



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 06:59 AM EDT

PDB ID : 7JPW
EMDB ID : EMD-22425
Title : Rabbit Cav1.1 in the presence of 100 micromolar (R)-(+)-Bay K8644 in nanodiscs at 3.2 Angstrom resolution
Authors : Yan, N.; Gao, S.
Deposited on : 2020-08-10
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

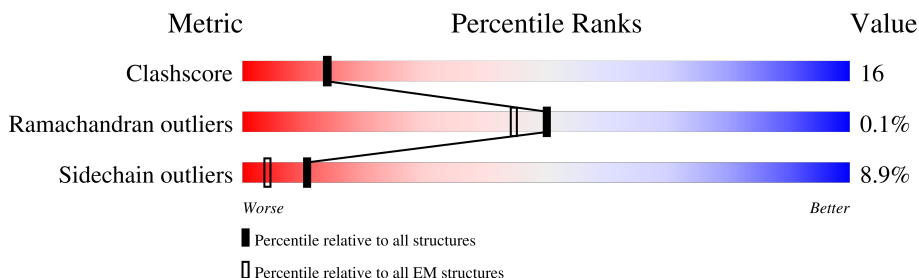
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1873	
2	E	222	
3	F	1105	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18583 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1115	Total	C	N	O	S	0	0
			9009	5976	1437	1537	59		

- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	169	Total	C	N	O	S	0	0
			1326	872	216	220	18		

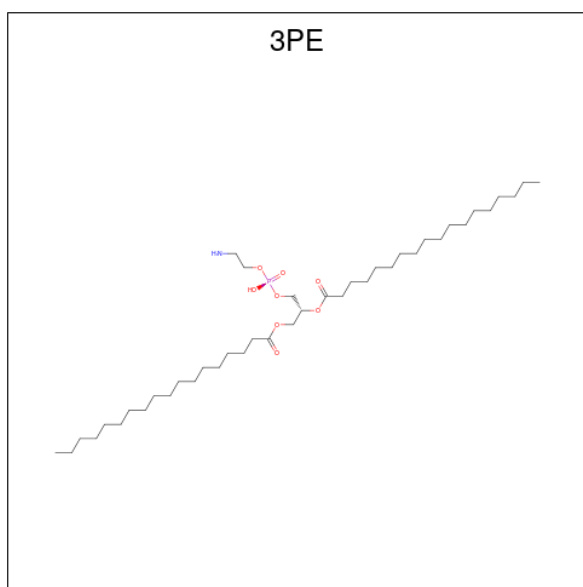
- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	973	Total	C	N	O	S	1	0
			7804	4942	1320	1510	32		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

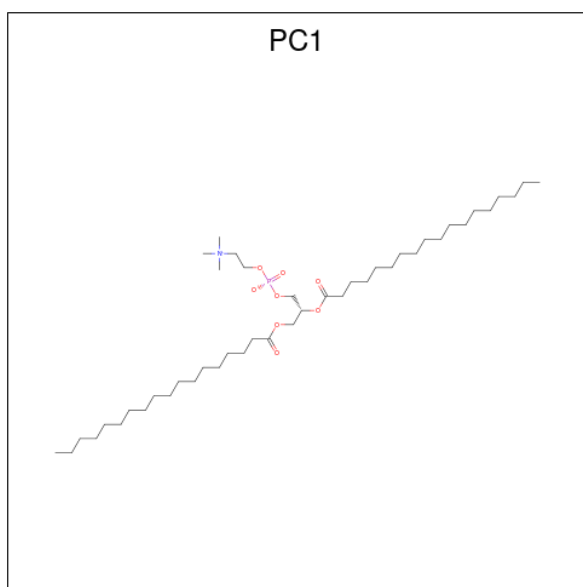
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	

- Molecule 5 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



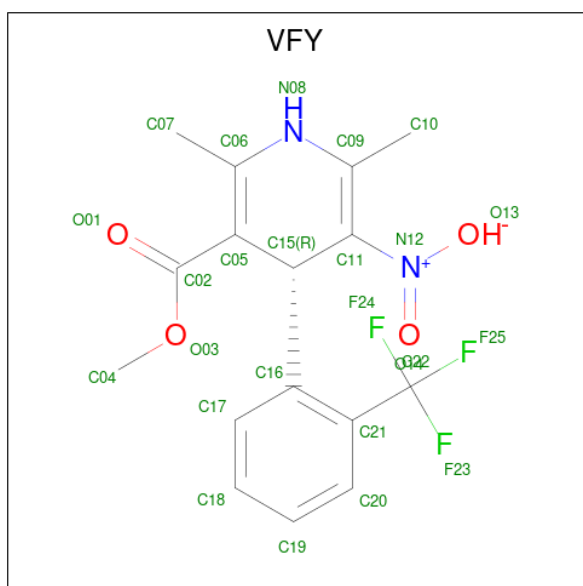
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
5	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
5	A	1	Total	C	N	O	P	0
			21	13	1	6	1	
5	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 7 is methyl (4 {R})-2,6-dimethyl-5-nitro-4-[2-(trifluoromethyl)phenyl]-1,4-dihydropyridine-3-carboxylate (three-letter code: VFY) (formula: $C_{16}H_{16}F_3N_2O_4$) (labeled as "Ligand of Interest" by depositor).

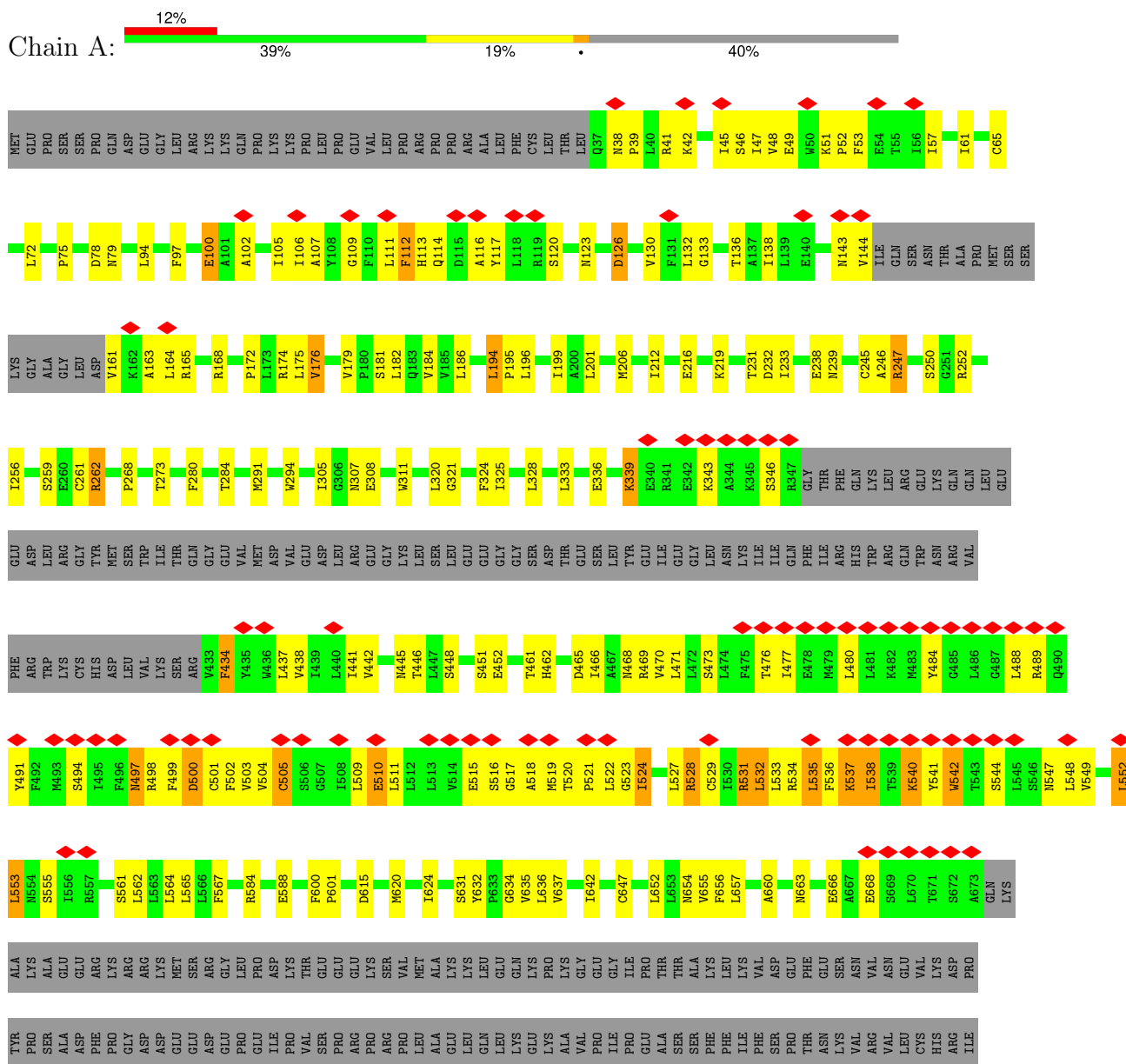


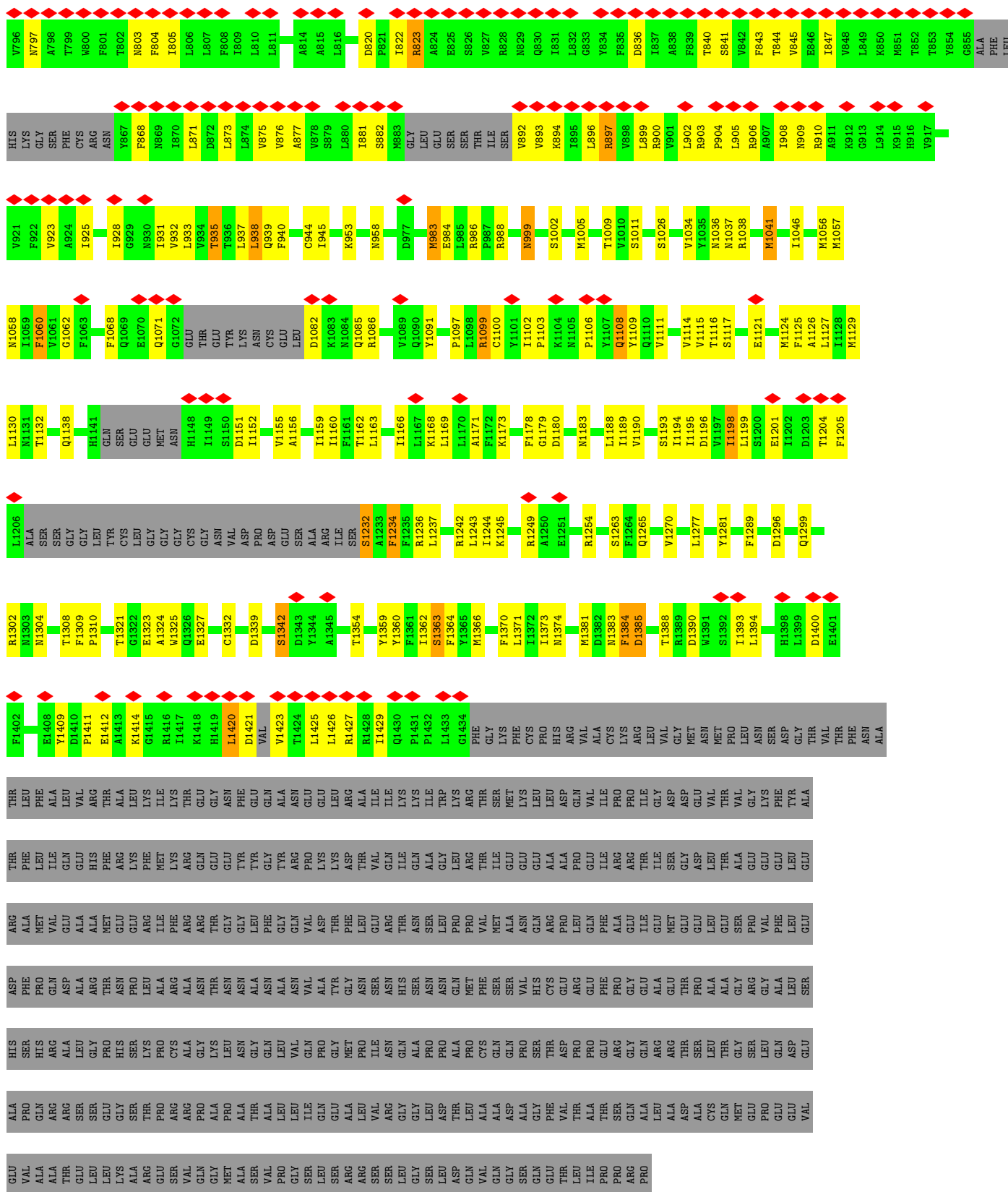
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	F	N	O	0
			25	16	3	2	4	

3 Residue-property plots

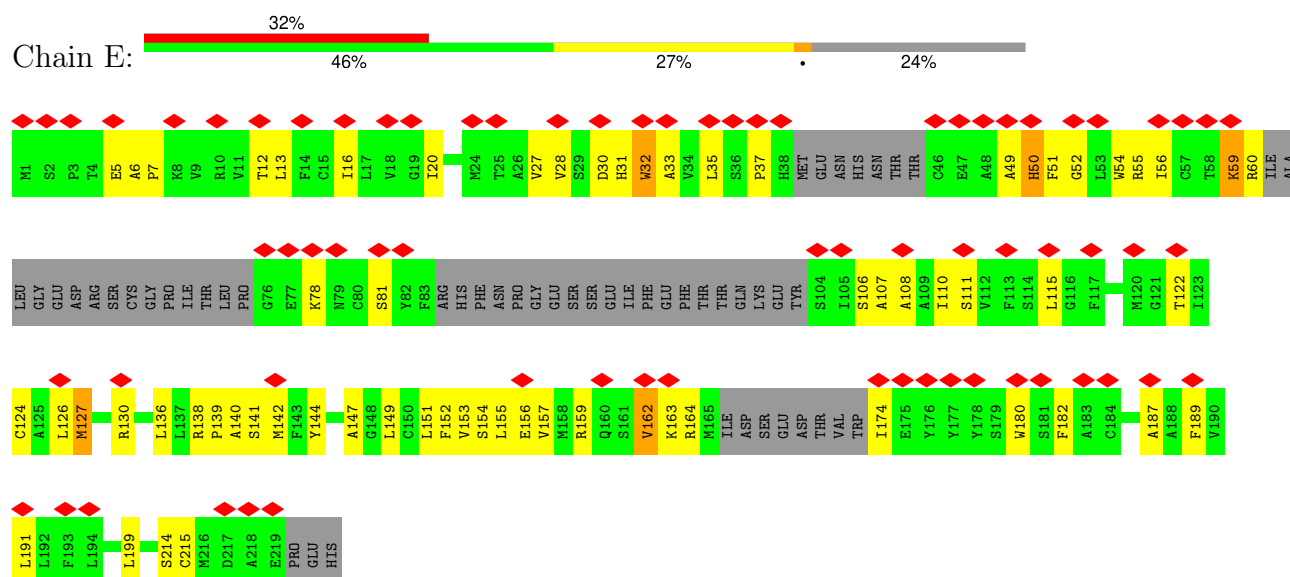
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Voltage-dependent L-type calcium channel subunit alpha-1S

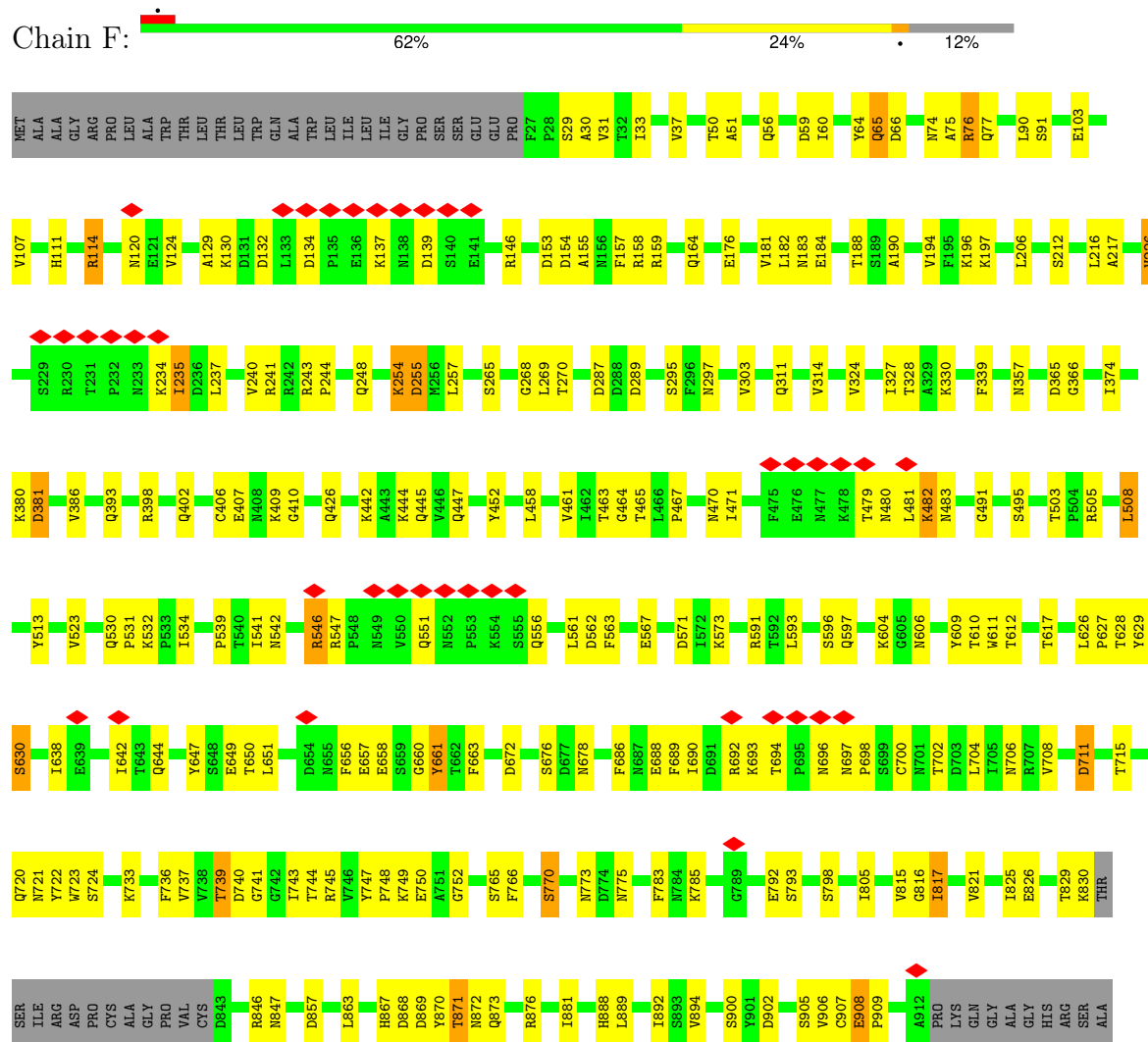


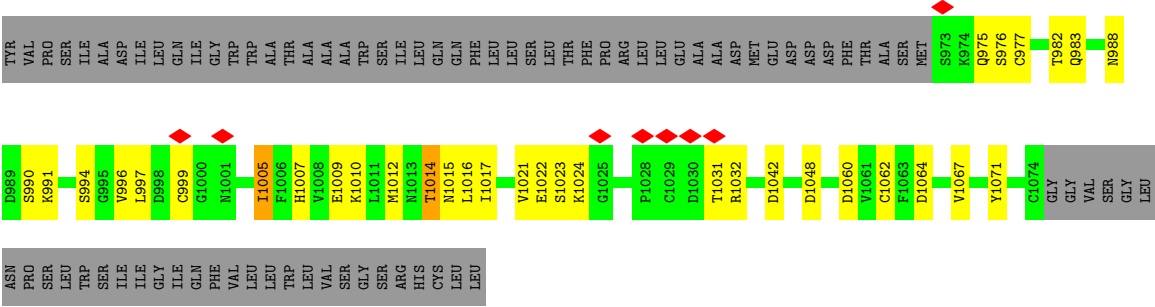


- Molecule 2: Voltage-dependent calcium channel gamma-1 subunit



• Molecule 3: Voltage-dependent calcium channel subunit alpha-2/delta-1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94695	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.145	Depositor
Minimum map value	-0.089	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.114, 1.114, 1.114	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: VFY, PC1, CA, 3PE

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	0.62	0/9233	0.53	0/12534
2	E	0.37	0/1358	0.51	0/1832
3	F	0.80	0/7974	0.58	0/10816
All	All	0.69	0/18565	0.55	0/25182

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9009	0	9145	312	0
2	E	1326	0	1345	45	0
3	F	7804	0	7617	171	0
4	A	1	0	0	0	0
5	A	364	0	524	89	0
6	A	54	0	88	18	0
7	A	25	0	0	5	0
All	All	18583	0	18719	579	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 16.

