
1	D	270	GLN
1	D	462	GLN
1	D	465	ASN
1	D	534	ASN

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Mol	Chain	Res	Type
1	D	585	ASN
1	D	749	HIS
1	D	771	HIS
1	D	875	ASN
1	D	932	ASN
1	D	1008	ASN
1	D	1036	ASN
2	E	83	ASN
2	E	91	GLN
2	E	153	ASN
2	E	162	ASN
2	E	164	GLN
2	E	184	GLN
2	E	202	HIS
2	F	83	ASN
2	F	91	GLN
2	F	162	ASN
2	F	164	GLN
2	F	184	GLN
2	F	202	HIS
2	G	83	ASN
2	G	91	GLN
2	G	125	ASN
2	G	153	ASN
2	G	162	ASN
2	G	164	GLN
2	G	184	GLN
2	G	202	HIS
2	H	91	GLN
2	H	125	ASN
2	H	153	ASN
2	H	162	ASN
2	H	164	GLN
2	H	184	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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
5	POV	A	1107	-	35,35,51	0.69	0	41,43,59	1.80	9 (21%)
5	POV	B	1104	-	45,45,51	0.68	1 (2%)	48,50,59	1.04	3 (6%)
5	POV	D	1101	-	14,14,51	1.02	1 (7%)	17,17,59	1.05	2 (11%)
5	POV	D	1104	-	32,32,51	0.57	0	35,37,59	0.80	1 (2%)
5	POV	D	1105	-	45,45,51	0.71	1 (2%)	48,50,59	0.94	4 (8%)
5	POV	C	1104	-	45,45,51	0.61	0	48,50,59	0.91	2 (4%)
5	POV	A	1108	-	41,41,51	0.55	0	43,43,59	1.30	4 (9%)
5	POV	B	1103	-	32,32,51	0.59	0	35,37,59	0.68	0
5	POV	A	1109	-	14,14,51	1.01	1 (7%)	17,17,59	1.05	2 (11%)
5	POV	C	1103	-	37,37,51	0.67	1 (2%)	43,45,59	1.72	6 (13%)

