



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:44 AM BST

PDB ID : 2ABM
Title : Crystal Structure of Aquaporin Z Tetramer Reveals both Open and Closed Water-conducting Channels
Authors : Jiang, J.; Daniels, B.V.; Fu, D.
Deposited on : 2005-07-15
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

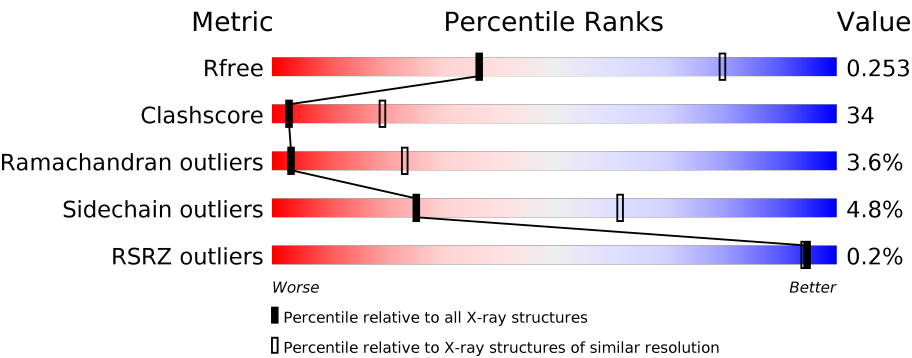
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	231	<div><div></div><div>47%48%...</div></div>
1	B	231	<div><div></div><div>48%45%... .</div></div>
1	C	231	<div><div></div><div>45%48%... .</div></div>
1	D	231	<div><div></div><div>40%52%6% .</div></div>
1	E	231	<div><div></div><div>43%50%... .</div></div>
1	F	231	<div><div></div><div>48%46%... .</div></div>

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Mol	Chain	Length	Quality of chain
1	G	231	
1	H	231	

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
2	BGL	A	609	X	-	-	-
2	BGL	E	608	X	-	-	-
3	POQ	A	600	X	-	-	-
4	PEE	F	607	-	-	-	X
5	PO4	B	626	-	-	X	-
5	PO4	F	636	-	-	X	-
5	PO4	G	635	-	-	-	X
6	3PG	C	627	X	-	-	-
6	3PG	G	637	X	-	-	X
7	AGA	C	629	-	X	-	-
7	AGA	G	639	-	X	-	X

2 Entry composition

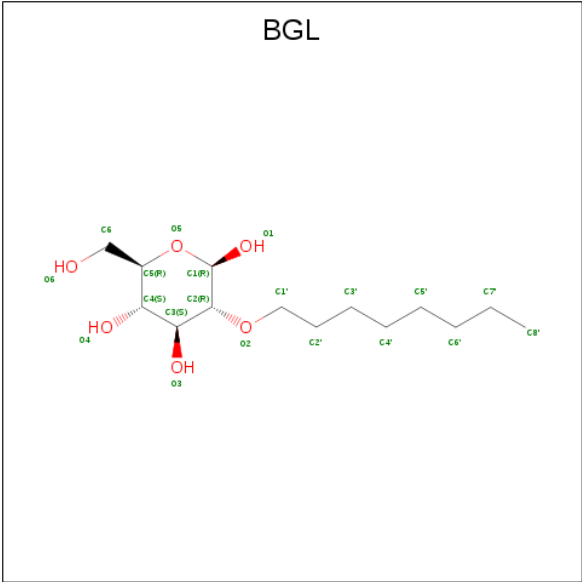
There are 8 unique types of molecules in this entry. The entry contains 13946 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aquaporin Z.

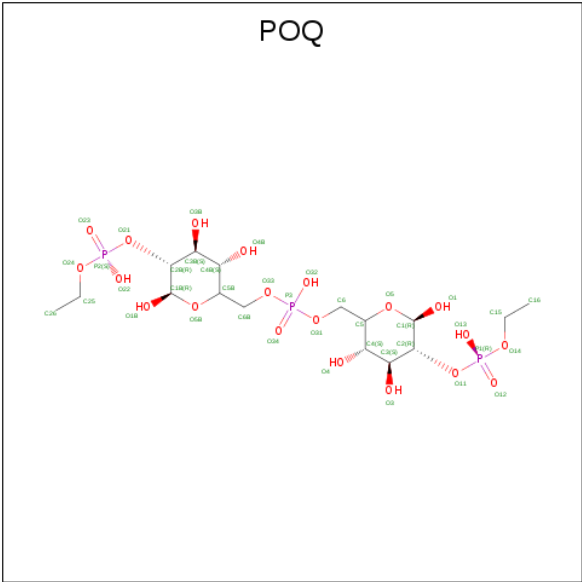
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1643	1095	265	278	5			
1	B	227	Total	C	N	O	S	0	0	0
			1643	1095	265	278	5			
1	C	227	Total	C	N	O	S	0	0	0
			1643	1095	265	278	5			
1	D	227	Total	C	N	O	S	0	0	0
			1643	1095	265	278	5			
1	E	227	Total	C	N	O	S	0	0	0
			1643	1095	265	278	5			
1	F	227	Total	C	N	O	S	0	0	0
			1643	1095	265	278	5			
1	G	227	Total	C	N	O	S	0	0	0
			1643	1095	265	278	5			
1	H	227	Total	C	N	O	S	0	0	0
			1643	1095	265	278	5			

- Molecule 2 is 2-O-octyl-beta-D-glucopyranose (three-letter code: BGL) (formula: C₁₄H₂₈O₆).



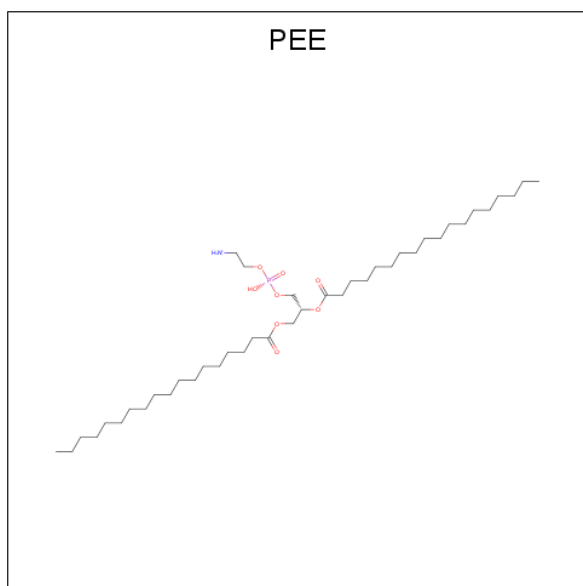
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	11	5		
2	B	1	Total	C	O	0	0
			18	12	6		
2	B	1	Total	C	O	0	0
			18	12	6		
2	E	1	Total	C	O	0	0
			16	11	5		

- Molecule 3 is BIS(((3S,4S,5R,6R)-5-(ETHYL(PHOSPHORYLOXY))-3,4,6-TRIHYDROXY-TETRAHYDRO-2H-PYRAN-2-YL)METHYL) HYDROGEN PHOSPHATE (three-letter code: POQ) (formula: C₁₆H₃₃O₂₀P₃).



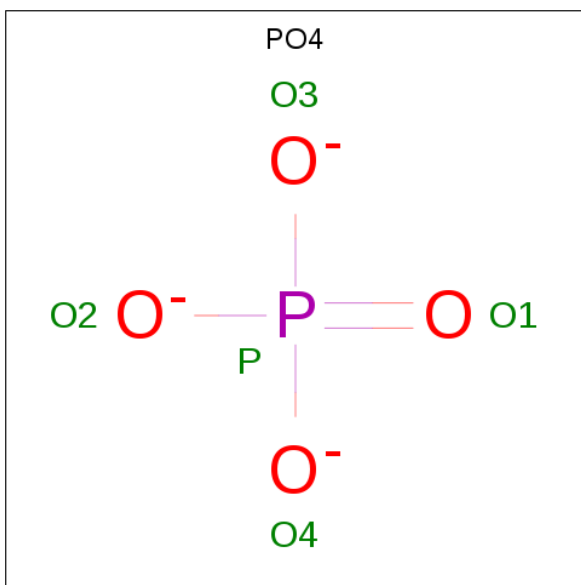
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			39	16	20	3		

- Molecule 4 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



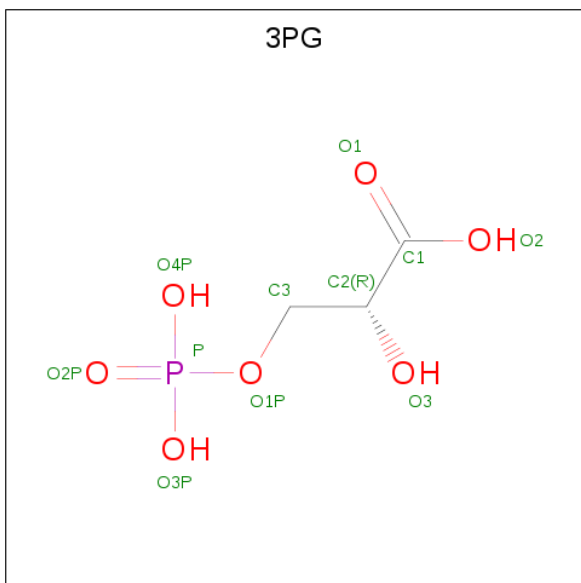
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			9	9		
4	B	1	Total	C	0	0
			14	14		
4	B	1	Total	C	0	0
			10	10		
4	E	1	Total	C	0	0
			16	16		
4	F	1	Total	C	0	0
			14	14		
4	F	1	Total	C	0	0
			10	10		
4	G	1	Total	C	0	0
			9	9		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



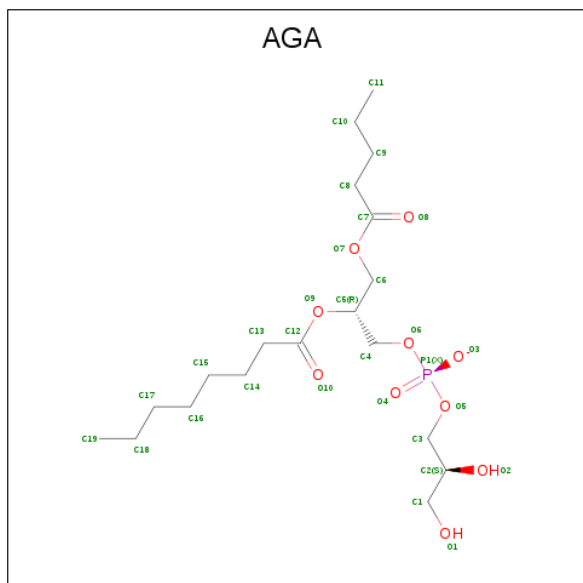
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is 3-PHOSPHOGLYCERIC ACID (three-letter code: 3PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	O	P	0	0
			11	3	7	1		
6	G	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 7 is (1S)-2-[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYL OCTANOATE (three-letter code: AGA) (formula: C₁₉H₃₆O₁₀P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			16	11	5		
7	G	1	Total	C	O	0	0
			16	11	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	69	Total	O	0	0
			69	69		
8	B	78	Total	O	0	0
			78	78		
8	C	69	Total	O	0	0
			69	69		
8	D	60	Total	O	0	0
			60	60		
8	E	65	Total	O	0	0
			65	65		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	68	Total 68	O 68	0	0
8	G	69	Total 69	O 69	0	0
8	H	61	Total 61	O 61	0	0

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

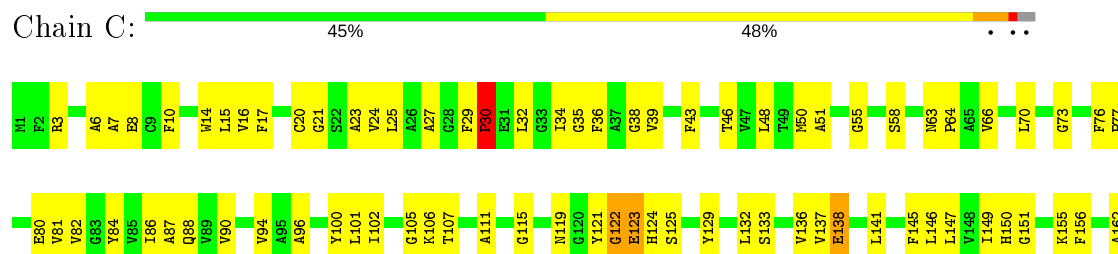
• Molecule 1: Aquaporin Z

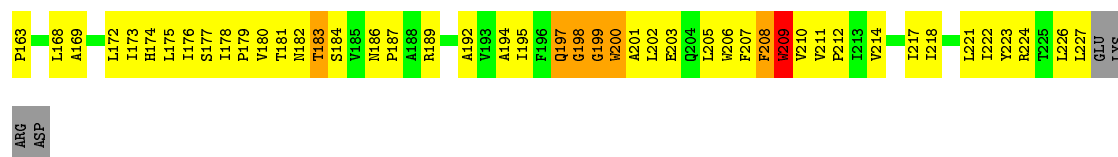


• Molecule 1: Aquaporin Z



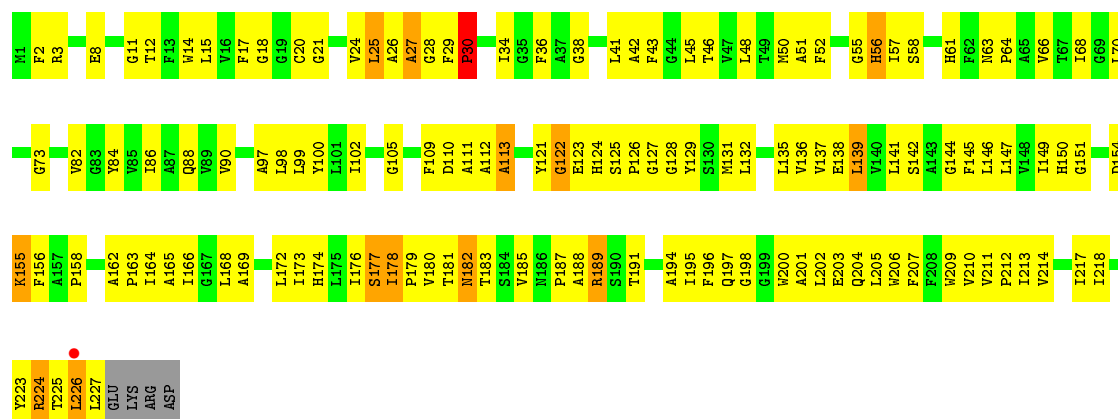
• Molecule 1: Aquaporin Z





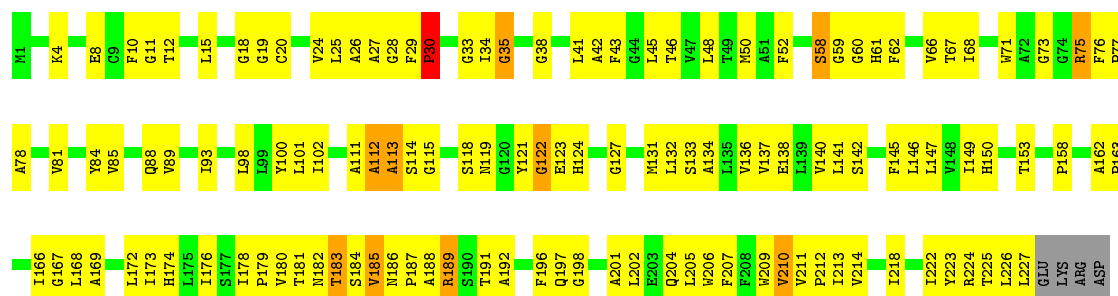
• Molecule 1: Aquaporin Z

Chain D: 40% 52% 6% .



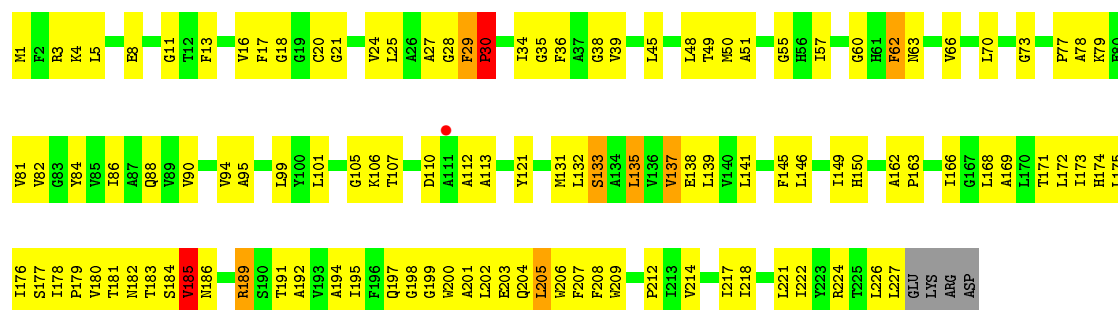
• Molecule 1: Aquaporin Z

Chain E: 43% 50% . .

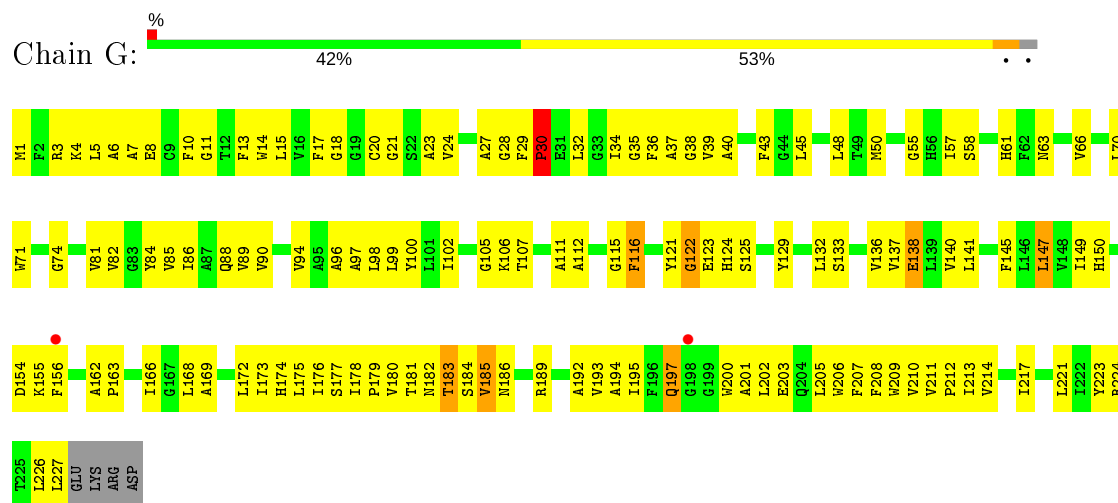


• Molecule 1: Aquaporin Z

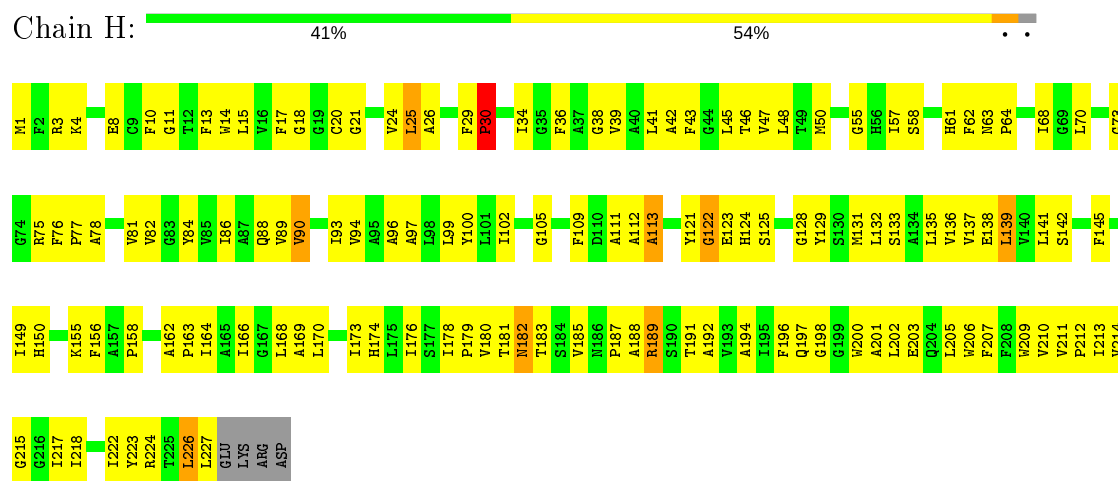
Chain F: 48% 46% . . .



• Molecule 1: Aquaporin Z



• Molecule 1: Aquaporin Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.15Å 119.15Å 380.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20 49.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (10.00-3.20) 99.9 (49.12-3.20)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.242 0.204 , 0.253	Depositor DCC
R_{free} test set	2306 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 79.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13946	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BGL, AGA, POQ, PEE, 3PG

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	0.47	0/1689	0.69	1/2305 (0.0%)
1	B	0.48	0/1689	0.71	1/2305 (0.0%)
1	C	0.42	0/1689	0.70	2/2305 (0.1%)
1	D	0.45	0/1689	0.68	1/2305 (0.0%)
1	E	0.44	0/1689	0.69	0/2305
1	F	0.46	0/1689	0.67	0/2305
1	G	0.44	0/1689	0.66	0/2305
1	H	0.43	0/1689	0.64	0/2305
All	All	0.45	0/13512	0.68	5/18440 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	ALA	N-CA-CB	5.63	117.98	110.10
1	C	208	PHE	O-C-N	5.24	131.09	122.70
1	C	209	TRP	CA-CB-CG	5.20	123.58	113.70
1	B	176	ILE	CB-CA-C	-5.10	101.40	111.60
1	A	58	SER	N-CA-CB	-5.01	102.98	110.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	196	PHE	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1643	0	1673	118	0
1	B	1643	0	1673	114	0
1	C	1643	0	1673	121	0
1	D	1643	0	1673	143	0
1	E	1643	0	1673	125	0
1	F	1643	0	1673	119	0
1	G	1643	0	1673	124	0
1	H	1643	0	1673	135	0
2	A	16	0	15	1	0
2	B	36	0	42	8	0
2	E	16	0	15	1	0
3	A	39	0	26	8	0
4	A	9	0	17	0	0
4	B	24	0	46	0	0
4	E	16	0	31	0	0
4	F	24	0	46	0	0
4	G	9	0	17	0	0
5	B	5	0	0	2	0
5	C	5	0	0	0	0
5	F	5	0	0	3	0
5	G	5	0	0	0	0
6	C	11	0	5	0	0
6	G	11	0	5	0	0
7	C	16	0	11	2	0
7	G	16	0	9	5	0
8	A	69	0	0	4	0
8	B	78	0	0	4	0
8	C	69	0	0	1	0
8	D	60	0	0	5	0
8	E	65	0	0	2	0
8	F	68	0	0	5	0
8	G	69	0	0	2	0
8	H	61	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13946	0	13669	932	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 34.