All (579) 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:502:PHE:HA	1:A:505:CYS:SG	1.35	1.65
1:A:647:CYS:SG	5:A:1905:3PE:C3I	2.04	1.43
1:A:502:PHE:CA	1:A:505:CYS:SG	2.14	1.33
5:A:1904:3PE:H2I1	7:A:1912:VFY:C04	1.64	1.25
1:A:1366:MET:CE	5:A:1904:3PE:H2A1	1.77	1.13
1:A:1366:MET:HE2	5:A:1904:3PE:H2A1	1.29	1.12
1:A:500:ASP:OD2	1:A:537:LYS:HE3	1.50	1.11
2:E:51:PHE:HA	2:E:56:ILE:HG22	1.31	1.06
1:A:501:CYS:O	1:A:505:CYS:SG	2.14	1.06
1:A:528:ARG:HH11	1:A:528:ARG:HB3	1.21	1.05
1:A:305:ILE:HD12	6:A:1909:PC1:H12	1.35	1.05
1:A:163:ALA:HB1	5:A:1906:3PE:H332	1.43	1.00
5:A:1911:3PE:H2H2	5:A:1911:3PE:H2C1	1.43	1.00
1:A:647:CYS:SG	5:A:1905:3PE:H3I1	2.02	0.99
5:A:1911:3PE:H3A1	5:A:1911:3PE:H2I1	1.43	0.98
5:A:1911:3PE:H2H2	5:A:1911:3PE:C2C	1.93	0.97
5:A:1911:3PE:H3A1	5:A:1911:3PE:C2I	1.97	0.95
5:A:1907:3PE:H361	5:A:1908:3PE:H251	1.48	0.95
1:A:500:ASP:OD1	1:A:537:LYS:CE	2.19	0.91
1:A:500:ASP:OD1	1:A:537:LYS:CD	2.20	0.90
5:A:1904:3PE:C2I	7:A:1912:VFY:C04	2.50	0.90
1:A:500:ASP:OD1	1:A:537:LYS:HD2	1.70	0.89
1:A:1370:PHE:HB2	5:A:1904:3PE:H2H1	1.54	0.88
1:A:501:CYS:C	1:A:505:CYS:HG	1.76	0.88
5:A:1907:3PE:C2C	5:A:1907:3PE:H272	2.03	0.88
5:A:1906:3PE:N	5:A:1906:3PE:O11	2.08	0.87
3:F:693:LYS:HE3	3:F:698:PRO:HD2	1.58	0.85
5:A:1911:3PE:O14	5:A:1911:3PE:N	2.08	0.85
2:E:31:HIS:HB3	2:E:180:TRP:HB3	1.58	0.85
1:A:51:LYS:HG2	1:A:52:PRO:HD2	1.58	0.85
1:A:1366:MET:HE2	5:A:1904:3PE:C2A	2.07	0.84
1:A:500:ASP:CG	1:A:537:LYS:HE3	1.98	0.84
5:A:1904:3PE:H221	5:A:1904:3PE:H31	1.58	0.84
1:A:528:ARG:HH11	1:A:528:ARG:CB	1.90	0.84
1:A:305:ILE:CD1	6:A:1909:PC1:H12	2.07	0.82
3:F:1010:LYS:HG3	3:F:1017:ILE:HG13	1.62	0.82
1:A:1046:ILE:HD13	5:A:1908:3PE:H262	1.62	0.81
6:A:1909:PC1:O32	6:A:1909:PC1:H242	1.80	0.81
2:E:51:PHE:HA	2:E:56:ILE:CG2	2.09	0.81
6:A:1909:PC1:H133	6:A:1909:PC1:P	2.20	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:PHE:C	1:A:505:CYS:SG	2.58	0.81
5:A:1911:3PE:H2I1	5:A:1911:3PE:H381	1.64	0.79
3:F:697:ASN:HB3	3:F:700:CYS:HB2	1.64	0.79
1:A:528:ARG:HA	1:A:531:ARG:HD3	1.64	0.79
2:E:124:CYS:HB2	2:E:140:ALA:HB2	1.63	0.79
1:A:438:VAL:HA	1:A:441:ILE:HD12	1.66	0.78
2:E:127:MET:SD	2:E:130:ARG:NH2	2.56	0.78
6:A:1909:PC1:H2E2	6:A:1909:PC1:H371	1.65	0.78
5:A:1905:3PE:O12	5:A:1905:3PE:N	2.17	0.78
2:E:32:TRP:HB2	2:E:182:PHE:HB2	1.65	0.77
1:A:1129:MET:HE1	5:A:1903:3PE:H2C2	1.67	0.77
1:A:601:PRO:HB3	5:A:1908:3PE:O22	1.85	0.77
1:A:522:LEU:HD22	1:A:1038:ARG:HE	1.49	0.76
3:F:658:GLU:O	3:F:720:GLN:NE2	2.18	0.76
3:F:386:VAL:O	3:F:410:GLY:HA3	1.85	0.76
1:A:1046:ILE:HD13	5:A:1908:3PE:C26	2.16	0.76
5:A:1904:3PE:H221	5:A:1904:3PE:C3	2.16	0.76
1:A:1366:MET:HE3	5:A:1904:3PE:H2D1	1.67	0.76
1:A:112:PHE:HB2	1:A:116:ALA:H	1.51	0.76
1:A:939:GLN:HE22	7:A:1912:VFY:C10	1.98	0.76
1:A:38:ASN:HB2	1:A:41:ARG:HE	1.50	0.75
1:A:937:LEU:O	1:A:937:LEU:HD12	1.87	0.75
3:F:243:ARG:HH21	3:F:556:GLN:HE21	1.35	0.74
5:A:1907:3PE:C36	5:A:1908:3PE:H251	2.16	0.74
3:F:792:GLU:N	3:F:792:GLU:OE1	2.20	0.74
1:A:503:VAL:CG2	1:A:534:ARG:HB2	2.20	0.72
1:A:931:ILE:O	1:A:935:THR:HG23	1.88	0.72
1:A:1178:PHE:O	2:E:138:ARG:NH1	2.22	0.72
1:A:500:ASP:CG	1:A:537:LYS:CE	2.59	0.71
1:A:503:VAL:HG22	1:A:534:ARG:HB2	1.71	0.71
3:F:444:LYS:NZ	3:F:467:PRO:O	2.23	0.71
1:A:562:LEU:HG	1:A:655:VAL:HG22	1.73	0.70
1:A:231:THR:O	1:A:262:ARG:NH1	2.24	0.70
1:A:1323:GLU:O	1:A:1325:TRP:N	2.25	0.70
3:F:711:ASP:OD2	3:F:743:ILE:HB	1.92	0.70
1:A:112:PHE:O	1:A:113:HIS:ND1	2.24	0.70
3:F:452:TYR:HH	3:F:463:THR:HG1	1.26	0.70
1:A:529:CYS:HB3	5:A:1910:3PE:H332	1.73	0.70
1:A:584:ARG:NH1	5:A:1906:3PE:O12	2.24	0.70
3:F:562:ASP:OD1	3:F:563:PHE:N	2.25	0.70
5:A:1911:3PE:H2I1	5:A:1911:3PE:C3A	2.19	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:MET:HG3	6:A:1909:PC1:H3F2	1.75	0.69
3:F:991:LYS:NZ	3:F:1012:MET:SD	2.61	0.69
3:F:402:GLN:O	3:F:406:CYS:SG	2.50	0.69
1:A:1129:MET:SD	5:A:1903:3PE:H2C1	2.33	0.68
1:A:1366:MET:CE	5:A:1904:3PE:H2D1	2.24	0.68
1:A:1041:MET:SD	5:A:1910:3PE:O12	2.50	0.68
1:A:1420:LEU:HA	1:A:1423:VAL:HG23	1.76	0.68
1:A:1132:THR:CG2	5:A:1903:3PE:H291	2.24	0.68
6:A:1909:PC1:H133	6:A:1909:PC1:O14	1.93	0.68
3:F:481:LEU:HG	3:F:482:LYS:H	1.59	0.68
1:A:1082:ASP:O	1:A:1086:ARG:NH1	2.27	0.67
1:A:206:MET:HG3	6:A:1909:PC1:C3F	2.24	0.67
3:F:297:ASN:ND2	3:F:330:LYS:O	2.27	0.67
1:A:632:TYR:HD1	5:A:1905:3PE:O32	1.77	0.66
5:A:1903:3PE:H222	5:A:1903:3PE:H322	1.75	0.66
5:A:1907:3PE:H341	5:A:1907:3PE:O32	1.94	0.66
3:F:702:THR:O	3:F:706:ASN:HB2	1.94	0.66
5:A:1911:3PE:H2H2	5:A:1911:3PE:C2D	2.26	0.66
1:A:503:VAL:HG22	1:A:534:ARG:CB	2.25	0.65
3:F:1014:THR:OG1	3:F:1015:ASN:N	2.28	0.65
1:A:531:ARG:NH1	1:A:531:ARG:HG2	2.12	0.65
1:A:102:ALA:HA	1:A:105:ILE:HG22	1.78	0.64
3:F:889:LEU:HD22	3:F:894:VAL:HG11	1.78	0.64
3:F:1005:ILE:H	3:F:1022:GLU:HG3	1.63	0.64
1:A:238:GLU:OE1	1:A:238:GLU:N	2.30	0.63
3:F:1023:SER:OG	3:F:1024:LYS:N	2.30	0.63
1:A:441:ILE:HG23	1:A:471:LEU:HD22	1.80	0.63
1:A:502:PHE:O	1:A:505:CYS:SG	2.57	0.63
1:A:836:ASP:O	1:A:840:THR:HG23	1.99	0.63
1:A:1234:PHE:HB3	6:A:1909:PC1:H231	1.80	0.63
1:A:1232:SER:O	1:A:1232:SER:OG	2.10	0.63
2:E:33:ALA:HB3	2:E:51:PHE:HB2	1.81	0.63
1:A:163:ALA:HB1	5:A:1906:3PE:C33	2.24	0.62
1:A:1366:MET:CE	5:A:1904:3PE:C2A	2.68	0.62
3:F:287:ASP:O	3:F:311:GLN:NE2	2.32	0.62
1:A:294:TRP:HE1	1:A:1321:THR:HG21	1.64	0.62
1:A:529:CYS:HA	1:A:532:LEU:HD12	1.81	0.62
3:F:737:VAL:HG22	3:F:815:VAL:HG12	1.79	0.62
3:F:656:PHE:HB3	3:F:749:LYS:HD2	1.81	0.62
3:F:206:LEU:HD13	3:F:458:LEU:HD21	1.81	0.62
1:A:528:ARG:HH11	1:A:528:ARG:CG	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:LEU:HD21	1:A:944:CYS:HB2	1.82	0.62
3:F:503:THR:O	3:F:503:THR:OG1	2.15	0.61
3:F:747:TYR:HB3	3:F:748:PRO:HD3	1.81	0.61
3:F:994:SER:HB3	3:F:1007:HIS:HD2	1.66	0.61
5:A:1903:3PE:O32	5:A:1903:3PE:H341	2.01	0.61
3:F:711:ASP:OD2	3:F:743:ILE:HG13	2.01	0.61
3:F:647:TYR:O	3:F:650:THR:OG1	2.17	0.61
1:A:642:ILE:HG22	5:A:1905:3PE:H3E2	1.83	0.60
3:F:908:GLU:OE1	3:F:908:GLU:HA	2.01	0.60
1:A:280:PHE:O	1:A:284:THR:HG22	2.01	0.60
1:A:1132:THR:HG22	5:A:1903:3PE:H291	1.83	0.60
3:F:696:ASN:OD1	3:F:698:PRO:HD3	2.01	0.60
1:A:531:ARG:CG	1:A:531:ARG:HH11	2.15	0.60
3:F:711:ASP:OD2	3:F:743:ILE:CB	2.49	0.60
1:A:660:ALA:HB1	1:A:1062:GLY:HA3	1.84	0.60
1:A:446:THR:OG1	1:A:535:LEU:HD13	2.02	0.60
1:A:477:ILE:HA	1:A:480:LEU:HD12	1.84	0.60
1:A:531:ARG:HG2	1:A:531:ARG:HH11	1.67	0.60
3:F:365:ASP:OD1	3:F:366:GLY:N	2.34	0.59
3:F:591:ARG:NH2	3:F:606:ASN:OD1	2.35	0.59
1:A:528:ARG:HB3	1:A:528:ARG:NH1	2.05	0.59
3:F:630:SER:O	3:F:630:SER:OG	2.15	0.59
1:A:45:ILE:HD11	1:A:106:ILE:HG13	1.84	0.59
1:A:75:PRO:HG2	3:F:265:SER:HA	1.84	0.59
1:A:245:CYS:SG	1:A:246:ALA:N	2.76	0.59
5:A:1902:3PE:H241	5:A:1902:3PE:O22	2.02	0.59
2:E:35:LEU:HG	2:E:49:ALA:HB3	1.84	0.59
3:F:217:ALA:HB2	3:F:240:VAL:HG21	1.85	0.59
6:A:1909:PC1:H392	6:A:1909:PC1:H2F1	1.84	0.59
1:A:1281:TYR:OH	1:A:1363:SER:OG	2.16	0.58
1:A:305:ILE:HD12	6:A:1909:PC1:C1	2.24	0.58
3:F:694:THR:HB	3:F:696:ASN:ND2	2.18	0.58
3:F:829:THR:HG21	3:F:846:ARG:HD3	1.84	0.58
1:A:939:GLN:NE2	7:A:1912:VFY:C10	2.66	0.58
3:F:546:ARG:NH2	3:F:547:ARG:O	2.35	0.57
3:F:184:GLU:O	3:F:188:THR:OG1	2.14	0.57
1:A:78:ASP:OD1	1:A:79:ASN:N	2.34	0.57
1:A:38:ASN:HD21	1:A:42:LYS:HE2	1.69	0.57
1:A:897:ARG:HA	1:A:900:ARG:HD3	1.85	0.57
1:A:1129:MET:SD	5:A:1903:3PE:C2C	2.92	0.56
3:F:711:ASP:OD1	3:F:739:THR:OG1	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:LEU:O	1:A:875:VAL:HG23	2.06	0.56
1:A:1201:GLU:O	1:A:1205:PHE:HB2	2.05	0.56
3:F:513:TYR:OH	3:F:567:GLU:OE1	2.21	0.56
3:F:688:GLU:O	3:F:692:ARG:CB	2.54	0.56
5:A:1908:3PE:O14	5:A:1908:3PE:H121	2.04	0.56
1:A:308:GLU:O	1:A:311:TRP:NE1	2.39	0.56
3:F:688:GLU:O	3:F:692:ARG:HB2	2.06	0.56
2:E:37:PRO:HG3	2:E:174:ILE:HD11	1.88	0.56
3:F:539:PRO:HD3	3:F:977:CYS:HB3	1.88	0.56
3:F:733:LYS:NZ	3:F:792:GLU:O	2.39	0.56
3:F:711:ASP:OD2	3:F:743:ILE:CG1	2.53	0.56
1:A:1060:PHE:HE2	1:A:1373:ILE:HD13	1.71	0.55
3:F:37:VAL:HG21	3:F:1009:GLU:HG2	1.88	0.55
1:A:906:ARG:O	1:A:910:ARG:NH1	2.39	0.55
1:A:1129:MET:HE3	5:A:1903:3PE:H2F1	1.87	0.55
3:F:481:LEU:HG	3:F:482:LYS:N	2.21	0.55
5:A:1906:3PE:H242	5:A:1906:3PE:H322	1.89	0.55
3:F:638:ILE:O	3:F:644:GLN:NE2	2.34	0.55
3:F:708:VAL:HG22	3:F:741:GLY:O	2.06	0.55
3:F:736:PHE:CZ	3:F:816:GLY:HA3	2.41	0.55
1:A:1189:ILE:HG21	1:A:1242:ARG:HG2	1.87	0.55
5:A:1905:3PE:O22	5:A:1905:3PE:H242	2.05	0.55
2:E:106:SER:O	2:E:110:ILE:HG13	2.06	0.55
3:F:821:VAL:O	3:F:825:ILE:HG13	2.07	0.55
3:F:164:GLN:O	3:F:196:LYS:NZ	2.36	0.55
1:A:501:CYS:C	1:A:505:CYS:SG	2.76	0.54
1:A:881:ILE:HD11	1:A:896:LEU:HD22	1.89	0.54
2:E:51:PHE:CA	2:E:56:ILE:HG22	2.22	0.54
3:F:176:GLU:O	3:F:176:GLU:HG2	2.08	0.54
1:A:500:ASP:OD1	1:A:537:LYS:HE2	2.04	0.54
1:A:902:LEU:HB2	1:A:905:LEU:HD13	1.88	0.54
1:A:841:SER:O	1:A:845:VAL:HG23	2.08	0.54
1:A:1099:ARG:NH2	1:A:1412:GLU:HB3	2.22	0.54
3:F:56:GLN:O	3:F:60:ILE:HG23	2.07	0.54
3:F:720:GLN:O	3:F:724:SER:OG	2.26	0.54
1:A:46:SER:HB2	1:A:107:ALA:HB1	1.88	0.54
1:A:502:PHE:N	1:A:505:CYS:SG	2.79	0.54
1:A:61:ILE:HD11	1:A:174:ARG:NH2	2.23	0.54
1:A:206:MET:CG	6:A:1909:PC1:C3F	2.85	0.54
5:A:1906:3PE:N	5:A:1906:3PE:P	2.81	0.53
1:A:877:ALA:O	1:A:881:ILE:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:ILE:O	1:A:1163:LEU:HG	2.08	0.53
1:A:1371:LEU:O	1:A:1374:ASN:HB3	2.08	0.53
3:F:739:THR:OG1	3:F:740:ASP:N	2.41	0.53
1:A:1339:ASP:O	1:A:1342:SER:OG	2.24	0.53
3:F:867:HIS:C	3:F:869:ASP:H	2.11	0.53
1:A:1190:VAL:O	1:A:1194:ILE:HG12	2.08	0.53
1:A:294:TRP:NE1	1:A:1321:THR:HG21	2.24	0.53
1:A:343:LYS:O	1:A:346:SER:OG	2.26	0.53
1:A:499:PHE:O	1:A:502:PHE:N	2.42	0.53
1:A:1129:MET:CE	5:A:1903:3PE:H2C2	2.37	0.53
5:A:1904:3PE:C3	5:A:1904:3PE:C22	2.86	0.53
2:E:151:LEU:O	2:E:154:SER:HB3	2.09	0.52
1:A:307:ASN:OD1	5:A:1911:3PE:H12	2.09	0.52
1:A:562:LEU:HD21	1:A:654:ASN:O	2.09	0.52
1:A:1129:MET:HE3	5:A:1903:3PE:C2F	2.39	0.52
3:F:64:TYR:O	3:F:66:ASP:N	2.43	0.52
3:F:1042:ASP:OD1	3:F:1042:ASP:N	2.40	0.52
1:A:1156:ALA:O	1:A:1160:ILE:HG13	2.10	0.52
5:A:1906:3PE:N	5:A:1906:3PE:O22	2.39	0.52
1:A:61:ILE:HD11	1:A:174:ARG:HH21	1.74	0.52
1:A:503:VAL:CG1	1:A:534:ARG:HB2	2.38	0.52
1:A:105:ILE:HD11	1:A:111:LEU:HG	1.91	0.52
1:A:519:MET:O	1:A:520:THR:OG1	2.28	0.52
3:F:715:THR:HG21	3:F:745:ARG:HG3	1.92	0.52
1:A:1108:GLN:OE1	1:A:1173:LYS:NZ	2.32	0.52
1:A:434:PHE:CE1	1:A:437:LEU:HD22	2.44	0.52
7:A:1912:VFY:O13	7:A:1912:VFY:F23	2.18	0.52
3:F:114:ARG:HH12	3:F:120:ASN:HB2	1.75	0.52
1:A:1198:ILE:HG22	1:A:1199:LEU:HD23	1.90	0.52
1:A:1179:GLY:HA2	2:E:138:ARG:HH12	1.75	0.51
2:E:107:ALA:HB2	2:E:157:VAL:HG11	1.93	0.51
1:A:176:VAL:HG21	1:A:186:LEU:HD12	1.92	0.51
5:A:1911:3PE:H2I1	5:A:1911:3PE:C38	2.39	0.51
3:F:75:ALA:HB2	3:F:626:LEU:HD12	1.93	0.51
1:A:567:PHE:HE1	5:A:1908:3PE:C29	2.23	0.51
1:A:466:ILE:HG22	1:A:469:ARG:HH21	1.75	0.51
1:A:634:GLY:O	1:A:637:VAL:HG22	2.10	0.51
1:A:847:ILE:HG21	1:A:873:LEU:HD13	1.91	0.51
2:E:110:ILE:HG21	2:E:153:VAL:HG13	1.93	0.51
1:A:1071:GLN:N	1:A:1071:GLN:OE1	2.44	0.51
2:E:55:ARG:CD	2:E:81:SER:HA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:303:VAL:HG23	3:F:327:ILE:HD11	1.92	0.51
1:A:1106:PRO:HA	1:A:1109:TYR:HB3	1.93	0.51
5:A:1906:3PE:P	5:A:1906:3PE:HN2	2.33	0.51
2:E:111:SER:O	2:E:115:LEU:HG	2.11	0.51
1:A:48:VAL:HG23	1:A:51:LYS:HD3	1.92	0.51
1:A:47:ILE:HG13	1:A:48:VAL:N	2.26	0.51
1:A:1180:ASP:HB3	1:A:1183:ASN:HD22	1.76	0.51
5:A:1905:3PE:N	5:A:1905:3PE:P	2.83	0.51
5:A:1906:3PE:N	5:A:1906:3PE:C1	2.73	0.51
2:E:187:ALA:O	2:E:191:LEU:HG	2.11	0.51
3:F:244:PRO:O	3:F:248:GLN:HB2	2.11	0.51
1:A:908:ILE:HD12	1:A:908:ILE:H	1.75	0.50
3:F:480:ASN:HA	3:F:483:ASN:HB2	1.93	0.50
3:F:530:GLN:HB3	3:F:531:PRO:HD2	1.92	0.50
1:A:206:MET:CG	6:A:1909:PC1:H3F1	2.40	0.50
1:A:1281:TYR:O	1:A:1360:TYR:OH	2.24	0.50
1:A:1046:ILE:HG21	5:A:1908:3PE:H262	1.93	0.50
1:A:510:GLU:HB2	1:A:527:LEU:HG	1.93	0.50
1:A:529:CYS:SG	1:A:945:ILE:HG23	2.51	0.50
1:A:442:VAL:HG11	1:A:538:ILE:HB	1.93	0.50
3:F:132:ASP:OD2	3:F:132:ASP:N	2.33	0.50
1:A:984:GLU:OE2	1:A:986:ARG:NH1	2.44	0.50
3:F:398:ARG:O	3:F:402:GLN:HG3	2.11	0.50
3:F:628:THR:O	3:F:629:TYR:CD2	2.64	0.50
1:A:516:SER:OG	1:A:517:GLY:N	2.44	0.50
1:A:1296:ASP:OD2	1:A:1302:ARG:NH1	2.42	0.50
3:F:243:ARG:NH2	3:F:556:GLN:HG3	2.27	0.50
3:F:704:LEU:O	3:F:708:VAL:HG23	2.12	0.50
3:F:876:ARG:HE	3:F:881:ILE:HG22	1.76	0.50
1:A:112:PHE:HB3	1:A:117:TYR:H	1.77	0.50
1:A:637:VAL:HG12	5:A:1906:3PE:H272	1.94	0.49
1:A:620:MET:O	1:A:624:ILE:HG13	2.12	0.49
1:A:958:ASN:HD22	1:A:988:ARG:HA	1.78	0.49
3:F:51:ALA:HB3	3:F:817:ILE:HD11	1.94	0.49
3:F:988:ASN:ND2	3:F:990:SER:OG	2.45	0.49
1:A:1103:PRO:HB2	1:A:1108:GLN:HE22	1.77	0.49
1:A:1426:LEU:HA	1:A:1429:ILE:HD12	1.95	0.49
1:A:1409:TYR:O	1:A:1411:PRO:HD3	2.13	0.49
3:F:857:ASP:OD1	3:F:857:ASP:N	2.45	0.49
1:A:503:VAL:HG13	1:A:534:ARG:HB2	1.94	0.49
1:A:928:ILE:O	1:A:928:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:VAL:HG11	2:E:115:LEU:HD21	1.94	0.49
1:A:61:ILE:HG13	1:A:97:PHE:CZ	2.48	0.49
6:A:1909:PC1:H371	6:A:1909:PC1:C2E	2.40	0.49
1:A:114:GLN:NE2	1:A:116:ALA:HB2	2.27	0.49
1:A:114:GLN:HG3	1:A:116:ALA:HB2	1.94	0.49
1:A:840:THR:O	1:A:844:THR:HG23	2.12	0.48
