Full wwPDB EM Validation Report ⓘ

Oct 20, 2024 – 11:38 AM EDT

PDB ID	:	7JPL
EMDB ID	:	EMD-22415
Title	:	Rabbit Cav1.1 in the presence of 10 micromolar (S)-(-)-Bay K8644 in nanodiscs at 3.4 Angstrom resolution
Authors	:	Yan, N.; Gao, S.
Deposited on	:	2020-08-09
Resolution	:	3.40 Å(reported)

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

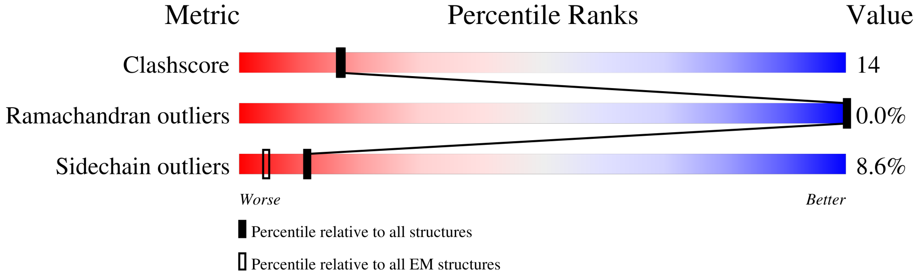
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

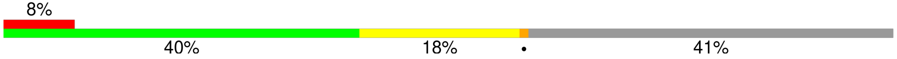
The reported resolution of this entry is 3.40 Å.

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 <=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 18565 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
			Total	C	N	O	S		
1	A	1114	8998	5970	1433	1536	59	0	0

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

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

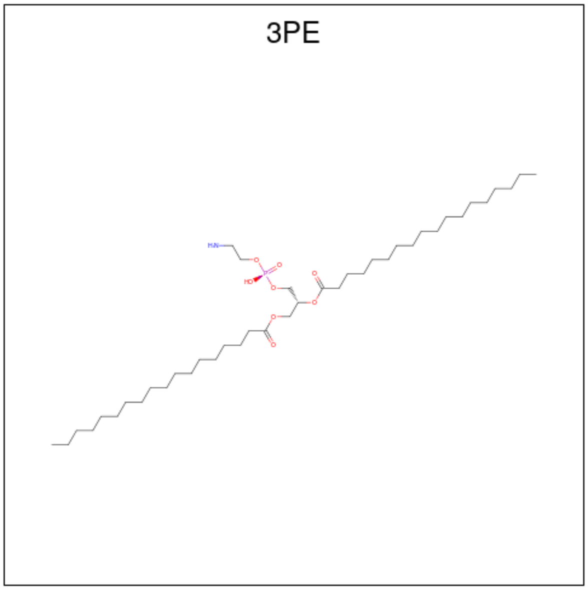
- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

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

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

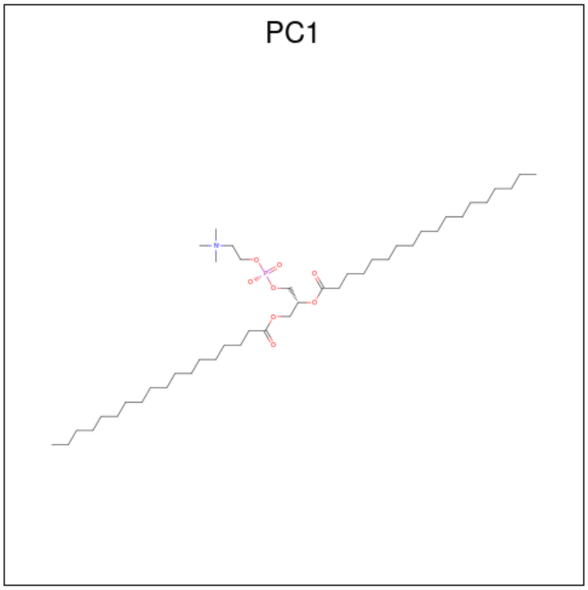
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
4	A	1	1	1	0

- Molecule 5 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



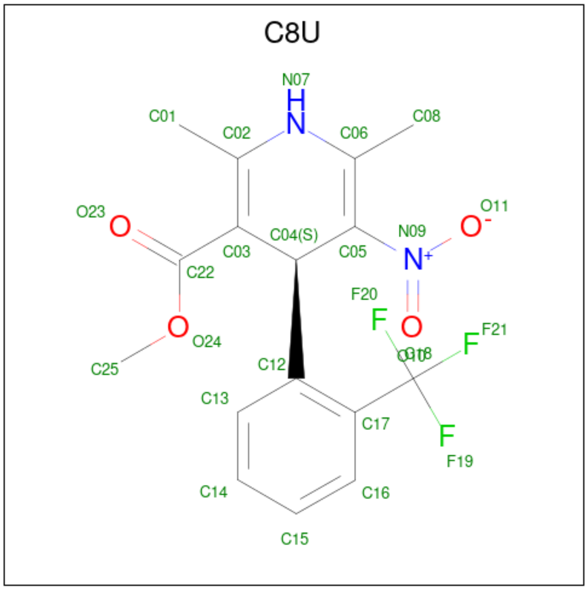
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 33	C 23	N 1	O 8	P 1	0
5	A	1	Total 36	C 26	N 1	O 8	P 1	0
5	A	1	Total 51	C 41	N 1	O 8	P 1	0
5	A	1	Total 51	C 41	N 1	O 8	P 1	0
5	A	1	Total 44	C 34	N 1	O 8	P 1	0
5	A	1	Total 38	C 28	N 1	O 8	P 1	0
5	A	1	Total 21	C 13	N 1	O 6	P 1	0
5	A	1	Total 32	C 22	N 1	O 8	P 1	0
5	A	1	Total 51	C 41	N 1	O 8	P 1	0

- 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 54 44 1 8 1	0

- Molecule 7 is methyl (4 {S})-2,6-dimethyl-5-nitro-4-[2-(trifluoromethyl)phenyl]-1,4-dihydropyridine-3-carboxylate (three-letter code: C8U) (formula: $C_{16}H_{15}F_3N_2O_4$) (labeled as "Ligand of Interest" by depositor).

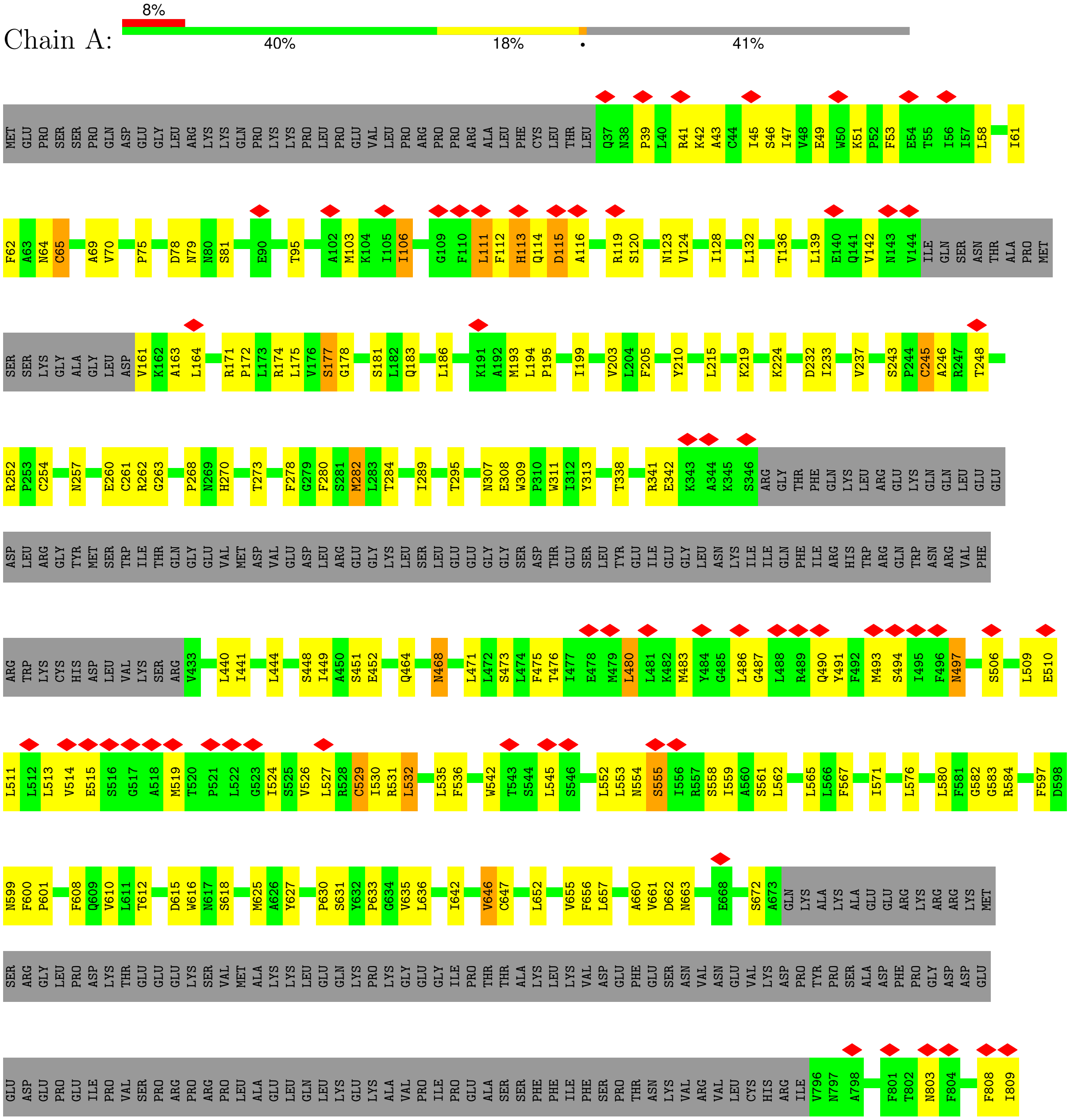


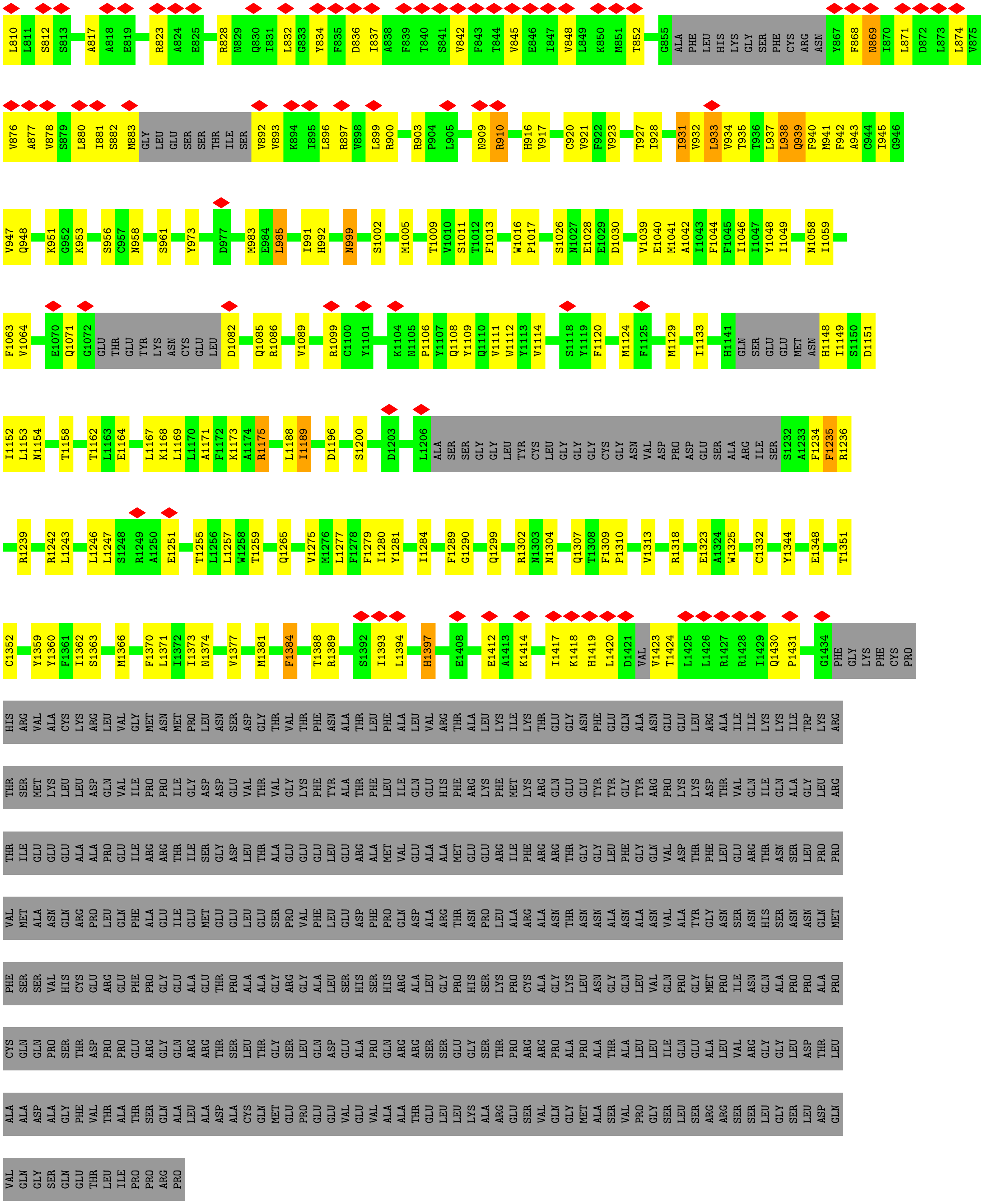
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C F N O 25 16 3 2 4	0

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 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.