All (932) 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)
7:G:639:AGA:C10	7:G:639:AGA:C9	1.76	1.64
2:B:605:BGL:C3'	2:B:605:BGL:C4'	1.74	1.57
2:B:605:BGL:C6'	2:B:605:BGL:C5'	1.80	1.56
2:B:604:BGL:C5'	2:B:604:BGL:C6'	1.79	1.54
7:G:639:AGA:O9	7:G:639:AGA:C5	1.63	1.46
7:C:629:AGA:O9	7:C:629:AGA:C5	1.64	1.42
7:C:629:AGA:O9	7:C:629:AGA:C12	1.66	1.41
3:A:600:POQ:O5	3:A:600:POQ:C1	1.69	1.40
7:G:639:AGA:O9	7:G:639:AGA:C12	1.67	1.40
3:A:600:POQ:O5B	3:A:600:POQ:C1B	1.69	1.39
3:A:600:POQ:C2	3:A:600:POQ:O11	1.79	1.30
3:A:600:POQ:O21	3:A:600:POQ:C2B	1.78	1.28
1:G:115:GLY:HA2	1:G:197:GLN:NE2	1.51	1.20
1:E:18:GLY:HA2	1:F:176:ILE:CD1	1.73	1.19
1:E:26:ALA:HB2	1:F:179:PRO:CG	1.79	1.12
1:E:26:ALA:HB2	1:F:179:PRO:HG2	1.09	1.08
1:E:18:GLY:HA2	1:F:176:ILE:HD11	1.29	1.06
1:D:24:VAL:HG23	1:D:25:LEU:HD13	1.37	1.05
2:B:605:BGL:C4'	2:B:605:BGL:C2'	2.41	0.97
1:G:115:GLY:HA2	1:G:197:GLN:HE22	1.03	0.96
1:F:11:GLY:HA2	1:F:50:MET:HG2	1.46	0.95
1:H:139:LEU:HD22	1:H:211:VAL:HG13	1.50	0.94
1:D:139:LEU:HD22	1:D:211:VAL:HG13	1.52	0.91
1:E:18:GLY:CA	1:F:176:ILE:HD11	1.99	0.91
1:E:18:GLY:HA2	1:F:176:ILE:HD13	1.53	0.89
1:A:11:GLY:HA2	1:A:50:MET:HG2	1.53	0.87
1:D:198:GLY:HA2	1:D:202:LEU:CD2	2.04	0.87
1:B:149:ILE:HG12	1:B:166:ILE:HD12	1.58	0.86
1:H:100:TYR:HE1	1:H:111:ALA:HB2	1.41	0.86
1:H:112:ALA:HA	1:H:197:GLN:HE21	1.40	0.86
1:G:133:SER:O	1:G:137:VAL:HG23	1.75	0.86
7:G:639:AGA:C10	7:G:639:AGA:C8	2.54	0.85
1:C:141:LEU:HD13	1:C:173:ILE:HG23	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PHE:HB3	8:A:1148:HOH:O	1.77	0.83
1:B:189:ARG:HD2	8:B:1202:HOH:O	1.78	0.83
1:F:189:ARG:HD2	8:F:643:HOH:O	1.79	0.83
1:C:84:TYR:O	1:C:88:GLN:HG3	1.79	0.82
1:F:45:LEU:O	1:F:49:THR:HG23	1.79	0.82
1:B:198:GLY:HA2	1:B:202:LEU:CD2	2.08	0.82
1:A:224:ARG:HG3	8:A:1115:HOH:O	1.78	0.82
1:E:11:GLY:HA2	1:E:50:MET:HG2	1.61	0.82
1:F:162:ALA:HB3	1:F:163:PRO:HD3	1.58	0.82
1:H:198:GLY:HA2	1:H:202:LEU:HD21	1.60	0.82
1:H:122:GLY:H	1:H:125:SER:HB2	1.43	0.81
1:D:12:THR:HG21	1:D:88:GLN:O	1.79	0.81
1:E:225:THR:HG22	1:E:226:LEU:HD23	1.62	0.81
1:D:213:ILE:O	1:D:217:ILE:HG12	1.79	0.81
1:D:198:GLY:HA2	1:D:202:LEU:HD21	1.59	0.81
2:B:605:BGL:C6'	2:B:605:BGL:C4'	2.58	0.80
1:E:102:ILE:HD13	1:F:137:VAL:HG13	1.62	0.80
1:G:210:VAL:O	1:G:214:VAL:HG23	1.80	0.80
1:E:68:ILE:HD12	1:E:213:ILE:HD12	1.65	0.79
1:A:84:TYR:O	1:A:88:GLN:HG3	1.83	0.79
1:B:11:GLY:HA2	1:B:50:MET:HG2	1.63	0.79
1:F:218:ILE:O	1:F:222:ILE:HG12	1.81	0.79
1:G:210:VAL:HG13	1:G:211:VAL:H	1.46	0.78
1:G:200:TRP:HA	1:G:203:GLU:HB2	1.63	0.78
2:B:604:BGL:C4'	2:B:604:BGL:C6'	2.61	0.78
1:C:90:VAL:O	1:C:94:VAL:HG23	1.84	0.78
1:D:141:LEU:HD13	1:D:173:ILE:HG23	1.64	0.78
1:B:3:ARG:HH11	1:D:227:LEU:HG	1.49	0.78
1:G:63:ASN:HD22	1:G:66:VAL:HG23	1.47	0.78
1:A:75:ARG:HH11	1:A:75:ARG:HG2	1.49	0.77
1:C:174:HIS:O	1:C:178:ILE:HG13	1.84	0.77
1:A:149:ILE:HG12	1:A:166:ILE:HD12	1.66	0.77
1:B:162:ALA:HB3	1:B:163:PRO:HD3	1.65	0.77
1:C:86:ILE:O	1:C:90:VAL:HG23	1.83	0.77
1:D:122:GLY:H	1:D:125:SER:HB2	1.49	0.77
1:D:178:ILE:HB	1:D:179:PRO:HD3	1.64	0.77
1:H:64:PRO:O	1:H:68:ILE:HG12	1.85	0.77
1:G:141:LEU:HD13	1:G:173:ILE:HG23	1.65	0.77
1:F:3:ARG:HH11	1:H:227:LEU:HG	1.50	0.77
1:B:149:ILE:HA	1:B:166:ILE:CD1	2.14	0.76
1:A:155:LYS:HG2	8:A:1131:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:LEU:H	1:D:226:LEU:HD12	1.51	0.76
1:C:24:VAL:HG12	1:C:24:VAL:O	1.84	0.76
1:D:73:GLY:HA3	1:D:150:HIS:NE2	2.02	0.75
1:D:122:GLY:C	1:D:124:HIS:H	1.88	0.75
1:E:211:VAL:HB	1:E:212:PRO:HD3	1.69	0.75
1:G:137:VAL:HG22	1:H:102:ILE:HD13	1.69	0.75
1:A:68:ILE:HD12	1:A:213:ILE:HD12	1.68	0.74
1:C:197:GLN:HG2	1:C:201:ALA:HB2	1.68	0.74
1:C:63:ASN:HD22	1:C:66:VAL:HG23	1.52	0.74
1:B:218:ILE:O	1:B:222:ILE:HG12	1.86	0.74
1:H:180:VAL:HG12	1:H:181:THR:HG23	1.69	0.74
1:H:24:VAL:HG23	1:H:25:LEU:HD13	1.69	0.74
1:H:73:GLY:HA3	1:H:150:HIS:NE2	2.03	0.74
1:H:100:TYR:CE1	1:H:111:ALA:HB2	2.23	0.74
1:D:112:ALA:HA	1:D:197:GLN:HE21	1.52	0.74
1:E:162:ALA:HB3	1:E:163:PRO:HD3	1.69	0.74
1:A:89:VAL:O	1:A:93:ILE:HG12	1.88	0.73
1:B:214:VAL:O	1:B:218:ILE:HG12	1.88	0.73
1:C:122:GLY:C	1:C:124:HIS:H	1.91	0.73
8:B:1211:HOH:O	1:D:227:LEU:HD11	1.88	0.73
1:F:82:VAL:O	1:F:86:ILE:HD13	1.88	0.73
1:A:85:VAL:O	1:A:89:VAL:HG23	1.89	0.72
1:C:115:GLY:HA2	1:C:197:GLN:NE2	2.04	0.72
1:B:82:VAL:O	1:B:86:ILE:HD13	1.88	0.72
1:G:84:TYR:O	1:G:88:GLN:HG3	1.89	0.72
1:B:198:GLY:HA2	1:B:202:LEU:HD21	1.70	0.72
3:A:600:POQ:H162	1:E:101:LEU:HD23	1.71	0.72
1:F:66:VAL:HA	1:F:146:LEU:HD21	1.70	0.72
1:H:198:GLY:HA2	1:H:202:LEU:CD2	2.19	0.71
1:C:226:LEU:O	1:C:227:LEU:HB2	1.89	0.71
1:D:226:LEU:O	1:D:227:LEU:HB2	1.90	0.71
1:B:137:VAL:HG23	1:B:138:GLU:H	1.54	0.71
1:C:82:VAL:O	1:C:86:ILE:HG12	1.90	0.71
1:H:122:GLY:C	1:H:124:HIS:H	1.94	0.71
1:B:198:GLY:HA2	1:B:202:LEU:HD23	1.73	0.71
1:C:197:GLN:HG2	1:C:201:ALA:CB	2.21	0.71
1:E:209:TRP:O	1:E:213:ILE:HG12	1.90	0.71
1:G:145:PHE:O	1:G:149:ILE:HG13	1.91	0.70
1:A:225:THR:HG22	1:A:226:LEU:HD23	1.74	0.70
1:F:21:GLY:O	1:F:25:LEU:HB2	1.91	0.70
1:F:199:GLY:HA3	5:F:636:PO4:P	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:ALA:HB3	1:G:163:PRO:HD3	1.72	0.70
1:G:226:LEU:O	1:G:227:LEU:HB2	1.91	0.70
1:B:131:MET:HE2	8:B:1278:HOH:O	1.91	0.70
1:F:208:PHE:O	1:F:212:PRO:HG3	1.91	0.70
1:D:139:LEU:CD2	1:D:211:VAL:HG13	2.21	0.70
1:D:29:PHE:CG	1:D:30:PRO:HD2	2.27	0.69
1:D:64:PRO:O	1:D:68:ILE:HG12	1.90	0.69
1:C:145:PHE:O	1:C:149:ILE:HG13	1.92	0.69
1:E:111:ALA:HB3	2:E:608:BGL:O3	1.92	0.69
1:C:162:ALA:HB3	1:C:163:PRO:HD3	1.74	0.69
1:A:211:VAL:HB	1:A:212:PRO:HD3	1.73	0.69
1:G:210:VAL:HG13	1:G:211:VAL:N	2.07	0.69
1:F:18:GLY:HA2	1:H:176:ILE:HD11	1.74	0.69
1:A:11:GLY:HA2	1:A:50:MET:CG	2.23	0.69
1:C:34:ILE:HB	1:C:38:GLY:HA3	1.73	0.69
1:E:112:ALA:HA	1:E:197:GLN:HE21	1.57	0.69
1:F:177:SER:O	1:F:178:ILE:C	2.29	0.69
1:H:226:LEU:HD12	1:H:226:LEU:H	1.57	0.69
1:D:223:TYR:O	1:D:227:LEU:HD13	1.93	0.69
2:B:605:BGL:C3'	2:B:605:BGL:C5'	2.68	0.68
1:A:18:GLY:HA2	1:B:176:ILE:CD1	2.22	0.68
1:G:211:VAL:HB	1:G:212:PRO:HD3	1.75	0.68
1:A:112:ALA:HA	1:A:197:GLN:HE21	1.58	0.68
1:D:155:LYS:HE3	1:D:156:PHE:CE1	2.29	0.68
1:H:210:VAL:O	1:H:214:VAL:HG23	1.94	0.68
1:A:66:VAL:HA	1:A:146:LEU:HD11	1.75	0.68
1:G:86:ILE:O	1:G:90:VAL:HG23	1.94	0.68
1:H:198:GLY:C	1:H:202:LEU:HD23	2.13	0.68
1:F:198:GLY:HA2	1:F:202:LEU:HD21	1.76	0.68
1:C:6:ALA:O	1:C:10:PHE:HD1	1.77	0.67
1:C:211:VAL:HB	1:C:212:PRO:HD3	1.77	0.67
1:C:178:ILE:N	1:C:179:PRO:CD	2.58	0.67
1:C:8:GLU:HG2	1:C:58:SER:HB2	1.76	0.67
1:C:115:GLY:HA2	1:C:197:GLN:HE22	1.59	0.67
1:A:101:LEU:HD21	1:F:226:LEU:HD11	1.75	0.67
1:D:68:ILE:HG22	1:D:217:ILE:HD11	1.77	0.67
1:E:198:GLY:HA2	1:E:202:LEU:CD1	2.25	0.67
1:E:42:ALA:O	1:E:46:THR:HG23	1.95	0.67
1:A:209:TRP:O	1:A:213:ILE:HG12	1.95	0.67
1:D:180:VAL:HG12	1:D:181:THR:HG23	1.76	0.67
1:H:20:CYS:O	1:H:24:VAL:HG22	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:LEU:HB3	1:G:3:ARG:HH21	1.60	0.67
1:C:63:ASN:ND2	1:C:66:VAL:HG23	2.09	0.66
1:F:198:GLY:HA2	1:F:202:LEU:CD2	2.25	0.66
1:F:199:GLY:HA3	5:F:636:PO4:O2	1.95	0.66
1:A:227:LEU:HB3	1:C:3:ARG:HH21	1.60	0.66
1:H:141:LEU:HD13	1:H:173:ILE:HG23	1.77	0.66
1:H:198:GLY:O	1:H:202:LEU:HD23	1.93	0.66
1:A:227:LEU:HD22	1:C:3:ARG:NH2	2.09	0.66
1:F:45:LEU:HD22	1:H:168:LEU:HB3	1.77	0.66
1:A:162:ALA:HB3	1:A:163:PRO:HD3	1.76	0.66
1:G:227:LEU:HD11	8:H:367:HOH:O	1.94	0.66
1:D:210:VAL:O	1:D:214:VAL:HG23	1.95	0.66
1:G:150:HIS:HB3	1:G:223:TYR:CD1	2.31	0.66
1:A:122:GLY:C	1:A:124:HIS:H	1.99	0.66
1:F:84:TYR:O	1:F:88:GLN:HG3	1.95	0.66
1:A:132:LEU:HD11	1:C:101:LEU:HD11	1.78	0.66
1:E:84:TYR:O	1:E:88:GLN:HG3	1.96	0.66
1:B:132:LEU:HD11	1:F:222:ILE:HD13	1.76	0.66
1:A:35:GLY:HA2	1:C:32:LEU:HD22	1.78	0.65
1:H:86:ILE:O	1:H:90:VAL:HG23	1.96	0.65
1:F:227:LEU:C	8:F:637:HOH:O	2.34	0.65
1:F:191:THR:HA	1:F:205:LEU:HD11	1.77	0.65
1:C:227:LEU:HG	1:D:3:ARG:CZ	2.26	0.65
1:A:102:ILE:HD13	1:B:137:VAL:HG13	1.78	0.65
1:D:135:LEU:HD12	1:D:139:LEU:HD23	1.79	0.65
1:F:149:ILE:HA	1:F:166:ILE:CD1	2.26	0.65
1:E:10:PHE:HB3	8:E:667:HOH:O	1.97	0.65
1:H:213:ILE:O	1:H:217:ILE:HG12	1.97	0.65
1:D:8:GLU:HG3	1:D:84:TYR:CD2	2.32	0.65
1:E:112:ALA:O	1:E:114:SER:N	2.30	0.65
1:G:122:GLY:C	1:G:124:HIS:H	1.98	0.65
1:C:180:VAL:HG12	1:C:181:THR:HG23	1.78	0.64
1:C:24:VAL:O	1:C:25:LEU:HD12	1.96	0.64
1:D:122:GLY:H	1:D:125:SER:CB	2.11	0.64
1:E:149:ILE:HG12	1:E:166:ILE:HD12	1.78	0.64
1:F:110:ASP:HB3	1:F:113:ALA:HB3	1.79	0.64
1:H:194:ALA:HA	1:H:201:ALA:HB1	1.78	0.64
1:H:68:ILE:HG22	1:H:217:ILE:HD11	1.80	0.64
1:B:84:TYR:O	1:B:88:GLN:HG3	1.98	0.64
1:G:168:LEU:HB3	1:H:45:LEU:HD22	1.80	0.64
1:H:132:LEU:O	1:H:136:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:GLU:HG3	1:D:84:TYR:CE2	2.33	0.63
1:G:82:VAL:O	1:G:86:ILE:HG12	1.98	0.63
1:G:98:LEU:O	1:G:102:ILE:HG13	1.99	0.63
1:G:227:LEU:HG	1:H:3:ARG:CZ	2.29	0.63
1:D:198:GLY:CA	1:D:202:LEU:CD2	2.77	0.63
1:A:37:ALA:HB2	1:C:34:ILE:HG22	1.80	0.63
1:F:21:GLY:HA2	1:F:99:LEU:HD11	1.80	0.63
1:E:198:GLY:HA2	1:E:202:LEU:HD12	1.81	0.62
1:H:198:GLY:CA	1:H:202:LEU:CD2	2.77	0.62
1:H:139:LEU:CD2	1:H:211:VAL:HG13	2.26	0.62
1:F:77:PRO:HB2	1:F:79:LYS:HG2	1.81	0.62
8:F:651:HOH:O	1:H:227:LEU:HD21	1.97	0.62
1:D:36:PHE:CG	1:D:178:ILE:HG21	2.35	0.62
1:F:149:ILE:HG12	1:F:166:ILE:HD12	1.82	0.62
1:F:18:GLY:HA2	1:H:176:ILE:CD1	2.29	0.62
1:D:29:PHE:CD1	1:D:30:PRO:HD2	2.35	0.62
1:A:133:SER:O	1:A:137:VAL:HG12	1.99	0.62
1:H:155:LYS:HE3	1:H:156:PHE:CE1	2.35	0.62
1:A:226:LEU:O	1:A:227:LEU:HB2	2.00	0.62
1:A:15:LEU:C	1:A:15:LEU:HD23	2.20	0.62
1:A:185:VAL:HG12	1:A:185:VAL:O	2.00	0.62
1:E:224:ARG:HG3	8:E:634:HOH:O	2.00	0.61
1:B:184:SER:O	1:B:185:VAL:HG12	1.99	0.61
1:C:210:VAL:HG13	1:C:211:VAL:H	1.64	0.61
1:F:60:GLY:HA2	1:F:62:PHE:CE2	2.35	0.61
1:G:137:VAL:HG11	1:G:177:SER:HB3	1.82	0.61
1:G:197:GLN:HG2	1:G:201:ALA:HB2	1.82	0.61
1:C:217:ILE:O	1:C:221:LEU:HG	2.00	0.61
1:A:2:PHE:CE1	1:B:226:LEU:HD22	2.35	0.61
1:D:177:SER:O	1:D:179:PRO:HD2	1.99	0.61
1:C:122:GLY:O	1:C:124:HIS:N	2.33	0.61
3:A:600:POQ:C5B	3:A:600:POQ:C1B	2.79	0.61
1:C:63:ASN:HB3	1:C:66:VAL:HG23	1.83	0.61
1:F:45:LEU:HD21	1:H:168:LEU:HD22	1.83	0.61
1:G:176:ILE:HD13	1:H:18:GLY:HA2	1.83	0.61
1:D:198:GLY:HA2	1:D:202:LEU:HD23	1.81	0.61
1:H:162:ALA:HB3	1:H:163:PRO:HD3	1.83	0.61
1:E:35:GLY:HA2	1:G:32:LEU:HD22	1.83	0.61
1:E:176:ILE:CD1	1:G:18:GLY:HA2	2.30	0.60
1:B:197:GLN:HB3	1:B:201:ALA:HB3	1.84	0.60
1:D:226:LEU:N	1:D:226:LEU:HD12	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:ILE:O	1:E:222:ILE:HG13	2.00	0.60
1:A:29:PHE:CG	1:A:30:PRO:HD2	2.37	0.60
1:B:149:ILE:HA	1:B:166:ILE:HD11	1.83	0.60
1:F:174:HIS:O	1:F:178:ILE:HG13	2.02	0.60
1:B:194:ALA:HB1	1:B:202:LEU:HD13	1.83	0.60
1:D:24:VAL:CG2	1:D:25:LEU:HD13	2.24	0.60
1:H:223:TYR:O	1:H:227:LEU:HD13	2.00	0.60
1:E:98:LEU:O	1:E:102:ILE:HG13	2.01	0.60
1:E:166:ILE:O	1:E:169:ALA:HB3	2.02	0.60
1:B:27:ALA:HB2	1:B:39:VAL:CG2	2.32	0.60
3:A:600:POQ:C5	3:A:600:POQ:C1	2.79	0.60
1:H:112:ALA:HA	1:H:197:GLN:NE2	2.16	0.60
1:B:21:GLY:O	1:B:25:LEU:HB2	2.02	0.59
1:G:132:LEU:O	1:G:136:VAL:HG23	2.02	0.59
1:B:198:GLY:CA	1:B:202:LEU:CD2	2.80	0.59
1:H:84:TYR:O	1:H:88:GLN:HG3	2.03	0.59
1:C:133:SER:O	1:C:137:VAL:HG23	2.03	0.59
1:D:174:HIS:O	1:D:178:ILE:HG13	2.03	0.59
1:G:63:ASN:OD1	1:G:186:ASN:HA	2.01	0.59
1:D:177:SER:O	1:D:179:PRO:N	2.35	0.59
1:E:137:VAL:HG11	1:E:180:VAL:HG11	1.83	0.59
1:G:155:LYS:HG3	1:G:156:PHE:CD1	2.38	0.59
1:G:23:ALA:HA	1:G:27:ALA:HB2	1.83	0.59
1:D:177:SER:O	1:D:179:PRO:CD	2.51	0.59
1:G:224:ARG:HD3	1:G:224:ARG:C	2.23	0.59
1:G:85:VAL:O	1:G:89:VAL:HG23	2.03	0.59
1:H:226:LEU:O	1:H:227:LEU:HB2	2.02	0.59
1:F:145:PHE:O	1:F:149:ILE:HG13	2.03	0.59
1:C:172:LEU:O	1:C:176:ILE:HG13	2.02	0.58
1:C:210:VAL:O	1:C:214:VAL:HG23	2.02	0.58
1:C:63:ASN:HB3	1:C:66:VAL:CG2	2.33	0.58
1:D:34:ILE:HB	1:D:38:GLY:HA3	1.85	0.58
1:A:93:ILE:HD13	1:A:192:ALA:HA	1.84	0.58
1:D:122:GLY:C	1:D:124:HIS:N	2.57	0.58
1:E:133:SER:OG	1:G:105:GLY:HA3	2.03	0.58
1:G:37:ALA:N	8:G:337:HOH:O	2.31	0.58
1:H:211:VAL:HB	1:H:212:PRO:HD3	1.85	0.58
1:A:162:ALA:O	1:A:166:ILE:HG12	2.04	0.58
1:C:63:ASN:OD1	1:C:186:ASN:HA	2.03	0.58
1:D:178:ILE:CB	1:D:179:PRO:HD3	2.33	0.58
1:B:70:LEU:HD23	1:B:150:HIS:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ILE:O	1:D:90:VAL:HG23	2.03	0.58
1:G:145:PHE:HB2	1:G:173:ILE:HD11	1.86	0.58
1:B:77:PRO:HB2	1:B:79:LYS:HG2	1.86	0.58
1:B:8:GLU:HG3	1:B:84:TYR:CD2	2.37	0.58
1:H:36:PHE:CD1	1:H:178:ILE:HG21	2.39	0.58
1:A:178:ILE:HB	1:A:179:PRO:HD3	1.85	0.57
1:C:24:VAL:CG1	1:C:24:VAL:O	2.52	0.57
1:C:175:LEU:HD11	1:D:41:LEU:HD23	1.86	0.57
1:G:122:GLY:O	1:G:123:GLU:HB2	2.04	0.57
1:C:122:GLY:C	1:C:124:HIS:N	2.58	0.57
1:D:73:GLY:O	1:D:224:ARG:HG3	2.04	0.57
1:C:200:TRP:HA	1:C:203:GLU:HB2	1.86	0.57
1:E:12:THR:OG1	1:E:62:PHE:HA	2.05	0.57
1:C:70:LEU:HD23	1:C:150:HIS:CE1	2.39	0.57
1:G:195:ILE:HA	1:G:202:LEU:HD11	1.86	0.57
1:H:112:ALA:O	1:H:113:ALA:HB3	2.04	0.57
1:A:137:VAL:HG11	1:A:180:VAL:HG11	1.86	0.57
1:B:132:LEU:O	1:B:136:VAL:HG23	2.04	0.57
1:B:141:LEU:HB3	1:B:173:ILE:HG23	1.86	0.57
1:E:185:VAL:HG12	1:E:185:VAL:O	2.04	0.57
1:C:178:ILE:H	1:C:179:PRO:CD	2.16	0.57
1:G:1:MET:O	1:G:5:LEU:HD23	2.04	0.57
1:A:187:PRO:HB3	1:A:209:TRP:HA	1.87	0.57
1:D:14:TRP:CD1	1:D:50:MET:HG2	2.39	0.57
1:H:29:PHE:CG	1:H:30:PRO:HD2	2.39	0.57
1:A:26:ALA:O	1:A:34:ILE:HG12	2.06	0.56
1:F:169:ALA:O	1:F:173:ILE:HG12	2.05	0.56
1:E:68:ILE:CD1	1:E:213:ILE:HD12	2.32	0.56
1:B:197:GLN:NE2	5:B:626:PO4:O2	2.35	0.56
1:E:20:CYS:O	1:E:24:VAL:HG23	2.06	0.56
1:G:155:LYS:HG3	1:G:156:PHE:CE1	2.40	0.56
1:G:115:GLY:CA	1:G:197:GLN:NE2	2.46	0.56
1:G:205:LEU:HD12	1:G:205:LEU:O	2.06	0.56
1:B:121:TYR:CE1	1:B:204:GLN:HB3	2.40	0.56
1:A:45:LEU:HD21	1:B:168:LEU:HD22	1.88	0.56
1:E:45:LEU:HD21	1:F:168:LEU:HD22	1.88	0.56
1:E:75:ARG:HH11	1:E:75:ARG:HG2	1.70	0.56
1:G:7:ALA:HB3	1:G:58:SER:HB3	1.85	0.56
1:C:150:HIS:HB3	1:C:223:TYR:CD1	2.40	0.56
1:E:66:VAL:HA	1:E:146:LEU:HD11	1.87	0.56
1:H:82:VAL:O	1:H:86:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:PHE:CG	1:C:30:PRO:HD2	2.41	0.56
1:H:11:GLY:HA3	1:H:62:PHE:CE2	2.41	0.56
1:B:106:LYS:HB2	1:D:129:TYR:CE1	2.40	0.56
1:B:17:PHE:HE1	1:D:141:LEU:HD21	1.70	0.56
1:D:100:TYR:HE1	1:D:111:ALA:HB2	1.70	0.56
1:G:63:ASN:ND2	1:G:66:VAL:HG23	2.18	0.56
1:C:8:GLU:HG2	1:C:58:SER:CB	2.36	0.56
1:D:84:TYR:O	1:D:88:GLN:HG3	2.05	0.56
1:H:206:TRP:CG	1:H:207:PHE:N	2.73	0.56
1:H:34:ILE:HB	1:H:38:GLY:HA3	1.88	0.56
1:B:137:VAL:HG23	1:B:138:GLU:N	2.21	0.56
1:C:227:LEU:HD11	8:D:1413:HOH:O	2.06	0.56
1:E:85:VAL:O	1:E:89:VAL:HG23	2.05	0.56
1:G:8:GLU:HG2	1:G:58:SER:HB2	1.88	0.56
8:F:651:HOH:O	1:H:227:LEU:HD11	2.05	0.56
1:A:149:ILE:HA	1:A:166:ILE:CD1	2.35	0.55
1:B:35:GLY:O	1:B:39:VAL:HG23	2.05	0.55
1:B:78:ALA:HA	1:B:81:VAL:HG23	1.88	0.55
1:F:171:THR:O	1:F:175:LEU:HG	2.06	0.55
1:B:24:VAL:HG23	1:B:25:LEU:HD13	1.88	0.55
1:E:122:GLY:O	1:E:123:GLU:CB	2.54	0.55
1:D:214:VAL:O	1:D:218:ILE:HG12	2.07	0.55
1:D:8:GLU:HG2	1:D:58:SER:HB2	1.88	0.55
1:G:112:ALA:O	1:G:197:GLN:OE1	2.25	0.55
1:E:162:ALA:O	1:E:166:ILE:HG12	2.06	0.55
1:C:177:SER:O	1:C:183:THR:OG1	2.22	0.54
1:C:48:LEU:HD23	1:C:48:LEU:C	2.27	0.54
1:E:29:PHE:CG	1:E:30:PRO:HD2	2.42	0.54
1:G:96:ALA:HB2	1:G:192:ALA:HB1	1.88	0.54
1:F:112:ALA:HA	1:F:197:GLN:HE21	1.72	0.54
1:F:112:ALA:O	1:F:197:GLN:NE2	2.40	0.54
1:F:8:GLU:HG3	1:F:84:TYR:CD2	2.42	0.54
1:A:45:LEU:CD2	1:B:168:LEU:HD22	2.37	0.54
1:D:43:PHE:CZ	1:D:189:ARG:NH1	2.76	0.54
1:B:222:ILE:HD13	1:F:132:LEU:HD11	1.88	0.54
1:G:147:LEU:O	1:G:147:LEU:HD12	2.07	0.54
1:B:90:VAL:O	1:B:94:VAL:HG23	2.07	0.54
1:B:45:LEU:HD22	1:D:168:LEU:HB3	1.89	0.54
1:B:145:PHE:O	1:B:149:ILE:HG13	2.07	0.54
1:D:197:GLN:HB3	1:D:201:ALA:HB3	1.88	0.54
1:H:78:ALA:HA	1:H:81:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HG2	1:A:75:ARG:NH1	2.19	0.54
1:D:187:PRO:HB3	1:D:209:TRP:CD2	2.43	0.54
1:F:149:ILE:HA	1:F:166:ILE:HD12	1.88	0.54
1:F:191:THR:O	1:F:195:ILE:HG12	2.07	0.54
1:B:198:GLY:CA	1:B:202:LEU:HD23	2.36	0.54
1:D:15:LEU:C	1:D:15:LEU:HD23	2.28	0.54
1:B:169:ALA:O	1:B:173:ILE:HG12	2.09	0.53
1:D:194:ALA:HA	1:D:201:ALA:HB1	1.88	0.53
1:E:138:GLU:OE1	1:E:184:SER:HB3	2.07	0.53
1:B:89:VAL:O	1:B:93:ILE:HG13	2.07	0.53
1:C:77:PRO:HB2	1:C:80:GLU:HG3	1.90	0.53
1:D:122:GLY:O	1:D:123:GLU:HB2	2.08	0.53
1:E:89:VAL:O	1:E:93:ILE:HG12	2.08	0.53
1:A:206:TRP:CG	1:A:207:PHE:N	2.75	0.53
1:B:132:LEU:HD11	1:F:222:ILE:CD1	2.39	0.53
1:G:209:TRP:O	1:G:213:ILE:HG13	2.08	0.53
1:E:119:ASN:HD22	1:E:182:ASN:HB3	1.73	0.53
1:F:121:TYR:CE1	1:F:204:GLN:HB3	2.44	0.53
1:G:122:GLY:C	1:G:124:HIS:N	2.62	0.53
1:C:187:PRO:HB3	1:C:209:TRP:CD2	2.44	0.53
1:C:24:VAL:C	1:C:25:LEU:HD12	2.28	0.53
1:F:135:LEU:O	1:F:139:LEU:HB2	2.08	0.53
1:G:121:TYR:HA	1:G:125:SER:HB2	1.89	0.53
1:A:48:LEU:C	1:A:48:LEU:HD23	2.29	0.53
1:A:18:GLY:HA2	1:B:176:ILE:HD11	1.89	0.53
1:D:121:TYR:O	1:D:122:GLY:O	2.27	0.53
1:E:58:SER:OG	1:E:59:GLY:N	2.42	0.53
1:E:206:TRP:CG	1:E:207:PHE:N	2.76	0.53
1:A:138:GLU:OE1	1:A:184:SER:HB3	2.10	0.52
1:B:14:TRP:CZ3	1:D:144:GLY:HA3	2.45	0.52
1:C:73:GLY:O	1:C:224:ARG:HG3	2.08	0.52
1:C:96:ALA:HB2	1:C:192:ALA:HB1	1.91	0.52
1:G:176:ILE:CD1	1:H:18:GLY:HA2	2.39	0.52
1:H:11:GLY:HA2	1:H:50:MET:HG3	1.91	0.52
1:B:51:ALA:O	1:B:55:GLY:HA3	2.10	0.52
1:E:27:ALA:HA	1:E:34:ILE:HG13	1.91	0.52
1:C:168:LEU:HB3	1:D:45:LEU:HD22	1.91	0.52
1:F:70:LEU:HD23	1:F:150:HIS:CE1	2.45	0.52
1:H:122:GLY:O	1:H:123:GLU:HB2	2.10	0.52
1:H:21:GLY:HA2	1:H:99:LEU:HD11	1.92	0.52
1:B:66:VAL:HA	1:B:146:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:TRP:CD1	1:G:50:MET:HG2	2.44	0.52
1:F:105:GLY:HA3	1:H:133:SER:OG	2.10	0.52
1:A:46:THR:O	1:A:50:MET:HB2	2.10	0.52
1:C:137:VAL:HG22	1:D:102:ILE:HD13	1.91	0.52
1:C:218:ILE:O	1:C:222:ILE:HG12	2.10	0.52
1:D:173:ILE:O	1:D:177:SER:OG	2.28	0.52
1:E:189:ARG:HG2	1:E:189:ARG:HH11	1.75	0.52
1:F:51:ALA:O	1:F:55:GLY:HA3	2.09	0.52
1:G:180:VAL:HG12	1:G:181:THR:HG23	1.91	0.52
1:H:135:LEU:HD12	1:H:139:LEU:HD23	1.91	0.52
1:G:210:VAL:CG1	1:G:211:VAL:H	2.21	0.52
1:A:26:ALA:HB2	1:B:179:PRO:HG2	1.92	0.52
1:E:4:LYS:HD3	1:E:84:TYR:OH	2.10	0.52
1:G:202:LEU:HD22	1:G:202:LEU:N	2.24	0.52
1:H:149:ILE:HA	1:H:166:ILE:HD11	1.91	0.52
1:F:29:PHE:CD2	1:H:36:PHE:HE2	2.28	0.52
1:B:51:ALA:HB3	1:B:163:PRO:HB3	1.93	0.51
1:C:51:ALA:HB3	1:C:163:PRO:HB3	1.92	0.51
1:C:169:ALA:O	1:C:173:ILE:HG13	2.10	0.51
1:D:185:VAL:O	1:D:185:VAL:HG12	2.11	0.51
1:E:26:ALA:CB	1:F:179:PRO:CG	2.71	0.51
1:G:15:LEU:HD23	1:G:15:LEU:C	2.31	0.51
1:C:121:TYR:HA	1:C:125:SER:HB2	1.91	0.51
1:E:149:ILE:HA	1:E:166:ILE:CD1	2.41	0.51
1:F:177:SER:O	1:F:180:VAL:N	2.43	0.51
1:E:48:LEU:HD23	1:E:48:LEU:C	2.30	0.51
1:F:1:MET:O	1:F:5:LEU:HD23	2.11	0.51
1:G:39:VAL:HG12	1:G:43:PHE:HD2	1.76	0.51
1:C:51:ALA:O	1:C:55:GLY:HA3	2.11	0.50
1:D:155:LYS:HG2	8:D:1455:HOH:O	2.10	0.50
1:B:46:THR:HG22	1:D:172:LEU:HD21	1.92	0.50
1:F:63:ASN:ND2	1:F:186:ASN:HB2	2.26	0.50
1:G:20:CYS:O	1:G:24:VAL:HG23	2.11	0.50
1:G:133:SER:OG	1:H:105:GLY:HA3	2.10	0.50
1:H:174:HIS:O	1:H:178:ILE:HG13	2.11	0.50
1:H:34:ILE:O	1:H:38:GLY:HA3	2.11	0.50
1:B:197:GLN:HG3	1:B:201:ALA:HB2	1.93	0.50
1:C:205:LEU:O	1:C:205:LEU:HD12	2.12	0.50
1:D:206:TRP:CG	1:D:207:PHE:N	2.80	0.50
1:G:179:PRO:HG2	1:H:26:ALA:HB2	1.94	0.50
1:A:102:ILE:HD13	1:B:137:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLY:HA3	1:B:171:THR:OG1	2.12	0.50
1:C:137:VAL:HG11	1:C:177:SER:HB3	1.94	0.50
1:F:206:TRP:CG	1:F:207:PHE:N	2.79	0.50
1:H:187:PRO:HB3	1:H:209:TRP:CD2	2.46	0.50
1:C:227:LEU:HD11	8:D:1420:HOH:O	2.11	0.50
1:F:36:PHE:N	8:F:652:HOH:O	2.45	0.50
1:B:191:THR:O	1:B:195:ILE:HG12	2.12	0.50
1:C:206:TRP:O	1:C:210:VAL:HG12	2.11	0.50
1:G:121:TYR:O	1:G:122:GLY:O	2.29	0.50
1:A:56:HIS:CE1	1:A:57:ILE:HD11	2.47	0.50
1:B:185:VAL:O	1:B:185:VAL:HG13	2.12	0.50
1:A:34:ILE:HG22	1:B:37:ALA:HB2	1.92	0.50
1:B:63:ASN:HB3	1:B:66:VAL:HB	1.94	0.50
1:E:136:VAL:O	1:E:140:VAL:HG23	2.11	0.50
1:H:78:ALA:HA	1:H:81:VAL:CG2	2.41	0.50
1:A:169:ALA:O	1:A:173:ILE:HG13	2.12	0.50
1:E:178:ILE:HB	1:E:179:PRO:HD3	1.94	0.50
1:H:149:ILE:HG12	1:H:166:ILE:HD13	1.93	0.50
1:H:210:VAL:HG13	1:H:211:VAL:H	1.77	0.50
1:H:218:ILE:O	1:H:222:ILE:HG12	2.11	0.50
1:A:111:ALA:HB3	2:A:609:BGL:O3	2.12	0.50
1:E:122:GLY:C	1:E:124:HIS:H	2.16	0.50
1:F:176:ILE:O	1:F:176:ILE:HG22	2.12	0.50
1:D:100:TYR:CE1	1:D:111:ALA:HB2	2.47	0.49
1:G:94:VAL:O	1:G:97:ALA:HB3	2.12	0.49