3:F:461:VAL:HG12	3:F:495:SER:HA	1.94	0.48
3:F:470:ASN:HD21	3:F:482:LYS:NZ	2.11	0.48
3:F:870:TYR:O	3:F:873:GLN:N	2.42	0.48
1:A:1277:LEU:HD22	1:A:1371:LEU:HD12	1.93	0.48
3:F:134:ASP:O	3:F:137:LYS:HG2	2.13	0.48
1:A:931:ILE:O	1:A:935:THR:CG2	2.60	0.48
1:A:1370:PHE:CB	5:A:1904:3PE:H2H1	2.37	0.48
1:A:1425:LEU:HD23	1:A:1425:LEU:H	1.78	0.48
5:A:1906:3PE:H272	5:A:1906:3PE:H241	1.62	0.48
3:F:597:GLN:HB3	3:F:765:SER:HB2	1.96	0.48
3:F:723:TRP:CH2	3:F:737:VAL:HG23	2.49	0.48
1:A:126:ASP:HB3	1:A:174:ARG:NH1	2.29	0.48
1:A:520:THR:O	1:A:523:GLY:N	2.45	0.48
3:F:33:ILE:HG21	3:F:1007:HIS:ND1	2.28	0.48
3:F:1031:THR:OG1	3:F:1032:ARG:N	2.47	0.48
1:A:111:LEU:HD23	1:A:112:PHE:CE1	2.48	0.48
1:A:109:GLY:HA3	1:A:113:HIS:HB3	1.95	0.48
1:A:179:VAL:HG21	1:A:182:LEU:HD13	1.96	0.48
1:A:219:LYS:NZ	1:A:1138:GLN:HE21	2.11	0.48
1:A:1242:ARG:O	1:A:1245:LYS:HG2	2.13	0.48
2:E:139:PRO:HA	2:E:142:MET:HE2	1.96	0.48
3:F:715:THR:HG22	3:F:745:ARG:HH21	1.77	0.48
3:F:1048:ASP:OD1	3:F:1048:ASP:N	2.47	0.48
5:A:1907:3PE:H372	5:A:1907:3PE:H3A1	1.67	0.48
2:E:159:ARG:O	2:E:162:VAL:HG12	2.14	0.48
1:A:113:HIS:CE1	1:A:114:GLN:HG2	2.48	0.48
1:A:953:LYS:HB3	1:A:1026:SER:HB2	1.95	0.48
2:E:141:SER:OG	2:E:142:MET:N	2.47	0.48
1:A:196:LEU:HD11	1:A:333:LEU:HG	1.96	0.47
1:A:518:ALA:HB1	1:A:524:ILE:HD11	1.96	0.47
1:A:805:ILE:HG23	1:A:843:PHE:HE2	1.79	0.47
5:A:1902:3PE:H2	5:A:1902:3PE:H221	1.68	0.47
3:F:289:ASP:OD1	3:F:289:ASP:N	2.47	0.47
1:A:231:THR:HG22	1:A:233:ILE:HG13	1.96	0.47
1:A:462:HIS:O	1:A:466:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:TRP:CD1	1:A:544:SER:HB3	2.49	0.47
1:A:1121:GLU:OE1	1:A:1249:ARG:HG2	2.13	0.47
5:A:1904:3PE:H351	5:A:1904:3PE:H382	1.52	0.47
3:F:593:LEU:HD23	3:F:604:LYS:HG2	1.96	0.47
2:E:136:LEU:HA	2:E:136:LEU:HD23	1.70	0.47
3:F:90:LEU:HD12	3:F:617:THR:HG21	1.96	0.47
1:A:45:ILE:HD12	1:A:46:SER:N	2.30	0.47
1:A:321:GLY:O	1:A:325:ILE:HB	2.14	0.47
1:A:600:PHE:HD2	5:A:1907:3PE:H32	1.79	0.47
1:A:999:ASN:ND2	1:A:1002:SER:H	2.13	0.47
1:A:1057:MET:O	1:A:1057:MET:HG3	2.15	0.47
3:F:381:ASP:OD1	3:F:381:ASP:N	2.40	0.47
3:F:442:LYS:O	3:F:445:GLN:NE2	2.48	0.47
3:F:686:PHE:O	3:F:690:ILE:HG12	2.15	0.47
1:A:935:THR:HG22	1:A:1056:MET:HE2	1.97	0.47
1:A:1129:MET:CE	5:A:1903:3PE:H2F2	2.45	0.47
1:A:320:LEU:O	1:A:324:PHE:HB3	2.14	0.47
1:A:476:THR:HG22	1:A:504:VAL:HG11	1.96	0.47
1:A:1385:ASP:OD1	1:A:1385:ASP:N	2.47	0.47
3:F:656:PHE:CB	3:F:749:LYS:HD2	2.45	0.47
1:A:280:PHE:CE2	5:A:1905:3PE:H12	2.50	0.47
1:A:1151:ASP:O	1:A:1155:VAL:HG23	2.14	0.47
6:A:1909:PC1:H282	6:A:1909:PC1:H2B2	1.57	0.46
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.72	0.46
3:F:909:PRO:HG3	3:F:975:GLN:HG2	1.97	0.46
1:A:143:ASN:OD1	1:A:143:ASN:N	2.37	0.46
1:A:488:LEU:HG	1:A:489:ARG:HH11	1.80	0.46
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.81	0.46
1:A:1116:THR:O	1:A:1116:THR:HG22	2.14	0.46
3:F:74:ASN:HB3	3:F:77:GLN:HB3	1.96	0.46
3:F:124:VAL:HG21	3:F:182:LEU:HD22	1.98	0.46
5:A:1907:3PE:H322	5:A:1907:3PE:H221	1.98	0.46
1:A:126:ASP:OD1	1:A:126:ASP:N	2.48	0.46
1:A:528:ARG:CG	1:A:528:ARG:NH1	2.73	0.46
1:A:1196:ASP:OD1	1:A:1236:ARG:HA	2.16	0.46
1:A:1299:GLN:O	1:A:1304:ASN:ND2	2.46	0.46
3:F:176:GLU:N	3:F:176:GLU:OE1	2.48	0.46
1:A:1310:PRO:HB3	5:A:1911:3PE:H322	1.98	0.46
5:A:1906:3PE:C1	5:A:1906:3PE:HN1	2.27	0.46
2:E:35:LEU:HD12	2:E:37:PRO:HD3	1.98	0.46
3:F:181:VAL:HG13	3:F:216:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:656:PHE:O	3:F:660:GLY:N	2.38	0.46
1:A:518:ALA:CB	1:A:524:ILE:HD11	2.46	0.46
1:A:1046:ILE:HD13	5:A:1908:3PE:H261	1.92	0.46
1:A:656:PHE:HB3	1:A:1058:ASN:HD22	1.81	0.46
2:E:144:TYR:O	2:E:147:ALA:HB3	2.16	0.46
1:A:1151:ASP:OD2	1:A:1152:ILE:N	2.49	0.45
5:A:1907:3PE:C2C	5:A:1907:3PE:C27	2.86	0.45
3:F:132:ASP:OD1	3:F:137:LYS:HG3	2.16	0.45
3:F:479:THR:HB	3:F:481:LEU:HD23	1.98	0.45
1:A:1005:MET:SD	1:A:1362:ILE:HD11	2.55	0.45
1:A:1324:ALA:HB1	1:A:1327:GLU:HG3	1.97	0.45
3:F:380:LYS:HE3	3:F:380:LYS:HB3	1.61	0.45
3:F:627:PRO:O	3:F:630:SER:HB3	2.17	0.45
3:F:826:GLU:O	3:F:830:LYS:HD3	2.16	0.45
1:A:238:GLU:HG2	1:A:239:ASN:N	2.31	0.45
1:A:466:ILE:O	1:A:470:VAL:HG13	2.17	0.45
1:A:544:SER:HA	1:A:547:ASN:ND2	2.31	0.45
1:A:820:ASP:OD2	1:A:823:ARG:HB2	2.15	0.45
1:A:983:MET:HG3	3:F:235:ILE:HD11	1.97	0.45
1:A:1359:TYR:O	1:A:1363:SER:HB3	2.16	0.45
3:F:663:PHE:HB2	3:F:744:THR:HB	1.97	0.45
1:A:126:ASP:O	1:A:130:VAL:HG23	2.16	0.45
1:A:291:MET:SD	1:A:1321:THR:HG23	2.57	0.45
1:A:532:LEU:HD21	1:A:944:CYS:CB	2.47	0.45
1:A:1309:PHE:HB3	1:A:1310:PRO:HD3	1.98	0.45
3:F:327:ILE:HD13	3:F:327:ILE:HA	1.74	0.45
1:A:256:ILE:O	1:A:259:SER:OG	2.34	0.45
2:E:199:LEU:HD23	2:E:199:LEU:HA	1.72	0.45
3:F:996:VAL:HG22	3:F:1005:ILE:HB	1.97	0.45
1:A:268:PRO:HD2	1:A:273:THR:O	2.16	0.45
1:A:94:LEU:HD21	1:A:133:GLY:C	2.37	0.45
1:A:186:LEU:HG	1:A:565:LEU:HD11	1.99	0.45
1:A:247:ARG:HB2	1:A:261:CYS:HB3	1.98	0.45
1:A:1384:PHE:O	1:A:1388:THR:OG1	2.32	0.45
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.85	0.45
2:E:54:TRP:CZ3	2:E:108:ALA:HB1	2.51	0.45
1:A:206:MET:HG3	6:A:1909:PC1:H3F1	1.94	0.45
3:F:33:ILE:O	3:F:37:VAL:HG13	2.17	0.45
1:A:238:GLU:HG2	1:A:239:ASN:HD22	1.82	0.45
3:F:846:ARG:NH1	3:F:868:ASP:HB2	2.32	0.45
3:F:1064:ASP:N	3:F:1064:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:HD23	1:A:333:LEU:HA	1.78	0.44
1:A:542:TRP:HA	1:A:542:TRP:CE3	2.52	0.44
1:A:65:CYS:SG	1:A:172:PRO:HG3	2.58	0.44
1:A:588:GLU:HG2	3:F:268:GLY:O	2.17	0.44
1:A:1111:VAL:HG23	1:A:1171:ALA:HB2	1.99	0.44
2:E:6:ALA:HB1	2:E:7:PRO:HD2	2.00	0.44
1:A:536:PHE:O	1:A:536:PHE:CD2	2.70	0.44
1:A:631:SER:O	1:A:635:VAL:HG22	2.18	0.44
5:A:1910:3PE:H282	5:A:1910:3PE:H252	1.72	0.44
2:E:152:PHE:O	2:E:155:LEU:HB2	2.17	0.44
3:F:65:GLN:HG3	3:F:805:ILE:HD12	1.99	0.44
3:F:736:PHE:CE2	3:F:816:GLY:HA3	2.53	0.44
1:A:548:LEU:HD12	1:A:549:VAL:N	2.32	0.44
3:F:254:LYS:HA	3:F:357:ASN:HB2	1.99	0.44
5:A:1910:3PE:H232	5:A:1910:3PE:H261	1.34	0.44
3:F:847:ASN:ND2	3:F:867:HIS:O	2.51	0.44
1:A:465:ASP:OD2	1:A:466:ILE:HG23	2.18	0.44
1:A:892:VAL:HG12	1:A:893:VAL:H	1.82	0.44
1:A:1366:MET:HE3	5:A:1904:3PE:H2A1	1.86	0.44
3:F:129:ALA:O	3:F:130:LYS:HG2	2.18	0.44
3:F:991:LYS:HE3	3:F:991:LYS:HB3	1.78	0.44
1:A:1363:SER:OG	1:A:1364:PHE:N	2.49	0.44
1:A:1390:ASP:OD2	1:A:1393:ILE:N	2.45	0.44
3:F:111:HIS:NE2	3:F:183:ASN:OD1	2.33	0.44
3:F:783:PHE:CE2	3:F:876:ARG:HD2	2.52	0.44
1:A:194:LEU:N	1:A:195:PRO:HD2	2.33	0.43
1:A:1169:LEU:HD23	1:A:1169:LEU:HA	1.81	0.43
2:E:16:ILE:O	2:E:20:ILE:HG13	2.18	0.43
2:E:163:LYS:HE2	2:E:163:LYS:HB3	1.81	0.43
3:F:888:HIS:O	3:F:892:ILE:HG23	2.17	0.43
1:A:45:ILE:HD12	1:A:46:SER:H	1.83	0.43
1:A:903:ARG:O	1:A:906:ARG:HG2	2.17	0.43
1:A:940:PHE:CD2	1:A:940:PHE:O	2.70	0.43
1:A:1115:VAL:HG13	1:A:1168:LYS:HE2	2.00	0.43
5:A:1911:3PE:H2C1	5:A:1911:3PE:C2H	2.31	0.43
3:F:64:TYR:C	3:F:66:ASP:H	2.20	0.43
2:E:122:THR:O	2:E:126:LEU:HG	2.19	0.43
3:F:471:ILE:HG13	3:F:471:ILE:O	2.18	0.43
3:F:721:ASN:OD1	3:F:721:ASN:N	2.50	0.43
3:F:870:TYR:O	3:F:872:ASN:N	2.52	0.43
1:A:138:ILE:HD13	1:A:138:ILE:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:59:LYS:HD2	2:E:59:LYS:HA	1.34	0.43
3:F:29:SER:OG	3:F:30:ALA:N	2.51	0.43
3:F:103:GLU:HG2	3:F:194:VAL:HG21	2.01	0.43
3:F:657:GLU:HA	3:F:749:LYS:HD3	2.01	0.43
1:A:45:ILE:CD1	1:A:107:ALA:HB2	2.49	0.43
5:A:1911:3PE:H2G1	5:A:1911:3PE:H2D1	1.57	0.43
3:F:50:THR:O	3:F:722:TYR:OH	2.33	0.43
3:F:863:LEU:HD12	3:F:1016:LEU:HD21	2.01	0.43
1:A:176:VAL:HG22	1:A:182:LEU:HB3	2.01	0.43
1:A:199:ILE:HD13	1:A:328:LEU:HB3	2.00	0.43
1:A:521:PRO:HA	1:A:524:ILE:HB	2.01	0.43
1:A:1159:ILE:HD13	1:A:1159:ILE:HA	1.83	0.43
2:E:153:VAL:O	2:E:156:GLU:HB2	2.19	0.43
1:A:549:VAL:O	1:A:553:LEU:HB3	2.19	0.43
2:E:27:VAL:HG23	2:E:28:VAL:H	1.83	0.43
1:A:903:ARG:N	1:A:904:PRO:HD2	2.33	0.43
5:A:1907:3PE:H322	5:A:1907:3PE:H31	1.86	0.43
5:A:1907:3PE:H221	5:A:1907:3PE:H31	2.00	0.43
3:F:234:LYS:HA	3:F:551:GLN:NE2	2.34	0.43
3:F:464:GLY:O	3:F:491:GLY:HA2	2.19	0.43
1:A:179:VAL:HG23	1:A:182:LEU:H	1.84	0.43
1:A:843:PHE:O	1:A:847:ILE:HG12	2.19	0.43
1:A:932:VAL:O	1:A:932:VAL:HG12	2.17	0.43
5:A:1911:3PE:HN2	5:A:1911:3PE:P	2.32	0.43
2:E:139:PRO:HA	2:E:142:MET:CE	2.49	0.43
3:F:750:GLU:H	3:F:750:GLU:CD	2.22	0.43
1:A:438:VAL:O	1:A:442:VAL:HG13	2.19	0.42
1:A:1263:SER:HB3	1:A:1383:ASN:HD21	1.82	0.42
2:E:55:ARG:HD2	2:E:81:SER:HA	2.00	0.42
3:F:539:PRO:HD3	3:F:977:CYS:CB	2.48	0.42
3:F:672:ASP:HB2	3:F:689:PHE:CE1	2.53	0.42
1:A:116:ALA:O	1:A:120:SER:HB2	2.19	0.42
1:A:212:ILE:O	1:A:216:GLU:HG2	2.20	0.42
1:A:1034:VAL:O	1:A:1037:ASN:HB2	2.19	0.42
1:A:1068:PHE:HB3	1:A:1381:MET:HG3	2.00	0.42
3:F:661:TYR:CD2	3:F:752:GLY:HA3	2.54	0.42
1:A:540:LYS:HD3	1:A:541:TYR:HD2	1.83	0.42
1:A:903:ARG:HG2	1:A:906:ARG:NH2	2.34	0.42
3:F:407:GLU:OE1	3:F:407:GLU:HA	2.19	0.42
1:A:503:VAL:HG13	1:A:534:ARG:HD2	2.01	0.42
3:F:442:LYS:HE3	3:F:442:LYS:HB2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:HE2	1:A:100:GLU:OE2	2.02	0.42
1:A:165:ARG:HG3	1:A:168:ARG:NH2	2.34	0.42
2:E:27:VAL:HG23	2:E:28:VAL:HG13	2.02	0.42
1:A:206:MET:CG	6:A:1909:PC1:H3F2	2.45	0.42
1:A:336:GLU:HA	1:A:339:LYS:HE3	2.02	0.42
1:A:1412:GLU:O	1:A:1414:LYS:HE2	2.20	0.42
3:F:773:ASN:OD1	3:F:773:ASN:N	2.51	0.42
1:A:57:ILE:HD11	1:A:100:GLU:HG3	2.02	0.42
1:A:1162:THR:O	1:A:1166:ILE:HG12	2.19	0.42
2:E:151:LEU:HD23	2:E:151:LEU:HA	1.79	0.42
1:A:114:GLN:HE21	1:A:116:ALA:HB2	1.85	0.42
1:A:117:TYR:CE2	1:A:123:ASN:HB3	2.55	0.42
1:A:445:ASN:HD21	1:A:534:ARG:HH21	1.68	0.42
5:A:1911:3PE:H2A1	5:A:1911:3PE:H2E2	2.02	0.42
2:E:33:ALA:HB3	2:E:51:PHE:CG	2.55	0.42
1:A:114:GLN:CG	1:A:116:ALA:HB2	2.50	0.42
1:A:1005:MET:O	1:A:1009:THR:HG23	2.19	0.42
1:A:1102:ILE:HG12	1:A:1411:PRO:HB3	2.01	0.42
1:A:894:LYS:HA	1:A:897:ARG:HD2	2.02	0.42
6:A:1909:PC1:H133	6:A:1909:PC1:O12	2.18	0.42
3:F:159:ARG:HH11	3:F:159:ARG:HD3	1.72	0.42
3:F:470:ASN:HD21	3:F:482:LYS:CE	2.33	0.42
3:F:743:ILE:HD13	3:F:743:ILE:HA	1.91	0.42
1:A:473:SER:O	1:A:476:THR:OG1	2.38	0.41
1:A:882:SER:O	1:A:882:SER:OG	2.27	0.41
1:A:1195:ILE:O	1:A:1199:LEU:HG	2.21	0.41
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.71	0.41
1:A:1129:MET:CE	5:A:1903:3PE:C2C	2.98	0.41
1:A:161:VAL:N	1:A:164:LEU:HD23	2.36	0.41
1:A:537:LYS:HZ2	1:A:538:ILE:HG23	1.86	0.41
1:A:542:TRP:HA	1:A:542:TRP:HE3	1.84	0.41
1:A:1085:GLN:H	1:A:1085:GLN:HG2	1.72	0.41
2:E:30:ASP:HA	2:E:52:GLY:HA2	2.01	0.41
3:F:642:ILE:H	3:F:642:ILE:HG12	1.73	0.41
3:F:676:SER:C	3:F:678:ASN:H	2.23	0.41
3:F:785:LYS:HB2	3:F:785:LYS:HE2	1.87	0.41
3:F:1021:VAL:HG22	3:F:1022:GLU:O	2.20	0.41
1:A:497:ASN:OD1	1:A:497:ASN:N	2.40	0.41
1:A:548:LEU:HD12	1:A:549:VAL:HG23	2.01	0.41
1:A:1126:ALA:O	1:A:1130:LEU:HG	2.21	0.41
1:A:1394:LEU:HD12	1:A:1394:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1412:GLU:HB2	1:A:1414:LYS:CD	2.50	0.41
2:E:50:HIS:O	2:E:56:ILE:HG22	2.21	0.41
3:F:447:GLN:O	3:F:464:GLY:HA2	2.20	0.41
3:F:766:PHE:O	3:F:770:SER:OG	2.30	0.41
3:F:889:LEU:HD23	3:F:889:LEU:HA	1.90	0.41
3:F:508:LEU:H	3:F:508:LEU:HG	1.73	0.41
1:A:1129:MET:HE1	5:A:1903:3PE:H2F2	2.02	0.41
3:F:197:LYS:HB2	3:F:197:LYS:HE3	1.89	0.41
1:A:111:LEU:HD23	1:A:112:PHE:HE1	1.85	0.41
3:F:107:VAL:HG11	3:F:190:ALA:HB3	2.02	0.41
3:F:153:ASP:OD1	3:F:154:ASP:N	2.54	0.41
1:A:181:SER:O	1:A:184:VAL:HG22	2.21	0.41
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.90	0.41
3:F:339:PHE:HB3	3:F:374:ILE:HG21	2.03	0.41
3:F:573:LYS:HE2	3:F:609:TYR:OH	2.21	0.41
3:F:1060:ASP:OD1	3:F:1060:ASP:N	2.49	0.41
1:A:555:SER:HA	1:A:663:ASN:OD1	2.20	0.41
5:A:1907:3PE:O22	5:A:1907:3PE:H11	2.21	0.41
3:F:155:ALA:C	3:F:157:PHE:H	2.24	0.41
3:F:226:VAL:H	3:F:226:VAL:HG22	1.65	0.41
3:F:409:LYS:HB3	3:F:409:LYS:HE2	1.78	0.41
3:F:534:ILE:HD11	3:F:561:LEU:HB2	2.02	0.41
3:F:902:ASP:OD2	3:F:905:SER:OG	2.38	0.41
3:F:146:ARG:HD3	3:F:146:ARG:HA	1.64	0.40
3:F:255:ASP:N	3:F:357:ASN:O	2.54	0.40
3:F:541:ILE:HD12	3:F:541:ILE:HA	1.80	0.40
3:F:672:ASP:HB2	3:F:689:PHE:HE1	1.86	0.40
1:A:38:ASN:HD22	1:A:41:ARG:NE	2.19	0.40
1:A:906:ARG:HB2	1:A:910:ARG:HH12	1.85	0.40
1:A:1103:PRO:CB	1:A:1108:GLN:HE22	2.34	0.40
3:F:626:LEU:HD23	3:F:626:LEU:HA	1.85	0.40
3:F:696:ASN:OD1	3:F:697:ASN:N	2.53	0.40
1:A:231:THR:HG22	1:A:232:ASP:N	2.36	0.40
1:A:548:LEU:O	1:A:552:LEU:N	2.36	0.40
1:A:624:ILE:HD13	1:A:624:ILE:HG21	1.85	0.40
1:A:635:VAL:HG21	5:A:1905:3PE:H31	2.04	0.40
1:A:1056:MET:HE3	1:A:1056:MET:HB3	1.98	0.40
2:E:149:LEU:O	2:E:152:PHE:HB3	2.21	0.40
3:F:234:LYS:HG2	3:F:551:GLN:HE22	1.87	0.40
1:A:38:ASN:HB2	1:A:39:PRO:HD2	2.04	0.40
1:A:567:PHE:CE1	5:A:1908:3PE:C29	3.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:PHE:O	1:A:909:ASN:ND2	2.55	0.40
1:A:1254:ARG:HE	1:A:1254:ARG:HB3	1.59	0.40
3:F:76:ARG:NH2	3:F:611:TRP:O	2.54	0.40
1:A:136:THR:HG22	1:A:164:LEU:HD12	2.04	0.40
1:A:186:LEU:O	1:A:186:LEU:HD23	2.21	0.40
2:E:37:PRO:HA	2:E:174:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1095/1873 (58%)	993 (91%)	101 (9%)	1 (0%)	48	80
2	E	159/222 (72%)	142 (89%)	17 (11%)	0	100	100
3	F	968/1105 (88%)	871 (90%)	96 (10%)	1 (0%)	48	80
All	All	2222/3200 (69%)	2006 (90%)	214 (10%)	2 (0%)	50	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	TRP
3	F	871	THR