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
5	POV	A	1107	-	-	19/39/39/55	-
5	POV	B	1104	-	-	23/47/47/55	-
5	POV	D	1101	-	-	6/13/13/55	-
5	POV	D	1104	-	-	18/36/36/55	-
5	POV	D	1105	-	-	18/47/47/55	-
5	POV	C	1104	-	-	25/49/49/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	POV	A	1108	-	-	19/43/43/55	-
5	POV	B	1103	-	-	19/36/36/55	-
5	POV	A	1109	-	-	7/13/13/55	-
5	POV	C	1103	-	-	17/41/41/55	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1105	POV	P-O12	3.04	1.66	1.54
5	A	1109	POV	P-O12	3.04	1.66	1.54
5	B	1104	POV	P-O12	3.02	1.66	1.54
5	D	1101	POV	P-O12	2.98	1.65	1.54
5	C	1103	POV	C15-N	-2.02	1.44	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1103	POV	C15-N-C14	-7.12	90.26	108.98
5	A	1107	POV	C15-N-C14	-6.85	90.98	108.98
5	A	1108	POV	C3-O31-C31	5.86	138.53	117.12
5	C	1103	POV	C15-N-C13	-4.73	96.56	108.98
5	C	1103	POV	C14-N-C13	3.86	119.10	108.98
5	A	1107	POV	C15-N-C13	-3.74	99.14	108.98
5	B	1104	POV	C34-C33-C32	3.71	126.75	113.13
5	A	1107	POV	C15-N-C12	-3.49	96.02	109.91
5	A	1107	POV	O21-C21-C22	3.37	118.77	111.48
5	D	1105	POV	O12-P-O11	-3.31	98.05	106.67
5	D	1105	POV	C3-O31-C31	3.00	128.08	117.12