1:A:100:TYR:CE1	1:A:111:ALA:HB2	2.47	0.49
1:C:34:ILE:HD12	1:C:38:GLY:C	2.32	0.49
1:E:132:LEU:C	1:E:132:LEU:HD13	2.33	0.49
1:F:133:SER:O	1:F:137:VAL:HG22	2.12	0.49
1:G:11:GLY:HA2	1:G:50:MET:HG3	1.94	0.49
1:H:46:THR:OG1	1:H:47:VAL:N	2.45	0.49
1:D:55:GLY:C	1:D:57:ILE:H	2.16	0.49
1:H:11:GLY:HA3	1:H:62:PHE:CD2	2.47	0.49
1:B:28:GLY:O	1:B:29:PHE:O	2.30	0.49
1:D:121:TYR:CE1	1:D:204:GLN:HB3	2.47	0.49
1:E:186:ASN:OD1	1:E:188:ALA:HB3	2.12	0.49
1:F:194:ALA:O	1:F:202:LEU:HD21	2.12	0.49
1:F:13:PHE:CE2	1:F:95:ALA:HA	2.48	0.49
1:H:122:GLY:N	1:H:125:SER:HB2	2.21	0.49
1:E:15:LEU:HD23	1:E:15:LEU:C	2.32	0.49
1:F:200:TRP:HA	1:F:203:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:TRP:CG	1:G:207:PHE:N	2.80	0.49
1:C:66:VAL:HG13	1:C:149:ILE:HD13	1.94	0.49
1:E:52:PHE:CZ	1:E:163:PRO:HB2	2.48	0.49
1:G:8:GLU:HG2	1:G:58:SER:CB	2.43	0.49
1:A:121:TYR:CE1	1:A:204:GLN:HB3	2.47	0.49
1:C:194:ALA:HB1	1:C:202:LEU:HD23	1.93	0.49
1:F:78:ALA:HA	1:F:81:VAL:HG23	1.93	0.49
1:A:73:GLY:HA3	1:A:150:HIS:NE2	2.27	0.49
1:C:14:TRP:CD1	1:C:50:MET:HG2	2.47	0.49
1:D:11:GLY:HA2	1:D:50:MET:HG3	1.95	0.49
1:D:211:VAL:HB	1:D:212:PRO:HD3	1.95	0.49
1:H:214:VAL:O	1:H:218:ILE:HG12	2.12	0.49
1:H:21:GLY:HA2	1:H:99:LEU:CD1	2.42	0.49
1:A:112:ALA:O	1:A:114:SER:N	2.46	0.49
1:A:19:GLY:HA3	1:A:43:PHE:CE1	2.48	0.49
1:F:202:LEU:N	1:F:202:LEU:HD22	2.27	0.49
1:G:169:ALA:O	1:G:173:ILE:HG13	2.12	0.49
1:G:185:VAL:O	1:G:185:VAL:HG12	2.13	0.49
1:H:155:LYS:HG2	8:H:522:HOH:O	2.13	0.49
1:E:112:ALA:O	1:E:113:ALA:HB3	2.13	0.49
1:G:4:LYS:HA	1:G:58:SER:HB3	1.95	0.49
1:H:8:GLU:HG2	1:H:58:SER:HB2	1.93	0.49
1:A:198:GLY:HA2	1:A:202:LEU:CD1	2.43	0.48
1:E:187:PRO:HB3	1:E:209:TRP:HA	1.95	0.48
1:E:93:ILE:HD13	1:E:192:ALA:HA	1.95	0.48
1:F:16:VAL:O	1:F:20:CYS:HB2	2.13	0.48
1:F:222:ILE:HG23	1:F:226:LEU:HD12	1.95	0.48
1:C:100:TYR:HE1	1:C:111:ALA:HB2	1.78	0.48
1:C:122:GLY:H	1:C:125:SER:HB2	1.79	0.48
1:F:112:ALA:HA	1:F:197:GLN:NE2	2.27	0.48
1:A:71:TRP:HE1	1:A:78:ALA:HB2	1.78	0.48
1:E:223:TYR:CE1	1:E:227:LEU:HD23	2.48	0.48
1:H:70:LEU:HD23	1:H:150:HIS:CE1	2.48	0.48
1:A:206:TRP:CD2	1:A:207:PHE:N	2.81	0.48
1:D:142:SER:HA	1:D:185:VAL:HG13	1.95	0.48
1:E:121:TYR:CE1	1:E:204:GLN:HB3	2.48	0.48
1:E:52:PHE:CE1	1:E:163:PRO:HG2	2.49	0.48
1:E:8:GLU:OE2	1:E:61:HIS:HB2	2.13	0.48
1:H:200:TRP:HA	1:H:203:GLU:HB2	1.95	0.48
1:F:3:ARG:NH1	1:H:227:LEU:HG	2.25	0.48
1:B:164:ILE:O	1:B:168:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:ILE:HD11	1:G:18:GLY:HA2	1.95	0.48
1:B:11:GLY:HA2	1:B:50:MET:CG	2.38	0.48
1:H:76:PHE:CD2	1:H:77:PRO:HD2	2.48	0.48
1:C:17:PHE:O	1:C:21:GLY:HA3	2.13	0.48
1:C:210:VAL:HG13	1:C:211:VAL:N	2.28	0.48
1:E:41:LEU:CD1	1:E:45:LEU:HG	2.44	0.48
1:E:46:THR:O	1:E:50:MET:HB2	2.14	0.48
1:H:226:LEU:HD12	1:H:226:LEU:N	2.26	0.48
1:B:132:LEU:CD1	1:F:222:ILE:HD13	2.44	0.48
1:H:122:GLY:C	1:H:124:HIS:N	2.62	0.48
1:H:48:LEU:HD12	1:H:164:ILE:HA	1.95	0.48
1:H:63:ASN:ND2	1:H:185:VAL:O	2.45	0.48
1:E:34:ILE:O	1:E:35:GLY:O	2.32	0.48
1:G:174:HIS:CD2	1:G:183:THR:HB	2.48	0.48
1:G:208:PHE:O	1:G:212:PRO:HG2	2.13	0.48
1:G:194:ALA:O	1:G:202:LEU:HD21	2.14	0.47
1:H:8:GLU:OE2	1:H:61:HIS:HB2	2.13	0.47
1:H:97:ALA:HA	1:H:196:PHE:CE2	2.50	0.47
1:A:217:ILE:O	1:A:221:LEU:HG	2.13	0.47
1:D:141:LEU:HB3	1:D:173:ILE:HG23	1.96	0.47
1:D:145:PHE:O	1:D:149:ILE:HG13	2.14	0.47
1:D:68:ILE:CG2	1:D:217:ILE:HD11	2.43	0.47
1:F:141:LEU:HB3	1:F:173:ILE:HG23	1.95	0.47
1:H:100:TYR:HE1	1:H:111:ALA:CB	2.20	0.47
1:B:110:ASP:HB3	1:B:113:ALA:HB3	1.97	0.47
1:C:7:ALA:HB3	1:C:58:SER:HB3	1.96	0.47
1:H:1:MET:HG3	1:H:4:LYS:HD2	1.97	0.47
1:F:29:PHE:CD2	1:H:36:PHE:CE2	3.02	0.47
1:B:4:LYS:HG2	1:B:57:ILE:O	2.13	0.47
1:C:122:GLY:H	1:C:125:SER:CB	2.28	0.47
1:D:125:SER:O	1:D:126:PRO:C	2.52	0.47
1:F:24:VAL:HG23	1:F:25:LEU:HD13	1.95	0.47
1:G:17:PHE:O	1:G:21:GLY:HA3	2.15	0.47
1:G:210:VAL:CG1	1:G:211:VAL:N	2.77	0.47
1:D:24:VAL:HG23	1:D:25:LEU:N	2.30	0.47
1:E:174:HIS:O	1:E:178:ILE:HG12	2.14	0.47
1:B:17:PHE:CE1	1:D:141:LEU:HD21	2.49	0.47
1:F:106:LYS:HB2	1:H:129:TYR:CE1	2.49	0.47
1:G:37:ALA:O	1:G:40:ALA:HB3	2.14	0.47
1:H:205:LEU:HD23	1:H:205:LEU:C	2.35	0.47
1:D:51:ALA:HB3	1:D:163:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:PHE:O	1:G:211:VAL:HG23	2.15	0.47
1:H:137:VAL:HG13	1:H:138:GLU:N	2.30	0.47
1:H:42:ALA:O	1:H:46:THR:HG23	2.15	0.47
1:H:48:LEU:C	1:H:48:LEU:HD23	2.35	0.47
1:B:28:GLY:O	1:B:29:PHE:C	2.53	0.47
1:B:73:GLY:HA3	1:B:150:HIS:NE2	2.29	0.47
1:D:137:VAL:HG13	1:D:138:GLU:N	2.29	0.47
1:F:63:ASN:O	1:F:66:VAL:N	2.46	0.47
1:A:76:PHE:CD2	1:A:77:PRO:HD2	2.50	0.47
1:C:76:PHE:CE1	1:C:80:GLU:HB2	2.50	0.47
1:E:11:GLY:HA2	1:E:50:MET:CG	2.41	0.47
1:E:141:LEU:HD13	1:E:173:ILE:HG23	1.96	0.47
1:G:175:LEU:HD11	1:H:41:LEU:HD23	1.96	0.47
1:H:15:LEU:C	1:H:15:LEU:HD23	2.34	0.47
1:A:121:TYR:CD2	1:A:131:MET:HB2	2.50	0.47
1:A:136:VAL:O	1:A:140:VAL:HG23	2.15	0.47
1:E:121:TYR:CD2	1:E:131:MET:HB2	2.50	0.47
1:G:100:TYR:HE1	1:G:111:ALA:HB2	1.79	0.47
1:H:122:GLY:O	1:H:124:HIS:N	2.46	0.47
1:H:39:VAL:HG12	1:H:43:PHE:HD2	1.80	0.47
1:H:55:GLY:C	1:H:57:ILE:H	2.18	0.47
1:A:58:SER:HB2	1:A:84:TYR:OH	2.15	0.46
1:D:198:GLY:CA	1:D:202:LEU:HD23	2.44	0.46
1:F:48:LEU:HD23	1:F:48:LEU:C	2.35	0.46
1:H:138:GLU:O	1:H:142:SER:OG	2.30	0.46
1:B:208:PHE:O	1:B:212:PRO:HG3	2.15	0.46
1:C:197:GLN:O	1:C:199:GLY:N	2.43	0.46
1:D:98:LEU:O	1:D:102:ILE:HG13	2.15	0.46
1:D:226:LEU:O	1:D:227:LEU:CB	2.62	0.46
1:F:194:ALA:HA	1:F:201:ALA:HB1	1.98	0.46
1:D:195:ILE:HA	1:D:202:LEU:HD11	1.97	0.46
1:E:206:TRP:CD2	1:E:207:PHE:N	2.84	0.46
1:H:125:SER:HB3	1:H:128:GLY:HA2	1.96	0.46
1:H:182:ASN:HD22	1:H:182:ASN:HA	1.49	0.46
1:A:2:PHE:HE1	1:B:226:LEU:HD22	1.79	0.46
1:G:137:VAL:CG1	1:G:177:SER:HB3	2.44	0.46
1:C:132:LEU:O	1:C:136:VAL:HG23	2.16	0.46
1:C:145:PHE:HB2	1:C:173:ILE:HD11	1.97	0.46
1:G:115:GLY:HA2	1:G:197:GLN:HE21	1.67	0.46
1:G:63:ASN:HB2	1:G:186:ASN:ND2	2.31	0.46
1:B:226:LEU:HD11	1:E:101:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ILE:HG22	1:D:217:ILE:CD1	2.44	0.46
1:E:68:ILE:O	1:E:71:TRP:HB3	2.15	0.46
8:B:1266:HOH:O	1:F:131:MET:HE1	2.15	0.46
1:G:136:VAL:O	1:G:140:VAL:HG23	2.16	0.46
1:G:125:SER:OG	1:G:180:VAL:O	2.21	0.46
1:A:20:CYS:HA	1:A:23:ALA:HB3	1.97	0.46
1:A:29:PHE:O	1:A:30:PRO:C	2.54	0.46
1:C:177:SER:C	1:C:183:THR:OG1	2.54	0.46
1:D:48:LEU:C	1:D:48:LEU:HD23	2.36	0.46
1:G:70:LEU:HD23	1:G:150:HIS:CE1	2.51	0.46
1:G:29:PHE:CD2	1:G:30:PRO:HD2	2.51	0.46
1:H:96:ALA:HB2	1:H:192:ALA:HB1	1.97	0.46
1:A:2:PHE:O	1:A:3:ARG:C	2.54	0.46
1:B:198:GLY:CA	1:B:202:LEU:HD21	2.43	0.46
1:F:60:GLY:HA2	1:F:62:PHE:CZ	2.50	0.46
1:G:172:LEU:O	1:G:176:ILE:HG13	2.16	0.46
1:B:50:MET:CE	1:B:54:VAL:HG13	2.46	0.46
1:A:172:LEU:HD21	1:C:46:THR:HG22	1.98	0.46
1:D:63:ASN:HB3	1:D:66:VAL:HB	1.98	0.46
1:H:191:THR:O	1:H:192:ALA:C	2.53	0.46
1:B:18:GLY:HA2	1:D:176:ILE:HD11	1.97	0.46
1:B:205:LEU:HD22	1:B:209:TRP:CD1	2.51	0.46
1:C:227:LEU:CG	8:D:1413:HOH:O	2.64	0.46
1:G:34:ILE:HB	1:G:38:GLY:HA3	1.98	0.46
1:A:71:TRP:NE1	1:A:78:ALA:HB2	2.31	0.45
1:B:15:LEU:HD23	1:B:15:LEU:C	2.36	0.45
1:B:187:PRO:HG3	1:B:212:PRO:HG2	1.97	0.45
1:C:35:GLY:O	1:C:39:VAL:HG23	2.16	0.45
1:C:76:PHE:CZ	1:C:80:GLU:HB2	2.51	0.45
1:B:49:THR:HG21	1:D:169:ALA:HA	1.97	0.45
1:D:70:LEU:HD23	1:D:70:LEU:HA	1.79	0.45
1:F:34:ILE:HB	1:F:38:GLY:HA3	1.98	0.45
1:H:121:TYR:O	1:H:122:GLY:O	2.33	0.45
1:H:14:TRP:CD1	1:H:50:MET:HG2	2.51	0.45
1:C:178:ILE:H	1:C:179:PRO:HD3	1.82	0.45
1:E:145:PHE:O	1:E:149:ILE:HG13	2.16	0.45
1:F:63:ASN:HB3	1:F:66:VAL:HB	1.98	0.45
1:A:122:GLY:C	1:A:124:HIS:N	2.68	0.45
1:D:200:TRP:HA	1:D:203:GLU:HB2	1.98	0.45
1:E:75:ARG:NH1	1:E:75:ARG:HG2	2.31	0.45
1:A:101:LEU:HD23	3:A:600:POQ:H262	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LEU:HB3	1:B:173:ILE:HD12	1.98	0.45
1:B:176:ILE:O	1:B:176:ILE:HG22	2.17	0.45
1:H:29:PHE:CD1	1:H:30:PRO:HD2	2.52	0.45
1:H:90:VAL:O	1:H:94:VAL:HG23	2.16	0.45
1:B:18:GLY:HA2	1:D:176:ILE:CD1	2.47	0.45
1:D:122:GLY:O	1:D:124:HIS:N	2.49	0.45
1:F:176:ILE:O	1:F:176:ILE:CG2	2.64	0.45
1:H:10:PHE:O	1:H:13:PHE:HB3	2.17	0.45
1:B:149:ILE:HA	1:B:166:ILE:HD12	1.98	0.45
1:E:76:PHE:HA	1:E:77:PRO:HD3	1.79	0.45
1:F:62:PHE:N	1:F:62:PHE:CD2	2.81	0.45
1:G:29:PHE:CG	1:G:30:PRO:HD2	2.51	0.45
1:G:39:VAL:HG12	1:G:43:PHE:CD2	2.51	0.45
7:G:639:AGA:O9	7:G:639:AGA:C4	2.54	0.45
1:G:6:ALA:O	1:G:10:PHE:HD1	1.99	0.45
1:A:213:ILE:O	1:A:217:ILE:HG13	2.17	0.45
1:C:133:SER:OG	1:D:105:GLY:HA3	2.16	0.45
1:D:112:ALA:O	1:D:113:ALA:HB3	2.16	0.45
1:F:4:LYS:HG2	1:F:57:ILE:O	2.16	0.45
1:D:127:GLY:N	1:D:179:PRO:O	2.47	0.45
1:D:64:PRO:HD3	1:D:188:ALA:HB2	1.98	0.45
1:E:121:TYR:O	1:E:122:GLY:O	2.35	0.45
1:H:198:GLY:C	1:H:202:LEU:CD2	2.84	0.45
1:A:149:ILE:HA	1:A:166:ILE:HD12	1.98	0.45
1:B:145:PHE:CE2	1:B:149:ILE:HD11	2.52	0.45
1:D:141:LEU:CD1	1:D:173:ILE:HG23	2.41	0.45
1:A:206:TRP:O	1:A:209:TRP:HB2	2.17	0.45
1:B:184:SER:C	1:B:186:ASN:H	2.19	0.45
1:F:198:GLY:HA2	1:F:202:LEU:HD23	1.98	0.45
1:G:174:HIS:O	1:G:178:ILE:HG13	2.17	0.45
2:B:604:BGL:H4'1	1:F:217:ILE:HG21	1.98	0.44
1:D:225:THR:HB	1:D:226:LEU:HD12	1.98	0.44
1:E:19:GLY:HA3	1:E:43:PHE:CE1	2.51	0.44
1:F:195:ILE:HD13	1:F:202:LEU:HD11	1.98	0.44
1:F:200:TRP:HA	1:F:203:GLU:CD	2.38	0.44
1:A:41:LEU:O	1:A:42:ALA:C	2.54	0.44
1:C:15:LEU:HD23	1:C:15:LEU:O	2.17	0.44
1:G:194:ALA:HA	1:G:201:ALA:HB1	1.99	0.44
1:H:210:VAL:HG13	1:H:211:VAL:N	2.32	0.44
1:A:129:TYR:CZ	1:C:106:LYS:HB2	2.52	0.44
1:A:191:THR:O	1:A:195:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:LEU:HA	1:C:149:ILE:HD12	1.99	0.44
1:D:207:PHE:CZ	1:D:211:VAL:HG21	2.51	0.44
1:E:29:PHE:HB3	1:E:33:GLY:HA2	1.98	0.44
1:F:162:ALA:O	1:F:166:ILE:HG12	2.18	0.44
1:A:144:GLY:O	1:A:148:VAL:HG23	2.17	0.44
1:B:50:MET:HE3	1:B:54:VAL:HG22	1.99	0.44
1:C:137:VAL:HG21	1:C:180:VAL:HG11	1.98	0.44
1:D:21:GLY:HA2	1:D:99:LEU:HD11	2.00	0.44
1:E:134:ALA:HB1	1:E:181:THR:HG22	1.98	0.44
1:E:46:THR:HG22	1:F:172:LEU:HD21	2.00	0.44
1:G:15:LEU:O	1:G:15:LEU:HD23	2.17	0.44
1:B:22:SER:HB2	1:B:34:ILE:HD11	2.00	0.44
1:B:63:ASN:H	1:B:88:GLN:NE2	2.15	0.44
1:D:197:GLN:HB3	1:D:201:ALA:CB	2.47	0.44
1:A:133:SER:OG	1:C:105:GLY:HA3	2.18	0.44
1:C:199:GLY:O	1:C:201:ALA:N	2.50	0.44
1:C:195:ILE:HA	1:C:202:LEU:HD21	1.99	0.44
1:E:115:GLY:O	1:E:118:SER:N	2.43	0.44
1:E:29:PHE:CD1	1:E:30:PRO:HD2	2.53	0.44
1:G:166:ILE:O	1:G:169:ALA:HB3	2.18	0.44
1:A:119:ASN:HD22	1:A:182:ASN:HB3	1.83	0.44
1:A:18:GLY:HA2	1:B:176:ILE:HD13	1.99	0.44
1:A:15:LEU:HA	1:A:46:THR:CB	2.48	0.44
1:H:178:ILE:HB	1:H:179:PRO:HD3	2.00	0.44
1:D:165:ALA:O	1:D:169:ALA:HB2	2.18	0.44
1:B:98:LEU:O	1:B:101:LEU:HB3	2.18	0.44
1:C:29:PHE:CD2	1:C:30:PRO:HD2	2.53	0.44
1:E:29:PHE:CD2	1:F:36:PHE:HE2	2.36	0.44
1:C:16:VAL:O	1:C:20:CYS:HB2	2.17	0.43
1:E:206:TRP:O	1:E:210:VAL:HG12	2.17	0.43
1:D:191:THR:HA	1:D:205:LEU:CD1	2.48	0.43
1:E:214:VAL:O	1:E:218:ILE:HG13	2.18	0.43
1:F:21:GLY:HA2	1:F:99:LEU:CD1	2.45	0.43
1:B:7:ALA:HB3	1:B:58:SER:HB3	2.00	0.43
1:A:187:PRO:HB2	1:A:209:TRP:CD2	2.53	0.43
1:B:112:ALA:HA	1:B:197:GLN:HE21	1.82	0.43
1:D:26:ALA:O	1:D:28:GLY:N	2.52	0.43
1:E:168:LEU:HB3	1:G:45:LEU:HD22	2.00	0.43
1:H:191:THR:HA	1:H:205:LEU:HD11	1.99	0.43
1:A:20:CYS:O	1:A:24:VAL:HG23	2.19	0.43
1:A:63:ASN:HB3	1:A:66:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:HIS:HB3	8:D:1412:HOH:O	2.17	0.43
1:E:147:LEU:HD13	1:E:147:LEU:O	2.19	0.43
1:H:169:ALA:O	1:H:173:ILE:HG13	2.18	0.43
1:A:101:LEU:O	1:A:101:LEU:HD13	2.19	0.43
1:A:147:LEU:O	1:A:147:LEU:HD13	2.19	0.43
1:D:166:ILE:O	1:D:169:ALA:HB3	2.19	0.43
1:E:73:GLY:HA3	1:E:150:HIS:NE2	2.34	0.43
1:E:119:ASN:ND2	1:E:183:THR:O	2.50	0.43
1:E:29:PHE:HB3	1:E:33:GLY:CA	2.48	0.43
1:E:81:VAL:O	1:E:85:VAL:HG23	2.18	0.43
1:F:28:GLY:O	1:F:29:PHE:C	2.57	0.43
1:G:36:PHE:CD1	1:G:178:ILE:HG21	2.53	0.43
1:G:23:ALA:HB2	1:G:39:VAL:HG11	2.00	0.43
1:A:101:LEU:HD21	1:F:226:LEU:CD1	2.45	0.43
1:A:136:VAL:HG12	1:C:102:ILE:HD11	2.00	0.43
1:D:36:PHE:CD1	1:D:178:ILE:HG21	2.53	0.43
1:D:2:PHE:O	1:D:3:ARG:C	2.57	0.43
1:F:90:VAL:O	1:F:94:VAL:HG23	2.18	0.43
1:G:178:ILE:N	1:G:179:PRO:CD	2.82	0.43
1:G:116:PHE:CD1	1:G:193:VAL:HG12	2.54	0.43
1:H:197:GLN:HB3	1:H:201:ALA:CB	2.49	0.43
1:B:194:ALA:HA	1:B:201:ALA:HB1	2.01	0.43
1:D:66:VAL:HA	1:D:146:LEU:HD11	2.00	0.43
1:D:217:ILE:O	1:D:218:ILE:C	2.57	0.43
1:D:82:VAL:O	1:D:86:ILE:HG12	2.19	0.43
1:A:129:TYR:CE1	1:C:106:LYS:HB2	2.54	0.43
1:A:227:LEU:HD22	1:C:3:ARG:HH21	1.81	0.43
1:E:223:TYR:O	1:E:227:LEU:HA	2.19	0.43
1:G:13:PHE:C	1:G:13:PHE:CD1	2.92	0.43
8:A:1112:HOH:O	1:B:36:PHE:N	2.51	0.43
1:D:206:TRP:O	1:D:210:VAL:HG12	2.19	0.43
1:D:8:GLU:OE2	1:D:61:HIS:HB2	2.19	0.43
1:E:181:THR:O	1:E:182:ASN:CB	2.67	0.43
1:E:71:TRP:HE1	1:E:78:ALA:HB2	1.84	0.43
1:F:185:VAL:HG13	1:F:185:VAL:O	2.19	0.43
1:B:29:PHE:CG	1:B:30:PRO:HD2	2.54	0.42
1:D:198:GLY:CA	1:D:202:LEU:HD21	2.41	0.42
1:F:101:LEU:CD2	1:H:136:VAL:HG21	2.49	0.42
1:A:149:ILE:O	1:A:153:THR:HG23	2.19	0.42
1:A:138:GLU:HB3	1:A:211:VAL:HG11	2.01	0.42
1:C:206:TRP:CD2	1:C:207:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:GLY:HA2	1:G:99:LEU:CD1	2.48	0.42
1:H:181:THR:O	1:H:182:ASN:HB2	2.19	0.42
1:H:64:PRO:CD	1:H:188:ALA:HB2	2.49	0.42
1:C:177:SER:C	1:C:183:THR:HG1	2.20	0.42
1:E:100:TYR:CE1	1:E:111:ALA:HB2	2.54	0.42
1:C:176:ILE:HD13	1:D:18:GLY:HA2	2.02	0.42
1:E:142:SER:HA	1:E:185:VAL:HG13	2.00	0.42
1:E:172:LEU:HD11	1:E:176:ILE:HD11	2.00	0.42
1:E:34:ILE:O	1:E:38:GLY:HA3	2.20	0.42
1:H:17:PHE:O	1:H:21:GLY:HA3	2.19	0.42
1:A:109:PHE:CG	1:A:110:ASP:N	2.87	0.42
1:A:121:TYR:O	1:A:122:GLY:O	2.36	0.42
1:A:170:LEU:HD12	1:A:170:LEU:HA	1.85	0.42
1:A:15:LEU:HA	1:A:46:THR:HB	2.01	0.42
1:D:164:ILE:HG22	1:D:168:LEU:HD12	2.02	0.42
1:E:28:GLY:O	1:E:29:PHE:C	2.56	0.42
1:F:17:PHE:HB2	1:F:95:ALA:HB1	2.01	0.42
1:F:184:SER:C	1:F:186:ASN:H	2.22	0.42
1:C:124:HIS:CE1	1:C:200:TRP:CG	3.07	0.42
1:C:138:GLU:OE2	1:C:184:SER:HB3	2.19	0.42
1:D:42:ALA:O	1:D:46:THR:HG23	2.20	0.42
1:F:202:LEU:H	1:F:202:LEU:HD22	1.83	0.42
1:G:206:TRP:CD2	1:G:207:PHE:N	2.87	0.42
1:H:121:TYR:CD2	1:H:131:MET:HB2	2.54	0.42
1:B:202:LEU:HD22	1:B:202:LEU:N	2.35	0.42
1:D:109:PHE:CG	1:D:110:ASP:N	2.88	0.42
1:D:125:SER:O	1:D:128:GLY:N	2.43	0.42
1:D:191:THR:HA	1:D:205:LEU:HD11	2.02	0.42
1:D:17:PHE:O	1:D:21:GLY:HA3	2.19	0.42
1:E:191:THR:HA	1:E:205:LEU:HD21	2.01	0.42
1:E:226:LEU:O	1:E:227:LEU:HB2	2.20	0.42
1:F:199:GLY:HA3	5:F:636:PO4:O4	2.20	0.42
1:F:194:ALA:O	1:F:202:LEU:CD2	2.68	0.42
1:D:121:TYR:HE1	1:D:204:GLN:HB3	1.83	0.42
1:F:121:TYR:HE1	1:F:204:GLN:HB3	1.83	0.42
1:G:178:ILE:O	1:G:182:ASN:HA	2.20	0.42
1:G:36:PHE:O	1:G:37:ALA:C	2.57	0.42
1:G:48:LEU:HD23	1:G:48:LEU:C	2.40	0.42
1:H:47:VAL:HG21	1:H:170:LEU:CD2	2.49	0.42
1:H:89:VAL:O	1:H:93:ILE:HG13	2.19	0.42
1:A:184:SER:C	1:A:186:ASN:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:GLU:HG3	1:A:84:TYR:CD2	2.55	0.42
1:A:8:GLU:OE2	1:A:61:HIS:HB2	2.19	0.42
1:B:223:TYR:O	1:B:227:LEU:HA	2.20	0.42
1:G:71:TRP:O	1:G:74:GLY:N	2.53	0.42
1:G:97:ALA:O	1:G:100:TYR:HB3	2.20	0.42
1:H:43:PHE:CZ	1:H:189:ARG:NH1	2.87	0.42
1:G:66:VAL:HG13	1:G:149:ILE:HD13	2.01	0.42
1:B:63:ASN:HB3	1:B:66:VAL:CG2	2.50	0.41
1:C:155:LYS:HG3	1:C:156:PHE:CD1	2.55	0.41
1:E:119:ASN:OD1	1:E:184:SER:HB2	2.19	0.41
1:E:29:PHE:CD2	1:F:36:PHE:CE2	3.07	0.41
1:F:73:GLY:HA3	1:F:150:HIS:NE2	2.35	0.41
1:E:127:GLY:O	1:G:106:LYS:HE2	2.20	0.41
1:G:224:ARG:HD3	1:G:224:ARG:O	2.18	0.41
1:C:36:PHE:N	8:C:1316:HOH:O	2.53	0.41
1:C:176:ILE:CD1	1:D:18:GLY:HA2	2.50	0.41
1:D:48:LEU:HD12	1:D:164:ILE:HA	2.02	0.41
1:D:21:GLY:HA2	1:D:99:LEU:CD1	2.50	0.41
1:E:15:LEU:HA	1:E:46:THR:HB	2.01	0.41
1:F:27:ALA:HB2	1:F:39:VAL:CG2	2.50	0.41
1:G:217:ILE:O	1:G:221:LEU:HG	2.20	0.41
1:H:68:ILE:CG2	1:H:217:ILE:HD11	2.48	0.41
1:A:145:PHE:O	1:A:149:ILE:HG13	2.20	0.41
1:D:97:ALA:HA	1:D:196:PHE:CE2	2.55	0.41
1:D:151:GLY:HA2	1:D:223:TYR:CE2	2.56	0.41
1:E:15:LEU:HA	1:E:46:THR:CB	2.50	0.41
1:E:191:THR:O	1:E:192:ALA:C	2.59	0.41
1:H:76:PHE:CG	1:H:77:PRO:HD2	2.55	0.41
1:A:210:VAL:HG22	1:A:211:VAL:N	2.35	0.41
1:A:50:MET:HB3	1:A:62:PHE:CE1	2.55	0.41
1:A:76:PHE:HA	1:A:77:PRO:HD3	1.81	0.41
1:B:100:TYR:HE1	1:B:111:ALA:HB2	1.85	0.41
1:B:13:PHE:HE2	1:B:94:VAL:HG12	1.86	0.41
1:C:15:LEU:HD23	1:C:15:LEU:C	2.40	0.41
1:A:101:LEU:C	1:A:101:LEU:HD13	2.40	0.41
1:A:224:ARG:O	1:A:224:ARG:HD3	2.20	0.41
1:A:63:ASN:HB3	1:A:66:VAL:CG2	2.51	0.41
1:C:23:ALA:HA	1:C:27:ALA:HB2	2.02	0.41
1:E:149:ILE:O	1:E:153:THR:HG23	2.20	0.41
1:E:210:VAL:HG12	1:E:210:VAL:H	1.60	0.41
1:E:52:PHE:CD1	1:E:163:PRO:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:LEU:HD22	1:F:209:TRP:CD1	2.55	0.41
1:G:125:SER:CB	1:G:129:TYR:H	2.33	0.41
1:H:191:THR:HA	1:H:205:LEU:CD1	2.51	0.41
1:A:144:GLY:HA3	1:C:14:TRP:CZ3	2.55	0.41
1:B:137:VAL:O	1:B:138:GLU:C	2.59	0.41
1:C:122:GLY:O	1:C:123:GLU:HB2	2.20	0.41
1:D:51:ALA:O	1:D:55:GLY:HA3	2.20	0.41
1:F:13:PHE:CD2	1:F:95:ALA:HB2	2.55	0.41
1:F:138:GLU:HG2	1:F:181:THR:HG21	2.03	0.41
1:G:138:GLU:OE2	1:G:184:SER:HB3	2.21	0.41
1:B:78:ALA:HA	1:B:81:VAL:CG2	2.49	0.41
1:D:177:SER:O	1:D:178:ILE:C	2.59	0.41
1:E:197:GLN:HB3	1:E:201:ALA:HB3	2.02	0.41
1:H:68:ILE:HG22	1:H:217:ILE:CD1	2.49	0.41
1:A:49:THR:HG21	1:B:169:ALA:HA	2.02	0.41
1:C:198:GLY:O	1:C:199:GLY:O	2.39	0.41
1:C:86:ILE:O	1:C:87:ALA:C	2.59	0.41
1:E:206:TRP:O	1:E:209:TRP:HB2	2.21	0.41
1:F:29:PHE:CG	1:F:30:PRO:HD2	2.56	0.41
1:H:125:SER:CB	1:H:129:TYR:H	2.33	0.41
1:H:145:PHE:CE2	1:H:149:ILE:HD11	2.56	0.41
1:A:121:TYR:HE1	1:A:204:GLN:HB3	1.86	0.41
1:A:187:PRO:HB3	1:A:208:PHE:O	2.20	0.41
1:A:70:LEU:HA	1:A:70:LEU:HD23	1.96	0.41
1:B:199:GLY:HA3	5:B:626:PO4:P	2.60	0.41
1:B:63:ASN:N	1:B:88:GLN:NE2	2.68	0.41
1:B:97:ALA:O	1:B:100:TYR:HB3	2.21	0.41
1:D:132:LEU:O	1:D:136:VAL:HG23	2.21	0.41
1:D:181:THR:O	1:D:182:ASN:HB2	2.20	0.41
1:E:67:THR:HG23	1:E:76:PHE:CE1	2.56	0.41
1:F:5:LEU:CD2	1:F:5:LEU:N	2.84	0.41
1:F:181:THR:O	1:F:182:ASN:CB	2.68	0.41
1:F:1:MET:CE	1:F:5:LEU:HD21	2.51	0.41
1:G:23:ALA:HB2	1:G:39:VAL:CG1	2.50	0.41
1:A:11:GLY:HA3	1:A:62:PHE:CE2	2.56	0.41
1:D:20:CYS:O	1:D:24:VAL:HG22	2.21	0.41
1:E:134:ALA:O	1:E:138:GLU:HB2	2.21	0.41
1:B:149:ILE:CG1	1:B:166:ILE:HD12	2.41	0.40
1:C:181:THR:O	1:C:182:ASN:CB	2.69	0.40
1:C:64:PRO:HG3	1:C:88:GLN:OE1	2.21	0.40
1:D:121:TYR:CD2	1:D:131:MET:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:GLU:HG2	1:E:58:SER:CB	2.50	0.40
1:F:162:ALA:CB	1:F:163:PRO:HD3	2.39	0.40
1:H:135:LEU:CD1	1:H:139:LEU:HD23	2.51	0.40
1:A:174:HIS:CE1	1:A:183:THR:HG21	2.56	0.40
1:A:205:LEU:HD22	1:A:205:LEU:O	2.21	0.40
1:B:1:MET:O	1:B:5:LEU:HD23	2.21	0.40
1:C:125:SER:CB	1:C:129:TYR:H	2.34	0.40
1:C:151:GLY:HA2	1:C:223:TYR:CZ	2.57	0.40
1:C:119:ASN:HB3	1:C:208:PHE:CZ	2.56	0.40
1:D:197:GLN:HG3	1:D:201:ALA:HB2	2.02	0.40
1:D:8:GLU:CG	1:D:84:TYR:CE2	3.02	0.40
1:F:214:VAL:O	1:F:218:ILE:HG12	2.21	0.40
1:G:154:ASP:OD1	1:G:156:PHE:HD1	2.04	0.40
1:C:176:ILE:O	1:C:176:ILE:HG22	2.21	0.40
1:D:162:ALA:HB3	1:D:163:PRO:HD3	2.02	0.40
1:E:149:ILE:HA	1:E:166:ILE:HD12	2.03	0.40
1:F:184:SER:O	1:F:185:VAL:HG12	2.21	0.40
1:G:36:PHE:N	8:G:337:HOH:O	2.55	0.40
1:H:198:GLY:CA	1:H:202:LEU:HD21	2.37	0.40
1:H:215:GLY:HA2	1:H:218:ILE:CG1	2.51	0.40
1:H:8:GLU:HG3	1:H:84:TYR:CD2	2.56	0.40
1:B:149:ILE:HG12	1:B:166:ILE:HG23	2.02	0.40
1:C:27:ALA:HA	1:C:34:ILE:HG13	2.04	0.40
1:D:137:VAL:HG11	1:D:180:VAL:HG11	2.04	0.40
1:D:147:LEU:HD12	1:D:223:TYR:HD2	1.87	0.40
1:D:52:PHE:CE2	1:D:163:PRO:HB2	2.56	0.40
1:E:176:ILE:HD13	1:G:18:GLY:HA2	1.99	0.40
1:E:60:GLY:HA2	1:E:62:PHE:CZ	2.57	0.40
1:G:28:GLY:O	1:G:29:PHE:C	2.58	0.40
1:G:55:GLY:C	1:G:57:ILE:H	2.25	0.40
1:G:61:HIS:CE1	1:G:70:LEU:HD12	2.56	0.40
1:H:75:ARG:HG3	1:H:75:ARG:NH1	2.37	0.40
1:B:129:TYR:CD2	1:B:180:VAL:HA	2.57	0.40
1:B:19:GLY:HA3	1:B:43:PHE:CD1	2.57	0.40
1:D:154:ASP:O	1:D:156:PHE:N	2.54	0.40
1:G:197:GLN:HG2	1:G:201:ALA:CB	2.51	0.40
1:H:63:ASN:C	1:H:63:ASN:OD1	2.60	0.40
1:H:24:VAL:HG21	1:H:99:LEU:HD21	2.03	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/231 (97%)	191 (85%)	26 (12%)	8 (4%)	3	23
1	B	225/231 (97%)	204 (91%)	13 (6%)	8 (4%)	3	23
1	C	225/231 (97%)	194 (86%)	22 (10%)	9 (4%)	3	21
1	D	225/231 (97%)	181 (80%)	35 (16%)	9 (4%)	3	21
1	E	225/231 (97%)	196 (87%)	19 (8%)	10 (4%)	2	19
1	F	225/231 (97%)	205 (91%)	14 (6%)	6 (3%)	5	30
1	G	225/231 (97%)	196 (87%)	22 (10%)	7 (3%)	4	26
1	H	225/231 (97%)	190 (84%)	28 (12%)	7 (3%)	4	26
All	All	1800/1848 (97%)	1557 (86%)	179 (10%)	64 (4%)	3	23