5.3.2 Protein sidechains [i](#)

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	981/1628 (60%)	880 (90%)	101 (10%)	6	25
2	E	143/192 (74%)	129 (90%)	14 (10%)	6	27
3	F	868/973 (89%)	805 (93%)	63 (7%)	11	41
All	All	1992/2793 (71%)	1814 (91%)	178 (9%)	10	31

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLU
1	A	72	LEU
1	A	100	GLU
1	A	112	PHE
1	A	126	ASP
1	A	132	LEU
1	A	144	VAL
1	A	175	LEU
1	A	176	VAL
1	A	194	LEU
1	A	201	LEU
1	A	247	ARG
1	A	250	SER
1	A	252	ARG
1	A	262	ARG
1	A	339	LYS
1	A	434	PHE
1	A	448	SER
1	A	451	SER
1	A	452	GLU
1	A	461	THR
1	A	468	ASN
1	A	484	TYR
1	A	491	TYR
1	A	494	SER
1	A	497	ASN
1	A	498	ARG
1	A	500	ASP
1	A	505	CYS
1	A	509	LEU
1	A	510	GLU
1	A	511	LEU
1	A	515	GLU
1	A	524	ILE

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Mol	Chain	Res	Type
1	A	528	ARG
1	A	531	ARG
1	A	532	LEU
1	A	535	LEU
1	A	537	LYS
1	A	538	ILE
1	A	540	LYS
1	A	552	LEU
1	A	553	LEU
1	A	561	SER
1	A	615	ASP
1	A	636	LEU
1	A	657	LEU
1	A	666	GLU
1	A	668	GLU
1	A	797	ASN
1	A	803	ASN
1	A	804	PHE
1	A	822	ILE
1	A	823	ARG
1	A	876	VAL
1	A	897	ARG
1	A	899	LEU
1	A	923	VAL
1	A	925	ILE
1	A	933	LEU
1	A	935	THR
1	A	938	LEU
1	A	983	MET
1	A	999	ASN
1	A	1011	SER
1	A	1036	ASN
1	A	1041	MET
1	A	1060	PHE
1	A	1091	TYR
1	A	1097	PRO
1	A	1099	ARG
1	A	1100	CYS
1	A	1108	GLN
1	A	1114	VAL
1	A	1117	SER
1	A	1124	MET

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Mol	Chain	Res	Type
1	A	1125	PHE
1	A	1127	LEU
1	A	1188	LEU
1	A	1193	SER
1	A	1198	ILE
1	A	1204	THR
1	A	1232	SER
1	A	1234	PHE
1	A	1237	LEU
1	A	1243	LEU
1	A	1244	ILE
1	A	1265	GLN
1	A	1270	VAL
1	A	1289	PHE
1	A	1308	THR
1	A	1332	CYS
1	A	1342	SER
1	A	1354	THR
1	A	1363	SER
1	A	1384	PHE
1	A	1385	ASP
1	A	1400	ASP
1	A	1420	LEU
1	A	1421	ASP
1	A	1427	ARG
2	E	5	GLU
2	E	12	THR
2	E	13	LEU
2	E	32	TRP
2	E	50	HIS
2	E	59	LYS
2	E	60	ARG
2	E	78	LYS
2	E	127	MET
2	E	162	VAL
2	E	164	ARG
2	E	189	PHE
2	E	214	SER
2	E	215	CYS
3	F	31	VAL
3	F	59	ASP
3	F	65	GLN

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Mol	Chain	Res	Type
3	F	76	ARG
3	F	91	SER
3	F	114	ARG
3	F	139	ASP
3	F	158	ARG
3	F	212	SER
3	F	226	VAL
3	F	235	ILE
3	F	237	LEU
3	F	241	ARG
3	F	254	LYS
3	F	255	ASP
3	F	257	LEU
3	F	269	LEU
3	F	270	THR
3	F	295	SER
3	F	314	VAL
3	F	324	VAL
3	F	328	THR
3	F	381	ASP
3	F	393	GLN
3	F	426	GLN
3	F	465	THR
3	F	482	LYS
3	F	505	ARG
3	F	508	LEU
3	F	523	VAL
3	F	532	LYS
3	F	542	ASN
3	F	546	ARG
3	F	571	ASP
3	F	596	SER
3	F	610	THR
3	F	612	THR
3	F	630	SER
3	F	649	GLU
3	F	651	LEU
3	F	661	TYR
3	F	711	ASP
3	F	739	THR
3	F	770	SER
3	F	775	ASN

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Mol	Chain	Res	Type
3	F	793	SER
3	F	798	SER
3	F	817	ILE
3	F	871	THR
3	F	900	SER
3	F	906	VAL
3	F	907	CYS
3	F	908	GLU
3	F	976	SER
3	F	982	THR
3	F	983	GLN
3	F	997	LEU
3	F	999	CYS
3	F	1005	ILE
3	F	1014	THR
3	F	1062	CYS
3	F	1067	VAL
3	F	1071	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	239	ASN
1	A	274	HIS
1	A	277	ASN
1	A	445	ASN
1	A	453	HIS
1	A	803	ASN
1	A	909	ASN
1	A	939	GLN
1	A	958	ASN
1	A	999	ASN
1	A	1058	ASN
1	A	1069	GLN
1	A	1084	ASN
1	A	1087	GLN
1	A	1138	GLN
1	A	1154	ASN
1	A	1183	ASN
1	A	1374	ASN
1	A	1383	ASN