5	C	1104	POV	O21-C21-C22	2.86	117.66	111.48
5	C	1103	POV	C15-N-C12	-2.81	98.73	109.91
5	A	1108	POV	O21-C21-C22	2.78	117.50	111.48
5	A	1109	POV	O13-P-O14	2.76	121.59	110.83
5	A	1107	POV	C13-N-C12	2.73	120.77	109.91
5	B	1104	POV	O13-P-O14	2.73	121.48	110.83
5	A	1107	POV	C14-N-C12	2.72	120.70	109.91
5	C	1103	POV	C13-N-C12	2.71	120.68	109.91
5	A	1107	POV	C14-N-C13	2.63	115.89	108.98
5	D	1105	POV	O13-P-O14	2.62	121.04	110.83
5	A	1108	POV	O31-C31-C32	2.62	119.81	111.83
5	C	1104	POV	O31-C31-O32	2.58	130.07	123.63
5	D	1101	POV	O13-P-O14	2.44	120.33	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1104	POV	O12-P-O11	-2.37	100.49	106.67
5	A	1107	POV	C3-O31-C31	2.31	125.57	117.12
5	A	1109	POV	O12-P-O11	-2.26	100.78	106.67
5	D	1101	POV	O12-P-O11	-2.23	100.86	106.67
5	A	1108	POV	O11-C1-C2	-2.22	106.08	111.77
5	D	1105	POV	C34-C33-C32	-2.13	105.31	113.13
5	A	1107	POV	O31-C31-C32	2.07	118.14	111.83
5	D	1104	POV	O21-C21-C22	2.07	115.95	111.48
5	C	1103	POV	O21-C21-C22	2.04	115.89	111.48

There are no chirality outliers.

All (171) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1107	POV	C1-O11-P-O14
5	A	1107	POV	C11-O12-P-O11
5	A	1107	POV	C11-O12-P-O13