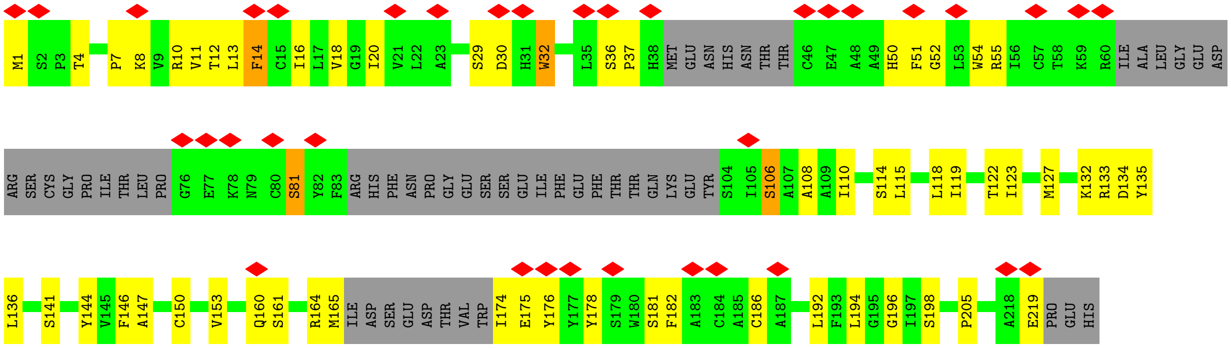
- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1S





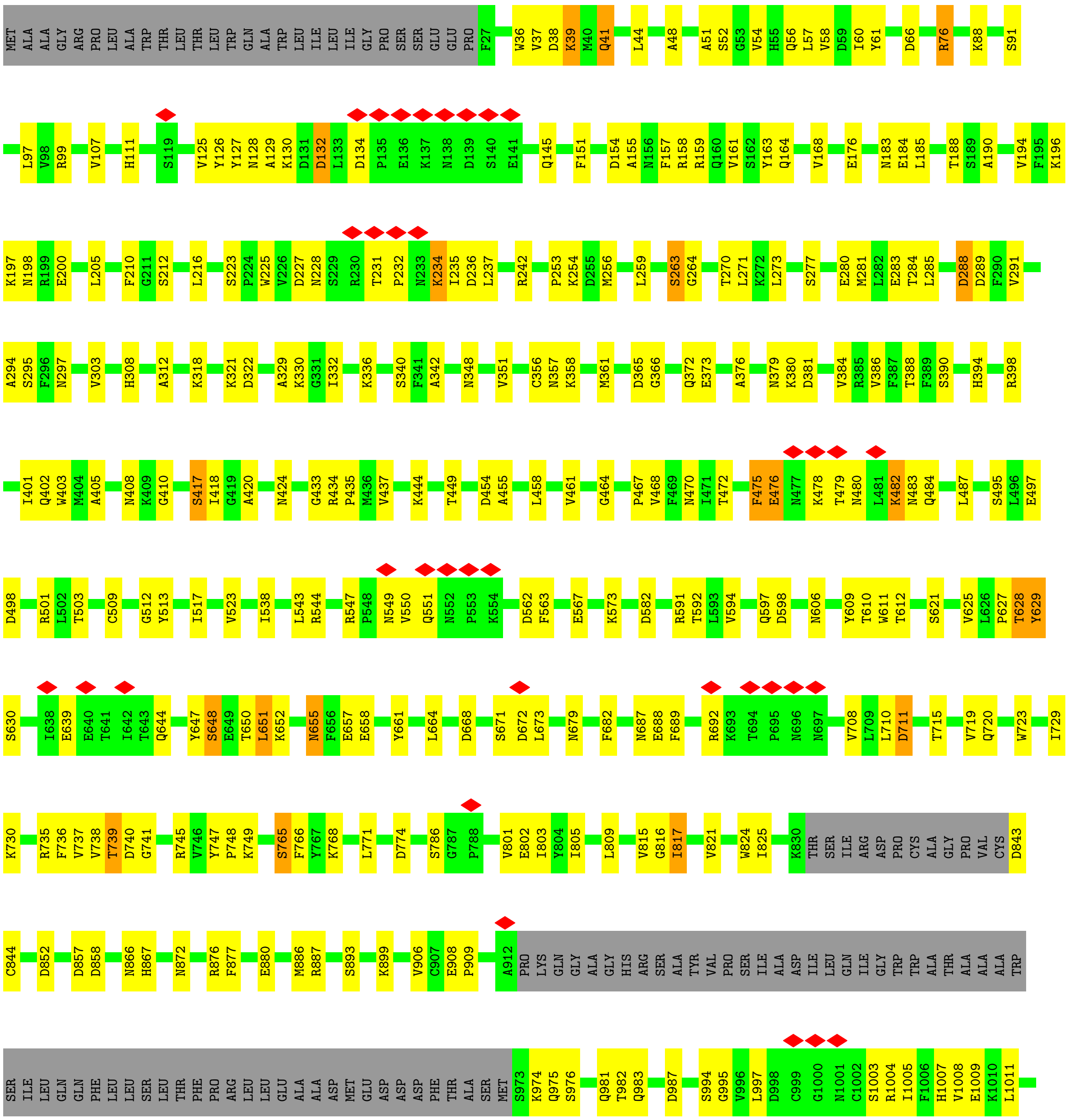
- Molecule 2: Voltage-dependent calcium channel gamma-1 subunit

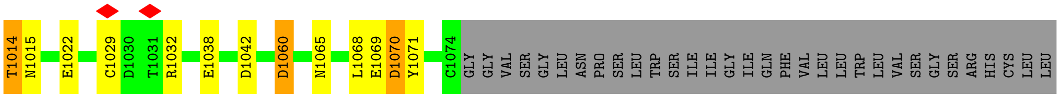
Chain E:



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

Chain F:




T1014
N1015
E1022
C1029
D1030
T1031
R1032
E1038
D1042
D1060
N1065
L1068
E1069
D1070
Y1071
C1074
GLY
GLY
VAL
SER
GLY
LEU
ASN
PRO
SER
LEU
TRP
SER
ILE
ILE
GLY
ILE
GLN
PHE
VAL
LEU
LEU
TRP
LEU
VAL
SER
GLY
SER
ARG
HIS
CYS
LEU
LEU

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53789	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 ($e^-/\text{Å}^2$)	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	0.159	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	311.91998, 311.91998, 311.91998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.114, 1.114, 1.114	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, C8U, 3PE, PC1

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	0.39	0/9222	0.47	0/12520
2	E	0.30	0/1358	0.45	0/1832
3	F	0.48	0/7974	0.50	0/10816
All	All	0.43	0/18554	0.48	0/25168

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 ⓘ

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	8998	0	9133	274	0
2	E	1326	0	1345	33	0
3	F	7804	0	7617	164	0
4	A	1	0	0	0	0
5	A	357	0	508	113	0
6	A	54	0	88	12	0
7	A	25	0	0	6	0
All	All	18565	0	18691	514	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 14.

All (514) 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:536:PHE:CE1	1:A:941:MET:HE1	1.37	1.58
1:A:646:VAL:CG1	5:A:1905:3PE:H3F1	1.37	1.50
1:A:536:PHE:HE1	1:A:941:MET:CE	1.20	1.50
5:A:1904:3PE:H371	7:A:1912:C8U:C25	1.50	1.41
1:A:536:PHE:CE1	1:A:941:MET:CE	1.99	1.33
1:A:282:MET:CE	5:A:1903:3PE:H371	1.74	1.16
1:A:646:VAL:HG12	5:A:1905:3PE:C3F	1.74	1.16
1:A:646:VAL:CG1	5:A:1905:3PE:C3F	2.24	1.15
5:A:1904:3PE:C37	7:A:1912:C8U:C25	2.25	1.14
1:A:282:MET:HE3	5:A:1903:3PE:H371	1.14	1.11
1:A:646:VAL:HG12	5:A:1905:3PE:H3F1	1.00	1.00
5:A:1911:3PE:H2I1	5:A:1911:3PE:C3A	1.90	0.99
5:A:1911:3PE:H3A1	5:A:1911:3PE:C2I	1.93	0.98
1:A:282:MET:HE3	5:A:1903:3PE:C37	1.92	0.98
1:A:163:ALA:CB	5:A:1906:3PE:H321	1.94	0.98
1:A:536:PHE:CD1	1:A:941:MET:HE1	1.99	0.98
5:A:1911:3PE:H2I1	5:A:1911:3PE:H3A1	0.98	0.96
3:F:386:VAL:O	3:F:410:GLY:HA3	1.67	0.93
1:A:536:PHE:CE1	1:A:941:MET:HE3	2.05	0.92
5:A:1903:3PE:H391	5:A:1905:3PE:H372	1.51	0.92
1:A:567:PHE:HE1	5:A:1908:3PE:C29	1.83	0.91
5:A:1904:3PE:H221	5:A:1904:3PE:H31	1.53	0.90
1:A:536:PHE:CD1	1:A:941:MET:CE	2.55	0.89
1:A:584:ARG:NH1	5:A:1906:3PE:O12	2.05	0.88
1:A:70:VAL:HG12	5:A:1907:3PE:H11	1.56	0.88
5:A:1903:3PE:H352	5:A:1905:3PE:H341	1.55	0.87
3:F:688:GLU:O	3:F:692:ARG:HB2	1.76	0.85
1:A:567:PHE:HZ	5:A:1907:3PE:H361	1.42	0.84
1:A:163:ALA:HB2	5:A:1906:3PE:H321	1.58	0.84
1:A:1044:PHE:HD1	5:A:1910:3PE:H221	1.42	0.84
1:A:536:PHE:HE1	1:A:941:MET:HE2	1.42	0.83
1:A:567:PHE:CE1	5:A:1908:3PE:C29	2.61	0.83
1:A:646:VAL:HG13	5:A:1905:3PE:H3F1	1.59	0.83
5:A:1904:3PE:H382	7:A:1912:C8U:C25	2.08	0.83
1:A:1420:LEU:O	1:A:1423:VAL:N	2.12	0.82
5:A:1904:3PE:C38	7:A:1912:C8U:C25	2.57	0.81
1:A:1046:ILE:CD1	5:A:1908:3PE:H262	2.11	0.81
5:A:1904:3PE:H31	5:A:1904:3PE:C22	2.08	0.81
1:A:646:VAL:HG11	5:A:1905:3PE:H3E2	1.63	0.80
1:A:646:VAL:HG11	5:A:1905:3PE:H3F1	1.56	0.80

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:163:ALA:HB1	5:A:1906:3PE:H321	1.63	0.78
1:A:112:PHE:O	1:A:113:HIS:ND1	2.16	0.78
1:A:567:PHE:CZ	5:A:1907:3PE:H361	2.18	0.78
1:A:1370:PHE:HB2	5:A:1904:3PE:H2H1	1.66	0.76
1:A:510:GLU:HB3	1:A:527:LEU:HD12	1.68	0.75
1:A:646:VAL:HG11	5:A:1905:3PE:C3E	2.15	0.75
1:A:245:CYS:SG	1:A:246:ALA:N	2.58	0.75
3:F:737:VAL:HG22	3:F:815:VAL:HG12	1.68	0.75
1:A:282:MET:CE	5:A:1903:3PE:C37	2.59	0.75
3:F:235:ILE:H	3:F:551:GLN:HG3	1.52	0.75
1:A:646:VAL:HG11	5:A:1905:3PE:C3F	2.15	0.74
5:A:1903:3PE:C39	5:A:1905:3PE:H372	2.18	0.73
5:A:1906:3PE:H122	5:A:1906:3PE:O14	1.89	0.72
3:F:711:ASP:OD2	3:F:739:THR:OG1	2.04	0.72
1:A:58:LEU:HD11	1:A:178:GLY:HA3	1.72	0.72
3:F:858:ASP:OD1	3:F:1015:ASN:ND2	2.19	0.72
1:A:571:ILE:HD13	5:A:1907:3PE:H262	1.71	0.71
5:A:1910:3PE:O14	5:A:1910:3PE:H32	1.90	0.71
1:A:45:ILE:HD11	1:A:106:ILE:HG22	1.72	0.71
1:A:309:TRP:CE3	6:A:1909:PC1:H252	2.26	0.70
3:F:164:GLN:O	3:F:196:LYS:NZ	2.24	0.70
1:A:1359:TYR:CD2	5:A:1904:3PE:H231	2.27	0.69
3:F:37:VAL:HG21	3:F:1009:GLU:HG2	1.75	0.69
1:A:449:ILE:HG21	1:A:535:LEU:HD11	1.76	0.68
1:A:1275:VAL:HG13	5:A:1911:3PE:H2G2	1.74	0.68
1:A:510:GLU:OE1	1:A:531:ARG:NH1	2.26	0.68
1:A:1046:ILE:HD13	5:A:1908:3PE:H262	1.76	0.68
1:A:341:ARG:NH2	1:A:661:VAL:O	2.26	0.68
1:A:601:PRO:HB3	5:A:1908:3PE:O22	1.95	0.67
1:A:1046:ILE:HD12	5:A:1908:3PE:H262	1.75	0.67
3:F:184:GLU:O	3:F:188:THR:OG1	2.08	0.67
3:F:644:GLN:O	3:F:648:SER:OG	2.13	0.67
1:A:232:ASP:OD2	3:F:544:ARG:NH1	2.28	0.66
3:F:283:GLU:OE2	3:F:321:LYS:NZ	2.24	0.66
3:F:739:THR:OG1	3:F:740:ASP:N	2.27	0.66
1:A:542:TRP:HB3	1:A:545:LEU:HB2	1.78	0.66
1:A:78:ASP:OD1	1:A:79:ASN:N	2.28	0.66
3:F:658:GLU:O	3:F:720:GLN:NE2	2.28	0.65
1:A:1277:LEU:HD22	1:A:1371:LEU:HD12	1.78	0.65
5:A:1910:3PE:H32	5:A:1910:3PE:P	2.36	0.65
3:F:994:SER:HB3	3:F:1007:HIS:HD2	1.61	0.65