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	PRO
1	A	183	THR
1	B	29	PHE
1	B	30	PRO
1	C	30	PRO
1	D	27	ALA
1	D	178	ILE
1	E	183	THR
1	F	29	PHE
1	F	30	PRO
1	G	30	PRO
1	A	122	GLY
1	B	185	VAL
1	C	122	GLY
1	C	183	THR
1	C	199	GLY
1	C	200	TRP

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Mol	Chain	Res	Type
1	D	30	PRO
1	D	122	GLY
1	D	183	THR
1	E	30	PRO
1	E	35	GLY
1	E	122	GLY
1	F	183	THR
1	F	185	VAL
1	G	81	VAL
1	G	122	GLY
1	G	183	THR
1	H	30	PRO
1	H	122	GLY
1	H	183	THR
1	B	35	GLY
1	B	42	ALA
1	C	198	GLY
1	D	155	LYS
1	E	113	ALA
1	G	116	PHE
1	B	183	THR
1	C	81	VAL
1	C	123	GLU
1	D	56	HIS
1	D	113	ALA
1	E	58	SER
1	E	112	ALA
1	E	167	GLY
1	H	113	ALA
1	A	58	SER
1	A	158	PRO
1	B	112	ALA
1	B	180	VAL
1	C	209	TRP
1	F	192	ALA
1	H	109	PHE
1	D	158	PRO
1	E	158	PRO
1	G	35	GLY
1	G	185	VAL
1	E	185	VAL
1	A	185	VAL