5	A	1107	POV	C32-C31-O31-C3
5	A	1107	POV	O32-C31-O31-C3
5	A	1108	POV	O22-C21-O21-C2
5	A	1109	POV	C1-O11-P-O13
5	B	1103	POV	C11-O12-P-O13
5	B	1103	POV	C22-C21-O21-C2
5	B	1103	POV	O22-C21-O21-C2
5	C	1103	POV	C1-O11-P-O14
5	C	1103	POV	O12-C11-C12-N
5	C	1103	POV	C12-C11-O12-P
5	C	1103	POV	C22-C21-O21-C2
5	C	1104	POV	C1-O11-P-O12
5	C	1104	POV	C11-O12-P-O11
5	C	1104	POV	C11-O12-P-O13
5	C	1104	POV	C11-O12-P-O14
5	D	1101	POV	C1-O11-P-O12
5	D	1101	POV	C1-O11-P-O14
5	D	1104	POV	C11-O12-P-O11
5	D	1104	POV	C11-O12-P-O13
5	D	1104	POV	C11-O12-P-O14
5	D	1104	POV	C22-C21-O21-C2
5	D	1105	POV	C1-O11-P-O12
5	D	1105	POV	C1-O11-P-O13
5	C	1103	POV	O22-C21-O21-C2
5	D	1104	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
5	A	1108	POV	C22-C21-O21-C2
5	A	1108	POV	C32-C31-O31-C3
5	A	1108	POV	O32-C31-O31-C3
5	C	1104	POV	C36-C37-C38-C39
5	B	1104	POV	C311-C310-C39-C38
5	C	1104	POV	C25-C26-C27-C28
5	D	1101	POV	C22-C21-O21-C2
5	A	1107	POV	C33-C34-C35-C36
5	A	1108	POV	C310-C311-C312-C313
5	A	1108	POV	C311-C310-C39-C38
5	A	1108	POV	C211-C212-C213-C214
5	A	1108	POV	C33-C34-C35-C36
5	B	1104	POV	C211-C212-C213-C214
5	D	1101	POV	C22-C23-C24-C25
5	A	1107	POV	C11-C12-N-C13