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:1313:VAL:HG12	5:A:1911:3PE:H362	1.79	0.64
3:F:747:TYR:HB3	3:F:748:PRO:HD3	1.79	0.64
1:A:338:THR:O	1:A:342:GLU:HG2	1.96	0.64
3:F:981:GLN:HG2	3:F:1038:GLU:HG3	1.79	0.64
1:A:529:CYS:O	5:A:1910:3PE:H352	1.98	0.64
3:F:472:THR:H	3:F:483:ASN:HD21	1.46	0.63
3:F:242:ARG:NH2	3:F:280:GLU:O	2.32	0.63
1:A:817:ALA:HB2	1:A:1279:PHE:HE1	1.63	0.63
1:A:112:PHE:HD2	1:A:115:ASP:H	1.46	0.63
3:F:273:LEU:O	3:F:277:SER:OG	2.14	0.63
1:A:64:ASN:OD1	1:A:171:ARG:NH1	2.29	0.62
3:F:228:ASN:HB2	3:F:232:PRO:HD3	1.81	0.62
3:F:652:LYS:O	3:F:655:ASN:ND2	2.32	0.62
1:A:307:ASN:OD1	5:A:1911:3PE:H12	2.00	0.62
5:A:1906:3PE:H112	5:A:1906:3PE:H12	1.82	0.62
1:A:633:PRO:CB	5:A:1906:3PE:H222	2.29	0.62
5:A:1910:3PE:O22	5:A:1910:3PE:H242	1.99	0.62
1:A:1281:TYR:O	1:A:1360:TYR:OH	2.18	0.62
1:A:1255:THR:O	1:A:1259:THR:HG23	2.00	0.62
1:A:132:LEU:O	1:A:136:THR:HG23	2.00	0.61
3:F:154:ASP:OD2	3:F:163:TYR:OH	2.17	0.61
3:F:651:LEU:O	3:F:687:ASN:ND2	2.32	0.61
3:F:227:ASP:HB2	3:F:236:ASP:HB3	1.80	0.61
1:A:1039:VAL:CG1	5:A:1908:3PE:O12	2.47	0.61
1:A:114:GLN:HG3	1:A:116:ALA:HB2	1.82	0.61
1:A:116:ALA:O	1:A:120:SER:OG	2.18	0.61
3:F:444:LYS:NZ	3:F:467:PRO:O	2.33	0.60
1:A:928:ILE:HG22	1:A:928:ILE:O	2.01	0.60
3:F:365:ASP:OD1	3:F:366:GLY:N	2.35	0.60
1:A:215:LEU:O	1:A:219:LYS:HB2	2.01	0.60
1:A:1039:VAL:HG13	5:A:1908:3PE:O12	2.01	0.60
1:A:62:PHE:CE1	5:A:1907:3PE:H281	2.37	0.60
1:A:536:PHE:CD1	1:A:941:MET:HE3	2.30	0.60
1:A:448:SER:O	1:A:464:GLN:NE2	2.35	0.59
5:A:1903:3PE:H3A2	5:A:1905:3PE:H392	1.84	0.59
3:F:318:LYS:NZ	3:F:322:ASP:OD2	2.32	0.59
3:F:597:GLN:OE1	3:F:768:LYS:NZ	2.31	0.59
1:A:932:VAL:HG12	1:A:932:VAL:O	2.02	0.59
3:F:259:LEU:HD13	3:F:342:ALA:HB2	1.83	0.59
3:F:498:ASP:OD1	3:F:501:ARG:NH2	2.35	0.59
2:E:37:PRO:HA	2:E:174:ILE:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:503:THR:O	3:F:503:THR:OG1	2.21	0.58
1:A:999:ASN:HD22	1:A:1002:SER:H	1.52	0.58
1:A:1366:MET:HE1	5:A:1904:3PE:H391	1.86	0.58
1:A:1323:GLU:O	1:A:1325:TRP:N	2.35	0.58
1:A:909:ASN:HB3	1:A:910:ARG:HH11	1.67	0.58
3:F:281:MET:O	3:F:284:THR:OG1	2.21	0.58
1:A:527:LEU:HD13	1:A:530:ILE:HD11	1.86	0.57
1:A:115:ASP:HB3	1:A:119:ARG:HB2	1.84	0.57
1:A:532:LEU:HD11	1:A:945:ILE:HG12	1.85	0.57
1:A:473:SER:HA	1:A:476:THR:HG22	1.86	0.57
3:F:51:ALA:HB3	3:F:817:ILE:HD11	1.85	0.57
1:A:1290:GLY:O	1:A:1307:GLN:NE2	2.38	0.57
3:F:127:TYR:HH	3:F:151:PHE:HZ	1.52	0.57
3:F:365:ASP:HB2	3:F:394:HIS:CD2	2.40	0.57
1:A:633:PRO:HB3	5:A:1906:3PE:C22	2.35	0.57
1:A:1275:VAL:HG13	5:A:1911:3PE:C2G	2.34	0.57
3:F:1014:THR:OG1	3:F:1015:ASN:N	2.38	0.57
1:A:210:TYR:O	1:A:313:TYR:OH	2.21	0.56
3:F:381:ASP:OD1	3:F:381:ASP:N	2.36	0.56
3:F:582:ASP:OD1	3:F:582:ASP:N	2.34	0.56
3:F:562:ASP:OD1	3:F:563:PHE:N	2.38	0.56
1:A:999:ASN:ND2	1:A:1002:SER:OG	2.37	0.56
1:A:552:LEU:HA	1:A:555:SER:HB2	1.88	0.56
2:E:55:ARG:HA	2:E:81:SER:O	2.06	0.56
3:F:480:ASN:HA	3:F:483:ASN:HB2	1.88	0.56
5:A:1903:3PE:O32	5:A:1903:3PE:H341	2.05	0.56
1:A:1106:PRO:HA	1:A:1109:TYR:HB3	1.88	0.55
3:F:76:ARG:NH2	3:F:611:TRP:O	2.39	0.55
3:F:715:THR:HB	3:F:745:ARG:HH21	1.71	0.55
1:A:947:VAL:O	1:A:951:LYS:HB2	2.06	0.55
3:F:297:ASN:ND2	3:F:330:LYS:O	2.38	0.55
3:F:1060:ASP:OD1	3:F:1060:ASP:N	2.32	0.55
1:A:280:PHE:O	1:A:284:THR:HG22	2.07	0.55
1:A:1133:ILE:HG12	5:A:1903:3PE:H282	1.89	0.55
5:A:1907:3PE:C2C	5:A:1907:3PE:H271	2.37	0.55
3:F:672:ASP:HB2	3:F:689:PHE:HE1	1.72	0.55
5:A:1910:3PE:P	5:A:1910:3PE:C3	2.94	0.55
3:F:99:ARG:NH1	3:F:198:ASN:OD1	2.37	0.55
3:F:597:GLN:HB3	3:F:765:SER:HB2	1.89	0.55
1:A:932:VAL:HG22	7:A:1912:C8U:F21	1.98	0.54
1:A:627:TYR:CD2	5:A:1906:3PE:H232	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:MET:SD	1:A:1362:ILE:HD11	2.47	0.54
1:A:880:LEU:HD22	1:A:883:MET:HA	1.89	0.54
3:F:373:GLU:H	3:F:373:GLU:CD	2.11	0.54
1:A:43:ALA:HB1	1:A:46:SER:OG	2.08	0.54
1:A:224:LYS:HA	1:A:263:GLY:HA2	1.90	0.54
1:A:939:GLN:HG3	1:A:939:GLN:O	2.07	0.54
5:A:1907:3PE:C2C	5:A:1907:3PE:C27	2.86	0.54
3:F:379:ASN:HD21	3:F:408:ASN:HD22	1.53	0.54
5:A:1904:3PE:H3I3	5:A:1904:3PE:H272	1.90	0.54
2:E:178:TYR:HB3	2:E:182:PHE:CG	2.43	0.54
1:A:486:LEU:HD22	1:A:491:TYR:HB2	1.89	0.54
5:A:1907:3PE:C2C	5:A:1907:3PE:C28	2.86	0.54
3:F:358:LYS:HB3	3:F:384:VAL:HG22	1.89	0.53
1:A:1418:LYS:NZ	1:A:1420:LEU:H	2.07	0.53
1:A:1175:ARG:HH21	2:E:133:ARG:HH11	1.57	0.53
3:F:168:VAL:HG11	3:F:185:LEU:HD21	1.90	0.53
5:A:1911:3PE:C2G	5:A:1911:3PE:C2C	2.85	0.53
3:F:538:ILE:HG13	3:F:1042:ASP:HB3	1.90	0.53
1:A:282:MET:HE1	5:A:1903:3PE:H382	1.90	0.52
1:A:309:TRP:CE3	6:A:1909:PC1:C25	2.91	0.52
1:A:928:ILE:CD1	1:A:1064:VAL:HG22	2.39	0.52
1:A:186:LEU:HD13	1:A:565:LEU:HD11	1.90	0.52
5:A:1902:3PE:O22	5:A:1902:3PE:H252	2.09	0.52
3:F:107:VAL:HG11	3:F:190:ALA:HB3	1.90	0.52
3:F:475:PHE:HD1	3:F:476:GLU:HG3	1.74	0.52
1:A:1373:ILE:O	1:A:1377:VAL:HG23	2.09	0.52
1:A:1041:MET:SD	5:A:1910:3PE:O12	2.67	0.52
1:A:112:PHE:HB2	1:A:115:ASP:HA	1.91	0.52
1:A:1234:PHE:HB3	6:A:1909:PC1:H221	1.91	0.52
2:E:133:ARG:HD2	2:E:135:TYR:HE1	1.75	0.52
1:A:295:THR:HG21	1:A:1318:ARG:HG3	1.92	0.52
3:F:513:TYR:OH	3:F:567:GLU:OE1	2.26	0.52
3:F:130:LYS:HB2	3:F:228:ASN:HA	1.92	0.52
1:A:1085:GLN:O	1:A:1089:VAL:HG22	2.10	0.52
1:A:636:LEU:HD21	5:A:1905:3PE:H321	1.92	0.51
5:A:1903:3PE:H321	5:A:1903:3PE:H222	1.92	0.51
1:A:452:GLU:OE1	1:A:948:GLN:NE2	2.34	0.51
3:F:176:GLU:OE1	3:F:176:GLU:N	2.41	0.51
1:A:61:ILE:HD11	1:A:171:ARG:HB3	1.92	0.51
1:A:232:ASP:OD1	1:A:262:ARG:NH1	2.41	0.51
1:A:627:TYR:CE2	5:A:1906:3PE:H232	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:461:VAL:HG12	3:F:495:SER:HA	1.91	0.51
1:A:309:TRP:C	6:A:1909:PC1:O32	2.48	0.51
1:A:834:TYR:O	1:A:837:ILE:HG13	2.09	0.51
1:A:939:GLN:NE2	1:A:1048:TYR:OH	2.43	0.51
3:F:1042:ASP:OD1	3:F:1042:ASP:N	2.42	0.51
1:A:932:VAL:HA	1:A:935:THR:HG22	1.91	0.51
1:A:309:TRP:HB3	6:A:1909:PC1:O32	2.11	0.51
1:A:920:CYS:HA	1:A:923:VAL:HG12	1.92	0.51
1:A:1099:ARG:NH1	2:E:219:GLU:OE1	2.34	0.51
3:F:57:LEU:HD23	3:F:801:VAL:HG21	1.91	0.51
3:F:893:SER:O	3:F:893:SER:OG	2.22	0.51
7:A:1912:C8U:O11	7:A:1912:C8U:F19	2.18	0.51
1:A:1348:GLU:HB3	1:A:1351:THR:HG21	1.93	0.51
5:A:1904:3PE:H221	5:A:1904:3PE:C3	2.28	0.51
3:F:509:CYS:SG	3:F:630:SER:HB2	2.50	0.51
1:A:917:VAL:O	1:A:921:VAL:HG13	2.11	0.51
3:F:194:VAL:HA	3:F:197:LYS:HG2	1.93	0.51
5:A:1911:3PE:C2G	5:A:1911:3PE:H2C1	2.39	0.51
1:A:874:LEU:O	1:A:878:VAL:HG22	2.10	0.50
1:A:916:HIS:O	1:A:916:HIS:ND1	2.44	0.50
3:F:56:GLN:O	3:F:60:ILE:HG23	2.11	0.50
3:F:291:VAL:HG12	3:F:312:ALA:HB2	1.94	0.50
3:F:908:GLU:HG3	3:F:974:LYS:HD3	1.93	0.50
1:A:61:ILE:HG12	1:A:174:ARG:HB2	1.93	0.50
1:A:1071:GLN:N	1:A:1071:GLN:OE1	2.44	0.50
3:F:398:ARG:O	3:F:402:GLN:HG3	2.11	0.50
1:A:309:TRP:O	6:A:1909:PC1:O32	2.30	0.50
3:F:995:GLY:O	3:F:1005:ILE:HG13	2.12	0.50
3:F:729:ILE:HG22	3:F:730:LYS:H	1.77	0.50
1:A:848:VAL:O	1:A:852:THR:N	2.45	0.50
2:E:36:SER:HB2	2:E:175:GLU:HB2	1.94	0.49
3:F:48:ALA:O	3:F:52:SER:OG	2.28	0.49
1:A:646:VAL:HG12	5:A:1905:3PE:H3F2	1.84	0.49
1:A:662:ASP:C	1:A:663:ASN:HD22	2.16	0.49
3:F:738:VAL:HG21	3:F:766:PHE:HZ	1.78	0.49
2:E:32:TRP:HB2	2:E:182:PHE:N	2.28	0.49
1:A:39:PRO:HG2	1:A:41:ARG:HE	1.78	0.49
1:A:921:VAL:HG12	1:A:1374:ASN:HD21	1.78	0.49
1:A:128:ILE:O	1:A:132:LEU:HD12	2.13	0.49
3:F:657:GLU:HG3	3:F:749:LYS:CD	2.43	0.49
1:A:1112:TRP:HA	1:A:1171:ALA:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:THR:O	1:A:1162:THR:OG1	2.28	0.49
3:F:111:HIS:NE2	3:F:183:ASN:OD1	2.32	0.48
3:F:736:PHE:CZ	3:F:816:GLY:HA3	2.48	0.48
1:A:633:PRO:HB3	5:A:1906:3PE:H222	1.93	0.48
1:A:828:ARG:O	1:A:832:LEU:HG	2.13	0.48
1:A:932:VAL:HA	1:A:935:THR:CG2	2.43	0.48
5:A:1907:3PE:H2	5:A:1907:3PE:O12	2.12	0.48
3:F:125:VAL:HA	3:F:145:GLN:O	2.14	0.48
3:F:417:SER:OG	3:F:418:ILE:N	2.44	0.48
1:A:582:GLY:HA2	1:A:597:PHE:O	2.14	0.48
5:A:1907:3PE:O32	5:A:1907:3PE:H342	2.11	0.48
2:E:16:ILE:O	2:E:20:ILE:HG13	2.14	0.48
2:E:164:ARG:HG3	2:E:165:MET:HG2	1.93	0.48
1:A:282:MET:CE	5:A:1903:3PE:H382	2.44	0.48
3:F:259:LEU:HD12	3:F:294:ALA:HB3	1.96	0.48
1:A:1039:VAL:HG11	5:A:1908:3PE:O12	2.13	0.48
1:A:163:ALA:HB2	5:A:1906:3PE:C32	2.37	0.48
1:A:625:MET:HE1	1:A:630:PRO:HD3	1.95	0.48
3:F:58:VAL:HG13	3:F:803:ILE:HG22	1.96	0.48
3:F:484:GLN:HE22	3:F:1070:ASP:N	2.11	0.48
1:A:1393:ILE:HG13	1:A:1394:LEU:H	1.79	0.48
3:F:591:ARG:NH2	3:F:606:ASN:OD1	2.47	0.48
1:A:842:VAL:O	1:A:845:VAL:HG22	2.14	0.48
1:A:1359:TYR:CE2	5:A:1904:3PE:H231	2.48	0.47
1:A:1363:SER:HA	5:A:1904:3PE:H291	1.96	0.47
3:F:176:GLU:O	3:F:176:GLU:HG2	2.14	0.47
3:F:547:ARG:HB2	3:F:550:VAL:HG13	1.95	0.47
1:A:205:PHE:HE2	1:A:1246:LEU:HD11	1.80	0.47
1:A:562:LEU:HG	1:A:655:VAL:HG22	1.96	0.47
1:A:809:ILE:HD12	1:A:810:LEU:N	2.29	0.47
1:A:1414:LYS:HD2	1:A:1414:LYS:HA	1.73	0.47
1:A:1418:LYS:HE3	1:A:1420:LEU:HB3	1.97	0.47
3:F:36:TRP:O	3:F:39:LYS:HG3	2.13	0.47
3:F:876:ARG:NE	3:F:880:GLU:OE2	2.48	0.47
1:A:1040:GLU:OE2	5:A:1910:3PE:H112	2.13	0.47
5:A:1902:3PE:H221	5:A:1902:3PE:H2	1.79	0.47
1:A:45:ILE:HD12	1:A:46:SER:N	2.29	0.47
3:F:253:PRO:O	3:F:356:CYS:HB3	2.15	0.47
3:F:263:SER:OG	3:F:264:GLY:N	2.48	0.47
1:A:897:ARG:O	1:A:900:ARG:HG2	2.15	0.47
5:A:1907:3PE:H281	5:A:1907:3PE:C2C	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1907:3PE:H111	5:A:1908:3PE:H112	1.97	0.47
6:A:1909:PC1:H131	2:E:160:GLN:HE22	1.79	0.47
1:A:39:PRO:HG2	1:A:41:ARG:HG3	1.97	0.47
1:A:660:ALA:HB1	1:A:1059:ILE:HA	1.96	0.47
1:A:1016:TRP:CD1	1:A:1017:PRO:HD3	2.50	0.47
2:E:144:TYR:O	2:E:147:ALA:HB3	2.15	0.47
2:E:194:LEU:O	2:E:198:SER:OG	2.25	0.47
3:F:256:MET:HE3	3:F:285:LEU:HD21	1.97	0.47
1:A:1412:GLU:HB3	1:A:1414:LYS:HD3	1.97	0.47
3:F:210:PHE:CE2	3:F:212:SER:HB3	2.50	0.46
3:F:497:GLU:O	3:F:501:ARG:HG3	2.15	0.46
3:F:647:TYR:O	3:F:650:THR:OG1	2.30	0.46
1:A:124:VAL:O	1:A:128:ILE:HG13	2.15	0.46
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.77	0.46
5:A:1910:3PE:H252	5:A:1910:3PE:H282	1.84	0.46
3:F:336:LYS:O	3:F:340:SER:OG	2.27	0.46
1:A:928:ILE:HD12	1:A:1064:VAL:CG2	2.45	0.46