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Mol	Chain	Res	Type
1	A	33	GLY
1	H	158	PRO
1	F	35	GLY
1	H	90	VAL
1	A	35	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/162 (98%)	152 (96%)	6 (4%)	33	67
1	B	158/162 (98%)	148 (94%)	10 (6%)	18	52
1	C	158/162 (98%)	150 (95%)	8 (5%)	24	60
1	D	158/162 (98%)	150 (95%)	8 (5%)	24	60
1	E	158/162 (98%)	153 (97%)	5 (3%)	39	71
1	F	158/162 (98%)	147 (93%)	11 (7%)	15	48
1	G	158/162 (98%)	152 (96%)	6 (4%)	33	67
1	H	158/162 (98%)	151 (96%)	7 (4%)	28	64
All	All	1264/1296 (98%)	1203 (95%)	61 (5%)	25	61

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	30	PRO
1	A	75	ARG
1	A	125	SER
1	A	189	ARG
1	A	210	VAL
1	B	25	LEU
1	B	30	PRO
1	B	107	THR
1	B	135	LEU

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Mol	Chain	Res	Type
1	B	137	VAL
1	B	185	VAL
1	B	189	ARG
1	B	205	LEU
1	B	221	LEU
1	B	224	ARG
1	C	30	PRO
1	C	43	PHE
1	C	107	THR
1	C	138	GLU
1	C	147	LEU
1	C	189	ARG
1	C	197	GLN
1	C	209	TRP
1	D	25	LEU
1	D	30	PRO
1	D	139	LEU
1	D	177	SER
1	D	182	ASN
1	D	189	ARG
1	D	224	ARG
1	D	226	LEU
1	E	25	LEU
1	E	30	PRO
1	E	75	ARG
1	E	189	ARG
1	E	210	VAL
1	F	30	PRO
1	F	62	PHE
1	F	107	THR
1	F	133	SER
1	F	135	LEU
1	F	137	VAL
1	F	185	VAL
1	F	189	ARG
1	F	205	LEU
1	F	221	LEU
1	F	224	ARG
1	G	30	PRO
1	G	107	THR
1	G	138	GLU
1	G	147	LEU

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Mol	Chain	Res	Type
1	G	189	ARG
1	G	197	GLN
1	H	25	LEU
1	H	30	PRO
1	H	139	LEU
1	H	182	ASN
1	H	189	ARG
1	H	224	ARG
1	H	226	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	88	GLN
1	C	197	GLN
1	D	182	ASN
1	G	197	GLN
1	H	182	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 ligands are modelled in this entry.

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
6	3PG	C	627	-	7,10,10	1.91	2 (28%)	10,14,14	3.53	3 (30%)
5	PO4	B	626	-	4,4,4	1.86	3 (75%)	6,6,6	0.41	0
4	PEE	B	602	-	13,13,50	0.26	0	12,12,55	0.88	0
6	3PG	G	637	-	7,10,10	2.19	3 (42%)	10,14,14	3.39	4 (40%)
2	BGL	B	604	-	18,18,20	2.74	8 (44%)	22,23,25	2.28	9 (40%)
7	AGA	G	639	-	14,14,29	6.39	8 (57%)	16,16,35	8.75	13 (81%)
3	POQ	A	600	-	40,40,40	5.29	29 (72%)	55,60,60	3.13	18 (32%)
4	PEE	A	612	-	8,8,50	0.89	0	7,7,55	1.03	1 (14%)
4	PEE	F	607	-	9,9,50	1.01	1 (11%)	8,8,55	1.29	1 (12%)
5	PO4	F	636	-	4,4,4	1.53	0	6,6,6	0.43	0
4	PEE	F	603	-	13,13,50	0.28	0	12,12,55	0.86	0
5	PO4	G	635	-	4,4,4	1.43	0	6,6,6	0.43	0
2	BGL	A	609	-	16,16,20	4.04	10 (62%)	19,21,25	3.43	10 (52%)
4	PEE	G	611	-	8,8,50	0.80	0	7,7,55	1.00	1 (14%)
5	PO4	C	625	-	4,4,4	1.82	1 (25%)	6,6,6	0.44	0
2	BGL	E	608	-	16,16,20	4.08	9 (56%)	19,21,25	3.47	10 (52%)
2	BGL	B	605	-	18,18,20	3.10	8 (44%)	22,23,25	2.36	9 (40%)
7	AGA	C	629	-	15,15,29	5.79	9 (60%)	17,17,35	6.28	14 (82%)
4	PEE	B	606	-	9,9,50	1.06	1 (11%)	8,8,55	1.31	1 (12%)
4	PEE	E	613	-	15,15,50	1.19	3 (20%)	14,14,55	2.14	4 (28%)

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
6	3PG	C	627	-	1/1/3/3	6/6/10/10	-
6	3PG	G	637	-	1/1/3/3	6/6/10/10	-
2	BGL	B	604	-	-	2/9/29/31	0/1/1/1
7	AGA	G	639	-	-	9/15/15/34	-
3	POQ	A	600	-	2/2/13/13	13/30/70/70	0/2/2/2
4	PEE	A	612	-	-	0/6/6/54	-
4	PEE	F	607	-	-	1/7/7/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEE	F	603	-	-	3/11/11/54	-
2	BGL	A	609	-	1/1/5/5	2/6/26/31	0/1/1/1
4	PEE	G	611	-	-	0/6/6/54	-
4	PEE	B	602	-	-	3/11/11/54	-
2	BGL	E	608	-	1/1/5/5	2/6/26/31	0/1/1/1
2	BGL	B	605	-	-	2/9/29/31	0/1/1/1
7	AGA	C	629	-	-	10/17/17/34	-
4	PEE	B	606	-	-	1/7/7/54	-
4	PEE	E	613	-	-	2/13/13/54	-

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	639	AGA	O8-C7	12.23	1.58	1.22
7	G	639	AGA	O9-C12	11.94	1.67	1.34
7	C	629	AGA	O8-C7	11.64	1.57	1.22
7	C	629	AGA	O9-C12	11.57	1.66	1.34
3	A	600	POQ	O5B-C1B	10.68	1.69	1.42
3	A	600	POQ	O5-C1	10.64	1.69	1.42
3	A	600	POQ	C1B-C2B	9.83	1.61	1.52
3	A	600	POQ	C1-C2	9.77	1.61	1.52
7	G	639	AGA	O7-C7	9.77	1.61	1.33
7	G	639	AGA	O9-C5	9.74	1.63	1.47
7	C	629	AGA	O7-C7	9.62	1.61	1.33
3	A	600	POQ	O11-C2	9.61	1.79	1.44
3	A	600	POQ	O21-C2B	9.56	1.78	1.44
2	B	605	BGL	C1-C2	9.04	1.60	1.52
2	E	608	BGL	O2-C2	8.82	1.58	1.43
3	A	600	POQ	C4B-C3B	7.77	1.72	1.52
2	A	609	BGL	O2-C2	7.74	1.56	1.43
3	A	600	POQ	O5B-C5B	7.55	1.62	1.44
3	A	600	POQ	O5-C5	7.40	1.62	1.44
3	A	600	POQ	C4-C3	7.40	1.71	1.52
2	A	609	BGL	C1-C2	7.31	1.59	1.52
2	B	604	BGL	C1-C2	7.16	1.58	1.52
7	C	629	AGA	O9-C5	6.97	1.64	1.46
2	A	609	BGL	O5-C1	6.96	1.60	1.42
2	E	608	BGL	O5-C1	6.56	1.59	1.42
2	A	609	BGL	O5-C5	6.04	1.58	1.44
7	C	629	AGA	C8-C7	-5.96	1.33	1.50
2	E	608	BGL	C1-C2	5.90	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	608	BGL	O5-C5	5.84	1.58	1.44
3	A	600	POQ	P3-O33	5.79	1.82	1.59
7	G	639	AGA	O10-C12	5.60	1.39	1.22
7	G	639	AGA	C8-C7	-5.57	1.34	1.50
7	C	629	AGA	O10-C12	5.50	1.38	1.22
3	A	600	POQ	O4-C4	4.75	1.54	1.43
3	A	600	POQ	P2-O21	4.69	1.72	1.60
3	A	600	POQ	P1-O11	4.54	1.72	1.60
6	G	637	3PG	O3-C2	4.47	1.53	1.42
2	B	605	BGL	C4-C5	4.46	1.62	1.53
2	E	608	BGL	O4-C4	4.46	1.53	1.43
3	A	600	POQ	P3-O31	4.41	1.77	1.59
2	B	604	BGL	C4-C5	4.28	1.62	1.53
3	A	600	POQ	O4B-C4B	4.27	1.53	1.43
6	C	627	3PG	O3-C2	4.24	1.52	1.42
2	B	605	BGL	C4'-C3'	4.10	1.74	1.51
3	A	600	POQ	P2-O23	4.06	1.65	1.50
2	B	604	BGL	C4'-C3'	4.04	1.74	1.51
2	E	608	BGL	C4-C3	3.97	1.62	1.52
2	A	609	BGL	C4-C3	3.80	1.62	1.52
2	A	609	BGL	O4-C4	3.79	1.51	1.43
3	A	600	POQ	C4-C5	3.78	1.61	1.53
3	A	600	POQ	C3B-C2B	3.77	1.62	1.52
2	B	605	BGL	C6'-C5'	3.72	1.80	1.49
2	B	604	BGL	C6'-C5'	3.66	1.79	1.49
3	A	600	POQ	C4B-C5B	3.45	1.60	1.53
3	A	600	POQ	C3-C2	3.40	1.61	1.52
3	A	600	POQ	P1-O12	3.38	1.62	1.50
3	A	600	POQ	P2-O24	3.37	1.72	1.59
3	A	600	POQ	P3-O32	3.33	1.70	1.55
2	E	608	BGL	C4-C5	3.22	1.60	1.52
3	A	600	POQ	P3-O34	3.21	1.62	1.50
7	G	639	AGA	C10-C9	3.18	1.76	1.49
3	A	600	POQ	P1-O14	3.05	1.71	1.59
2	E	608	BGL	C3-C2	3.00	1.60	1.52
7	C	629	AGA	C10-C9	2.97	1.74	1.49
2	B	604	BGL	C3-C2	2.78	1.59	1.52
7	G	639	AGA	C6-C5	2.78	1.57	1.50
2	B	605	BGL	C4-C3	2.77	1.59	1.52
2	A	609	BGL	O3-C3	2.69	1.49	1.43
2	B	605	BGL	O2-C2	2.62	1.47	1.43
2	A	609	BGL	C4-C5	2.60	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	608	BGL	O3-C3	2.59	1.49	1.43
2	A	609	BGL	C3-C2	2.54	1.59	1.52
4	B	606	PEE	C22-C21	2.51	1.65	1.51
2	B	605	BGL	C3-C2	2.51	1.59	1.52
3	A	600	POQ	C6-C5	2.46	1.59	1.51
4	E	613	PEE	C19-C18	2.42	1.65	1.51
4	F	607	PEE	C22-C21	2.40	1.65	1.51
4	E	613	PEE	C20-C19	-2.28	1.38	1.51
2	A	609	BGL	O1-C1	2.28	1.46	1.39
3	A	600	POQ	C6B-C5B	2.26	1.58	1.51
6	G	637	3PG	P-O3P	2.25	1.63	1.54
7	C	629	AGA	C6-C5	2.20	1.57	1.50
4	E	613	PEE	C21-C20	2.19	1.63	1.51
2	B	604	BGL	C6-C5	2.18	1.59	1.51
7	C	629	AGA	C4-C5	-2.16	1.45	1.51
2	B	604	BGL	C4-C3	2.15	1.57	1.52
5	B	626	PO4	P-O3	-2.13	1.48	1.54
6	C	627	3PG	P-O3P	2.12	1.63	1.54
5	B	626	PO4	P-O2	-2.10	1.48	1.54
2	B	604	BGL	O4-C4	-2.09	1.38	1.43
6	G	637	3PG	P-O2P	2.08	1.57	1.50
2	B	605	BGL	C6-C5	2.07	1.58	1.51
5	B	626	PO4	P-O4	-2.06	1.48	1.54
5	C	625	PO4	P-O4	-2.04	1.48	1.54
3	A	600	POQ	P1-O13	2.02	1.64	1.55