5	D	1104	POV	C31-C32-C33-C34
5	A	1107	POV	C21-C22-C23-C24
5	C	1104	POV	C31-C32-C33-C34
5	D	1101	POV	O22-C21-O21-C2
5	D	1104	POV	C21-C22-C23-C24
5	D	1105	POV	C36-C37-C38-C39
5	C	1104	POV	C32-C33-C34-C35
5	C	1103	POV	C11-C12-N-C13
5	A	1109	POV	C21-C22-C23-C24
5	D	1105	POV	C311-C310-C39-C38
5	C	1103	POV	C11-C12-N-C15
5	D	1105	POV	C22-C23-C24-C25
5	C	1104	POV	C23-C24-C25-C26
5	D	1104	POV	C36-C37-C38-C39
5	B	1104	POV	C25-C26-C27-C28
5	A	1107	POV	C23-C24-C25-C26
5	A	1109	POV	C22-C21-O21-C2
5	C	1104	POV	C311-C312-C313-C314
5	B	1103	POV	C32-C33-C34-C35
5	A	1108	POV	C25-C26-C27-C28
5	D	1104	POV	C22-C23-C24-C25
5	D	1105	POV	C21-C22-C23-C24
5	B	1104	POV	C214-C215-C216-C217
5	C	1104	POV	C213-C214-C215-C216
5	B	1103	POV	C34-C35-C36-C37
5	C	1104	POV	C22-C23-C24-C25
5	A	1108	POV	C37-C38-C39-C310

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Mol	Chain	Res	Type	Atoms
5	B	1103	POV	C22-C23-C24-C25
5	A	1108	POV	C29-C210-C211-C212
5	C	1104	POV	C313-C314-C315-C316
5	A	1108	POV	C21-C22-C23-C24
5	C	1104	POV	C32-C31-O31-C3
5	B	1104	POV	C310-C311-C312-C313
5	C	1104	POV	C34-C35-C36-C37
5	C	1104	POV	C24-C25-C26-C27
5	A	1107	POV	C32-C33-C34-C35
5	B	1104	POV	C212-C213-C214-C215