3:F:857:ASP:OD1	3:F:857:ASP:N	2.46	0.46
1:A:817:ALA:HB2	1:A:1279:PHE:CE1	2.47	0.46
3:F:434:ARG:HB2	3:F:435:PRO:HD3	1.98	0.46
1:A:1417:ILE:HD12	1:A:1418:LYS:O	2.15	0.46
5:A:1904:3PE:H2I3	5:A:1904:3PE:H2F2	1.64	0.46
3:F:373:GLU:OE1	3:F:373:GLU:N	2.36	0.46
3:F:909:PRO:HG3	3:F:975:GLN:HG2	1.98	0.46
3:F:630:SER:O	3:F:630:SER:OG	2.29	0.46
2:E:123:ILE:HG22	2:E:127:MET:HE1	1.98	0.46
2:E:115:LEU:O	2:E:119:ILE:HG13	2.16	0.46
3:F:887:ARG:NH2	3:F:1032:ARG:O	2.26	0.46
1:A:49:GLU:OE2	1:A:103:MET:HG2	2.16	0.45
1:A:1149:ILE:O	1:A:1153:LEU:HD12	2.16	0.45
3:F:271:LEU:HD22	3:F:329:ALA:HB2	1.98	0.45
3:F:899:LYS:HG2	3:F:982:THR:HG23	1.98	0.45
1:A:194:LEU:N	1:A:195:PRO:HD2	2.31	0.45
1:A:559:ILE:O	1:A:559:ILE:HG22	2.16	0.45
3:F:475:PHE:CD1	3:F:476:GLU:HG3	2.52	0.45
3:F:821:VAL:O	3:F:825:ILE:HG13	2.16	0.45
1:A:1430:GLN:HB3	1:A:1431:PRO:CD	2.46	0.45
3:F:657:GLU:HG3	3:F:749:LYS:HD3	1.97	0.45
1:A:278:PHE:CE2	5:A:1903:3PE:H261	2.51	0.45
1:A:631:SER:O	1:A:635:VAL:HG22	2.16	0.45
1:A:1381:MET:HA	1:A:1384:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:155:ALA:C	3:F:157:PHE:H	2.20	0.45
3:F:254:LYS:HA	3:F:357:ASN:HB2	1.97	0.45
1:A:656:PHE:CB	1:A:1058:ASN:HD22	2.30	0.45
2:E:54:TRP:CH2	2:E:108:ALA:HB1	2.51	0.45
1:A:657:LEU:O	1:A:661:VAL:HG22	2.17	0.45
1:A:554:ASN:O	1:A:558:SER:HB2	2.15	0.45
5:A:1903:3PE:H322	5:A:1903:3PE:H31	1.78	0.45
5:A:1911:3PE:H2A1	5:A:1911:3PE:H2D2	1.74	0.45
2:E:150:CYS:O	2:E:153:VAL:HG22	2.17	0.45
1:A:509:LEU:O	1:A:513:LEU:HB2	2.17	0.45
1:A:656:PHE:HB3	1:A:1058:ASN:HD22	1.82	0.45
2:E:122:THR:HG23	2:E:123:ILE:HD13	1.99	0.45
1:A:877:ALA:O	1:A:881:ILE:HG23	2.17	0.45
3:F:129:ALA:O	3:F:130:LYS:HG2	2.17	0.45
1:A:69:ALA:CB	5:A:1907:3PE:O22	2.66	0.44
1:A:1196:ASP:HB2	1:A:1235:PHE:HB3	2.00	0.44
2:E:14:PHE:O	2:E:18:VAL:HG23	2.17	0.44
1:A:869:ASN:OD1	1:A:869:ASN:N	2.37	0.44
1:A:163:ALA:CB	5:A:1906:3PE:C32	2.83	0.44
1:A:233:ILE:HD13	3:F:547:ARG:HG2	2.00	0.44
3:F:270:THR:HG21	3:F:365:ASP:HB3	1.98	0.44
1:A:1120:PHE:O	1:A:1124:MET:HG2	2.17	0.44
3:F:479:THR:OG1	3:F:480:ASN:N	2.49	0.44
1:A:254:CYS:SG	1:A:261:CYS:HB2	2.58	0.44
1:A:1013:PHE:HE1	1:A:1049:ILE:HG23	1.83	0.44
2:E:8:LYS:O	2:E:12:THR:HG23	2.18	0.44
3:F:289:ASP:OD1	3:F:289:ASP:N	2.50	0.44
3:F:627:PRO:O	3:F:630:SER:HB3	2.18	0.44
3:F:673:LEU:H	3:F:673:LEU:HD23	1.82	0.44
1:A:1188:LEU:HD12	2:E:146:PHE:CE2	2.53	0.44
1:A:1359:TYR:HD2	5:A:1904:3PE:H252	1.81	0.44
3:F:159:ARG:HH11	3:F:223:SER:HB3	1.83	0.44
3:F:844:CYS:HB3	3:F:866:ASN:ND2	2.33	0.44
1:A:260:GLU:OE2	1:A:262:ARG:HD3	2.17	0.44
1:A:892:VAL:HG12	1:A:893:VAL:H	1.82	0.44
1:A:1082:ASP:O	1:A:1086:ARG:NH2	2.51	0.44
1:A:440:LEU:O	1:A:444:LEU:HG	2.17	0.44
1:A:808:PHE:O	1:A:812:SER:OG	2.27	0.44
1:A:836:ASP:OD2	1:A:903:ARG:NH1	2.51	0.44
3:F:512:GLY:HA2	3:F:625:VAL:O	2.18	0.44
1:A:1299:GLN:O	1:A:1304:ASN:ND2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:197:LYS:HA	3:F:200:GLU:HG2	2.00	0.44
1:A:282:MET:CE	5:A:1903:3PE:C38	2.95	0.43
1:A:1251:GLU:H	1:A:1251:GLU:HG2	1.66	0.43
3:F:232:PRO:HB2	3:F:234:LYS:HD3	2.00	0.43
3:F:1004:ARG:HB3	3:F:1022:GLU:HB2	2.00	0.43
1:A:177:SER:HA	1:A:183:GLN:HE21	1.82	0.43
1:A:1251:GLU:O	1:A:1255:THR:HG22	2.18	0.43
3:F:308:HIS:CD2	3:F:351:VAL:HG11	2.53	0.43
3:F:454:ASP:OD1	3:F:455:ALA:N	2.51	0.43
3:F:478:LYS:HB2	3:F:478:LYS:HE2	1.73	0.43
3:F:598:ASP:N	3:F:598:ASP:OD1	2.51	0.43
1:A:953:LYS:HG2	1:A:1028:GLU:O	2.17	0.43
3:F:44:LEU:HD11	3:F:824:TRP:CZ2	2.54	0.43
1:A:480:LEU:HA	1:A:483:MET:HG2	2.01	0.43
5:A:1911:3PE:C2C	5:A:1911:3PE:H2G1	2.48	0.43
3:F:372:GLN:HG3	3:F:403:TRP:CH2	2.53	0.43
1:A:39:PRO:HD2	1:A:41:ARG:HH11	1.84	0.43
3:F:719:VAL:HG22	3:F:723:TRP:CE3	2.54	0.43
1:A:172:PRO:HA	1:A:175:LEU:HD12	2.00	0.43
1:A:939:GLN:HE21	1:A:939:GLN:HB2	1.49	0.43
1:A:953:LYS:HB3	1:A:1026:SER:HB2	1.99	0.43
2:E:118:LEU:HD21	2:E:192:LEU:HD11	2.01	0.43
1:A:1430:GLN:HB3	1:A:1431:PRO:HD2	1.99	0.43
3:F:130:LYS:HB3	3:F:225:TRP:HB3	2.01	0.43
3:F:484:GLN:HE22	3:F:1070:ASP:HB2	1.84	0.43
3:F:802:GLU:HG3	3:F:809:LEU:HD11	2.01	0.43
1:A:62:PHE:HE1	5:A:1907:3PE:H281	1.79	0.43
1:A:555:SER:HA	1:A:663:ASN:OD1	2.18	0.43
2:E:7:PRO:O	2:E:11:VAL:HG13	2.19	0.43
2:E:134:ASP:OD1	2:E:134:ASP:N	2.47	0.43
3:F:154:ASP:HB2	3:F:161:VAL:HG22	2.01	0.43
1:A:270:HIS:HB2	1:A:625:MET:HE3	2.00	0.43
1:A:580:LEU:O	1:A:584:ARG:HD2	2.19	0.43
1:A:636:LEU:HD21	5:A:1905:3PE:C32	2.48	0.43
1:A:1148:HIS:O	1:A:1152:ILE:HG12	2.19	0.43
1:A:1189:ILE:HG21	1:A:1242:ARG:HG2	2.00	0.43
3:F:388:THR:OG1	3:F:405:ALA:HB2	2.19	0.43
3:F:1069:GLU:HB3	3:F:1071:TYR:CD2	2.54	0.43
1:A:973:TYR:HE1	3:F:235:ILE:HG21	1.84	0.42
1:A:1366:MET:CE	5:A:1904:3PE:H391	2.48	0.42
1:A:1257:LEU:HD23	1:A:1257:LEU:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:470:ASN:HD21	3:F:482:LYS:HE3	1.84	0.42
3:F:664:LEU:H	3:F:679:ASN:HD21	1.67	0.42
3:F:688:GLU:O	3:F:692:ARG:CB	2.58	0.42
1:A:111:LEU:HG	1:A:112:PHE:CD1	2.54	0.42
1:A:483:MET:O	1:A:487:GLY:N	2.38	0.42
3:F:420:ALA:HB1	3:F:424:ASN:ND2	2.34	0.42
3:F:88:LYS:HB2	3:F:88:LYS:HE3	1.63	0.42
3:F:388:THR:HB	3:F:401:ILE:HG23	2.01	0.42
1:A:115:ASP:N	1:A:115:ASP:OD1	2.52	0.42
1:A:199:ILE:O	1:A:203:VAL:HG23	2.18	0.42
1:A:219:LYS:HB3	1:A:219:LYS:HE2	1.87	0.42
1:A:608:PHE:O	1:A:612:THR:HG23	2.20	0.42
2:E:106:SER:O	2:E:110:ILE:HG13	2.19	0.42
1:A:41:ARG:HD2	1:A:42:LYS:N	2.35	0.42
1:A:633:PRO:HB3	5:A:1906:3PE:H221	2.02	0.42
1:A:558:SER:O	1:A:559:ILE:HD13	2.20	0.42
1:A:652:LEU:HD23	1:A:652:LEU:HA	1.78	0.42
1:A:933:LEU:HA	1:A:933:LEU:HD13	1.70	0.42
1:A:1234:PHE:HB3	6:A:1909:PC1:H232	2.01	0.42
6:A:1909:PC1:H232	6:A:1909:PC1:H262	1.89	0.42
5:A:1911:3PE:H291	5:A:1911:3PE:H262	1.42	0.42
3:F:126:TYR:CE2	3:F:128:ASN:HB2	2.55	0.42
3:F:877:PHE:CZ	3:F:886:MET:HE2	2.55	0.42
1:A:468:ASN:OD1	1:A:531:ARG:NH2	2.45	0.42
1:A:576:LEU:HD21	5:A:1906:3PE:H2C1	2.02	0.42
1:A:599:ASN:OD1	1:A:599:ASN:N	2.52	0.42
1:A:600:PHE:HB3	1:A:601:PRO:HD3	2.01	0.42
3:F:242:ARG:NH2	3:F:284:THR:HG23	2.34	0.42
3:F:468:VAL:HG12	3:F:487:LEU:HD12	2.01	0.42
1:A:139:LEU:O	1:A:142:VAL:HG12	2.19	0.41
1:A:630:PRO:HA	1:A:635:VAL:HG13	2.02	0.41
1:A:931:ILE:HD12	1:A:931:ILE:HA	1.66	0.41
3:F:132:ASP:OD2	3:F:231:THR:HG21	2.20	0.41
1:A:45:ILE:HB	1:A:103:MET:HG3	2.02	0.41
1:A:940:PHE:O	1:A:940:PHE:CG	2.73	0.41
1:A:1005:MET:O	1:A:1009:THR:HG23	2.21	0.41
1:A:1236:ARG:O	1:A:1239:ARG:HG2	2.21	0.41
1:A:1389:ARG:HD3	1:A:1397:HIS:HE1	1.85	0.41
3:F:185:LEU:HG	3:F:216:LEU:HD21	2.02	0.41
3:F:723:TRP:CE3	3:F:747:TYR:HB2	2.56	0.41
1:A:75:PRO:HB3	1:A:583:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:VAL:HG13	1:A:616:TRP:HB2	2.03	0.41
1:A:642:ILE:O	1:A:646:VAL:HB	2.20	0.41
1:A:1418:LYS:HZ2	1:A:1420:LEU:H	1.67	0.41
2:E:135:TYR:CZ	2:E:136:LEU:HG	2.56	0.41
3:F:573:LYS:HE2	3:F:609:TYR:OH	2.19	0.41
3:F:628:THR:O	3:F:629:TYR:CD2	2.73	0.41
1:A:513:LEU:HD12	1:A:513:LEU:HA	1.91	0.41
1:A:615:ASP:OD1	1:A:618:SER:OG	2.33	0.41
3:F:433:GLY:O	3:F:437:VAL:HG23	2.20	0.41
3:F:1065:ASN:O	3:F:1065:ASN:ND2	2.53	0.41
1:A:514:VAL:HG23	1:A:515:GLU:OE1	2.21	0.41
1:A:928:ILE:CD1	1:A:1064:VAL:CG2	2.99	0.41
1:A:1111:VAL:O	1:A:1114:VAL:HG12	2.21	0.41
2:E:32:TRP:HB3	2:E:181:SER:HB3	2.03	0.41
3:F:771:LEU:HD23	3:F:771:LEU:HA	1.90	0.41
1:A:584:ARG:NH1	5:A:1906:3PE:P	2.93	0.41
1:A:928:ILE:HD12	1:A:1064:VAL:HG22	2.03	0.41
5:A:1904:3PE:H3D2	5:A:1904:3PE:H3G2	1.79	0.41
2:E:30:ASP:HA	2:E:52:GLY:HA3	2.03	0.41
1:A:524:ILE:HD12	1:A:524:ILE:HA	1.82	0.41
3:F:97:LEU:HD11	3:F:464:GLY:O	2.20	0.41
1:A:1280:ILE:O	1:A:1284:ILE:HG13	2.20	0.41
1:A:1384:PHE:O	1:A:1388:THR:OG1	2.38	0.41
1:A:1418:LYS:HG2	1:A:1419:HIS:N	2.36	0.41
2:E:10:ARG:HA	2:E:13:LEU:HG	2.02	0.41
2:E:13:LEU:HA	2:E:16:ILE:HB	2.02	0.41
3:F:234:LYS:HD3	3:F:234:LYS:H	1.84	0.41
3:F:288:ASP:OD2	3:F:288:ASP:N	2.54	0.41
1:A:210:TYR:OH	6:A:1909:PC1:H3A1	2.20	0.41
1:A:497:ASN:OD1	1:A:497:ASN:N	2.54	0.41
1:A:553:LEU:HD23	1:A:553:LEU:O	2.21	0.41
3:F:470:ASN:HD21	3:F:482:LYS:NZ	2.19	0.41
3:F:664:LEU:HD23	3:F:682:PHE:HE2	1.86	0.41
1:A:268:PRO:HD2	1:A:273:THR:O	2.20	0.41
1:A:529:CYS:HA	1:A:532:LEU:HD21	2.03	0.41
3:F:987:ASP:OD1	3:F:987:ASP:N	2.54	0.41
1:A:490:GLN:HA	1:A:493:MET:HE3	2.02	0.40
1:A:1042:ALA:O	1:A:1046:ILE:HG13	2.21	0.40
2:E:127:MET:HG3	2:E:136:LEU:HD13	2.01	0.40
3:F:54:VAL:HG22	3:F:815:VAL:HG21	2.03	0.40
3:F:805:ILE:HD13	3:F:805:ILE:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:LEU:O	1:A:1173:LYS:N	2.50	0.40
1:A:1309:PHE:HB3	1:A:1310:PRO:HD3	2.03	0.40
5:A:1903:3PE:H352	5:A:1905:3PE:C34	2.38	0.40
5:A:1907:3PE:H112	5:A:1908:3PE:H111	2.02	0.40
5:A:1911:3PE:H2C1	5:A:1911:3PE:C2H	2.51	0.40
2:E:160:GLN:HE21	2:E:160:GLN:HB2	1.54	0.40
3:F:376:ALA:O	3:F:380:LYS:HB2	2.22	0.40
1:A:65:CYS:SG	5:A:1907:3PE:H282	2.61	0.40
1:A:441:ILE:HG23	1:A:471:LEU:HD23	2.04	0.40
3:F:44:LEU:HD23	3:F:44:LEU:HA	1.85	0.40
3:F:454:ASP:HB3	3:F:458:LEU:H	1.87	0.40
3:F:655:ASN:H	3:F:655:ASN:HD22	1.68	0.40
1:A:308:GLU:O	1:A:311:TRP:NE1	2.55	0.40
1:A:633:PRO:HB2	5:A:1906:3PE:H222	2.00	0.40
1:A:943:ALA:O	1:A:947:VAL:HG23	2.21	0.40
5:A:1907:3PE:H371	5:A:1907:3PE:H341	1.79	0.40
6:A:1909:PC1:H322	6:A:1909:PC1:H32	1.83	0.40
3:F:41:GLN:HB2	3:F:1011:LEU:HD23	2.02	0.40
3:F:708:VAL:HG22	3:F:741:GLY:O	2.22	0.40
1:A:985:LEU:HD23	1:A:985:LEU:HA	1.80	0.40
1:A:1168:LYS:HB2	1:A:1168:LYS:HE3	1.78	0.40
6:A:1909:PC1:H112	6:A:1909:PC1:H152	1.79	0.40
2:E:141:SER:OG	2:E:196:GLY:O	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1094/1873 (58%)	1017 (93%)	77 (7%)	0	100	100
2	E	159/222 (72%)	143 (90%)	15 (9%)	1 (1%)	22	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	968/1105 (88%)	876 (90%)	92 (10%)	0	100	100
All	All	2221/3200 (69%)	2036 (92%)	184 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	205	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	980/1628 (60%)	889 (91%)	91 (9%)	7	25
2	E	143/192 (74%)	129 (90%)	14 (10%)	6	23
3	F	868/973 (89%)	801 (92%)	67 (8%)	10	33
All	All	1991/2793 (71%)	1819 (91%)	172 (9%)	11	29