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	639	AGA	C5-O9-C12	28.16	154.11	117.88
7	C	629	AGA	C5-O9-C12	13.93	152.08	117.79
7	G	639	AGA	O9-C12-O10	-9.32	101.17	123.70
7	C	629	AGA	O9-C12-O10	-9.26	101.32	123.70
7	C	629	AGA	C9-C8-C7	9.11	151.78	114.34
7	G	639	AGA	C9-C8-C7	8.87	150.79	114.34
3	A	600	POQ	P1-O11-C2	8.30	149.59	119.41
3	A	600	POQ	P2-O21-C2B	8.28	149.53	119.41
2	A	609	BGL	C1'-O2-C2	8.08	133.60	114.32
7	C	629	AGA	O7-C6-C5	7.99	131.69	108.43
2	E	608	BGL	C1'-O2-C2	7.97	133.33	114.32
7	G	639	AGA	O7-C6-C5	7.94	131.25	108.38
6	C	627	3PG	P-O1P-C3	7.76	139.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	629	AGA	C6-C5-C4	-7.68	93.82	111.80
6	G	637	3PG	P-O1P-C3	7.62	139.27	118.30
3	A	600	POQ	C6-C5-C4	7.35	127.43	112.09
3	A	600	POQ	O5B-C5B-C6B	7.31	121.42	106.67
3	A	600	POQ	O5-C5-C6	7.22	121.23	106.67
3	A	600	POQ	C6B-C5B-C4B	7.21	127.14	112.09
2	A	609	BGL	O5-C5-C6	6.92	121.65	106.70
7	G	639	AGA	C4-C5-C6	-6.75	93.24	112.63
2	E	608	BGL	O5-C5-C6	6.70	121.18	106.70
6	C	627	3PG	O1P-C3-C2	6.06	125.42	107.94
6	G	637	3PG	O1P-C3-C2	5.67	124.31	107.94
2	E	608	BGL	C6-C5-C4	5.65	123.51	113.07
3	A	600	POQ	O32-P3-O34	-5.62	84.46	112.24
2	A	609	BGL	C6-C5-C4	5.37	122.99	113.07
7	C	629	AGA	O7-C7-C8	5.35	128.71	111.91
2	E	608	BGL	O2-C1'-C2'	5.29	128.11	109.56
7	C	629	AGA	C6-O7-C7	5.27	136.63	117.12
7	G	639	AGA	O10-C12-C13	-5.24	103.30	123.73
7	G	639	AGA	O7-C7-C8	5.23	128.33	111.91
7	C	629	AGA	O6-C4-C5	5.23	125.65	111.78
2	A	609	BGL	O2-C1'-C2'	5.10	127.44	109.56
7	C	629	AGA	O10-C12-C13	-5.08	103.92	123.73
7	G	639	AGA	C6-O7-C7	4.94	135.41	117.12
3	A	600	POQ	O33-P3-O34	-4.80	90.30	109.07
4	E	613	PEE	C20-C19-C18	4.74	138.51	114.42
7	C	629	AGA	C14-C13-C12	4.67	133.54	114.34
6	C	627	3PG	O3-C2-C3	-4.63	95.51	110.40
2	B	605	BGL	O5-C5-C4	-4.44	101.62	109.69
7	G	639	AGA	C14-C13-C12	4.36	132.24	114.34
6	G	637	3PG	O3-C2-C3	-4.30	96.58	110.40
2	B	604	BGL	O5-C5-C4	-4.25	101.98	109.69
4	E	613	PEE	C21-C20-C19	4.20	135.75	114.42
7	C	629	AGA	O8-C7-C8	-4.10	107.75	123.73
2	B	604	BGL	C1'-O2-C2	4.09	124.06	114.32
7	C	629	AGA	C15-C14-C13	4.07	130.08	112.67
7	G	639	AGA	O9-C12-C13	4.07	120.28	111.50
2	B	605	BGL	C1'-O2-C2	4.05	123.99	114.32
7	G	639	AGA	C15-C14-C13	4.05	129.99	112.67
2	B	605	BGL	C4'-C3'-C2'	-3.96	94.34	114.42
7	G	639	AGA	O8-C7-C8	-3.87	108.62	123.73
3	A	600	POQ	O21-C2B-C3B	3.83	117.58	108.66
3	A	600	POQ	O11-C2-C3	3.78	117.46	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	POQ	C4-C3-C2	3.78	118.31	109.68
2	B	604	BGL	C4'-C3'-C2'	-3.77	95.30	114.42
2	E	608	BGL	C3-C4-C5	-3.66	104.07	109.77
3	A	600	POQ	C4B-C3B-C2B	3.43	117.52	109.68
2	B	605	BGL	C6-C5-C4	3.36	120.88	113.00
2	A	609	BGL	O5-C5-C4	3.25	115.36	109.52
2	E	608	BGL	O5-C5-C4	3.23	115.31	109.52
7	C	629	AGA	O9-C12-C13	3.22	118.44	111.50
7	C	629	AGA	C10-C9-C8	-3.13	99.30	112.67
2	B	605	BGL	O4-C4-C3	3.07	117.44	110.35
2	B	604	BGL	C6-C5-C4	3.05	120.15	113.00
2	B	604	BGL	C3-C4-C5	-3.05	104.80	110.24
3	A	600	POQ	O3-C3-C4	-3.04	103.32	110.35
2	B	605	BGL	O6-C6-C5	3.04	121.71	111.29
2	B	604	BGL	O4-C4-C3	3.01	117.31	110.35
7	G	639	AGA	C10-C9-C8	-3.00	99.82	112.67
2	B	604	BGL	O6-C6-C5	2.97	121.48	111.29
2	B	605	BGL	C3-C4-C5	-2.95	104.98	110.24
2	B	605	BGL	C1-O5-C5	-2.94	108.12	113.66
2	A	609	BGL	C3'-C2'-C1'	-2.93	100.52	113.49
3	A	600	POQ	O31-P3-O34	-2.92	97.68	109.07
3	A	600	POQ	O31-C6-C5	-2.89	99.06	108.99
2	E	608	BGL	C4-C3-C2	2.81	116.09	109.68
2	A	609	BGL	C4-C3-C2	2.80	116.06	109.68
4	E	613	PEE	C24-C23-C22	-2.77	100.38	114.42
3	A	600	POQ	O3B-C3B-C4B	-2.75	104.00	110.35
4	E	613	PEE	C17-C16-C15	-2.74	100.52	114.42
2	A	609	BGL	O3-C3-C4	-2.72	104.06	110.35
2	A	609	BGL	C3-C4-C5	-2.71	105.55	109.77
2	E	608	BGL	O3-C3-C4	-2.70	104.12	110.35
2	B	604	BGL	O3-C3-C2	2.68	117.05	109.94
3	A	600	POQ	O32-P3-O33	-2.66	95.41	107.75
2	B	604	BGL	C1-O5-C5	-2.62	108.71	113.66
2	A	609	BGL	O4-C4-C3	2.60	116.35	110.35
2	E	608	BGL	C3'-C2'-C1'	-2.59	102.02	113.49
4	B	606	PEE	C27-C26-C25	2.51	132.47	113.42
3	A	600	POQ	O4-C4-C3	-2.48	104.61	110.35
4	F	607	PEE	C27-C26-C25	2.46	132.09	113.42
2	B	605	BGL	O3-C3-C2	2.34	116.14	109.94
6	G	637	3PG	O1P-P-O2P	2.25	112.78	106.47
4	G	611	PEE	C24-C23-C22	-2.17	103.40	114.42
2	E	608	BGL	O4-C4-C3	2.16	115.34	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	612	PEE	C24-C23-C22	-2.11	103.72	114.42

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	627	3PG	C2
6	G	637	3PG	C2
3	A	600	POQ	C5B
3	A	600	POQ	C5
2	A	609	BGL	C5
2	E	608	BGL	C5

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	627	3PG	C1-C2-C3-O1P
6	C	627	3PG	O3-C2-C3-O1P
6	C	627	3PG	C3-O1P-P-O3P
6	C	627	3PG	C3-O1P-P-O4P
7	G	639	AGA	O10-C12-O9-C5
7	G	639	AGA	C13-C12-O9-C5
6	G	637	3PG	C1-C2-C3-O1P
6	G	637	3PG	O3-C2-C3-O1P
6	G	637	3PG	C3-O1P-P-O2P
6	G	637	3PG	C3-O1P-P-O3P
6	G	637	3PG	C3-O1P-P-O4P
3	A	600	POQ	C3-C2-O11-P1
3	A	600	POQ	C4-C5-C6-O31
3	A	600	POQ	O5-C5-C6-O31
3	A	600	POQ	C6B-O33-P3-O32
3	A	600	POQ	C3B-C2B-O21-P2
3	A	600	POQ	C4B-C5B-C6B-O33
3	A	600	POQ	O5B-C5B-C6B-O33
7	C	629	AGA	O10-C12-O9-C5
7	C	629	AGA	C13-C12-O9-C5
7	C	629	AGA	C5-C6-O7-C7
4	E	613	PEE	C19-C20-C21-C22
7	G	639	AGA	C4-C5-O9-C12
4	E	613	PEE	C17-C18-C19-C20
2	B	604	BGL	O2-C1'-C2'-C3'
2	B	605	BGL	O2-C1'-C2'-C3'
3	A	600	POQ	C6-O31-P3-O33

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Mol	Chain	Res	Type	Atoms
7	G	639	AGA	C8-C7-O7-C6
6	G	637	3PG	C2-C3-O1P-P
2	E	608	BGL	O2-C1'-C2'-C3'
2	A	609	BGL	O2-C1'-C2'-C3'
4	F	603	PEE	C16-C17-C18-C19
7	G	639	AGA	C5-C6-O7-C7
7	G	639	AGA	O8-C7-O7-C6
4	B	602	PEE	C16-C17-C18-C19
7	C	629	AGA	C8-C7-O7-C6
4	F	603	PEE	C15-C16-C17-C18
4	F	607	PEE	C24-C25-C26-C27
6	C	627	3PG	C3-O1P-P-O2P
4	B	602	PEE	C15-C16-C17-C18
7	C	629	AGA	O8-C7-O7-C6
4	B	602	PEE	C14-C15-C16-C17
4	F	603	PEE	C14-C15-C16-C17
7	G	639	AGA	C4-C5-C6-O7
7	G	639	AGA	O9-C5-C6-O7
4	B	606	PEE	C24-C25-C26-C27
2	E	608	BGL	C3-C2-O2-C1'
2	A	609	BGL	C3-C2-O2-C1'
3	A	600	POQ	C5-C6-O31-P3
7	C	629	AGA	C4-C5-C6-O7
7	C	629	AGA	O9-C5-C6-O7
6	C	627	3PG	C2-C3-O1P-P
3	A	600	POQ	C5B-C6B-O33-P3
3	A	600	POQ	C6-O31-P3-O34
7	C	629	AGA	C4-C5-O9-C12
3	A	600	POQ	C15-O14-P1-O11
3	A	600	POQ	C25-O24-P2-O21
7	G	639	AGA	C12-C13-C14-C15
2	B	604	BGL	C3-C2-O2-C1'
2	B	605	BGL	C3-C2-O2-C1'
7	C	629	AGA	C12-C13-C14-C15
7	C	629	AGA	O10-C12-C13-C14

There are no ring outliers.

9 monomers are involved in 30 short contacts:

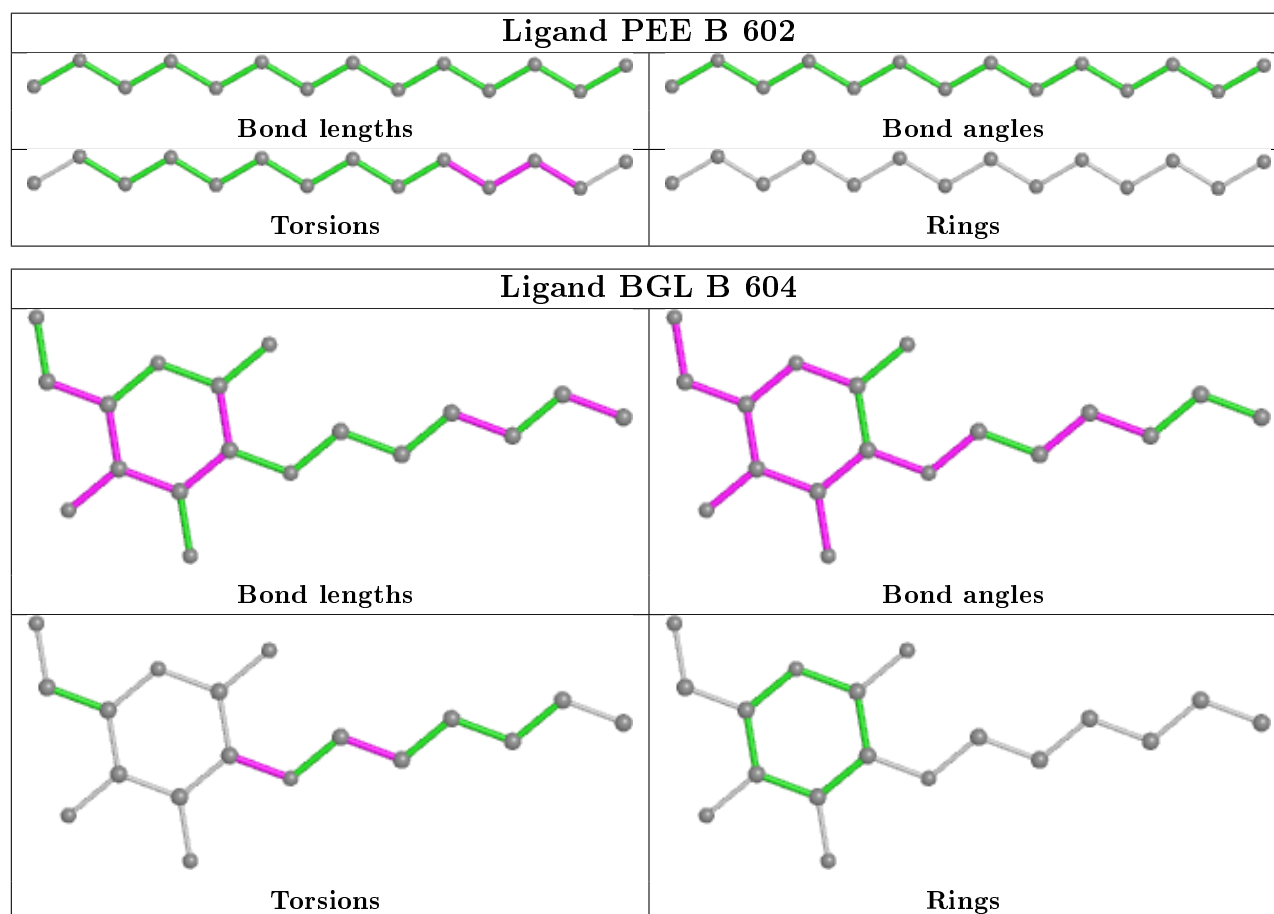
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	626	PO4	2	0
2	B	604	BGL	3	0