5	B	1104	POV	C213-C214-C215-C216
5	B	1103	POV	C37-C38-C39-C310
5	B	1103	POV	C24-C25-C26-C27
5	B	1104	POV	C23-C24-C25-C26
5	C	1104	POV	C310-C311-C312-C313
5	D	1105	POV	C26-C27-C28-C29
5	A	1109	POV	O22-C21-O21-C2
5	D	1105	POV	O11-C1-C2-C3
5	B	1104	POV	C22-C23-C24-C25
5	A	1108	POV	C23-C24-C25-C26
5	B	1104	POV	C22-C21-O21-C2
5	A	1108	POV	C32-C33-C34-C35
5	B	1104	POV	C35-C36-C37-C38
5	D	1105	POV	C1-O11-P-O14
5	B	1104	POV	C21-C22-C23-C24
5	C	1103	POV	C33-C34-C35-C36
5	B	1104	POV	C32-C31-O31-C3
5	A	1108	POV	C215-C216-C217-C218
5	C	1104	POV	C37-C38-C39-C310
5	D	1104	POV	C37-C38-C39-C310
5	B	1103	POV	O21-C2-C3-O31
5	B	1104	POV	C26-C27-C28-C29
5	D	1105	POV	C33-C34-C35-C36
5	C	1104	POV	C311-C310-C39-C38
5	D	1104	POV	C24-C25-C26-C27
5	B	1103	POV	C12-C11-O12-P
5	D	1105	POV	C213-C214-C215-C216
5	B	1103	POV	C1-C2-C3-O31
5	B	1104	POV	O11-C1-C2-O21
5	D	1105	POV	O11-C1-C2-O21
5	B	1103	POV	C31-C32-C33-C34
5	C	1103	POV	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
5	A	1107	POV	C37-C38-C39-C310
5	B	1104	POV	O32-C31-O31-C3
5	C	1104	POV	O32-C31-O31-C3
5	B	1104	POV	C29-C210-C211-C212
5	A	1108	POV	C39-C310-C311-C312
5	B	1104	POV	C32-C33-C34-C35