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Mol	Chain	Res	Type
1	A	1398	HIS
2	E	209	GLN
3	F	56	GLN
3	F	164	GLN
3	F	165	HIS
3	F	357	ASN
3	F	470	ASN
3	F	511	ASN
3	F	542	ASN
3	F	551	GLN
3	F	556	GLN
3	F	679	ASN
3	F	685	ASN
3	F	720	GLN
3	F	847	ASN
3	F	988	ASN
3	F	1039	GLN
3	F	1065	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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$
7	VFY	A	1912	-	24,26,26	3.75	7 (29%)	32,39,39	2.63	8 (25%)
5	3PE	A	1902	-	32,32,50	1.15	2 (6%)	35,37,55	1.20	4 (11%)
5	3PE	A	1904	-	42,42,50	1.00	2 (4%)	45,47,55	1.12	3 (6%)
5	3PE	A	1906	-	43,43,50	1.00	2 (4%)	46,48,55	1.10	3 (6%)
5	3PE	A	1905	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
5	3PE	A	1907	-	37,37,50	1.07	2 (5%)	40,42,55	1.11	3 (7%)
5	3PE	A	1903	-	50,50,50	0.92	2 (4%)	53,55,55	1.07	3 (5%)
5	3PE	A	1908	-	20,20,50	1.05	1 (5%)	22,23,55	1.00	1 (4%)
5	3PE	A	1910	-	31,31,50	1.17	2 (6%)	34,36,55	1.17	2 (5%)
5	3PE	A	1911	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
6	PC1	A	1909	-	53,53,53	0.94	2 (3%)	59,61,61	1.02	3 (5%)

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
7	VFY	A	1912	-	-	6/18/40/40	0/2/2/2
5	3PE	A	1902	-	-	12/36/36/54	-
5	3PE	A	1904	-	-	25/46/46/54	-
5	3PE	A	1906	-	-	31/47/47/54	-
5	3PE	A	1905	-	-	29/54/54/54	-
5	3PE	A	1907	-	-	25/41/41/54	-
5	3PE	A	1903	-	-	22/54/54/54	-
5	3PE	A	1908	-	-	11/21/21/54	-
5	3PE	A	1910	-	-	18/35/35/54	-
5	3PE	A	1911	-	-	25/54/54/54	-
6	PC1	A	1909	-	-	35/57/57/57	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1912	VFY	C06-C05	15.28	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1912	VFY	C06-N08	5.13	1.45	1.38
7	A	1912	VFY	C09-N08	4.82	1.44	1.38
5	A	1906	3PE	O31-C31	4.36	1.46	1.33
5	A	1907	3PE	O31-C31	4.30	1.45	1.33
5	A	1910	3PE	O31-C31	4.29	1.45	1.33
5	A	1903	3PE	O31-C31	4.27	1.45	1.33
5	A	1902	3PE	O31-C31	4.26	1.45	1.33
6	A	1909	PC1	O31-C31	4.25	1.45	1.33
5	A	1905	3PE	O31-C31	4.25	1.45	1.33
5	A	1908	3PE	O21-C21	4.23	1.45	1.33
5	A	1904	3PE	O31-C31	4.20	1.45	1.33
5	A	1911	3PE	O31-C31	4.20	1.45	1.33
6	A	1909	PC1	O21-C21	4.12	1.45	1.34
5	A	1904	3PE	O21-C21	4.11	1.45	1.34
5	A	1906	3PE	O21-C21	4.11	1.45	1.34
5	A	1907	3PE	O21-C21	4.10	1.45	1.34
5	A	1902	3PE	O21-C21	4.10	1.45	1.34
5	A	1905	3PE	O21-C21	4.08	1.45	1.34
5	A	1910	3PE	O21-C21	4.07	1.45	1.34
5	A	1911	3PE	O21-C21	4.06	1.45	1.34
5	A	1903	3PE	O21-C21	4.05	1.45	1.34
7	A	1912	VFY	O03-C02	3.04	1.40	1.33
7	A	1912	VFY	C02-C05	3.02	1.53	1.47
7	A	1912	VFY	O14-N12	-2.89	1.17	1.22
7	A	1912	VFY	O03-C04	-2.26	1.40	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1912	VFY	C07-C06-C05	-8.40	119.26	127.61
7	A	1912	VFY	C10-C09-N08	5.46	119.76	113.42
7	A	1912	VFY	C07-C06-N08	5.04	119.28	113.42
5	A	1905	3PE	O21-C21-C22	4.42	121.05	111.48
5	A	1904	3PE	O21-C21-C22	4.41	121.02	111.48
7	A	1912	VFY	C09-N08-C06	-4.24	119.50	123.44
7	A	1912	VFY	O03-C02-C05	4.23	120.09	112.31
5	A	1902	3PE	O21-C21-C22	4.14	120.44	111.48
5	A	1903	3PE	O21-C21-C22	4.04	120.22	111.48
5	A	1910	3PE	O21-C21-C22	3.98	120.08	111.48
5	A	1911	3PE	O21-C21-C22	3.94	120.00	111.48
5	A	1906	3PE	O21-C21-C22	3.94	120.00	111.48
7	A	1912	VFY	C11-C15-C05	3.93	113.49	108.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1907	3PE	O21-C21-C22	3.90	119.91	111.48
6	A	1909	PC1	O21-C21-C22	3.88	119.88	111.48
5	A	1911	3PE	O31-C31-C32	2.97	120.90	111.83
6	A	1909	PC1	O31-C31-C32	2.92	120.73	111.83
5	A	1905	3PE	O31-C31-C32	2.89	120.66	111.83
5	A	1908	3PE	O21-C21-C22	2.89	120.64	111.83
5	A	1903	3PE	O31-C31-C32	2.86	120.55	111.83
5	A	1904	3PE	O31-C31-C32	2.78	120.32	111.83
5	A	1903	3PE	C2-O21-C21	-2.76	111.18	117.80
5	A	1906	3PE	O31-C31-C32	2.76	120.26	111.83
5	A	1910	3PE	O31-C31-C32	2.73	120.17	111.83
5	A	1907	3PE	O31-C31-C32	2.69	120.04	111.83
5	A	1902	3PE	O31-C31-C32	2.69	120.03	111.83
5	A	1902	3PE	C2-O21-C21	-2.53	111.74	117.80
7	A	1912	VFY	O01-C02-C05	-2.49	119.94	125.20
5	A	1911	3PE	C2-O21-C21	-2.26	112.38	117.80
5	A	1907	3PE	C2-O21-C21	-2.15	112.65	117.80
5	A	1906	3PE	C2-O21-C21	-2.13	112.70	117.80
6	A	1909	PC1	C2-O21-C21	-2.12	112.72	117.80
5	A	1905	3PE	O21-C21-O22	-2.09	118.82	123.70
5	A	1904	3PE	O21-C21-O22	-2.08	118.84	123.70
5	A	1902	3PE	O21-C21-O22	-2.04	118.93	123.70
7	A	1912	VFY	C15-C05-C06	-2.00	118.58	120.86

There are no chirality outliers.

All (239) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1902	3PE	O22-C21-O21-C2
5	A	1902	3PE	C22-C21-O21-C2
5	A	1903	3PE	C22-C21-O21-C2
5	A	1904	3PE	C1-O11-P-O12
5	A	1904	3PE	C1-O11-P-O14
5	A	1904	3PE	C11-O13-P-O11
5	A	1904	3PE	C11-O13-P-O12
5	A	1904	3PE	C11-O13-P-O14
5	A	1904	3PE	O22-C21-O21-C2
5	A	1904	3PE	C22-C21-O21-C2
5	A	1905	3PE	C1-O11-P-O13
5	A	1905	3PE	C1-O11-P-O14
5	A	1905	3PE	O22-C21-O21-C2
5	A	1905	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
5	A	1906	3PE	C11-O13-P-O12
5	A	1906	3PE	C12-C11-O13-P
5	A	1907	3PE	C1-O11-P-O12
5	A	1907	3PE	C1-O11-P-O13
5	A	1907	3PE	C11-O13-P-O11
5	A	1907	3PE	C11-O13-P-O14
5	A	1907	3PE	O13-C11-C12-N
5	A	1907	3PE	C32-C31-O31-C3
5	A	1907	3PE	C22-C21-O21-C2
5	A	1908	3PE	C1-O11-P-O12
5	A	1908	3PE	C1-O11-P-O13
5	A	1908	3PE	C1-O11-P-O14
5	A	1908	3PE	C11-O13-P-O12
5	A	1908	3PE	C12-C11-O13-P
5	A	1910	3PE	C11-O13-P-O12
5	A	1910	3PE	O13-C11-C12-N
6	A	1909	PC1	C11-O13-P-O12
6	A	1909	PC1	C11-O13-P-O11
6	A	1909	PC1	O21-C2-C3-O31
7	A	1912	VFY	C05-C02-O03-C04
7	A	1912	VFY	O01-C02-O03-C04
5	A	1907	3PE	O32-C31-O31-C3
5	A	1906	3PE	O32-C31-O31-C3
7	A	1912	VFY	O01-C02-C05-C06
7	A	1912	VFY	O03-C02-C05-C06
5	A	1903	3PE	O22-C21-O21-C2
5	A	1907	3PE	O22-C21-O21-C2
5	A	1906	3PE	C32-C31-O31-C3
6	A	1909	PC1	C32-C31-O31-C3
5	A	1903	3PE	C32-C31-O31-C3
5	A	1910	3PE	C25-C26-C27-C28
5	A	1903	3PE	O32-C31-O31-C3
6	A	1909	PC1	O32-C31-O31-C3
5	A	1906	3PE	C22-C21-O21-C2
5	A	1906	3PE	O22-C21-O21-C2
5	A	1902	3PE	C33-C34-C35-C36
5	A	1904	3PE	C32-C31-O31-C3
5	A	1910	3PE	C32-C31-O31-C3
5	A	1911	3PE	C2D-C2E-C2F-C2G
5	A	1904	3PE	C35-C36-C37-C38
5	A	1910	3PE	C23-C24-C25-C26
5	A	1906	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
5	A	1911	3PE	C31-C32-C33-C34
5	A	1904	3PE	O32-C31-O31-C3
5	A	1910	3PE	O32-C31-O31-C3
5	A	1908	3PE	C22-C21-O21-C2
5	A	1910	3PE	C22-C21-O21-C2
5	A	1910	3PE	O22-C21-O21-C2
5	A	1907	3PE	C28-C29-C2A-C2B
5	A	1905	3PE	C31-C32-C33-C34
6	A	1909	PC1	C28-C29-C2A-C2B
5	A	1911	3PE	C22-C21-O21-C2
5	A	1904	3PE	C36-C37-C38-C39
5	A	1903	3PE	C22-C23-C24-C25
5	A	1904	3PE	C28-C29-C2A-C2B
5	A	1905	3PE	C3D-C3E-C3F-C3G
5	A	1905	3PE	C3E-C3F-C3G-C3H
6	A	1909	PC1	C23-C24-C25-C26
5	A	1908	3PE	O22-C21-O21-C2
5	A	1911	3PE	C33-C34-C35-C36
5	A	1904	3PE	C2B-C2C-C2D-C2E
5	A	1911	3PE	C2C-C2D-C2E-C2F
5	A	1903	3PE	C3A-C3B-C3C-C3D
5	A	1903	3PE	C3D-C3E-C3F-C3G
5	A	1904	3PE	C33-C34-C35-C36
5	A	1905	3PE	C29-C2A-C2B-C2C
5	A	1911	3PE	O22-C21-O21-C2
5	A	1907	3PE	C1-C2-C3-O31
5	A	1911	3PE	C21-C22-C23-C24
5	A	1904	3PE	C2E-C2F-C2G-C2H
5	A	1906	3PE	C2A-C2B-C2C-C2D
6	A	1909	PC1	C2A-C2B-C2C-C2D
5	A	1902	3PE	C25-C26-C27-C28
5	A	1910	3PE	C28-C29-C2A-C2B
6	A	1909	PC1	C34-C35-C36-C37
5	A	1902	3PE	C35-C36-C37-C38
5	A	1907	3PE	C25-C26-C27-C28
5	A	1903	3PE	C2D-C2E-C2F-C2G
5	A	1907	3PE	C23-C24-C25-C26
5	A	1905	3PE	C3A-C3B-C3C-C3D
5	A	1906	3PE	C35-C36-C37-C38
6	A	1909	PC1	C36-C37-C38-C39
5	A	1906	3PE	C2B-C2C-C2D-C2E
5	A	1906	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
6	A	1909	PC1	C29-C2A-C2B-C2C
5	A	1906	3PE	C31-C32-C33-C34
5	A	1911	3PE	C28-C29-C2A-C2B
5	A	1902	3PE	C27-C28-C29-C2A
5	A	1905	3PE	C27-C28-C29-C2A
5	A	1907	3PE	C24-C25-C26-C27
6	A	1909	PC1	C33-C34-C35-C36
6	A	1909	PC1	C25-C26-C27-C28
5	A	1905	3PE	O11-C1-C2-O21
5	A	1902	3PE	C24-C25-C26-C27
5	A	1908	3PE	C22-C23-C24-C25
5	A	1907	3PE	C22-C23-C24-C25
5	A	1905	3PE	C3C-C3D-C3E-C3F
5	A	1911	3PE	C29-C2A-C2B-C2C
5	A	1903	3PE	C38-C39-C3A-C3B
5	A	1904	3PE	C23-C24-C25-C26
5	A	1906	3PE	C32-C33-C34-C35
5	A	1911	3PE	C2A-C2B-C2C-C2D
6	A	1909	PC1	C39-C3A-C3B-C3C
5	A	1911	3PE	C22-C23-C24-C25
6	A	1909	PC1	C32-C33-C34-C35
6	A	1909	PC1	C2B-C2C-C2D-C2E
7	A	1912	VFY	O03-C02-C05-C15
5	A	1904	3PE	C2C-C2D-C2E-C2F
7	A	1912	VFY	O01-C02-C05-C15
5	A	1904	3PE	C21-C22-C23-C24
5	A	1906	3PE	C1-C2-C3-O31
6	A	1909	PC1	C1-C2-C3-O31
5	A	1905	3PE	C2A-C2B-C2C-C2D
5	A	1906	3PE	C37-C38-C39-C3A
5	A	1905	3PE	C32-C31-O31-C3
5	A	1911	3PE	C32-C31-O31-C3
5	A	1911	3PE	C23-C24-C25-C26
6	A	1909	PC1	C2C-C2D-C2E-C2F
5	A	1902	3PE	C23-C24-C25-C26
5	A	1911	3PE	C3B-C3C-C3D-C3E
5	A	1904	3PE	C32-C33-C34-C35
5	A	1903	3PE	C27-C28-C29-C2A
5	A	1903	3PE	C36-C37-C38-C39
5	A	1911	3PE	C3C-C3D-C3E-C3F
5	A	1903	3PE	C3B-C3C-C3D-C3E
5	A	1903	3PE	C3E-C3F-C3G-C3H

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Mol	Chain	Res	Type	Atoms
5	A	1906	3PE	C29-C2A-C2B-C2C
5	A	1906	3PE	O21-C2-C3-O31
5	A	1911	3PE	C39-C3A-C3B-C3C
5	A	1906	3PE	C2F-C2G-C2H-C2I
5	A	1907	3PE	C29-C2A-C2B-C2C
5	A	1906	3PE	C38-C39-C3A-C3B
5	A	1903	3PE	C39-C3A-C3B-C3C
6	A	1909	PC1	C2E-C2F-C2G-C2H
5	A	1905	3PE	C34-C35-C36-C37
6	A	1909	PC1	O11-C1-C2-C3
5	A	1904	3PE	C29-C2A-C2B-C2C
5	A	1910	3PE	C33-C34-C35-C36
5	A	1911	3PE	O32-C31-O31-C3
5	A	1911	3PE	C34-C35-C36-C37
5	A	1905	3PE	O32-C31-O31-C3
5	A	1905	3PE	C39-C3A-C3B-C3C
5	A	1902	3PE	C1-C2-C3-O31
5	A	1904	3PE	C1-C2-C3-O31
6	A	1909	PC1	C2F-C2G-C2H-C2I
5	A	1902	3PE	O21-C2-C3-O31
5	A	1904	3PE	O21-C2-C3-O31
5	A	1905	3PE	O21-C2-C3-O31
5	A	1906	3PE	C34-C35-C36-C37
5	A	1903	3PE	C3F-C3G-C3H-C3I
5	A	1910	3PE	C22-C23-C24-C25
6	A	1909	PC1	C24-C25-C26-C27
5	A	1905	3PE	O11-C1-C2-C3
5	A	1904	3PE	C25-C26-C27-C28
5	A	1907	3PE	C1-C2-O21-C21
5	A	1906	3PE	C25-C26-C27-C28
6	A	1909	PC1	C3A-C3B-C3C-C3D
5	A	1903	3PE	C1-C2-C3-O31
5	A	1905	3PE	C1-C2-C3-O31
5	A	1905	3PE	C12-C11-O13-P
5	A	1911	3PE	C12-C11-O13-P
6	A	1909	PC1	C12-C11-O13-P
5	A	1903	3PE	O21-C2-C3-O31
5	A	1910	3PE	O21-C2-C3-O31
5	A	1907	3PE	C36-C37-C38-C39
6	A	1909	PC1	O13-C11-C12-N
5	A	1905	3PE	C23-C24-C25-C26
5	A	1903	3PE	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
6	A	1909	PC1	C3F-C3G-C3H-C3I
5	A	1902	3PE	O11-C1-C2-C3
5	A	1903	3PE	C28-C29-C2A-C2B
5	A	1907	3PE	C2-C1-O11-P
5	A	1902	3PE	O11-C1-C2-O21
5	A	1907	3PE	O11-C1-C2-O21
5	A	1911	3PE	O11-C1-C2-O21
6	A	1909	PC1	O11-C1-C2-O21
5	A	1907	3PE	C37-C38-C39-C3A
5	A	1907	3PE	O21-C2-C3-O31
5	A	1905	3PE	C38-C39-C3A-C3B
5	A	1905	3PE	C2F-C2G-C2H-C2I
5	A	1908	3PE	C23-C24-C25-C26
5	A	1903	3PE	C1-O11-P-O14
5	A	1903	3PE	C11-O13-P-O14
5	A	1904	3PE	C1-O11-P-O13
5	A	1905	3PE	C1-O11-P-O12
5	A	1905	3PE	O13-C11-C12-N
5	A	1906	3PE	C11-O13-P-O11
5	A	1906	3PE	C11-O13-P-O14
5	A	1908	3PE	C11-O13-P-O11
5	A	1910	3PE	C11-O13-P-O11
6	A	1909	PC1	C11-C12-N-C15
5	A	1905	3PE	C28-C29-C2A-C2B
6	A	1909	PC1	C37-C38-C39-C3A
5	A	1904	3PE	C2F-C2G-C2H-C2I
5	A	1903	3PE	C2B-C2C-C2D-C2E
5	A	1906	3PE	O11-C1-C2-O21
5	A	1908	3PE	C26-C27-C28-C29
5	A	1911	3PE	O21-C2-C3-O31
5	A	1905	3PE	C24-C25-C26-C27
6	A	1909	PC1	C11-C12-N-C14
5	A	1906	3PE	C28-C29-C2A-C2B
5	A	1906	3PE	C24-C25-C26-C27
5	A	1911	3PE	C32-C33-C34-C35
5	A	1905	3PE	C2-C1-O11-P
5	A	1907	3PE	O11-C1-C2-C3
5	A	1907	3PE	C33-C34-C35-C36
6	A	1909	PC1	C11-C12-N-C13
5	A	1910	3PE	C1-C2-C3-O31
5	A	1911	3PE	C1-C2-C3-O31
5	A	1906	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	1906	3PE	C33-C34-C35-C36
5	A	1910	3PE	C2-C1-O11-P
6	A	1909	PC1	O21-C21-C22-C23
5	A	1906	3PE	C23-C24-C25-C26
5	A	1906	3PE	C2D-C2E-C2F-C2G
5	A	1910	3PE	C32-C33-C34-C35
5	A	1911	3PE	C2B-C2C-C2D-C2E
5	A	1910	3PE	O31-C31-C32-C33
5	A	1911	3PE	O11-C1-C2-C3
5	A	1906	3PE	C1-C2-O21-C21
6	A	1909	PC1	C3C-C3D-C3E-C3F
6	A	1909	PC1	C35-C36-C37-C38
6	A	1909	PC1	O22-C21-C22-C23
5	A	1910	3PE	O32-C31-C32-C33
5	A	1907	3PE	C27-C28-C29-C2A