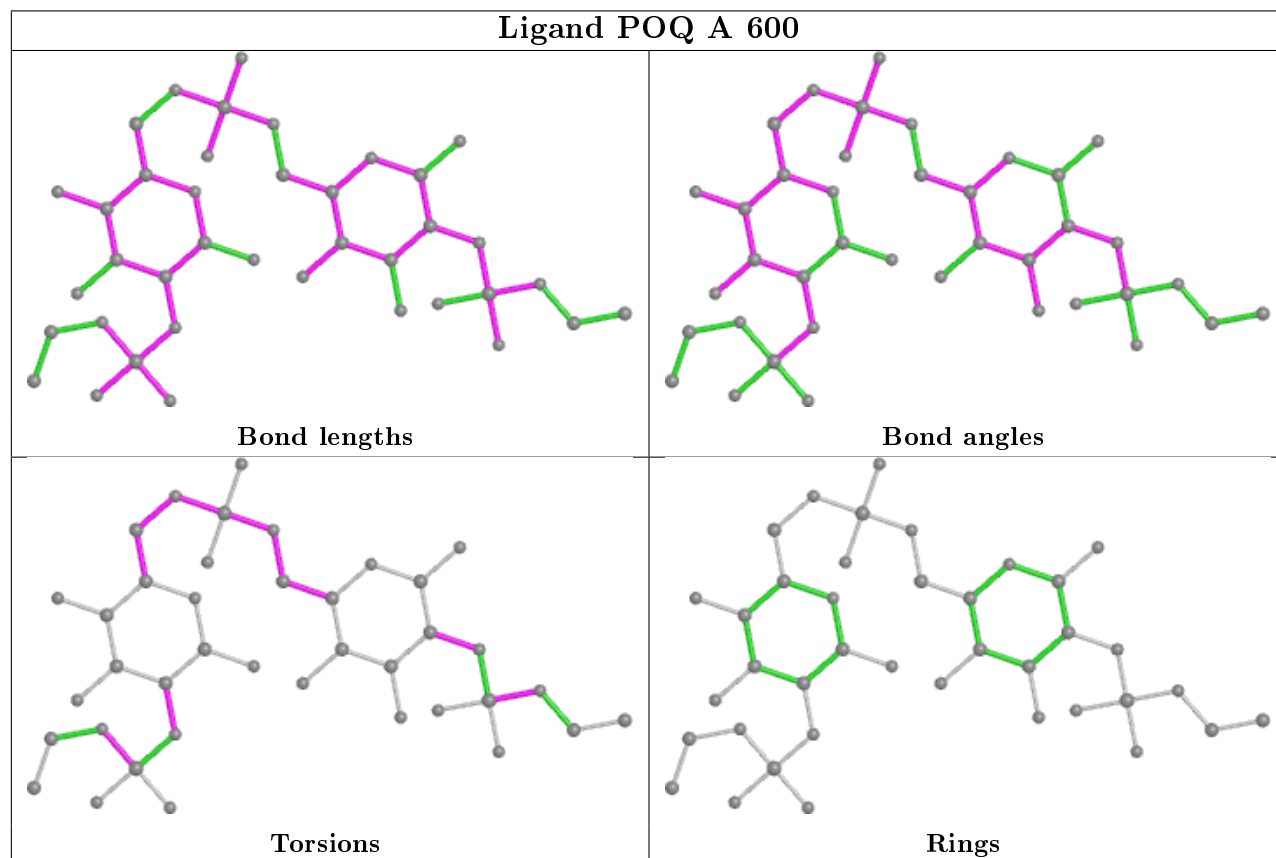
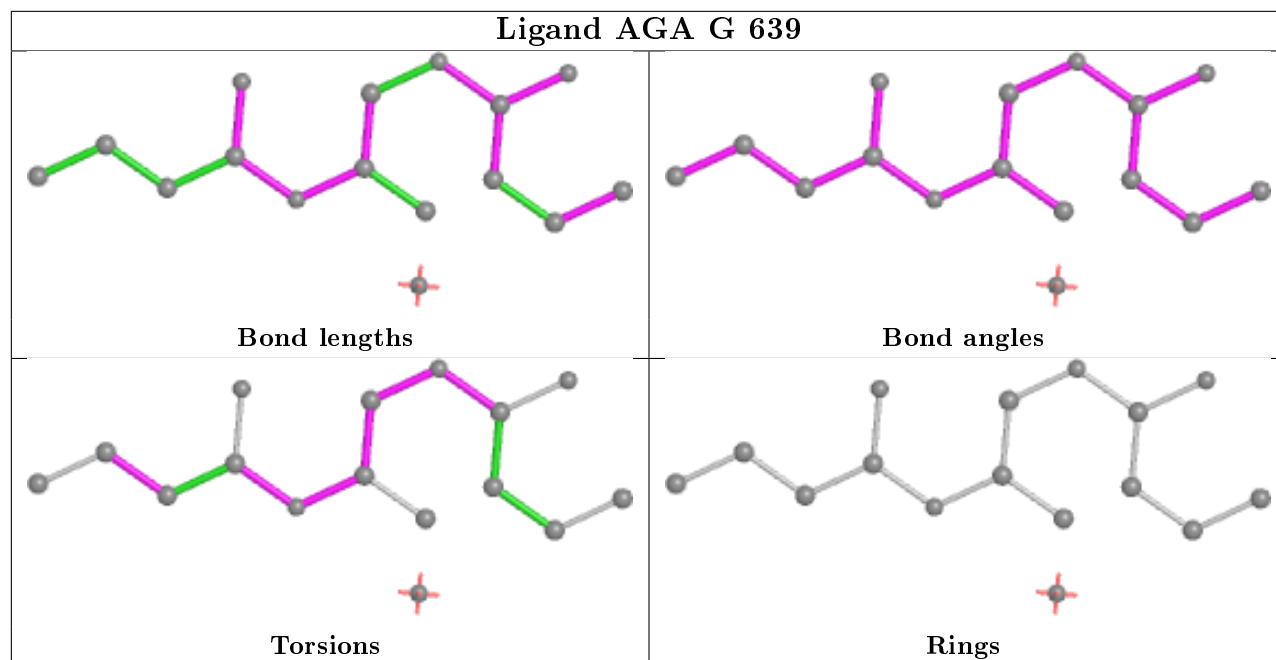
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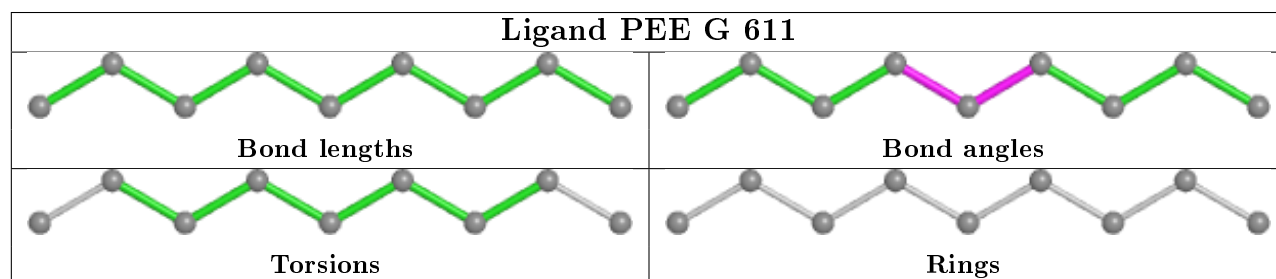
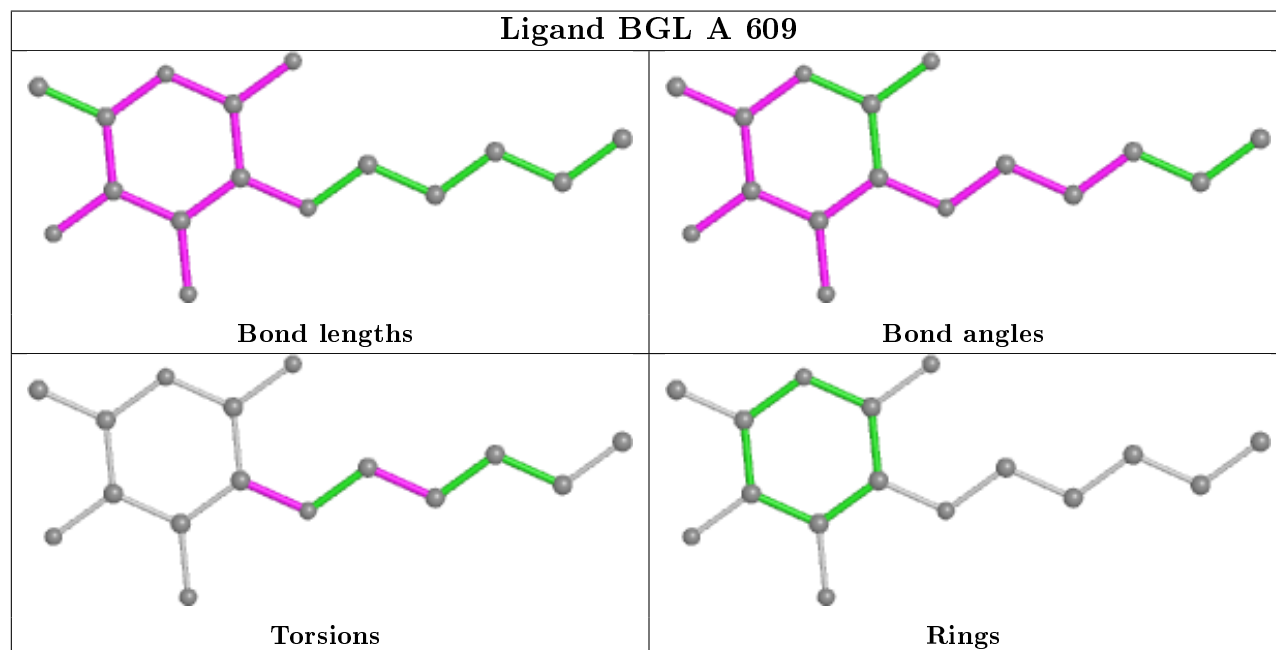
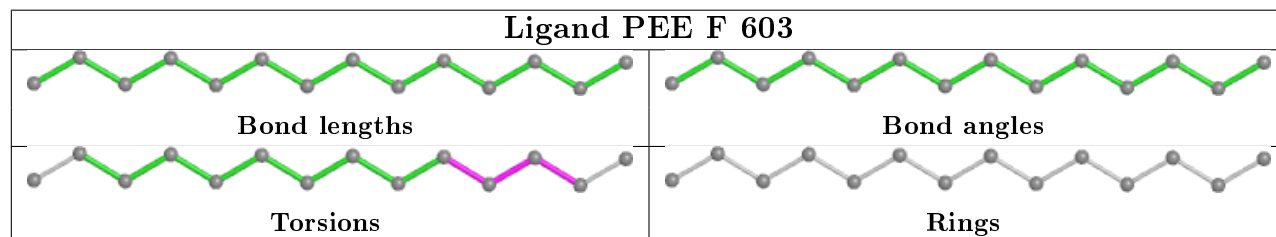
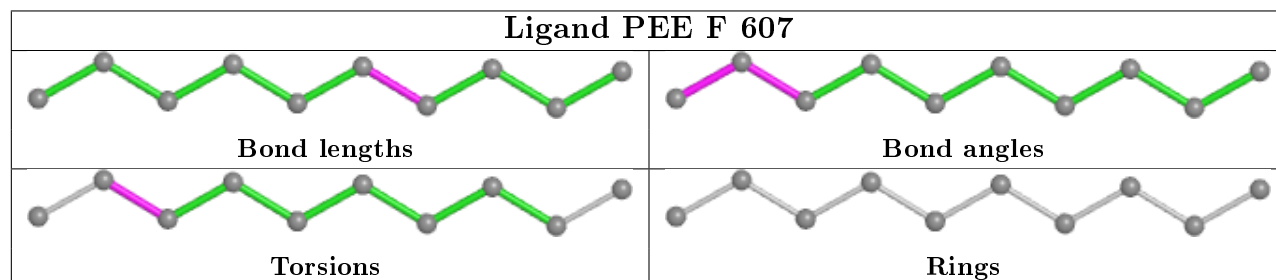
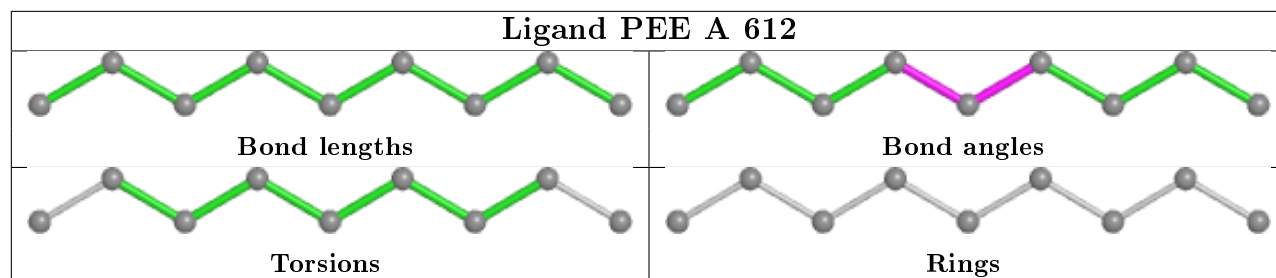
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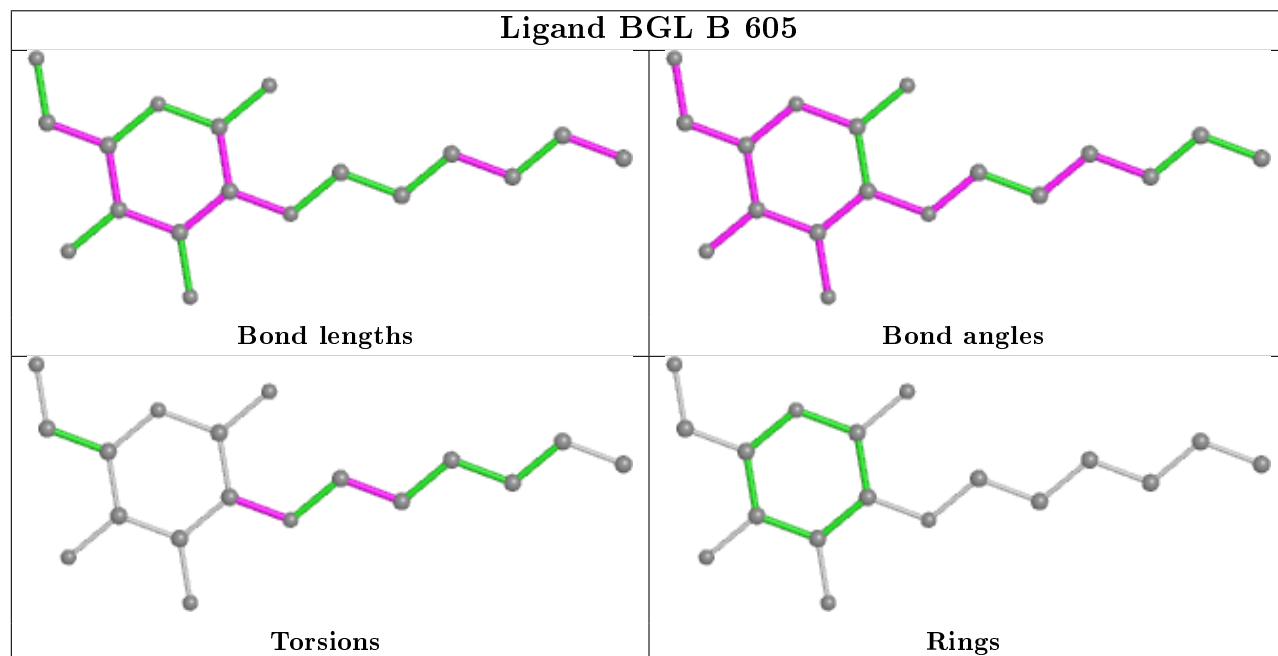
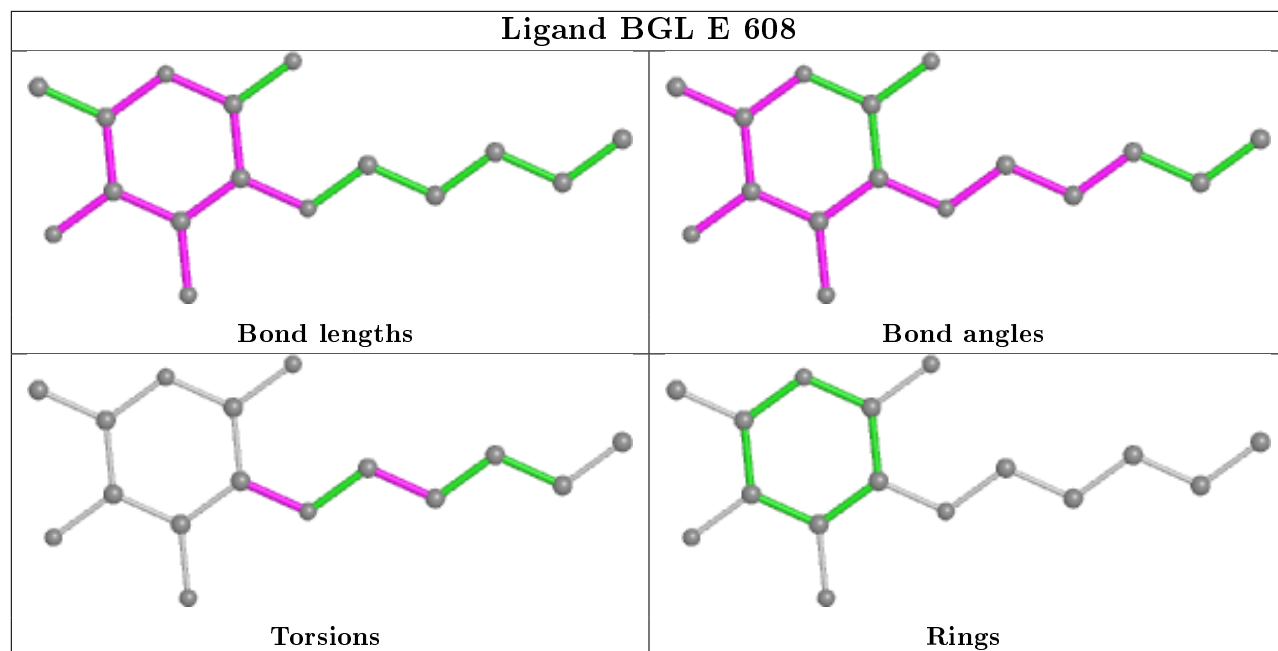
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	639	AGA	5	0
3	A	600	POQ	8	0
5	F	636	PO4	3	0
2	A	609	BGL	1	0
2	E	608	BGL	1	0
2	B	605	BGL	5	0
7	C	629	AGA	2	0

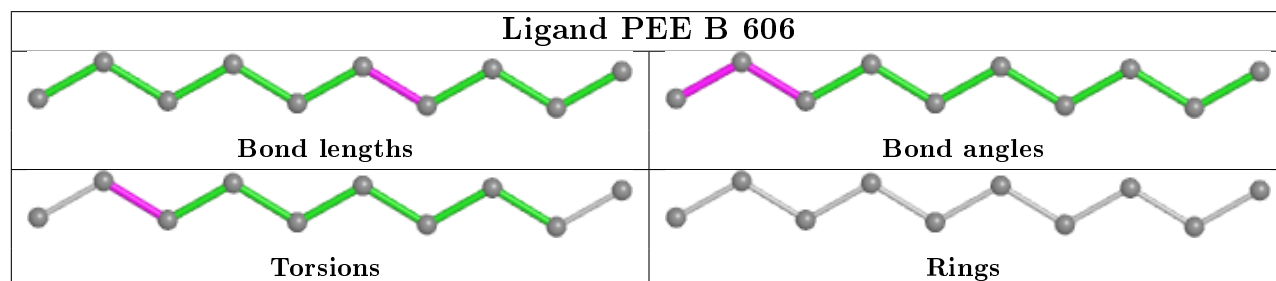
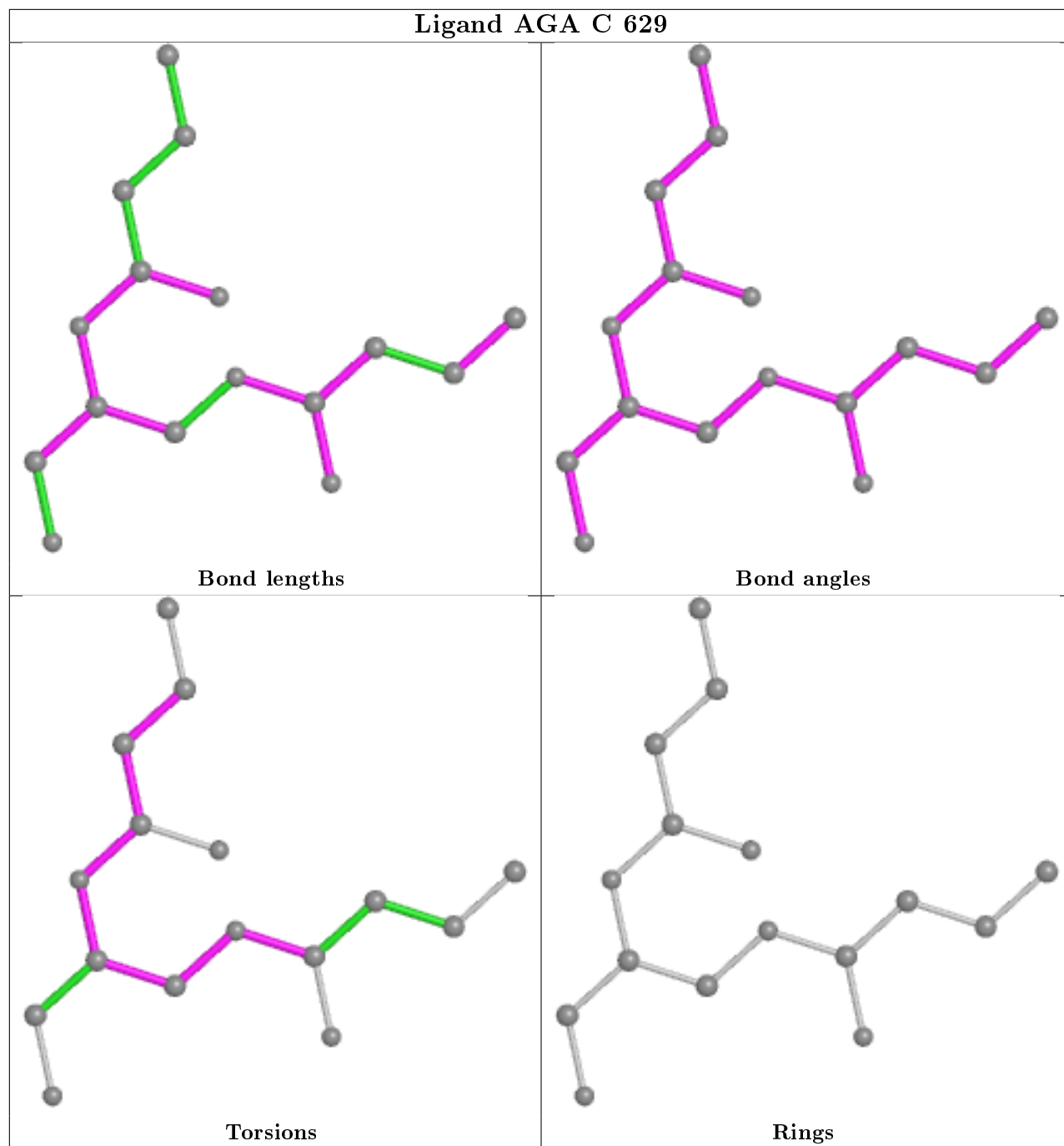
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

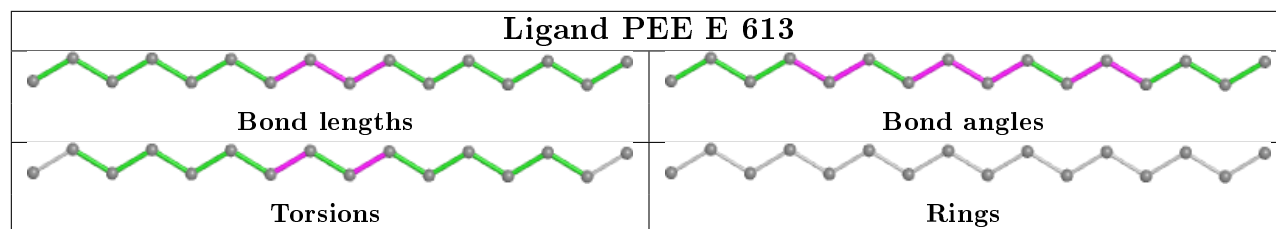












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/231 (98%)	-0.73	0 100 100	15, 32, 51, 66	0
1	B	227/231 (98%)	-0.65	0 100 100	14, 28, 48, 74	0
1	C	227/231 (98%)	-0.64	0 100 100	18, 38, 57, 77	0
1	D	227/231 (98%)	-0.58	1 (0%) 92 89	17, 37, 52, 78	0
1	E	227/231 (98%)	-0.61	0 100 100	16, 34, 53, 67	0
1	F	227/231 (98%)	-0.70	1 (0%) 92 89	15, 29, 50, 75	0
1	G	227/231 (98%)	-0.43	2 (0%) 84 75	21, 42, 59, 80	0
1	H	227/231 (98%)	-0.57	0 100 100	20, 38, 52, 77	0
All	All	1816/1848 (98%)	-0.61	4 (0%) 95 94	14, 35, 54, 80	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	156	PHE	2.3
1	G	198	GLY	2.2
1	F	111	ALA	2.0
1	D	226	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

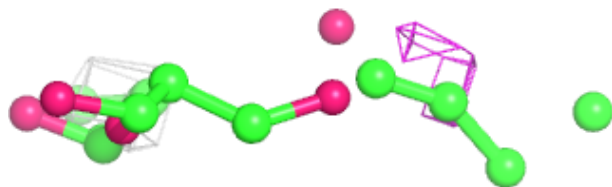
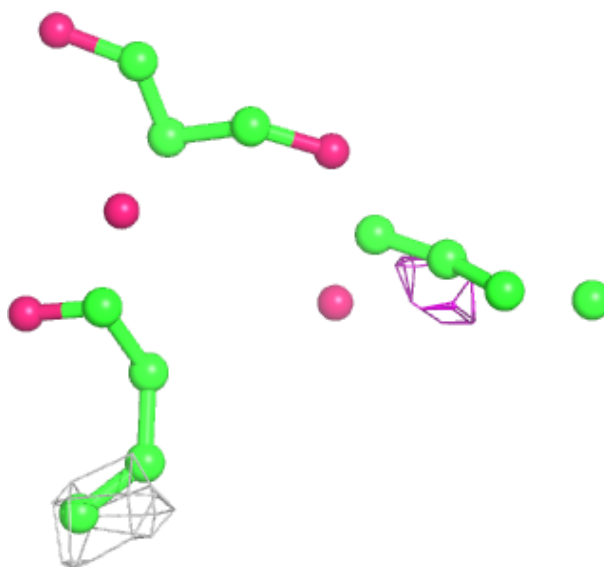
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	G	635	5/5	0.50	0.79	68,68,69,70	5
6	3PG	G	637	11/11	0.68	0.69	54,57,60,60	5
7	AGA	G	639	16/30	0.68	1.24	40,48,61,61	9
4	PEE	F	607	10/51	0.73	0.52	35,40,42,42	0
4	PEE	B	606	10/51	0.78	0.37	35,37,40,40	0
2	BGL	B	605	18/20	0.84	0.35	40,78,81,82	0
4	PEE	B	602	14/51	0.84	0.33	36,39,48,49	0
4	PEE	E	613	16/51	0.84	0.26	35,41,45,46	0
5	PO4	B	626	5/5	0.85	0.35	29,29,30,31	5
7	AGA	C	629	16/30	0.85	0.40	38,44,52,52	9
6	3PG	C	627	11/11	0.86	0.30	42,49,51,52	5
4	PEE	F	603	14/51	0.88	0.30	37,41,47,48	0
5	PO4	C	625	5/5	0.88	0.24	54,54,55,56	5
5	PO4	F	636	5/5	0.90	0.31	38,39,40,40	5
2	BGL	B	604	18/20	0.91	0.28	46,74,79,79	0
2	BGL	E	608	16/20	0.91	0.26	33,40,42,45	0
4	PEE	G	611	9/51	0.91	0.32	45,46,50,50	0
3	POQ	A	600	39/39	0.92	0.19	34,64,67,70	1
2	BGL	A	609	16/20	0.93	0.22	38,42,45,46	0
4	PEE	A	612	9/51	0.95	0.29	40,42,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