5	A	1109	POV	C1-O11-P-O12
5	B	1103	POV	C21-C22-C23-C24
5	D	1104	POV	C1-C2-O21-C21
5	A	1108	POV	C1-C2-C3-O31
5	A	1108	POV	O21-C2-C3-O31
5	B	1104	POV	O22-C21-O21-C2
5	B	1103	POV	C33-C34-C35-C36
5	C	1104	POV	O11-C1-C2-O21
5	B	1103	POV	C311-C310-C39-C38
5	C	1103	POV	C1-C2-C3-O31
5	A	1107	POV	C1-O11-P-O12
5	A	1107	POV	C1-O11-P-O13
5	A	1107	POV	C11-O12-P-O14
5	B	1103	POV	C11-O12-P-O11
5	B	1103	POV	C11-O12-P-O14
5	C	1103	POV	C11-O12-P-O14
5	C	1104	POV	C1-O11-P-O14
5	A	1107	POV	C3-C2-O21-C21
5	D	1105	POV	C312-C313-C314-C315
5	B	1104	POV	C215-C216-C217-C218
5	C	1103	POV	C37-C38-C39-C310
5	D	1104	POV	C35-C36-C37-C38
5	D	1104	POV	C25-C26-C27-C28
5	A	1109	POV	O21-C21-C22-C23
5	A	1107	POV	C2-C1-O11-P
5	B	1104	POV	O21-C2-C3-O31
5	D	1105	POV	O21-C2-C3-O31
5	D	1105	POV	C311-C312-C313-C314
5	B	1104	POV	C311-C312-C313-C314
5	A	1107	POV	O21-C2-C3-O31
5	D	1104	POV	O21-C2-C3-O31
5	A	1108	POV	C34-C35-C36-C37
5	C	1104	POV	C312-C313-C314-C315
5	C	1103	POV	C2-C1-O11-P
5	D	1101	POV	O21-C21-C22-C23
5	B	1103	POV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
5	D	1104	POV	C23-C24-C25-C26
5	C	1103	POV	C39-C310-C311-C312
5	C	1103	POV	C31-C32-C33-C34
5	D	1105	POV	O22-C21-O21-C2