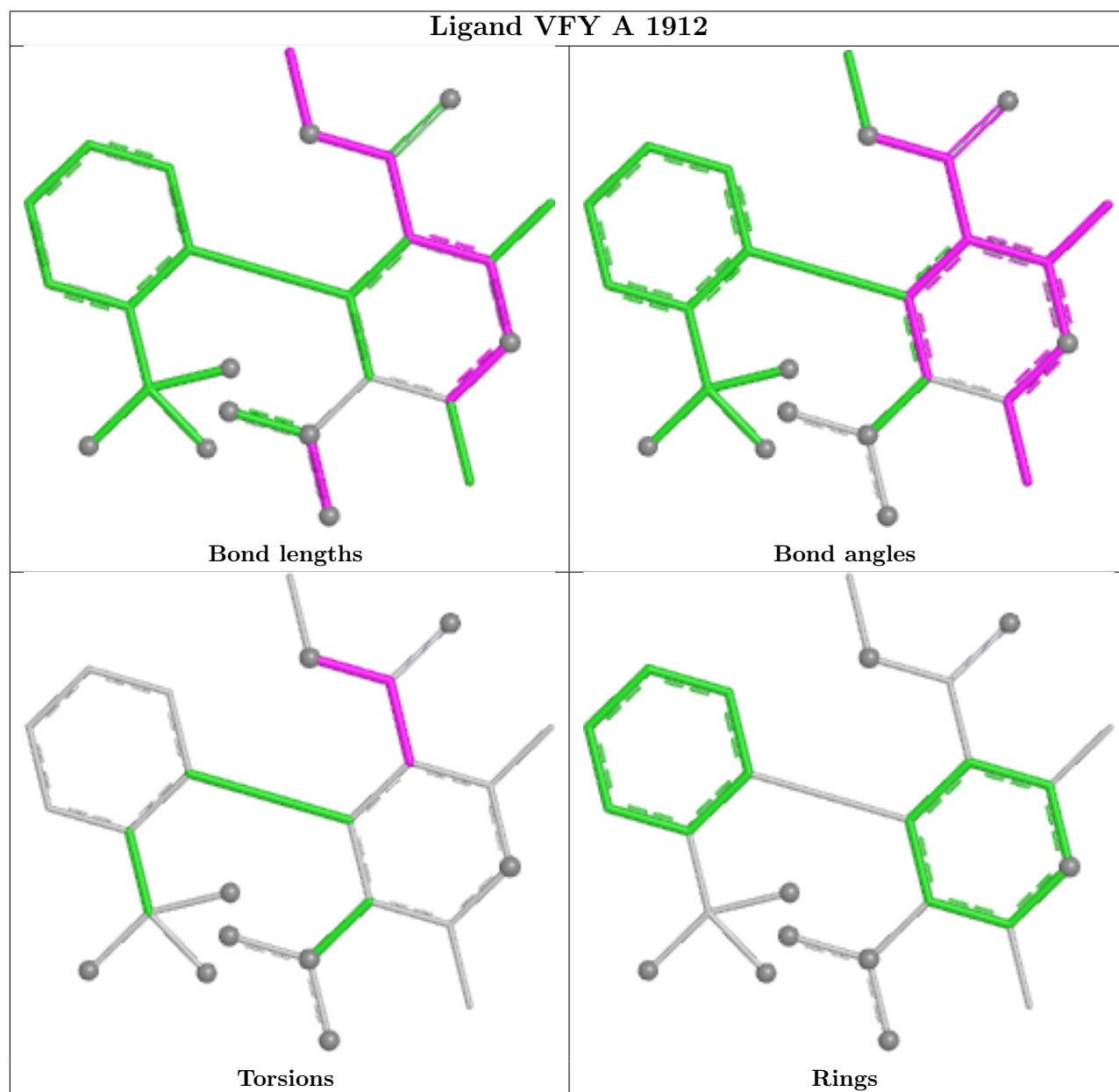
There are no ring outliers.

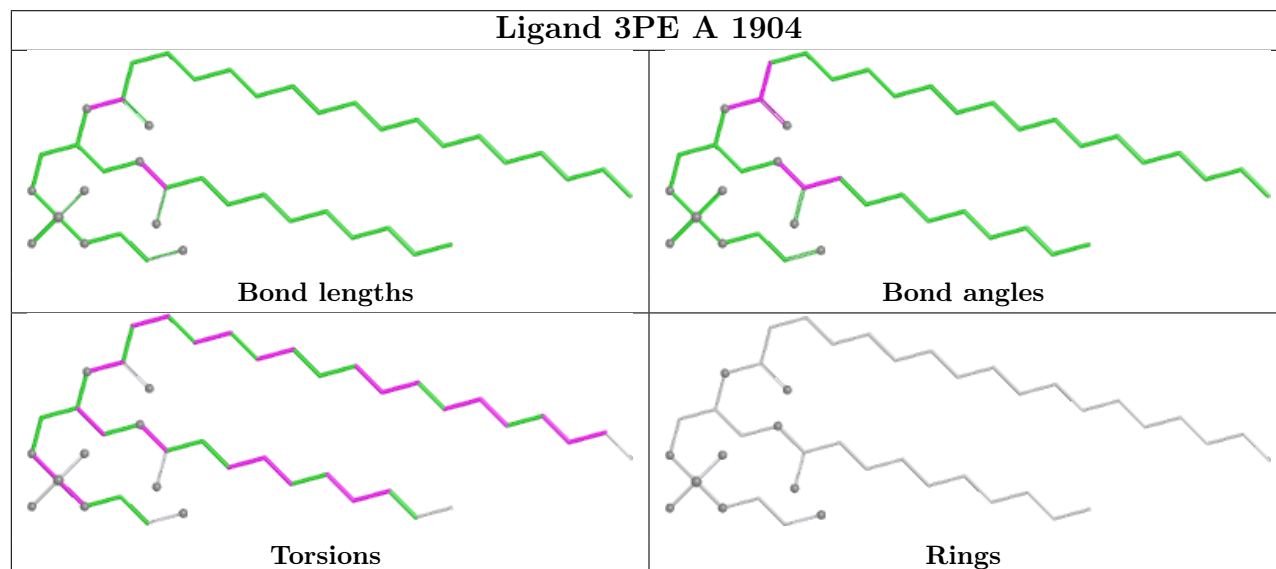
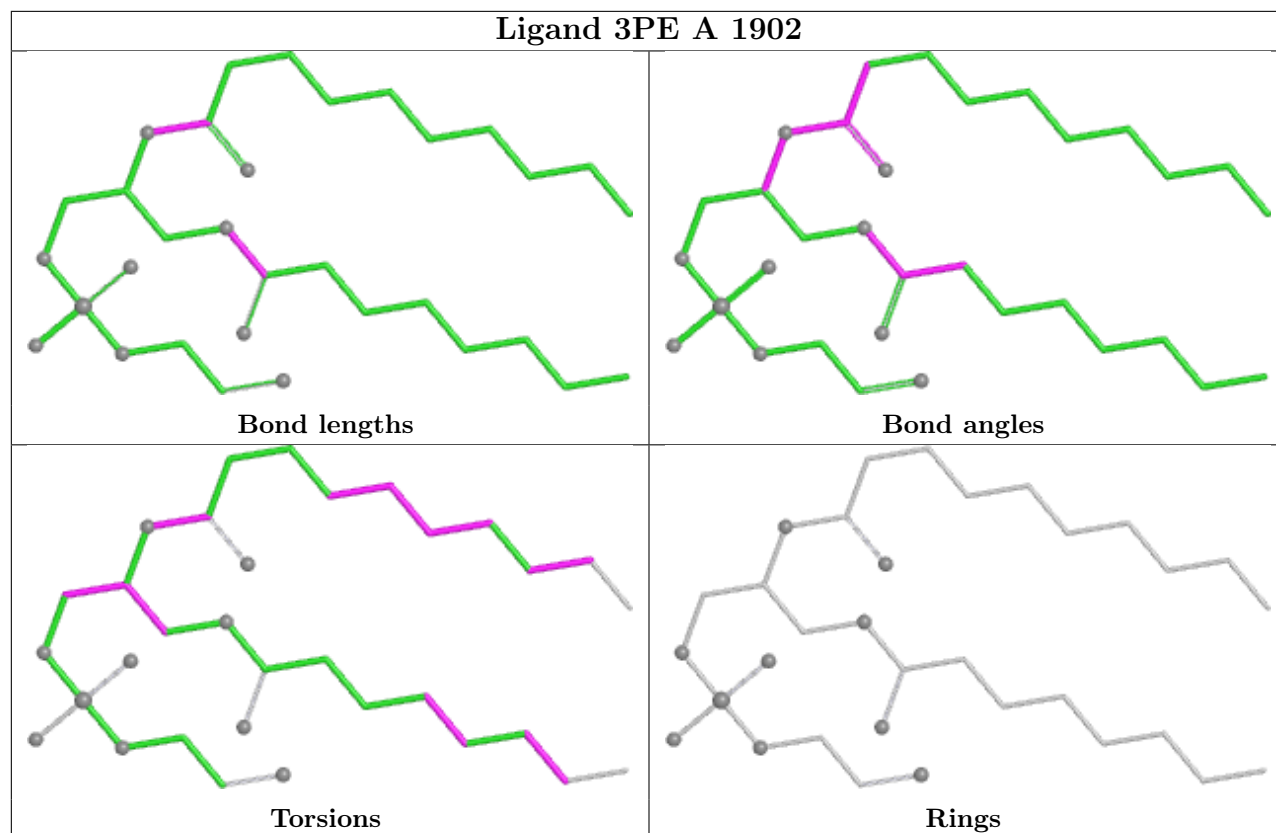
11 monomers are involved in 110 short contacts:

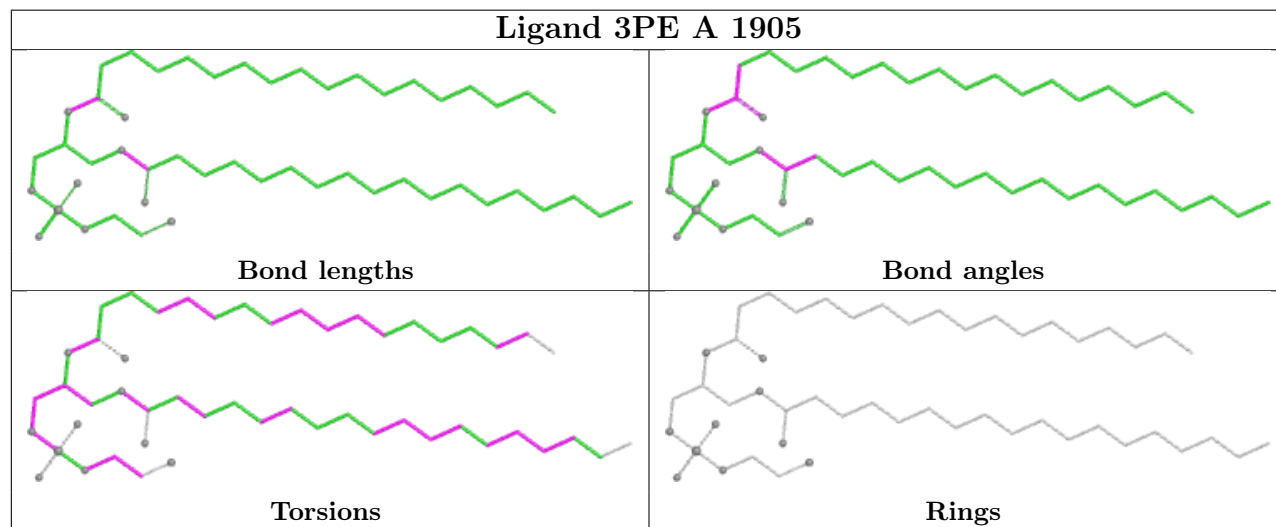
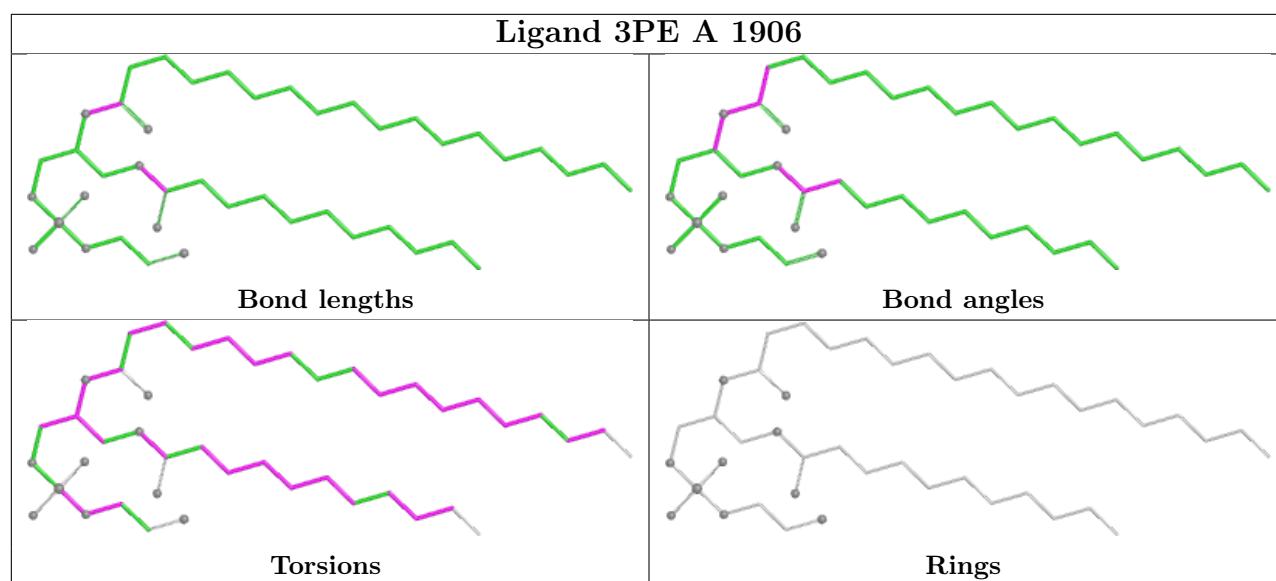
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1912	VFY	5	0
5	A	1902	3PE	2	0
5	A	1904	3PE	15	0
5	A	1906	3PE	12	0
5	A	1905	3PE	9	0
5	A	1907	3PE	11	0
5	A	1903	3PE	13	0
5	A	1908	3PE	10	0
5	A	1910	3PE	4	0
5	A	1911	3PE	15	0
6	A	1909	PC1	18	0

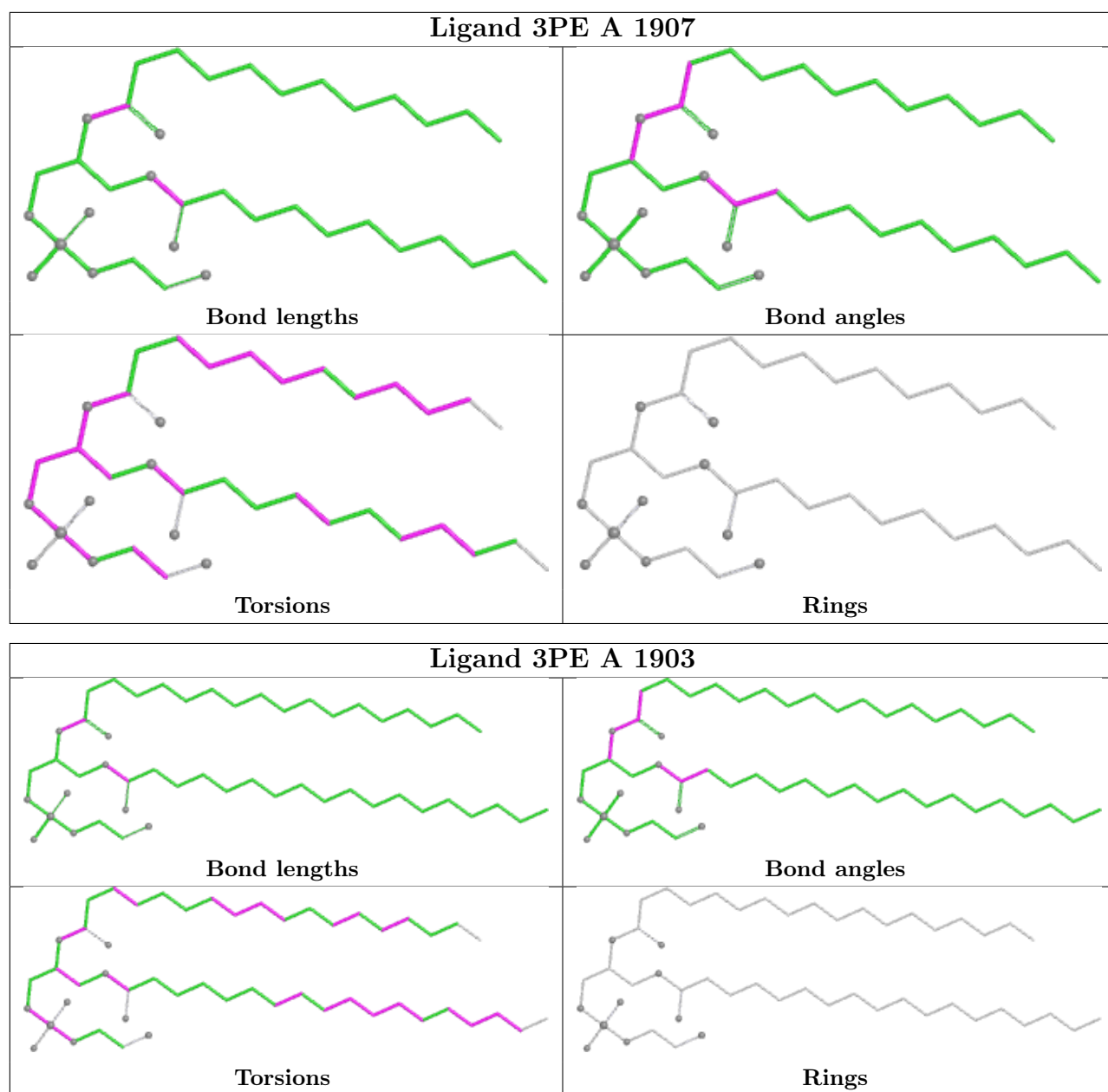
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