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	51	LYS
1	A	53	PHE
1	A	65	CYS
1	A	81	SER
1	A	95	THR
1	A	106	ILE
1	A	111	LEU
1	A	113	HIS
1	A	115	ASP
1	A	123	ASN
1	A	161	VAL
1	A	164	LEU
1	A	177	SER

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Mol	Chain	Res	Type
1	A	181	SER
1	A	193	MET
1	A	237	VAL
1	A	243	SER
1	A	245	CYS
1	A	248	THR
1	A	252	ARG
1	A	257	ASN
1	A	282	MET
1	A	289	ILE
1	A	451	SER
1	A	468	ASN
1	A	475	PHE
1	A	480	LEU
1	A	494	SER
1	A	497	ASN
1	A	506	SER
1	A	511	LEU
1	A	519	MET
1	A	526	VAL
1	A	529	CYS
1	A	532	LEU
1	A	555	SER
1	A	561	SER
1	A	646	VAL
1	A	647	CYS
1	A	672	SER
1	A	803	ASN
1	A	823	ARG
1	A	868	PHE
1	A	869	ASN
1	A	871	LEU
1	A	876	VAL
1	A	882	SER
1	A	896	LEU
1	A	899	LEU
1	A	910	ARG
1	A	927	THR
1	A	931	ILE
1	A	933	LEU
1	A	934	VAL
1	A	937	LEU

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Mol	Chain	Res	Type
1	A	938	LEU
1	A	939	GLN
1	A	942	PHE
1	A	956	SER
1	A	958	ASN
1	A	961	SER
1	A	983	MET
1	A	985	LEU
1	A	991	ILE
1	A	992	HIS
1	A	999	ASN
1	A	1011	SER
1	A	1030	ASP
1	A	1063	PHE
1	A	1108	GLN
1	A	1129	MET
1	A	1151	ASP
1	A	1154	ASN
1	A	1164	GLU
1	A	1167	LEU
1	A	1175	ARG
1	A	1189	ILE
1	A	1200	SER
1	A	1235	PHE
1	A	1243	LEU
1	A	1247	LEU
1	A	1265	GLN
1	A	1289	PHE
1	A	1302	ARG
1	A	1332	CYS
1	A	1344	TYR
1	A	1352	CYS
1	A	1384	PHE
1	A	1397	HIS
1	A	1424	THR
2	E	1	MET
2	E	4	THR
2	E	14	PHE
2	E	29	SER
2	E	32	TRP
2	E	50	HIS
2	E	51	PHE

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Mol	Chain	Res	Type
2	E	81	SER
2	E	106	SER
2	E	114	SER
2	E	132	LYS
2	E	161	SER
2	E	176	TYR
2	E	186	CYS
3	F	38	ASP
3	F	39	LYS
3	F	41	GLN
3	F	61	TYR
3	F	66	ASP
3	F	76	ARG
3	F	91	SER
3	F	132	ASP
3	F	134	ASP
3	F	158	ARG
3	F	205	LEU
3	F	234	LYS
3	F	237	LEU
3	F	263	SER
3	F	288	ASP
3	F	295	SER
3	F	303	VAL
3	F	332	ILE
3	F	348	ASN
3	F	361	MET
3	F	390	SER
3	F	417	SER
3	F	449	THR
3	F	475	PHE
3	F	476	GLU
3	F	482	LYS
3	F	517	ILE
3	F	523	VAL
3	F	543	LEU
3	F	549	ASN
3	F	592	THR
3	F	594	VAL
3	F	610	THR
3	F	612	THR
3	F	621	SER

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Mol	Chain	Res	Type
3	F	628	THR
3	F	629	TYR
3	F	639	GLU
3	F	648	SER
3	F	651	LEU
3	F	655	ASN
3	F	661	TYR
3	F	668	ASP
3	F	671	SER
3	F	710	LEU
3	F	711	ASP
3	F	735	ARG
3	F	739	THR
3	F	765	SER
3	F	774	ASP
3	F	786	SER
3	F	817	ILE
3	F	843	ASP
3	F	852	ASP
3	F	867	HIS
3	F	872	ASN
3	F	906	VAL
3	F	976	SER
3	F	983	GLN
3	F	997	LEU
3	F	1003	SER
3	F	1008	VAL
3	F	1014	THR
3	F	1029	CYS
3	F	1060	ASP
3	F	1068	LEU
3	F	1070	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	A	453	HIS
1	A	464	GLN
1	A	663	ASN
1	A	797	ASN
1	A	803	ASN

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Mol	Chain	Res	Type
1	A	939	GLN
1	A	999	ASN
1	A	1058	ASN
1	A	1087	GLN
1	A	1108	GLN
1	A	1110	GLN
1	A	1138	GLN
1	A	1305	ASN
1	A	1311	GLN
1	A	1374	ASN
2	E	160	GLN
3	F	164	GLN
3	F	169	HIS
3	F	408	ASN
3	F	447	GLN
3	F	450	ASN
3	F	470	ASN
3	F	484	GLN
3	F	655	ASN
3	F	679	ASN
3	F	697	ASN
3	F	706	ASN
3	F	866	ASN
3	F	872	ASN
3	F	1007	HIS
3	F	1052	GLN
3	F	1065	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#\|Z\| > 2$
5	3PE	A	1907	-	37,37,50	1.07	2 (5%)	40,42,55	1.16	3 (7%)
6	PC1	A	1909	-	53,53,53	0.94	2 (3%)	59,61,61	1.00	3 (5%)
5	3PE	A	1904	-	50,50,50	0.93	2 (4%)	53,55,55	1.04	2 (3%)
7	C8U	A	1912	-	24,26,26	4.13	8 (33%)	32,39,39	2.57	9 (28%)
5	3PE	A	1910	-	31,31,50	1.17	2 (6%)	34,36,55	1.23	3 (8%)
5	3PE	A	1905	-	50,50,50	0.93	2 (4%)	53,55,55	1.08	3 (5%)
5	3PE	A	1902	-	32,32,50	1.14	2 (6%)	35,37,55	1.22	3 (8%)
5	3PE	A	1908	-	20,20,50	1.03	1 (5%)	22,23,55	0.97	1 (4%)
5	3PE	A	1911	-	50,50,50	0.92	2 (4%)	53,55,55	1.04	3 (5%)
5	3PE	A	1903	-	35,35,50	1.10	2 (5%)	38,40,55	1.16	3 (7%)
5	3PE	A	1906	-	43,43,50	0.99	2 (4%)	46,48,55	1.11	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3PE	A	1907	-	-	20/41/41/54	-
6	PC1	A	1909	-	-	31/57/57/57	-
5	3PE	A	1904	-	-	36/54/54/54	-
7	C8U	A	1912	-	-	8/18/40/40	0/2/2/2
5	3PE	A	1910	-	-	14/35/35/54	-
5	3PE	A	1905	-	-	32/54/54/54	-
5	3PE	A	1902	-	-	19/36/36/54	-
5	3PE	A	1908	-	-	11/21/21/54	-
5	3PE	A	1911	-	-	30/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3PE	A	1903	-	-	23/39/39/54	-
5	3PE	A	1906	-	-	20/47/47/54	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1912	C8U	C02-C03	14.09	1.52	1.35
7	A	1912	C8U	O10-N09	10.27	1.40	1.22
7	A	1912	C8U	C06-N07	5.54	1.45	1.38
7	A	1912	C8U	C02-N07	4.69	1.44	1.38
5	A	1910	3PE	O31-C31	4.33	1.46	1.33
5	A	1905	3PE	O31-C31	4.32	1.45	1.33
5	A	1907	3PE	O31-C31	4.31	1.45	1.33
5	A	1906	3PE	O31-C31	4.29	1.45	1.33
5	A	1903	3PE	O31-C31	4.26	1.45	1.33
6	A	1909	PC1	O31-C31	4.24	1.45	1.33
5	A	1904	3PE	O31-C31	4.24	1.45	1.33
5	A	1902	3PE	O31-C31	4.19	1.45	1.33
5	A	1911	3PE	O31-C31	4.17	1.45	1.33
5	A	1904	3PE	O21-C21	4.14	1.46	1.34
5	A	1908	3PE	O21-C21	4.13	1.45	1.33
5	A	1902	3PE	O21-C21	4.11	1.45	1.34
5	A	1903	3PE	O21-C21	4.11	1.45	1.34
5	A	1907	3PE	O21-C21	4.10	1.45	1.34
5	A	1911	3PE	O21-C21	4.08	1.45	1.34
6	A	1909	PC1	O21-C21	4.08	1.45	1.34
5	A	1905	3PE	O21-C21	4.06	1.45	1.34
5	A	1910	3PE	O21-C21	4.04	1.45	1.34
5	A	1906	3PE	O21-C21	4.02	1.45	1.34
7	A	1912	C8U	C22-C03	3.32	1.53	1.47
7	A	1912	C8U	O24-C22	3.30	1.40	1.33
7	A	1912	C8U	O11-N09	-2.58	1.18	1.35
7	A	1912	C8U	O24-C25	-2.13	1.40	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1912	C8U	C01-C02-C03	-7.77	119.88	127.61
7	A	1912	C8U	C01-C02-N07	5.63	119.96	113.42
7	A	1912	C8U	C08-C06-N07	5.37	119.67	113.42
5	A	1905	3PE	O21-C21-C22	4.60	121.43	111.48
5	A	1904	3PE	O21-C21-C22	4.28	120.73	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1902	3PE	O21-C21-C22	4.22	120.62	111.48
5	A	1907	3PE	O21-C21-C22	4.22	120.61	111.48
7	A	1912	C8U	O24-C22-C03	4.19	120.02	112.31
5	A	1903	3PE	O21-C21-C22	4.12	120.39	111.48
5	A	1910	3PE	O21-C21-C22	4.11	120.38	111.48
5	A	1906	3PE	O21-C21-C22	3.99	120.11	111.48
5	A	1911	3PE	O21-C21-C22	3.94	120.00	111.48
6	A	1909	PC1	O21-C21-C22	3.84	119.79	111.48
7	A	1912	C8U	C05-C04-C03	3.79	113.33	108.62
7	A	1912	C8U	C06-N07-C02	-3.45	120.23	123.44
5	A	1911	3PE	O31-C31-C32	2.94	120.78	111.83
6	A	1909	PC1	O31-C31-C32	2.91	120.70	111.83
5	A	1903	3PE	O31-C31-C32	2.87	120.60	111.83
5	A	1907	3PE	O31-C31-C32	2.84	120.49	111.83
5	A	1902	3PE	O31-C31-C32	2.84	120.48	111.83
5	A	1905	3PE	O31-C31-C32	2.83	120.46	111.83
5	A	1910	3PE	O31-C31-C32	2.75	120.23	111.83
5	A	1906	3PE	O31-C31-C32	2.75	120.22	111.83
5	A	1904	3PE	O31-C31-C32	2.71	120.11	111.83
5	A	1906	3PE	C2-O21-C21	-2.65	111.44	117.80
5	A	1908	3PE	O21-C21-C22	2.65	119.92	111.83
5	A	1910	3PE	C2-O21-C21	-2.59	111.61	117.80
7	A	1912	C8U	C12-C04-C05	-2.56	108.70	112.52
7	A	1912	C8U	O23-C22-C03	-2.45	120.03	125.20
7	A	1912	C8U	C04-C05-N09	2.41	119.57	116.37
5	A	1907	3PE	C2-O21-C21	-2.33	112.22	117.80
5	A	1902	3PE	C2-O21-C21	-2.30	112.29	117.80
5	A	1905	3PE	O21-C21-O22	-2.19	118.58	123.70
5	A	1911	3PE	C2-O21-C21	-2.17	112.60	117.80
6	A	1909	PC1	C2-O21-C21	-2.15	112.65	117.80
5	A	1903	3PE	C2-O21-C21	-2.13	112.70	117.80