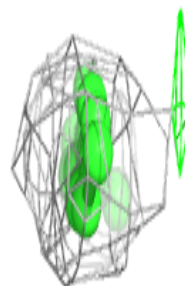
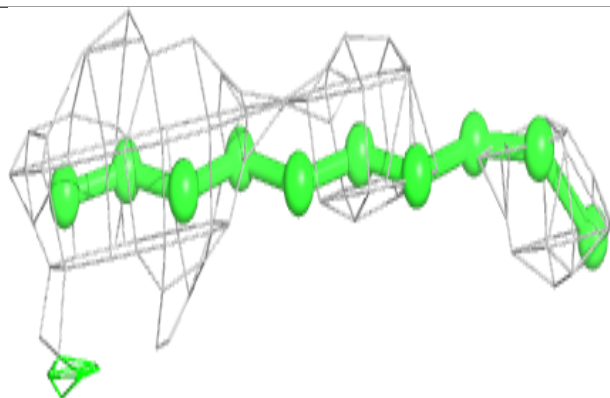
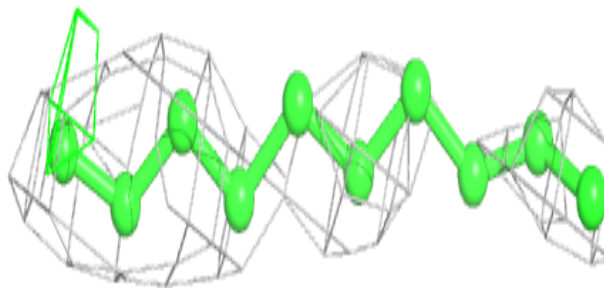
Electron density around AGA G 639:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

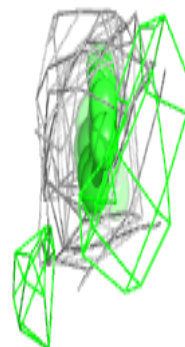
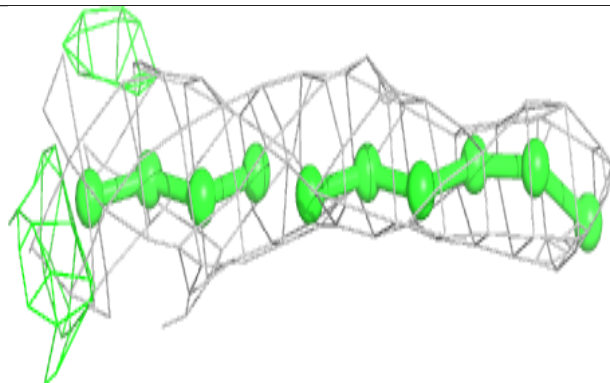
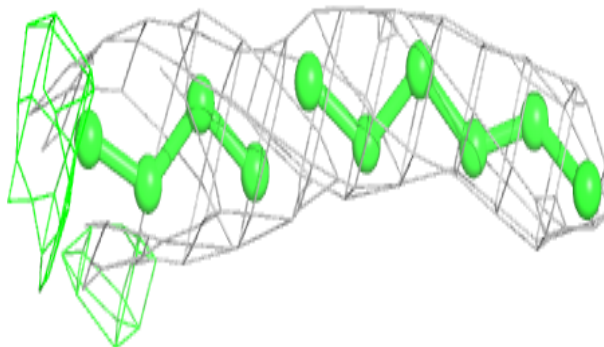


Electron density around PEE F 607:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

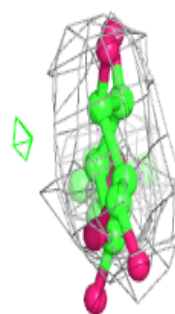
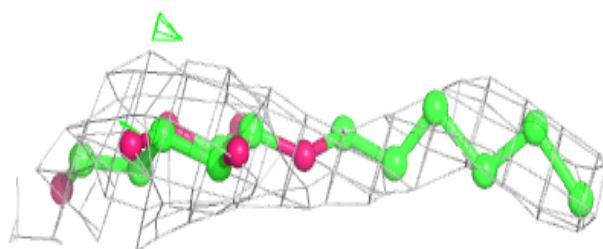
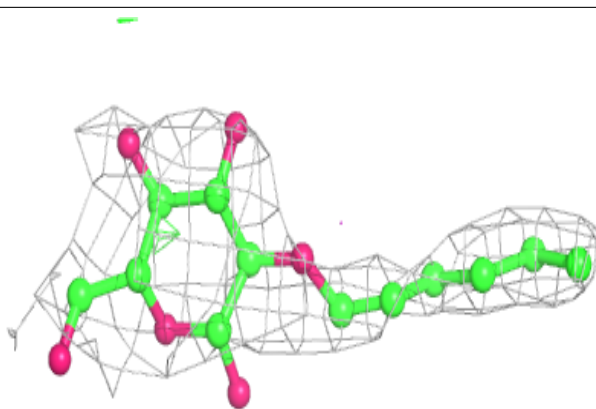
**Electron density around PEE B 606:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

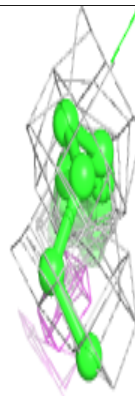
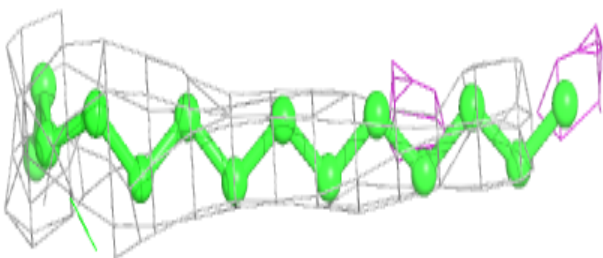
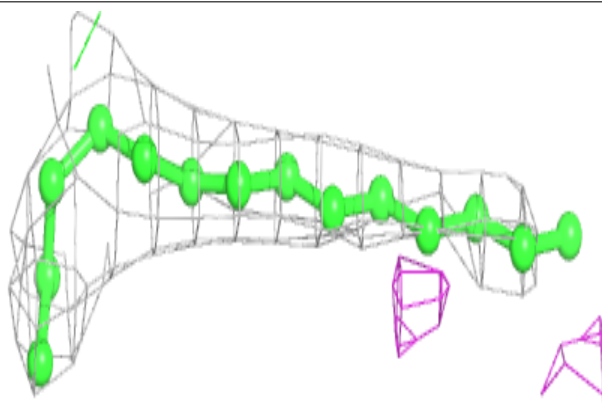


Electron density around BGL B 605:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

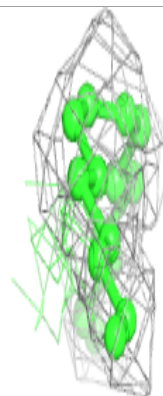
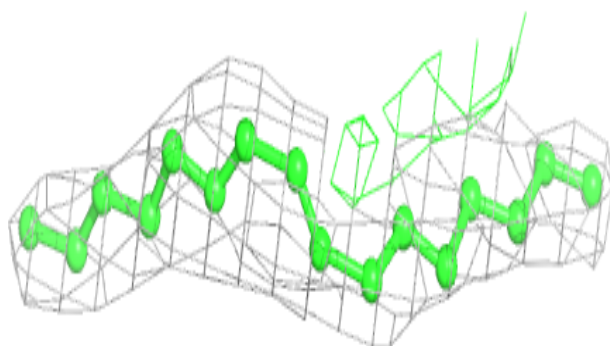
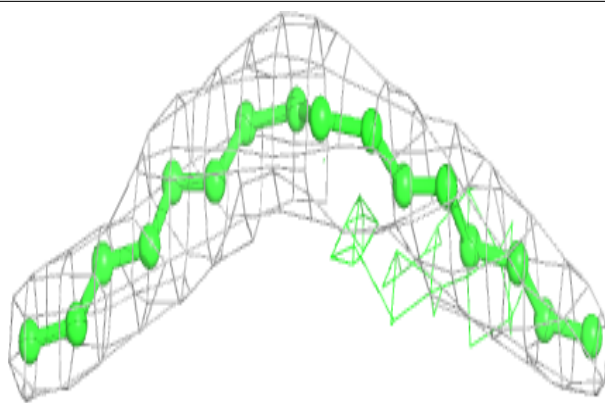
**Electron density around PEE B 602:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



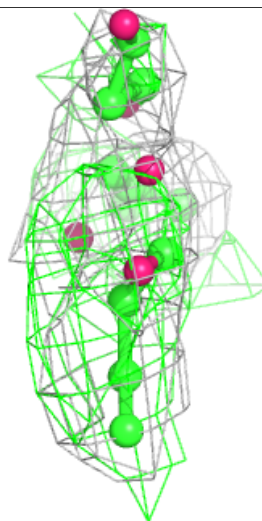
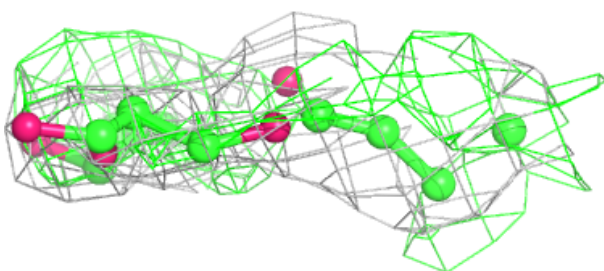
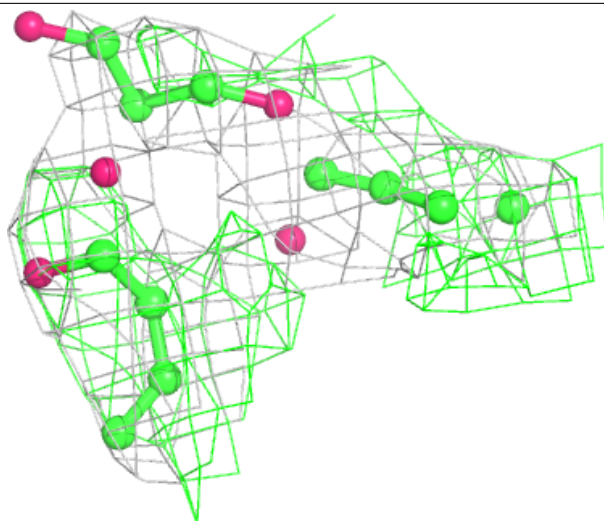
Electron density around PEE E 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



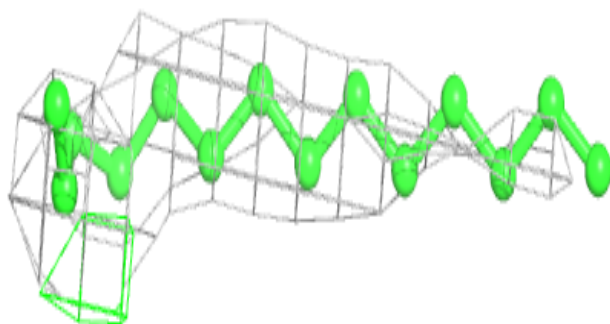
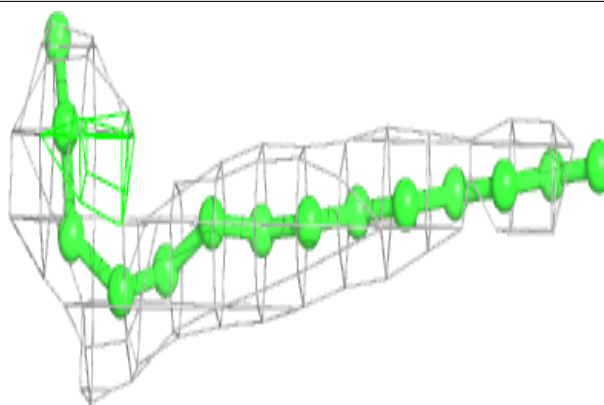
Electron density around AGA C 629:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

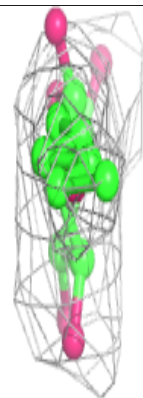
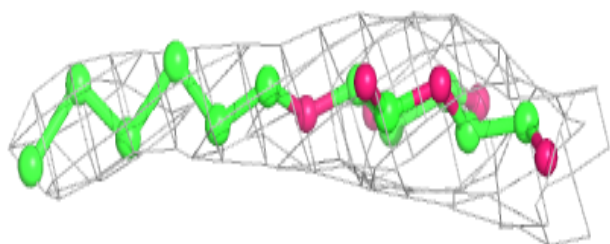
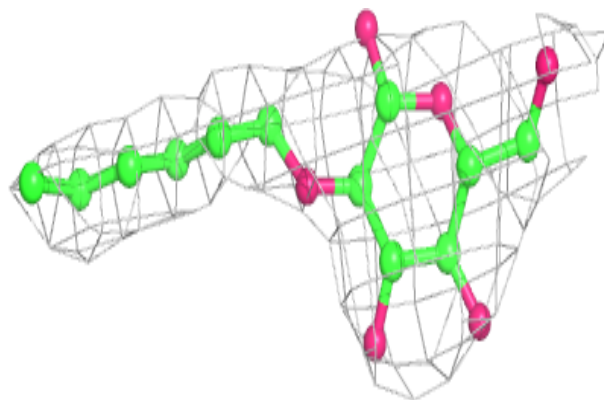


Electron density around PEE F 603:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

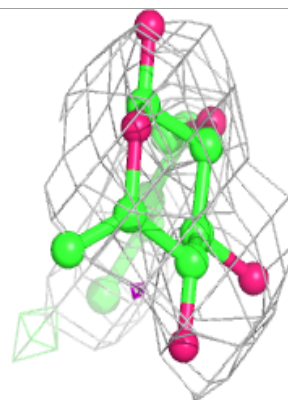
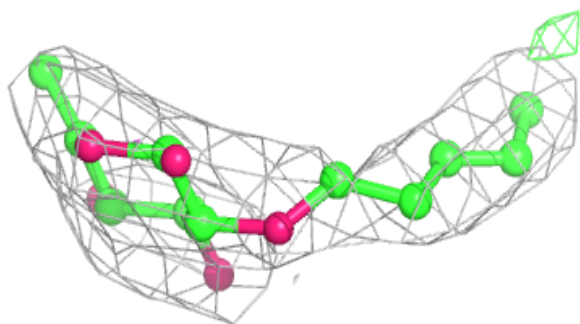
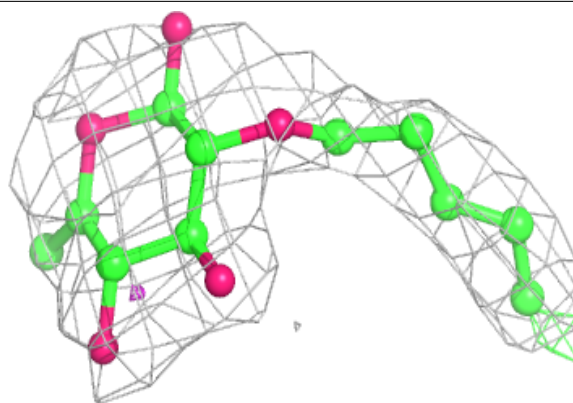
**Electron density around BGL B 604:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

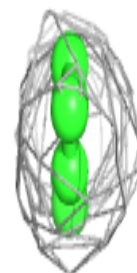
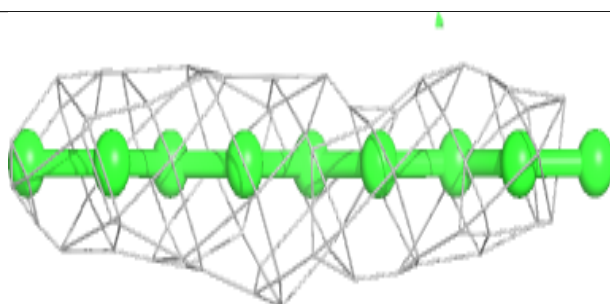
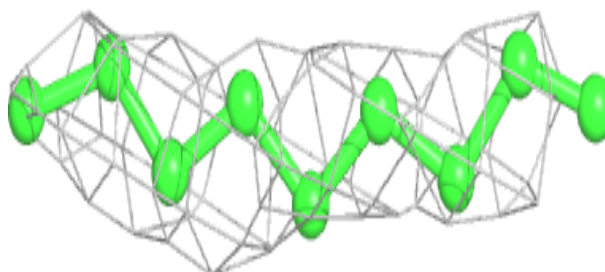


Electron density around BGL E 608:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

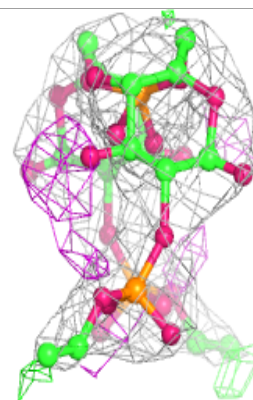
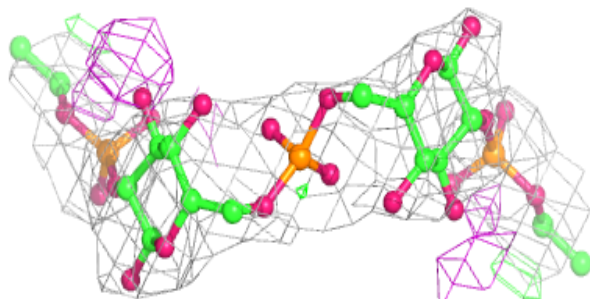
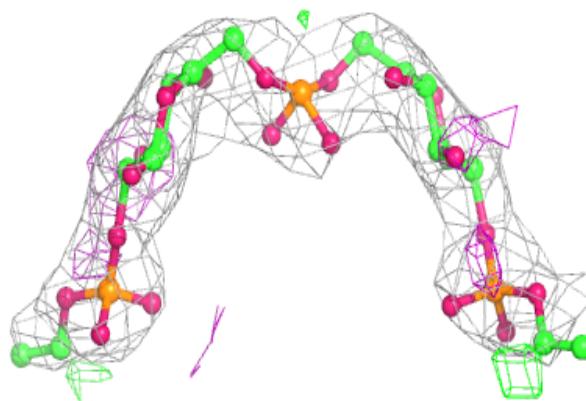
**Electron density around PEE G 611:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

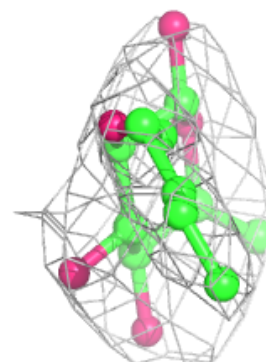
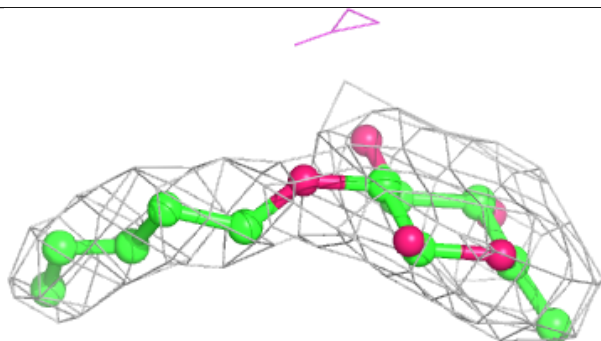
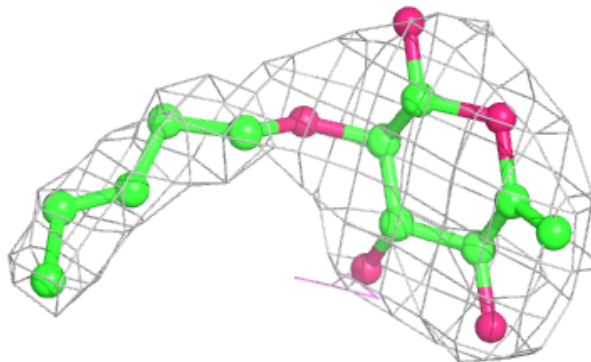


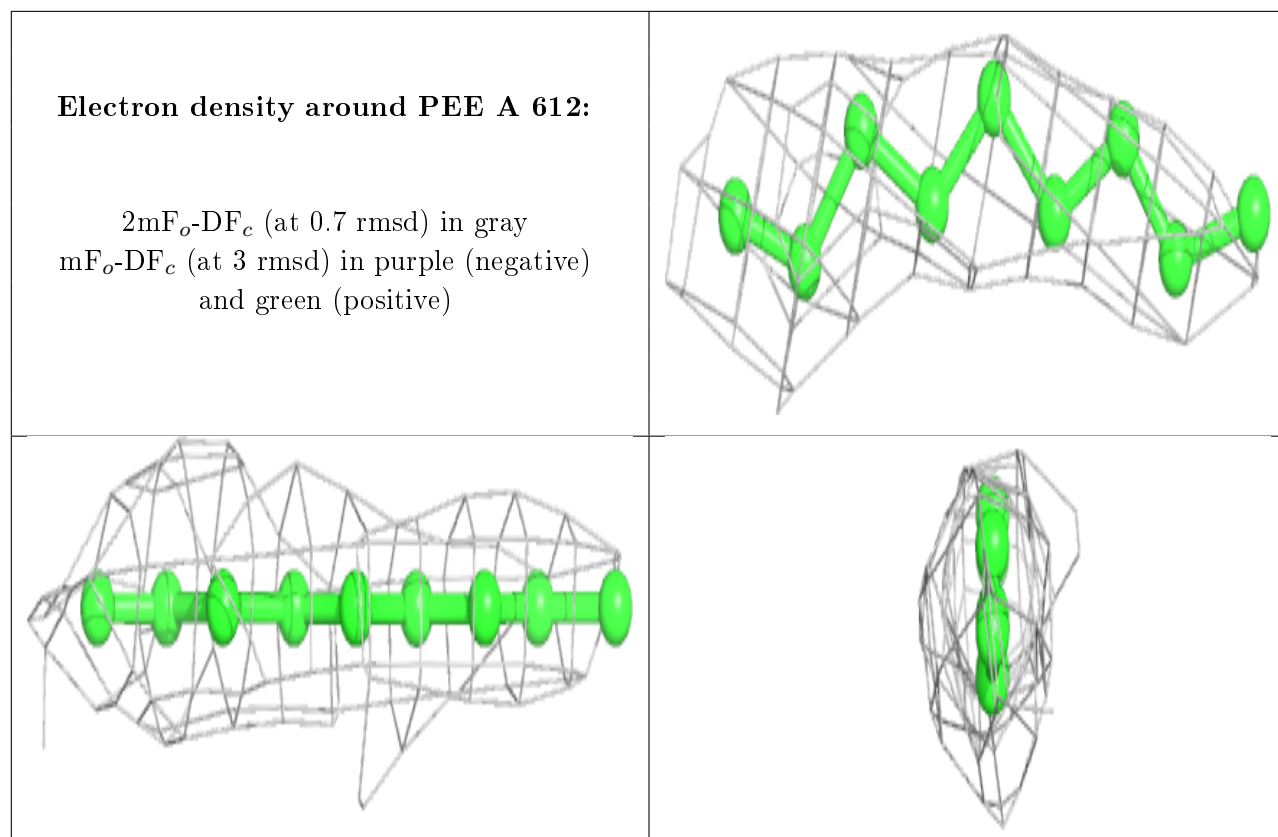
Electron density around POQ A 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around BGL A 609:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.