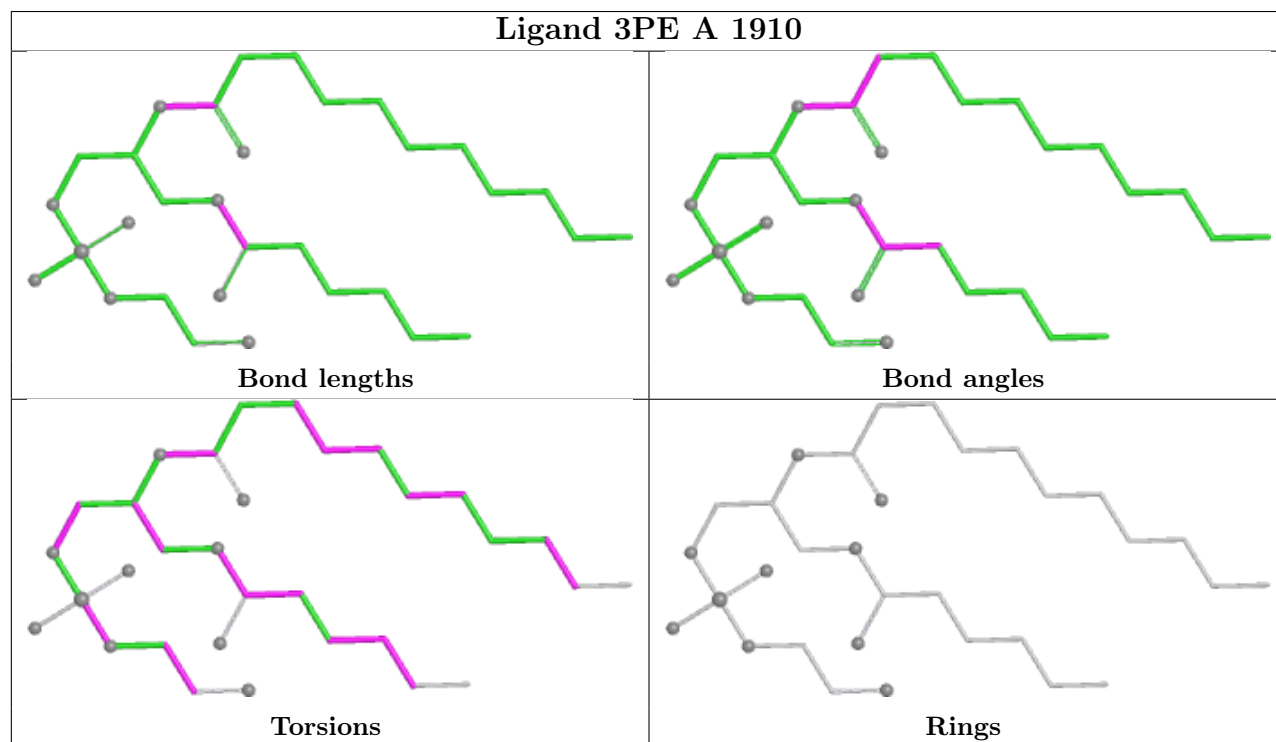
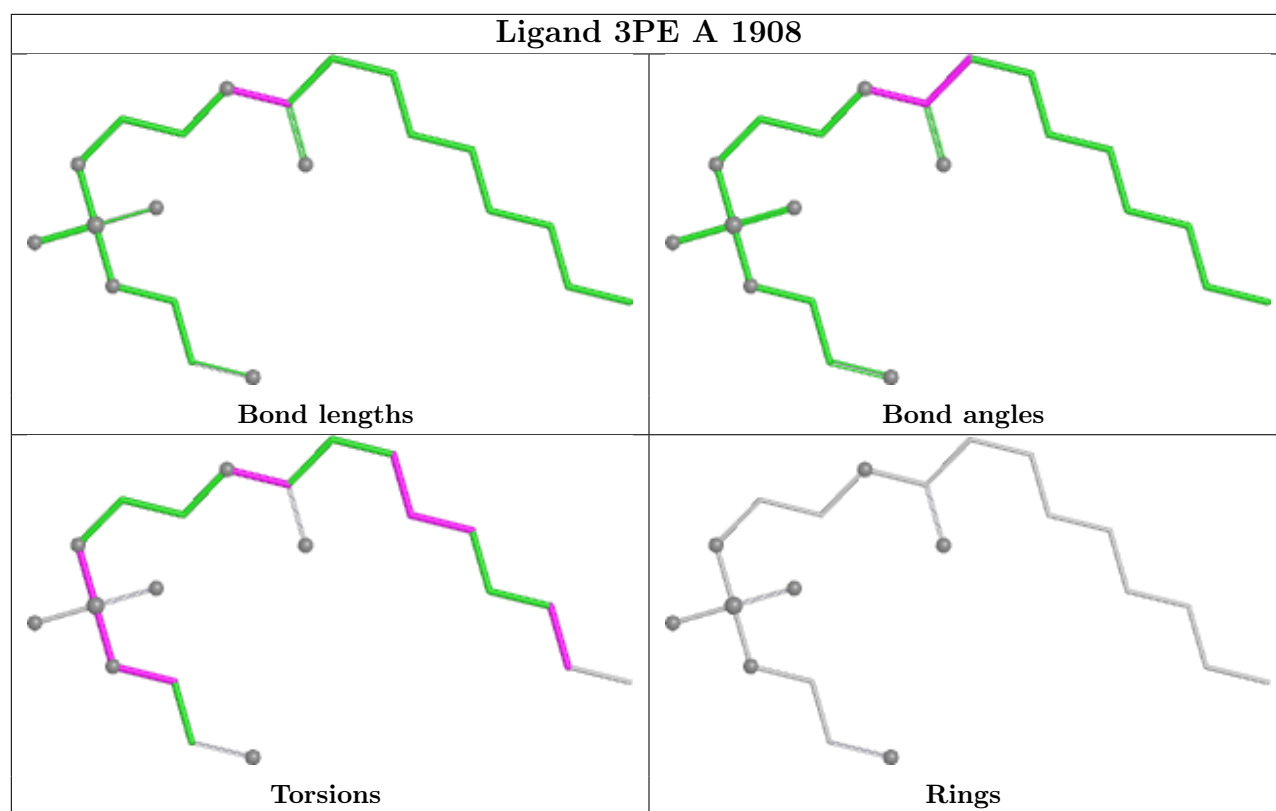
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

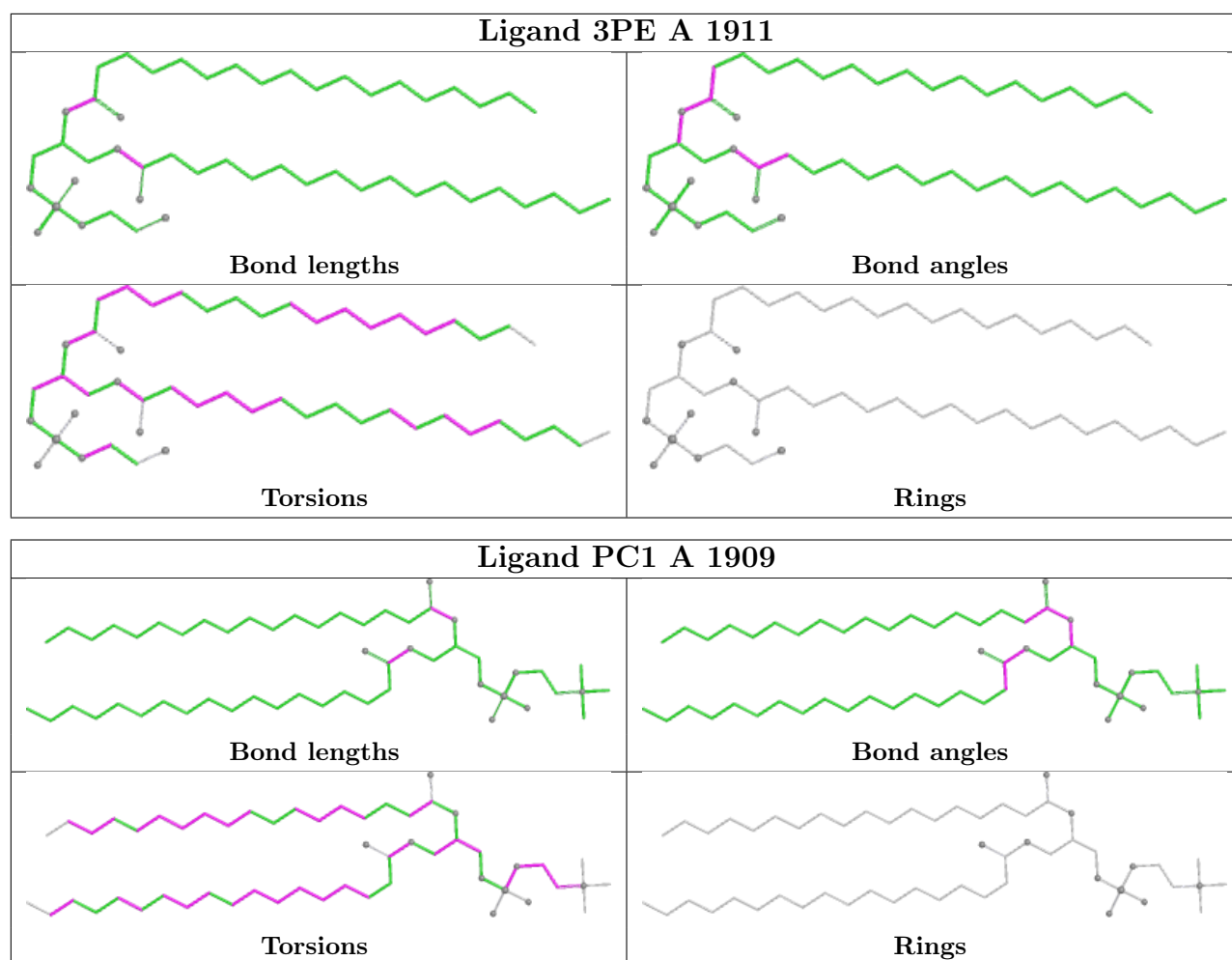












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

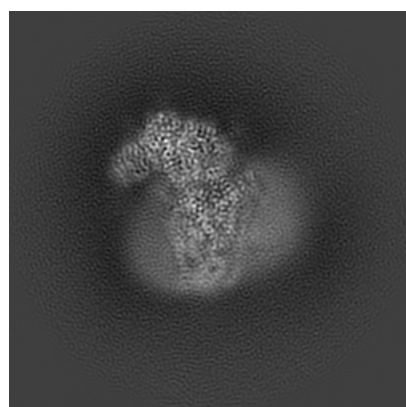
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22425. These allow visual inspection of the internal detail of the map and identification of artifacts.

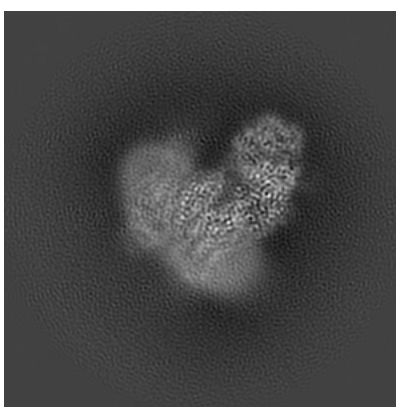
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

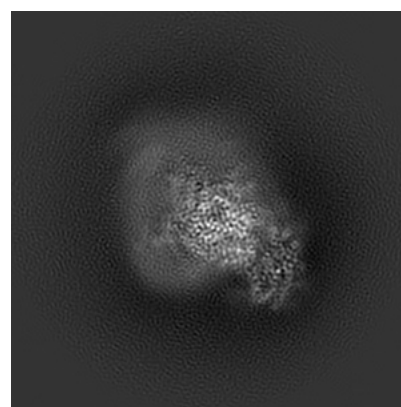
6.1.1 Primary map



X



Y

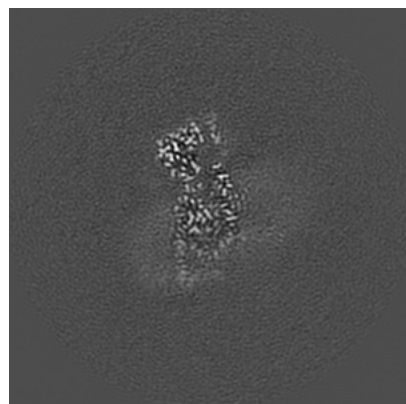


Z

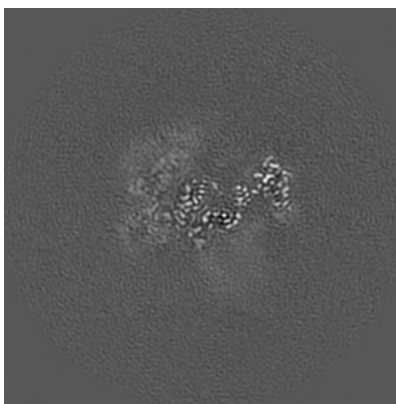
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

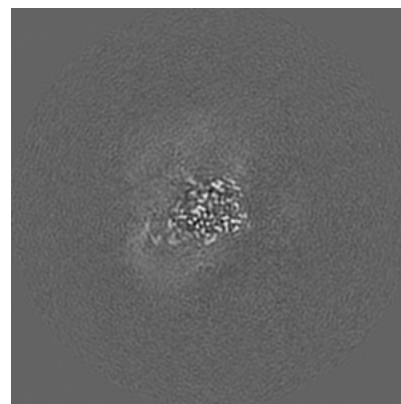
6.2.1 Primary map



X Index: 140



Y Index: 140

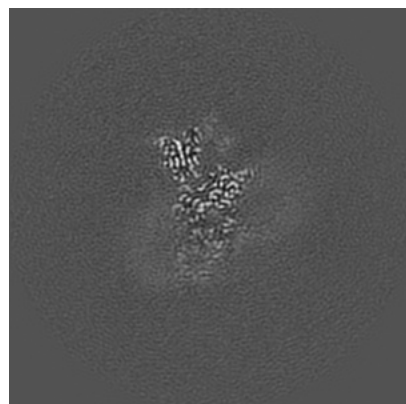


Z Index: 140

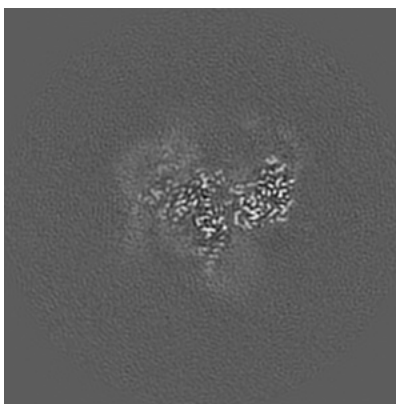
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

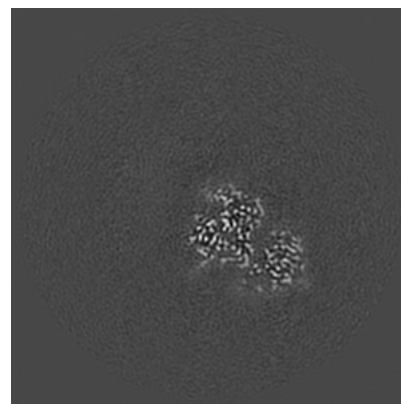
6.3.1 Primary map



X Index: 136



Y Index: 130

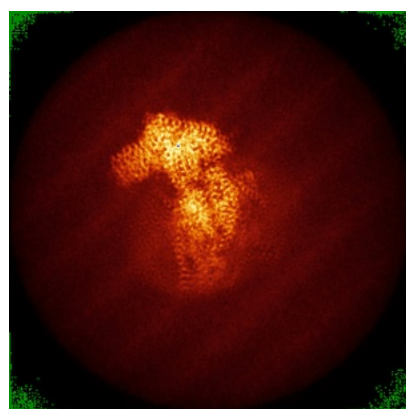


Z Index: 185

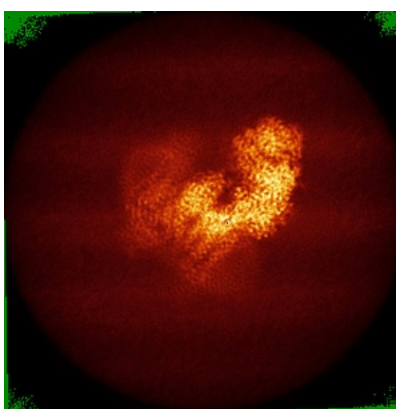
The images above show the largest variance slices of the map in three orthogonal directions.