There are no chirality outliers.

All (244) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1902	3PE	C11-O13-P-O11
5	A	1902	3PE	O13-C11-C12-N
5	A	1902	3PE	O22-C21-O21-C2
5	A	1902	3PE	C22-C21-O21-C2
5	A	1903	3PE	C1-O11-P-O12
5	A	1903	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
5	A	1903	3PE	C1-O11-P-O14
5	A	1903	3PE	C11-O13-P-O11
5	A	1903	3PE	C11-O13-P-O12
5	A	1903	3PE	C11-O13-P-O14
5	A	1903	3PE	O32-C31-O31-C3
5	A	1903	3PE	C32-C31-O31-C3
5	A	1903	3PE	C22-C21-O21-C2
5	A	1904	3PE	C1-O11-P-O12
5	A	1904	3PE	C11-O13-P-O11
5	A	1904	3PE	O22-C21-O21-C2
5	A	1904	3PE	C22-C21-O21-C2
5	A	1905	3PE	C1-O11-P-O12
5	A	1905	3PE	C1-O11-P-O13
5	A	1905	3PE	C1-O11-P-O14
5	A	1905	3PE	C11-O13-P-O11
5	A	1905	3PE	O22-C21-O21-C2
5	A	1905	3PE	C22-C21-O21-C2
5	A	1906	3PE	C12-C11-O13-P
5	A	1907	3PE	C11-O13-P-O14
5	A	1907	3PE	C2-C1-O11-P
5	A	1908	3PE	C1-O11-P-O12
5	A	1908	3PE	C1-O11-P-O13
5	A	1908	3PE	C11-O13-P-O14
5	A	1908	3PE	C12-C11-O13-P
5	A	1908	3PE	O13-C11-C12-N
5	A	1908	3PE	O11-C1-C2-O21
5	A	1910	3PE	C1-O11-P-O13
5	A	1910	3PE	C12-C11-O13-P
5	A	1911	3PE	C11-O13-P-O11
5	A	1911	3PE	C11-O13-P-O14
6	A	1909	PC1	C11-O13-P-O14
6	A	1909	PC1	C1-O11-P-O12
6	A	1909	PC1	C1-O11-P-O13
6	A	1909	PC1	O13-C11-C12-N
6	A	1909	PC1	O32-C31-O31-C3
6	A	1909	PC1	C32-C31-O31-C3
7	A	1912	C8U	C02-C03-C22-O24
5	A	1907	3PE	O32-C31-O31-C3
7	A	1912	C8U	C03-C22-O24-C25
5	A	1907	3PE	C32-C31-O31-C3
5	A	1906	3PE	O32-C31-O31-C3
7	A	1912	C8U	C02-C03-C22-O23

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Mol	Chain	Res	Type	Atoms
5	A	1903	3PE	O22-C21-O21-C2
5	A	1904	3PE	C32-C31-O31-C3
5	A	1905	3PE	C32-C31-O31-C3
5	A	1906	3PE	C32-C31-O31-C3
7	A	1912	C8U	O23-C22-O24-C25
5	A	1904	3PE	O32-C31-O31-C3
5	A	1905	3PE	O32-C31-O31-C3
5	A	1911	3PE	C26-C27-C28-C29
5	A	1907	3PE	C28-C29-C2A-C2B
6	A	1909	PC1	C23-C24-C25-C26
5	A	1911	3PE	C28-C29-C2A-C2B
5	A	1911	3PE	C2C-C2D-C2E-C2F
5	A	1904	3PE	C3D-C3E-C3F-C3G
5	A	1910	3PE	C25-C26-C27-C28
5	A	1905	3PE	C21-C22-C23-C24
6	A	1909	PC1	C31-C32-C33-C34
5	A	1907	3PE	C21-C22-C23-C24
7	A	1912	C8U	C04-C03-C22-O23
5	A	1910	3PE	C32-C31-O31-C3
5	A	1906	3PE	C22-C21-O21-C2
5	A	1907	3PE	C22-C21-O21-C2
5	A	1907	3PE	O22-C21-O21-C2
5	A	1904	3PE	C2A-C2B-C2C-C2D
7	A	1912	C8U	C04-C03-C22-O24
5	A	1905	3PE	C2-C1-O11-P
6	A	1909	PC1	C2E-C2F-C2G-C2H
5	A	1906	3PE	O22-C21-O21-C2
5	A	1907	3PE	C22-C23-C24-C25
5	A	1907	3PE	C25-C26-C27-C28
5	A	1905	3PE	C26-C27-C28-C29
5	A	1905	3PE	C29-C2A-C2B-C2C
5	A	1904	3PE	C2E-C2F-C2G-C2H
5	A	1905	3PE	C28-C29-C2A-C2B
5	A	1911	3PE	C25-C26-C27-C28
5	A	1905	3PE	C27-C28-C29-C2A
5	A	1906	3PE	C32-C33-C34-C35
5	A	1905	3PE	C31-C32-C33-C34
5	A	1902	3PE	C22-C23-C24-C25
5	A	1904	3PE	C39-C3A-C3B-C3C
5	A	1903	3PE	C25-C26-C27-C28
5	A	1905	3PE	C32-C33-C34-C35
5	A	1910	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
5	A	1906	3PE	C33-C34-C35-C36
6	A	1909	PC1	C3A-C3B-C3C-C3D
5	A	1902	3PE	C24-C25-C26-C27
5	A	1910	3PE	C26-C27-C28-C29
6	A	1909	PC1	C25-C26-C27-C28
6	A	1909	PC1	C38-C39-C3A-C3B
6	A	1909	PC1	C3C-C3D-C3E-C3F
5	A	1903	3PE	C37-C38-C39-C3A
5	A	1904	3PE	C34-C35-C36-C37
5	A	1904	3PE	C28-C29-C2A-C2B
5	A	1911	3PE	C3B-C3C-C3D-C3E
5	A	1911	3PE	C3C-C3D-C3E-C3F
6	A	1909	PC1	C35-C36-C37-C38
5	A	1910	3PE	C23-C24-C25-C26
5	A	1906	3PE	C35-C36-C37-C38
5	A	1910	3PE	C28-C29-C2A-C2B
5	A	1902	3PE	C34-C35-C36-C37
5	A	1906	3PE	C23-C24-C25-C26
5	A	1903	3PE	C36-C37-C38-C39
5	A	1905	3PE	C2A-C2B-C2C-C2D
5	A	1906	3PE	C34-C35-C36-C37
5	A	1911	3PE	C33-C34-C35-C36
6	A	1909	PC1	C32-C33-C34-C35
5	A	1904	3PE	C2F-C2G-C2H-C2I
5	A	1905	3PE	C3E-C3F-C3G-C3H
5	A	1911	3PE	C38-C39-C3A-C3B
5	A	1904	3PE	C32-C33-C34-C35
5	A	1903	3PE	C22-C23-C24-C25
5	A	1904	3PE	C25-C26-C27-C28
5	A	1906	3PE	C2B-C2C-C2D-C2E
5	A	1904	3PE	C23-C24-C25-C26
5	A	1910	3PE	C22-C21-O21-C2
5	A	1911	3PE	C22-C21-O21-C2
5	A	1908	3PE	C21-C22-C23-C24
5	A	1903	3PE	C33-C34-C35-C36
5	A	1906	3PE	C22-C23-C24-C25
5	A	1902	3PE	C26-C27-C28-C29
5	A	1906	3PE	C2A-C2B-C2C-C2D
5	A	1905	3PE	C3D-C3E-C3F-C3G
5	A	1906	3PE	C36-C37-C38-C39
5	A	1907	3PE	C23-C24-C25-C26
5	A	1911	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
5	A	1904	3PE	C35-C36-C37-C38
5	A	1907	3PE	C32-C33-C34-C35
5	A	1902	3PE	C32-C33-C34-C35
6	A	1909	PC1	C36-C37-C38-C39
5	A	1911	3PE	C22-C23-C24-C25
5	A	1904	3PE	C22-C23-C24-C25
5	A	1910	3PE	O22-C21-O21-C2
5	A	1902	3PE	C31-C32-C33-C34
5	A	1910	3PE	C32-C33-C34-C35
5	A	1905	3PE	C1-C2-C3-O31
5	A	1905	3PE	C34-C35-C36-C37
5	A	1904	3PE	C3A-C3B-C3C-C3D
6	A	1909	PC1	C3D-C3E-C3F-C3G
6	A	1909	PC1	C29-C2A-C2B-C2C
5	A	1904	3PE	C2D-C2E-C2F-C2G
5	A	1911	3PE	C31-C32-C33-C34
5	A	1904	3PE	C3-C2-O21-C21
5	A	1905	3PE	C39-C3A-C3B-C3C
5	A	1903	3PE	O11-C1-C2-O21
6	A	1909	PC1	O11-C1-C2-O21
5	A	1904	3PE	C37-C38-C39-C3A
6	A	1909	PC1	C37-C38-C39-C3A
5	A	1908	3PE	C26-C27-C28-C29
5	A	1902	3PE	C32-C31-O31-C3
5	A	1906	3PE	C2E-C2F-C2G-C2H
5	A	1910	3PE	C33-C34-C35-C36
5	A	1904	3PE	C3F-C3G-C3H-C3I
5	A	1904	3PE	C2C-C2D-C2E-C2F
5	A	1911	3PE	C32-C31-O31-C3
5	A	1910	3PE	C2-C1-O11-P
5	A	1904	3PE	O11-C1-C2-C3
5	A	1911	3PE	C23-C24-C25-C26
5	A	1904	3PE	C31-C32-C33-C34
5	A	1911	3PE	C3D-C3E-C3F-C3G
5	A	1911	3PE	C3E-C3F-C3G-C3H
5	A	1906	3PE	C24-C25-C26-C27
6	A	1909	PC1	C21-C22-C23-C24
6	A	1909	PC1	C33-C34-C35-C36
5	A	1902	3PE	C1-C2-C3-O31
5	A	1907	3PE	C1-C2-C3-O31
5	A	1905	3PE	C3B-C3C-C3D-C3E
5	A	1907	3PE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
5	A	1911	3PE	C2E-C2F-C2G-C2H
5	A	1911	3PE	C3F-C3G-C3H-C3I
5	A	1902	3PE	C27-C28-C29-C2A
5	A	1904	3PE	C36-C37-C38-C39
6	A	1909	PC1	O21-C21-C22-C23
5	A	1903	3PE	O21-C2-C3-O31
5	A	1905	3PE	O21-C2-C3-O31
5	A	1907	3PE	C27-C28-C29-C2A
5	A	1903	3PE	C27-C28-C29-C2A
5	A	1908	3PE	C23-C24-C25-C26
5	A	1902	3PE	O32-C31-O31-C3
5	A	1905	3PE	C3A-C3B-C3C-C3D
5	A	1902	3PE	C33-C34-C35-C36
5	A	1911	3PE	O32-C31-O31-C3
5	A	1911	3PE	C2F-C2G-C2H-C2I
5	A	1907	3PE	C3-C2-O21-C21
5	A	1906	3PE	C2C-C2D-C2E-C2F
5	A	1904	3PE	O11-C1-C2-O21
5	A	1905	3PE	O11-C1-C2-O21
5	A	1911	3PE	O11-C1-C2-O21
5	A	1903	3PE	C1-C2-C3-O31
5	A	1907	3PE	O21-C2-C3-O31
5	A	1904	3PE	C2B-C2C-C2D-C2E
5	A	1902	3PE	C35-C36-C37-C38
5	A	1902	3PE	C25-C26-C27-C28
7	A	1912	C8U	C04-C05-N09-O10
6	A	1909	PC1	C39-C3A-C3B-C3C
5	A	1903	3PE	O11-C1-C2-C3
6	A	1909	PC1	O11-C1-C2-C3
5	A	1902	3PE	O21-C2-C3-O31
5	A	1908	3PE	C22-C21-O21-C2
5	A	1902	3PE	C11-O13-P-O14
5	A	1904	3PE	C1-O11-P-O13
5	A	1904	3PE	C1-O11-P-O14
5	A	1904	3PE	C11-O13-P-O14
5	A	1904	3PE	O13-C11-C12-N
5	A	1905	3PE	C11-O13-P-O14
5	A	1907	3PE	C1-O11-P-O14
5	A	1910	3PE	C1-O11-P-O14
5	A	1911	3PE	O13-C11-C12-N
6	A	1909	PC1	C1-O11-P-O14
6	A	1909	PC1	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
5	A	1905	3PE	C2E-C2F-C2G-C2H
5	A	1906	3PE	C27-C28-C29-C2A
5	A	1911	3PE	C27-C28-C29-C2A
5	A	1908	3PE	O22-C21-O21-C2
5	A	1904	3PE	C26-C27-C28-C29
5	A	1907	3PE	C37-C38-C39-C3A
5	A	1906	3PE	O11-C1-C2-O21
5	A	1906	3PE	C2F-C2G-C2H-C2I
5	A	1903	3PE	C34-C35-C36-C37
5	A	1903	3PE	C26-C27-C28-C29
6	A	1909	PC1	C28-C29-C2A-C2B
5	A	1905	3PE	O11-C1-C2-C3
5	A	1911	3PE	O11-C1-C2-C3
5	A	1904	3PE	C33-C34-C35-C36
5	A	1905	3PE	C2F-C2G-C2H-C2I
6	A	1909	PC1	C2A-C2B-C2C-C2D
5	A	1911	3PE	C32-C33-C34-C35
6	A	1909	PC1	O22-C21-C22-C23
5	A	1911	3PE	O21-C21-C22-C23
7	A	1912	C8U	C06-C05-N09-O10
6	A	1909	PC1	C3F-C3G-C3H-C3I
5	A	1911	3PE	C2D-C2E-C2F-C2G
5	A	1907	3PE	C29-C2A-C2B-C2C
5	A	1903	3PE	C23-C24-C25-C26
5	A	1911	3PE	C2A-C2B-C2C-C2D
5	A	1905	3PE	O31-C31-C32-C33
5	A	1905	3PE	O32-C31-C32-C33
5	A	1904	3PE	C27-C28-C29-C2A