5	C	1104	POV	C29-C210-C211-C212
5	B	1104	POV	C39-C310-C311-C312
5	D	1105	POV	C22-C21-O21-C2
5	A	1107	POV	C11-C12-N-C15
5	C	1103	POV	C11-C12-N-C14
5	D	1104	POV	C26-C27-C28-C29
5	D	1105	POV	C2-C1-O11-P
5	C	1103	POV	C311-C310-C39-C38
5	B	1103	POV	O21-C21-C22-C23
5	A	1109	POV	O11-C1-C2-O21
5	C	1104	POV	C210-C211-C212-C213
5	A	1107	POV	O22-C21-O21-C2
5	D	1104	POV	O21-C21-C22-C23

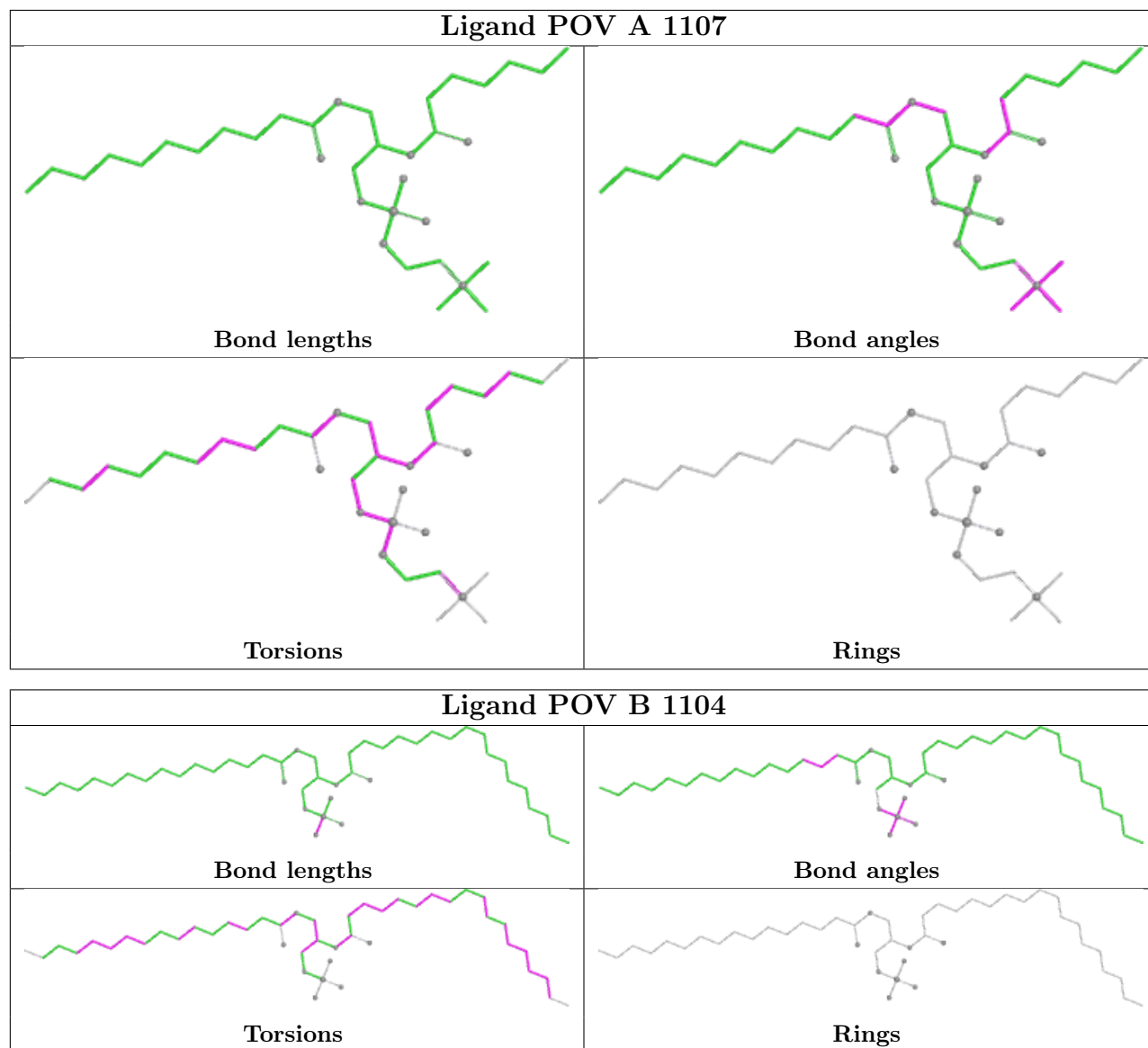
There are no ring outliers.

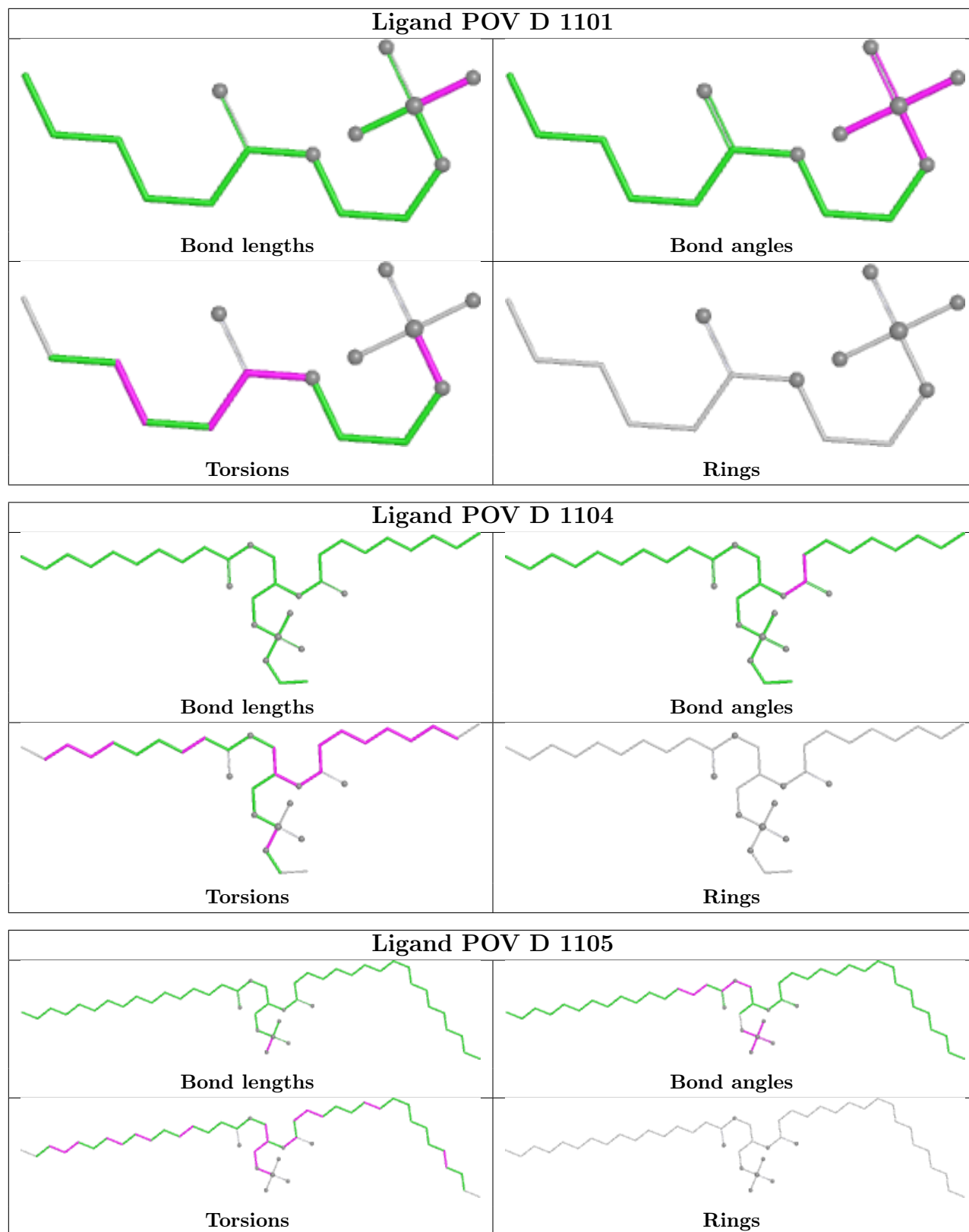
10 monomers are involved in 85 short contacts:

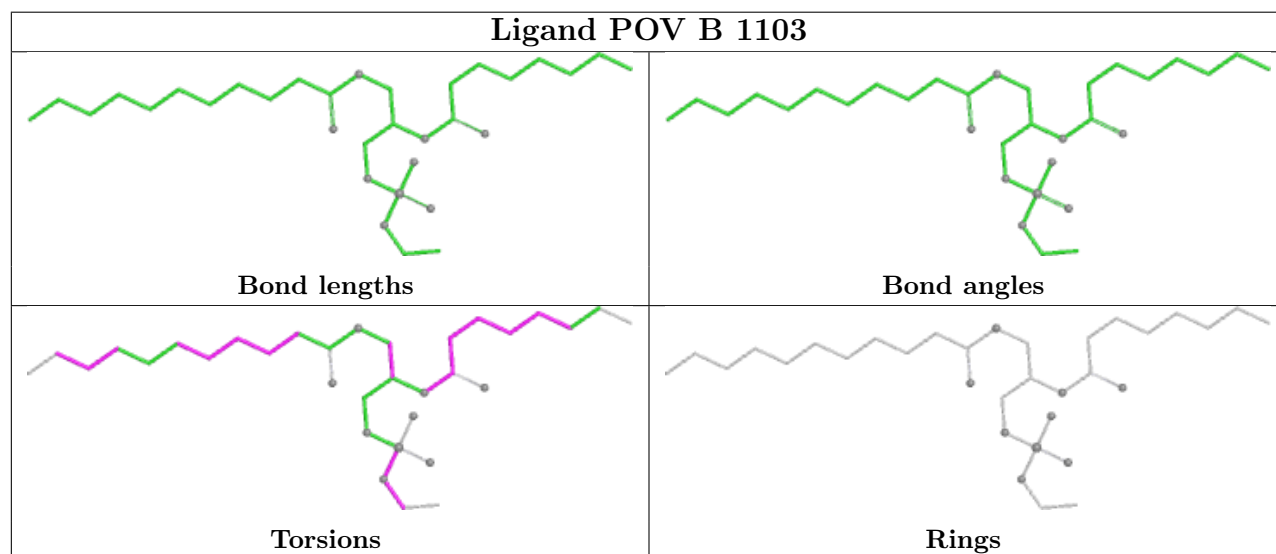
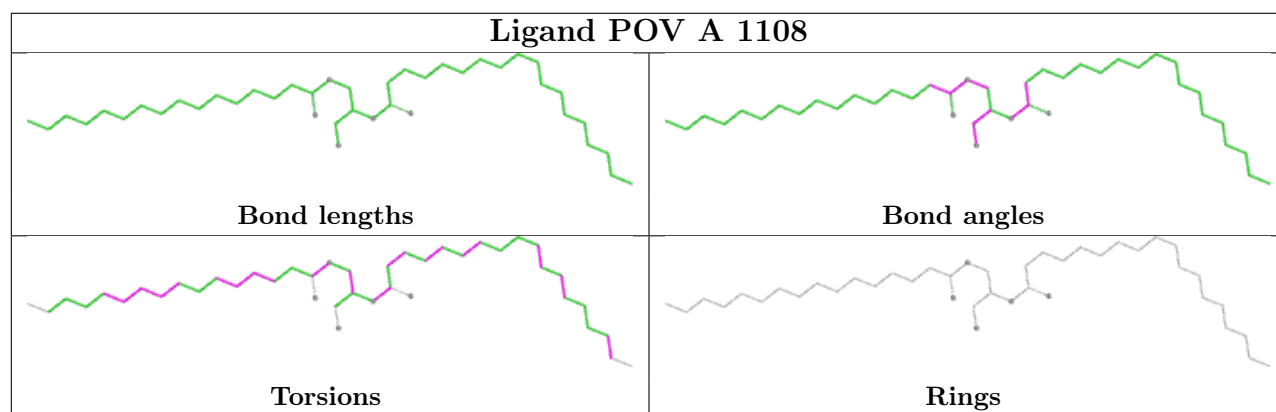
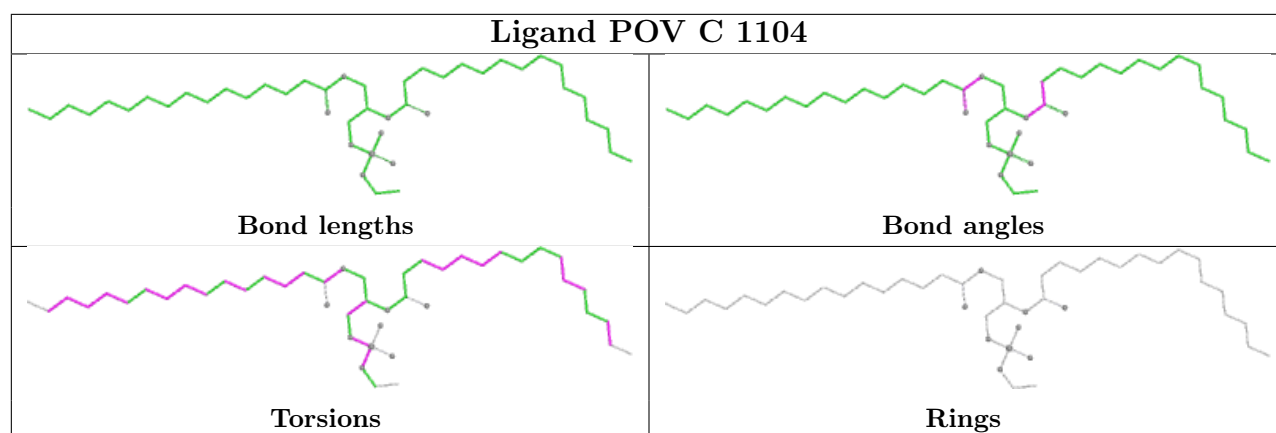
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1107	POV	13	0
5	B	1104	POV	5	0
5	D	1101	POV	4	0
5	D	1104	POV	6	0
5	D	1105	POV	2	0
5	C	1104	POV	5	0
5	A	1108	POV	24	0
5	B	1103	POV	8	0
5	A	1109	POV	1	0
5	C	1103	POV	17	0

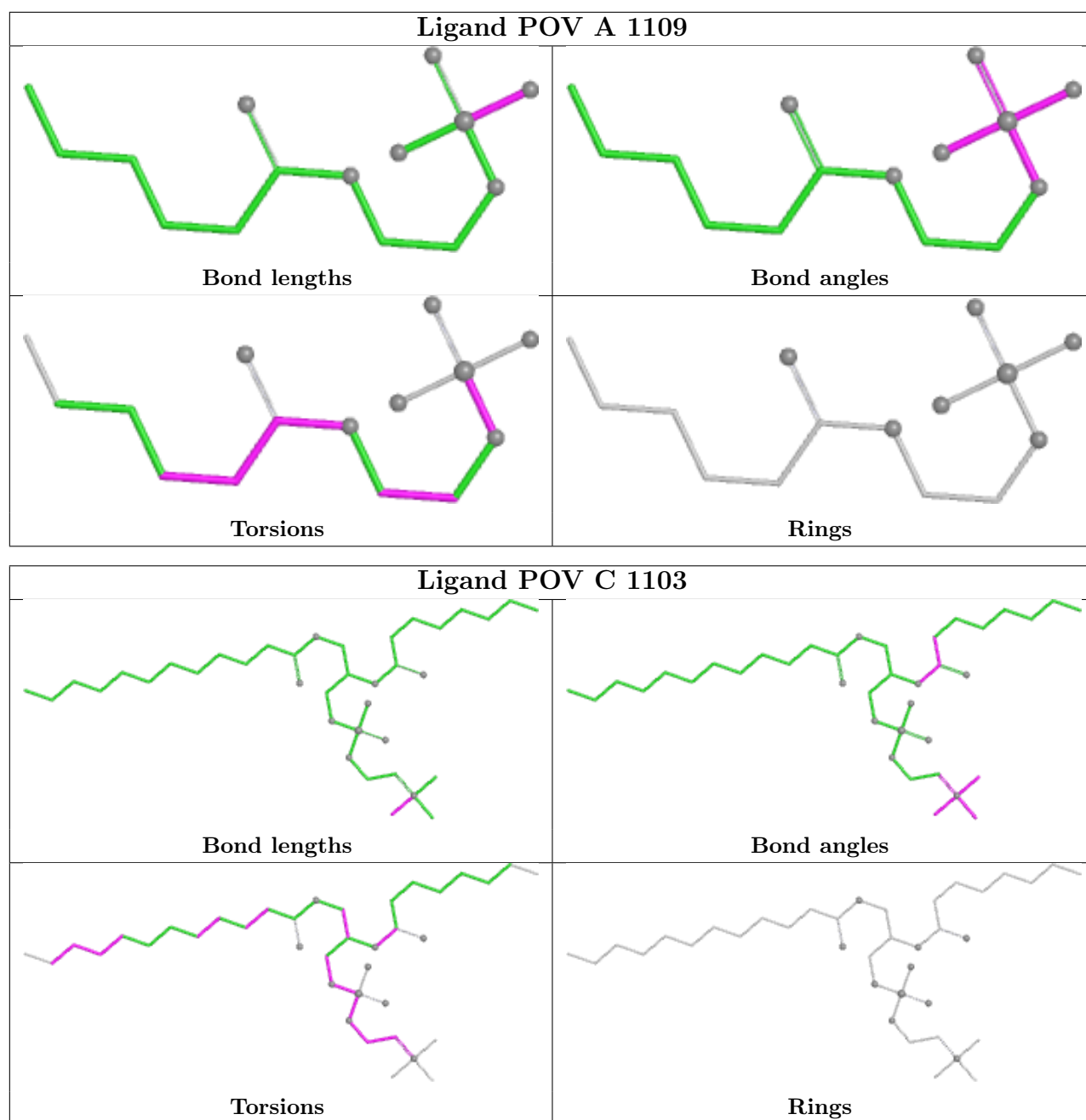
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [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

This section contains visualisations of the EMDB entry EMD-46416. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.