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

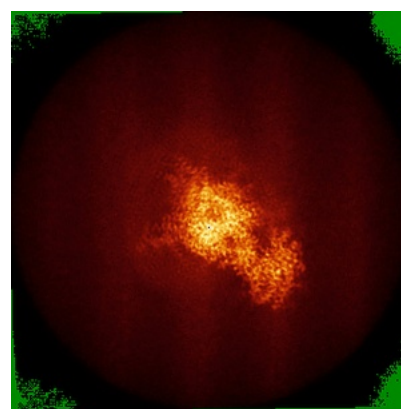
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

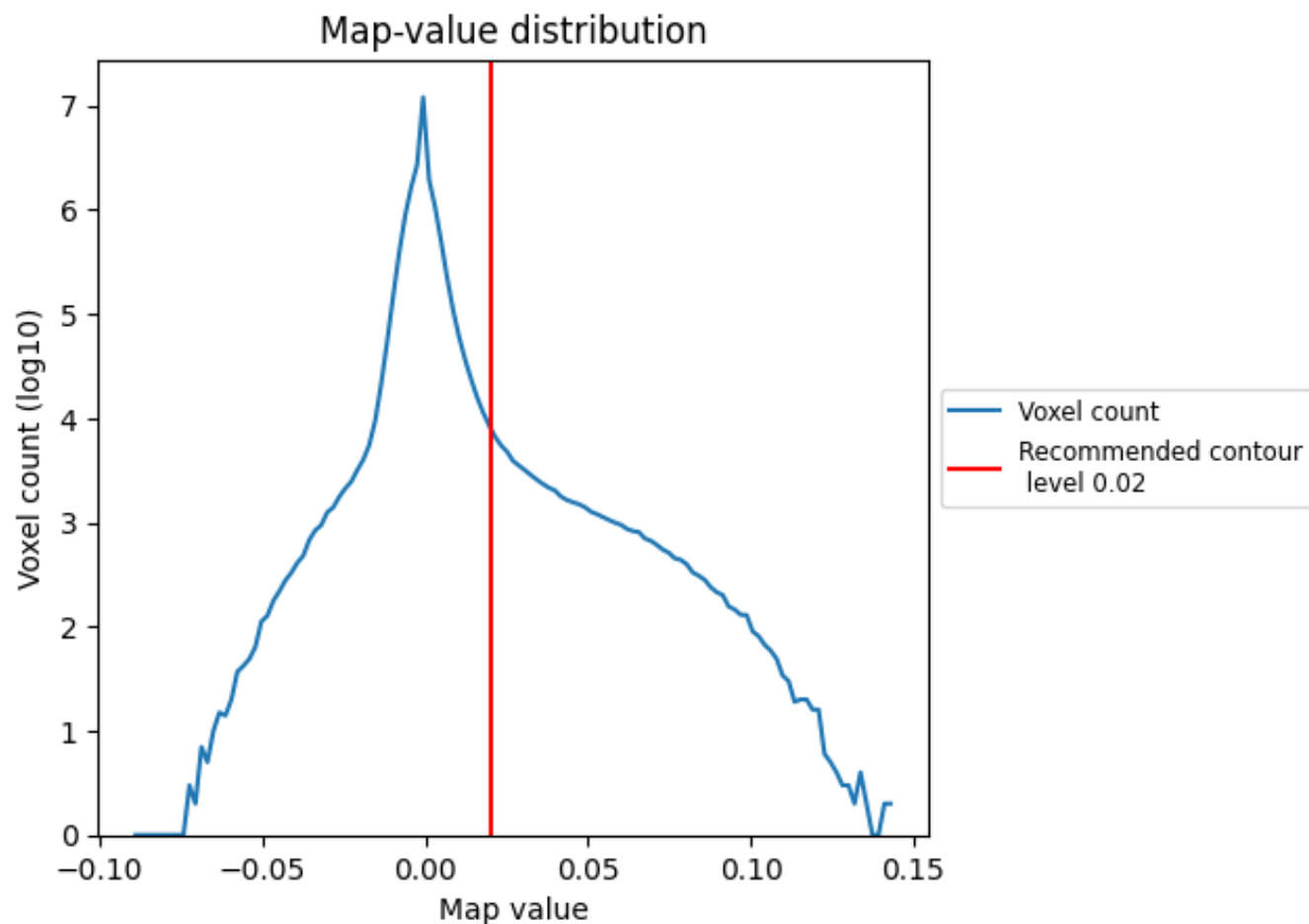
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

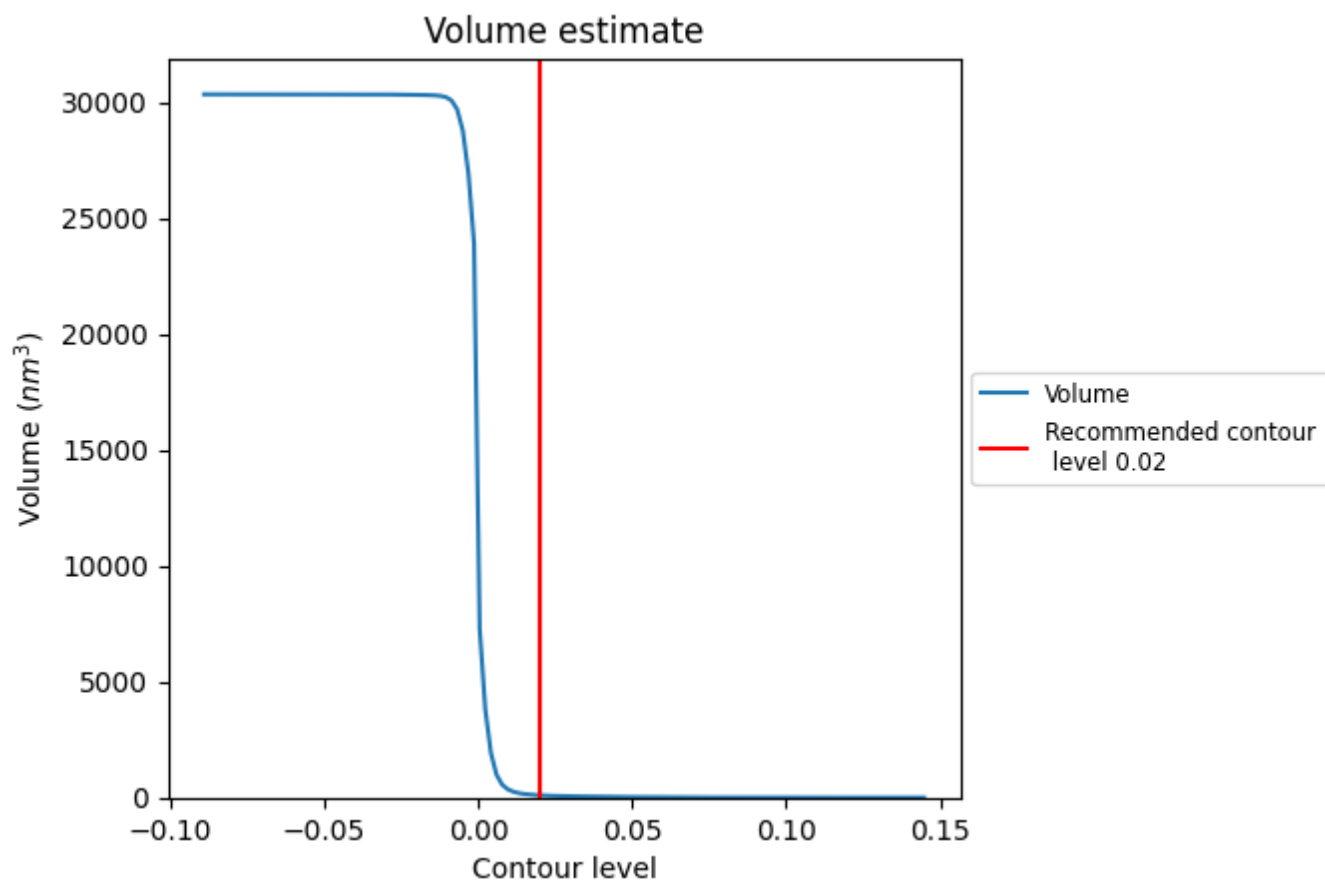
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

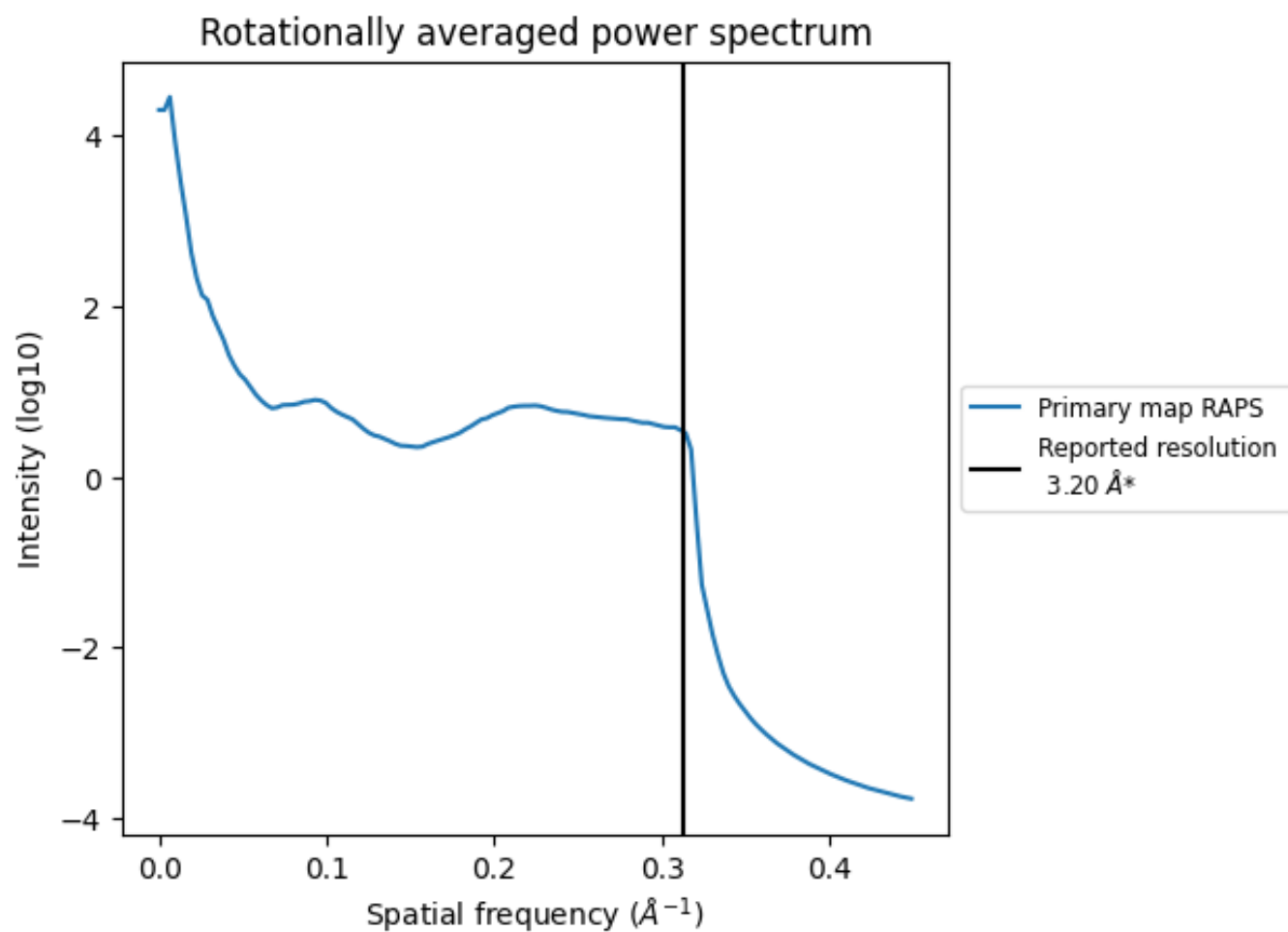
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 97 nm^3 ; this corresponds to an approximate mass of 88 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



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

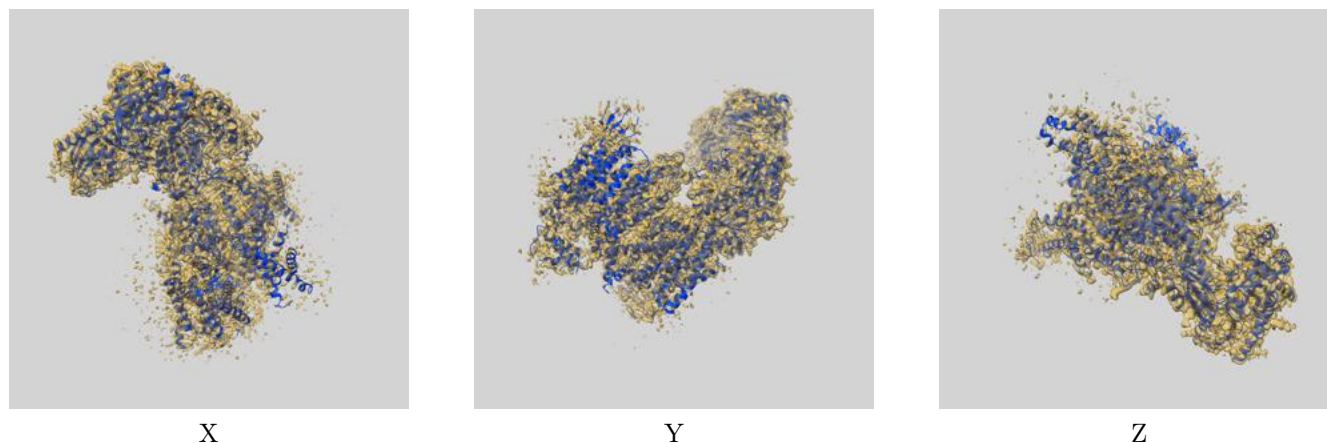
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

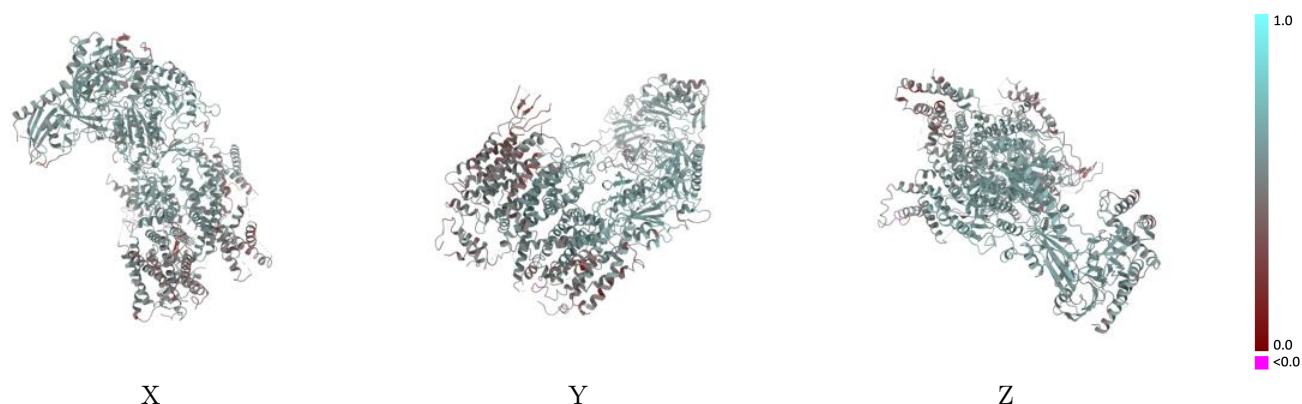
This section contains information regarding the fit between EMDB map EMD-22425 and PDB model 7JPW. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



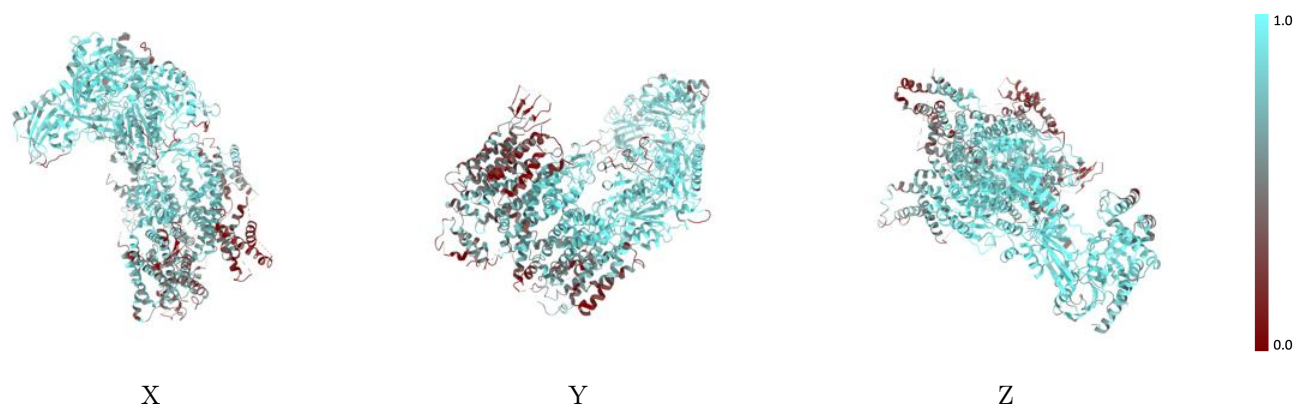
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



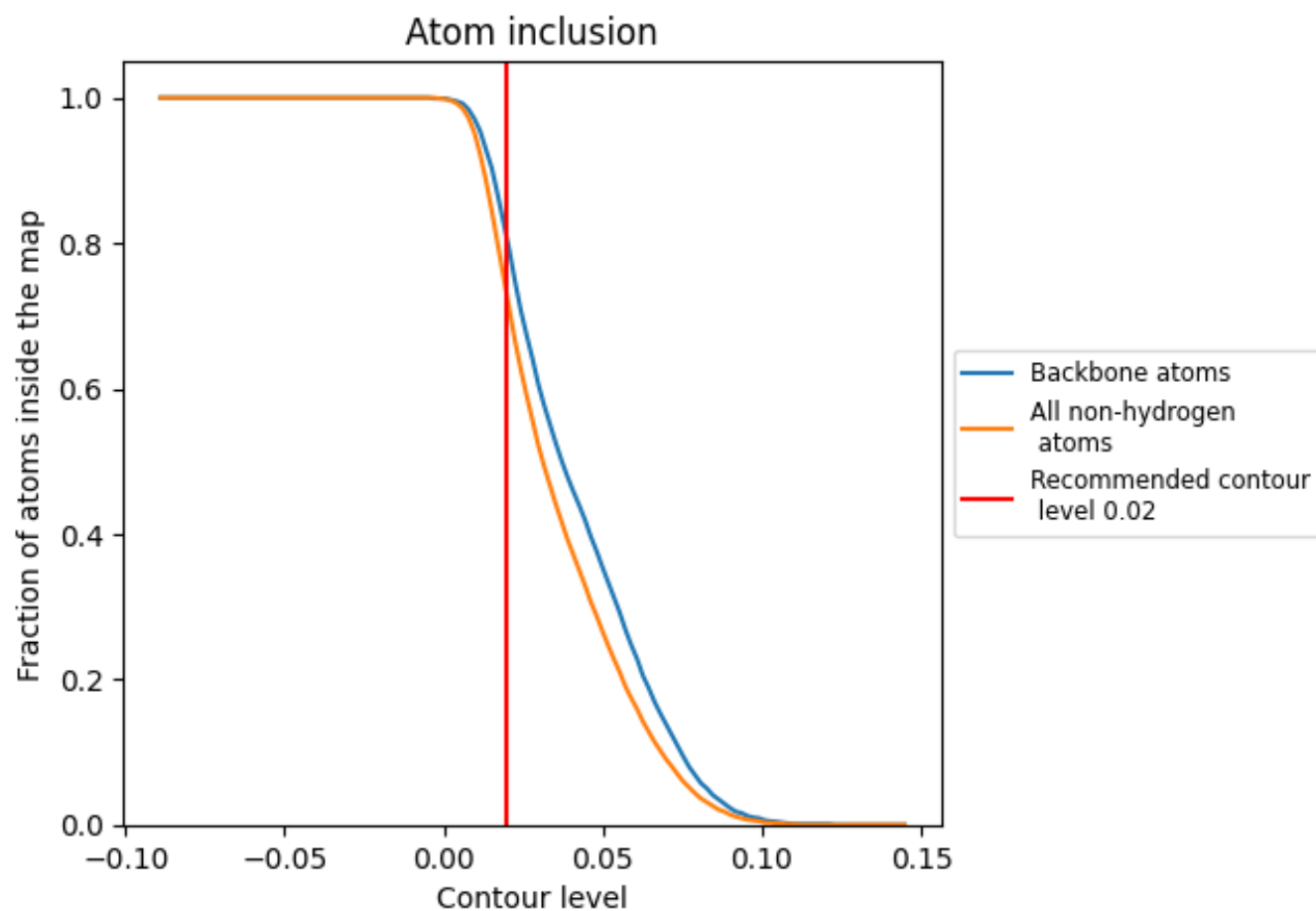
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7260	<div></div> 0.5430
A	<div></div> 0.6630	<div></div> 0.5320
E	<div></div> 0.4620	<div></div> 0.4460
F	<div></div> 0.8460	<div></div> 0.5720