There are no ring outliers.

11 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1907	3PE	17	0
6	A	1909	PC1	12	0
5	A	1904	3PE	17	0
7	A	1912	C8U	6	0
5	A	1910	3PE	9	0
5	A	1905	3PE	17	0
5	A	1902	3PE	2	0
5	A	1908	3PE	11	0
5	A	1911	3PE	13	0

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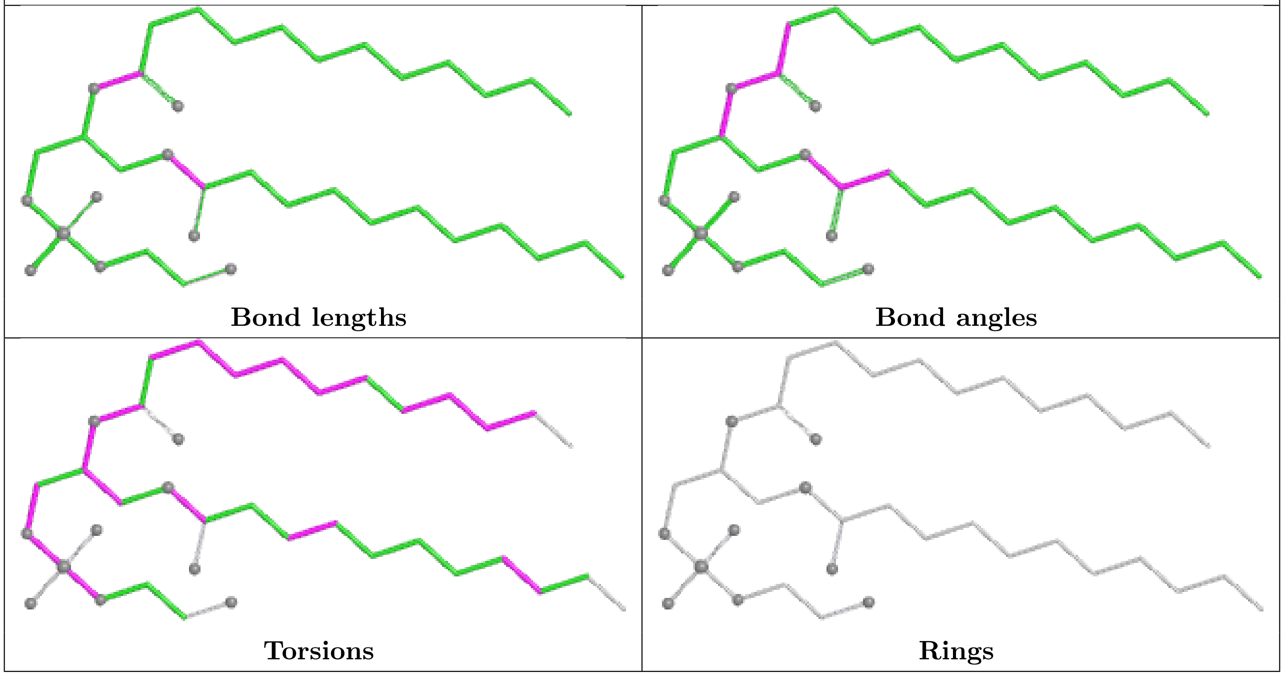
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1903	3PE	17	0
5	A	1906	3PE	17	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 3PE A 1907



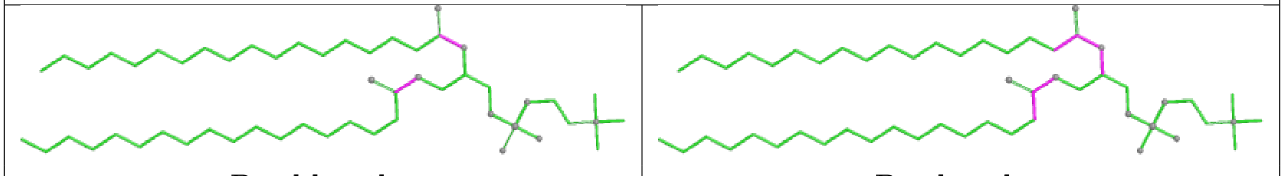
Bond lengths

Bond angles

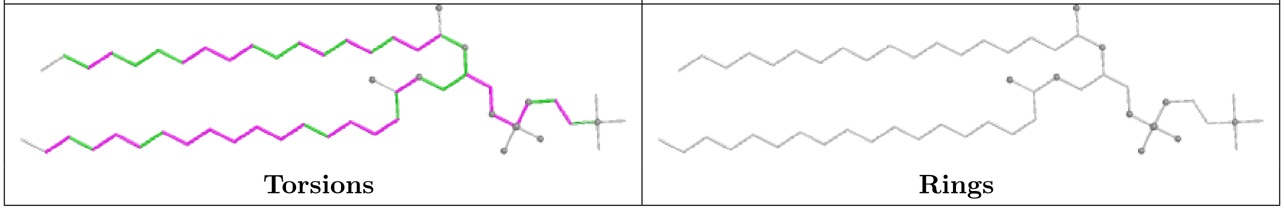
Torsions

Rings

Ligand PC1 A 1909

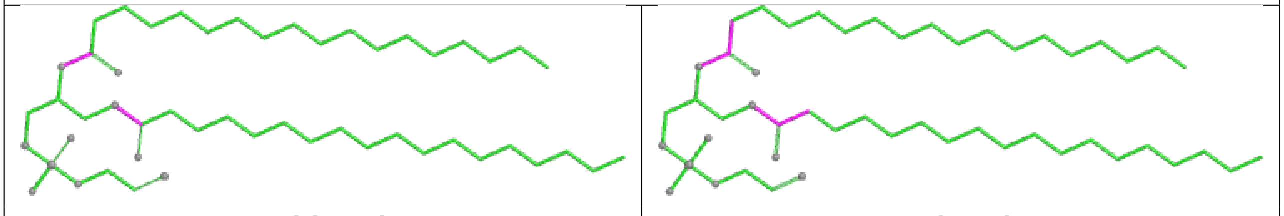


Bond lengths **Bond angles**

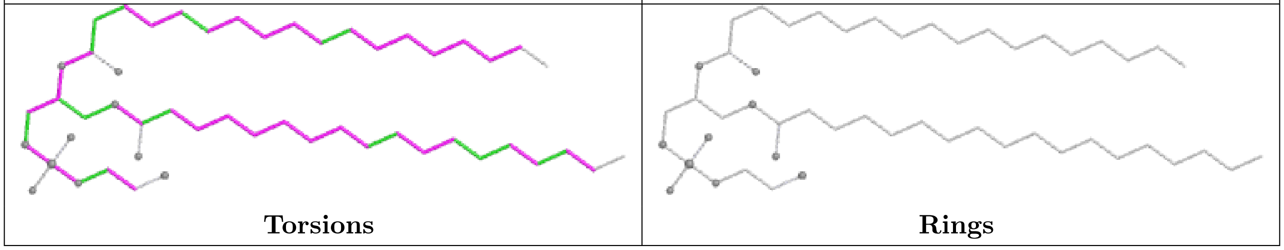


Torsions **Rings**

Ligand 3PE A 1904

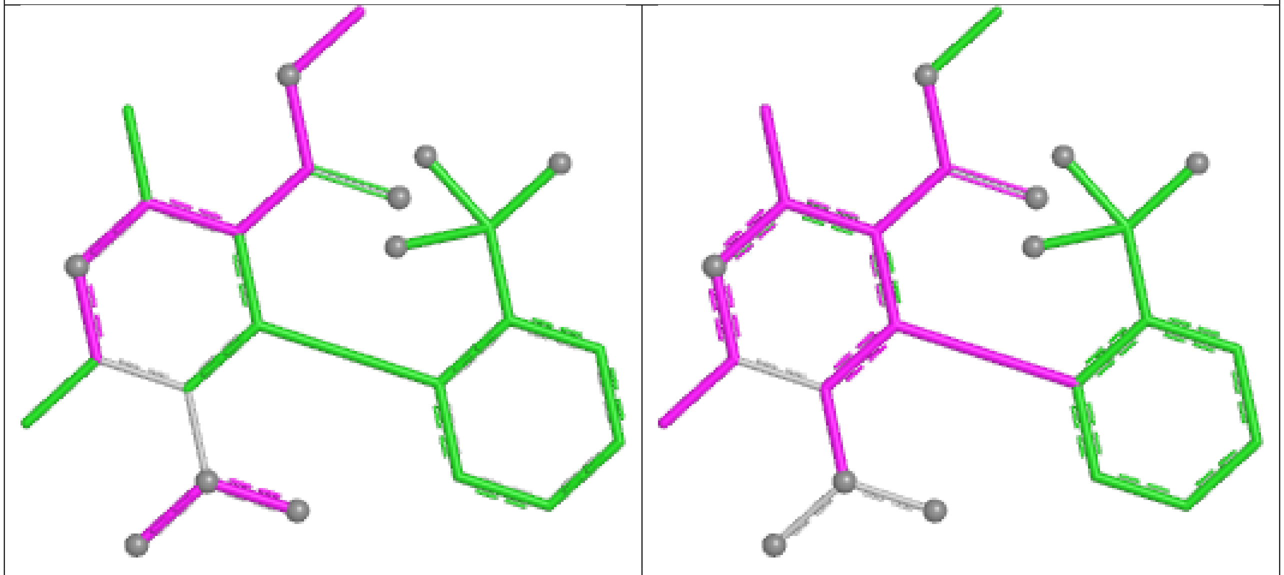


Bond lengths **Bond angles**



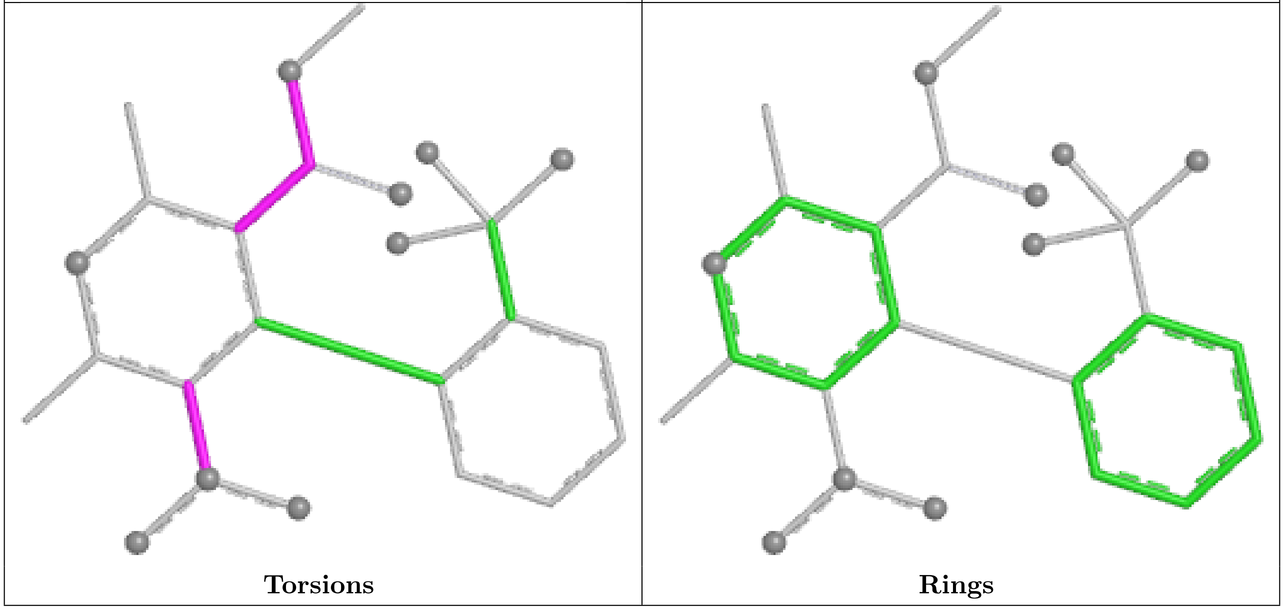
Torsions **Rings**

Ligand C8U A 1912



Bond lengths

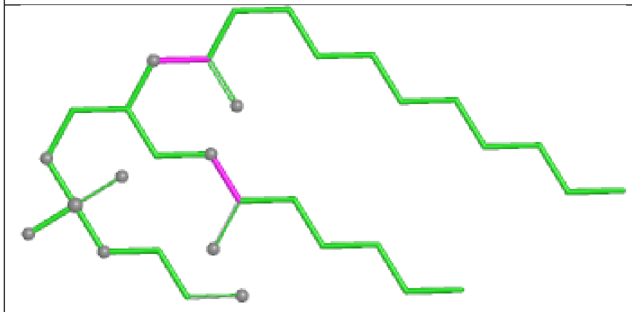
Bond angles



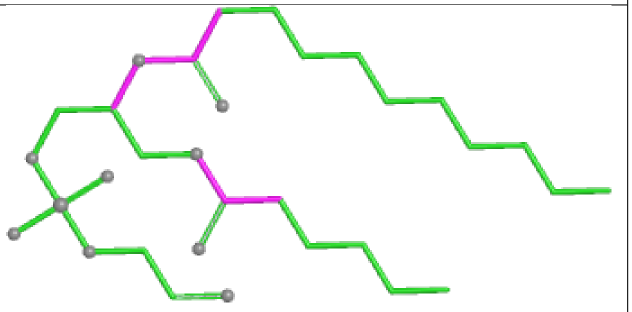
Torsions

Rings

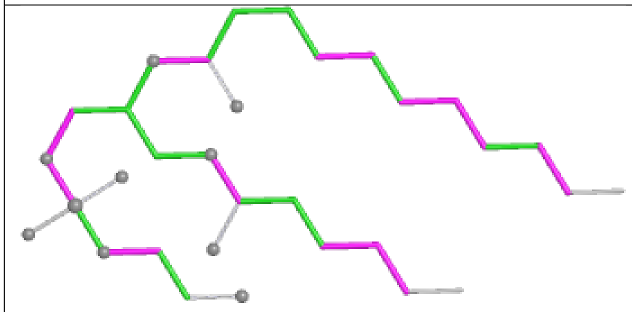
Ligand 3PE A 1910



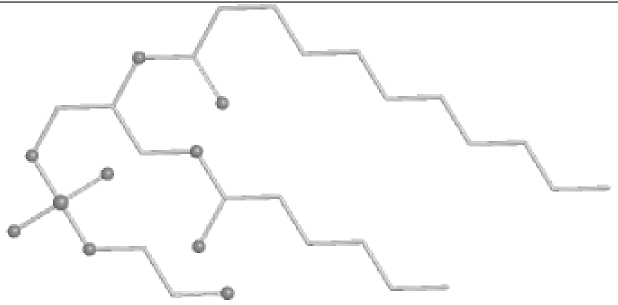
Bond lengths



Bond angles

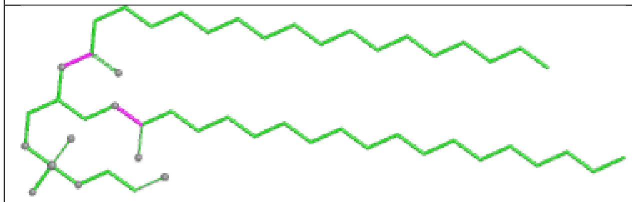


Torsions

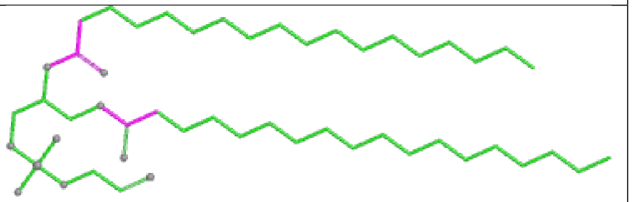


Rings

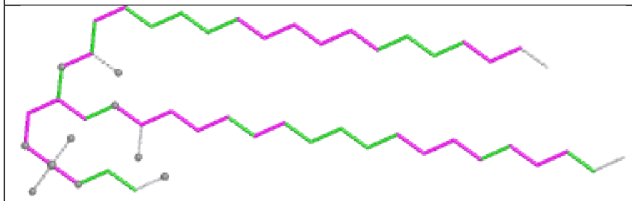
Ligand 3PE A 1905



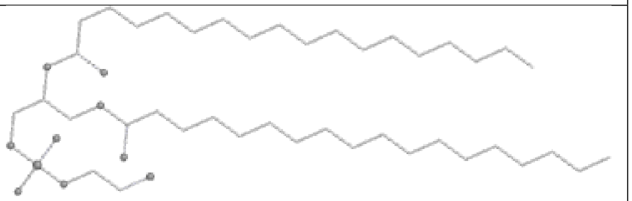
Bond lengths



Bond angles

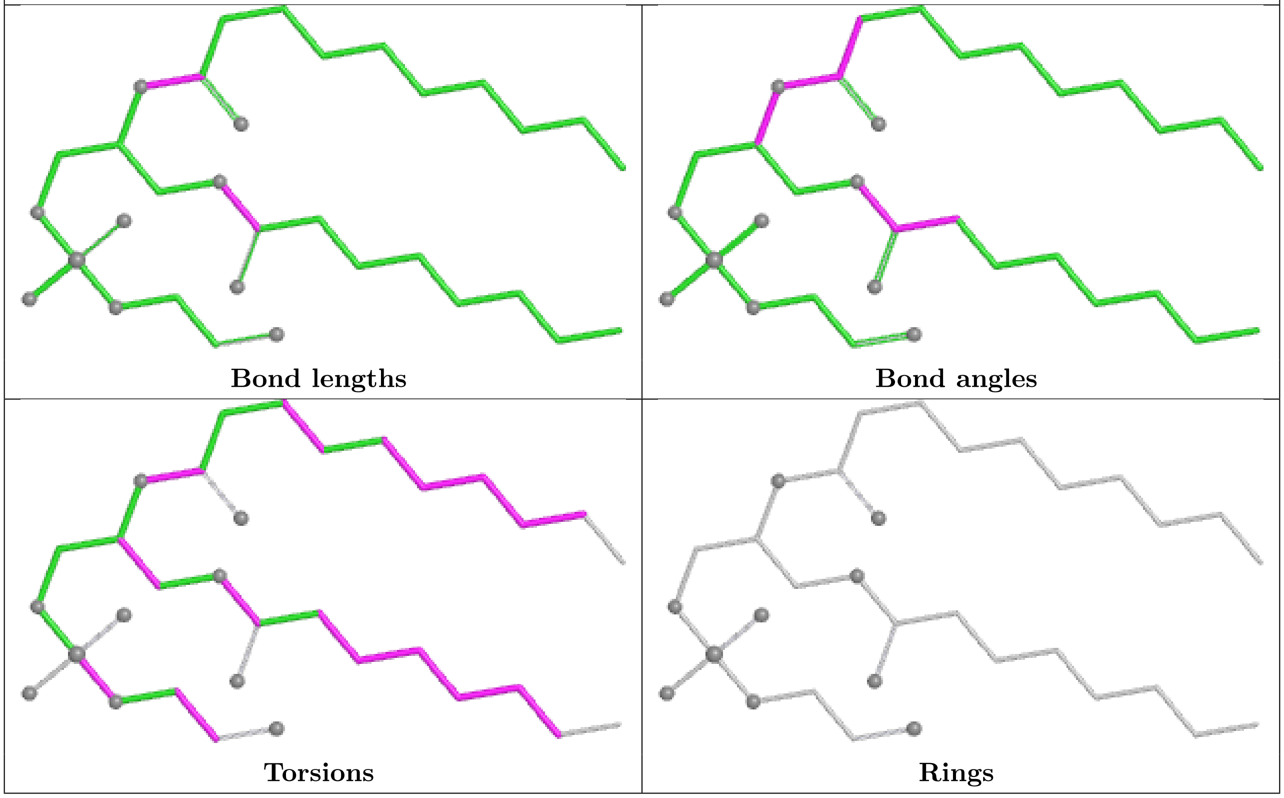


Torsions

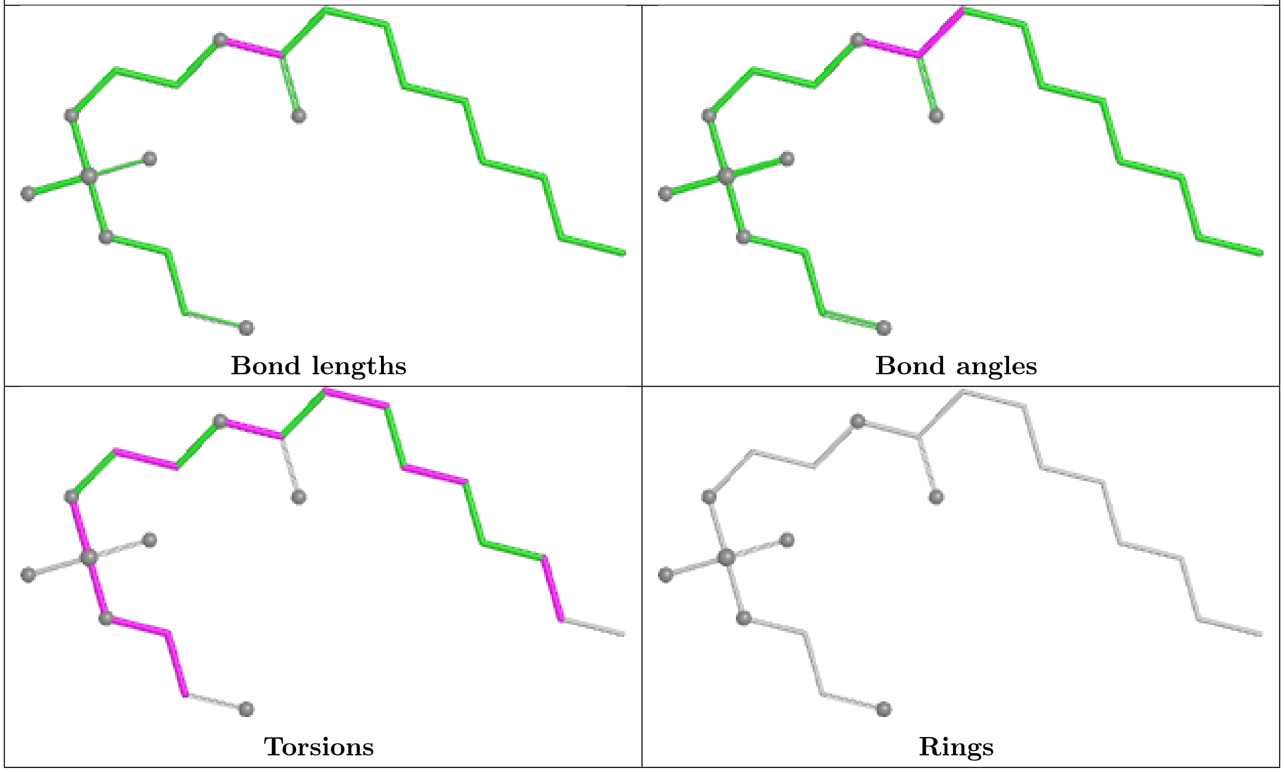


Rings

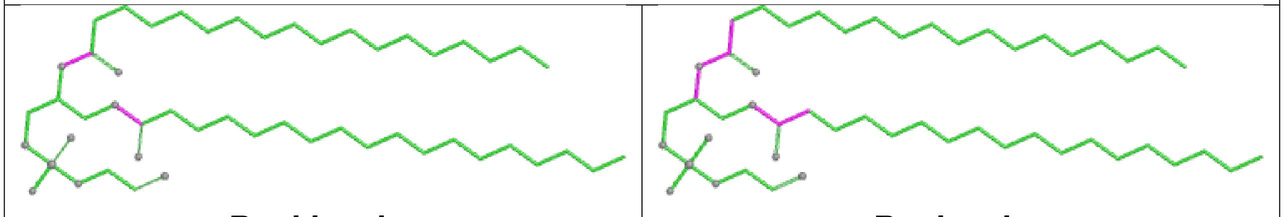
Ligand 3PE A 1902



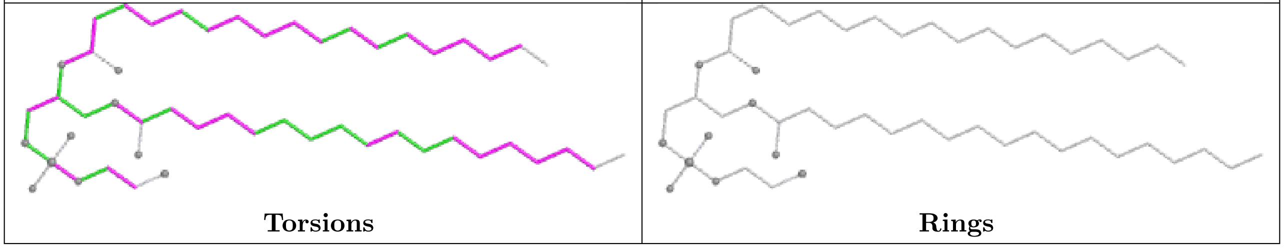
Ligand 3PE A 1908



Ligand 3PE A 1911

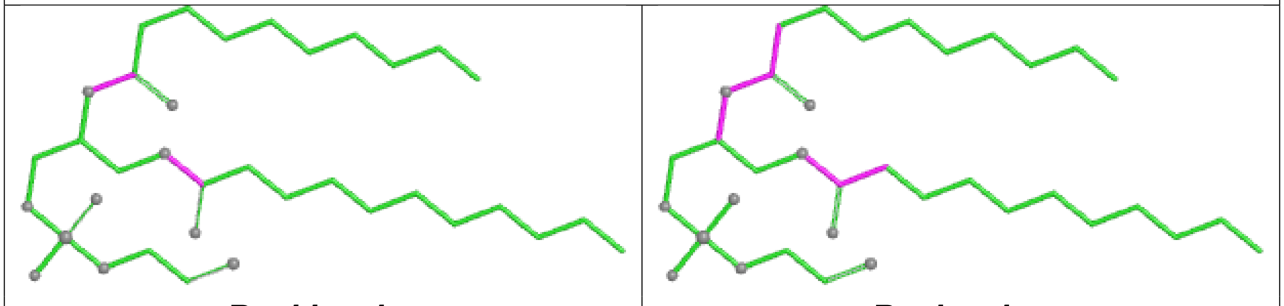


Bond lengths **Bond angles**

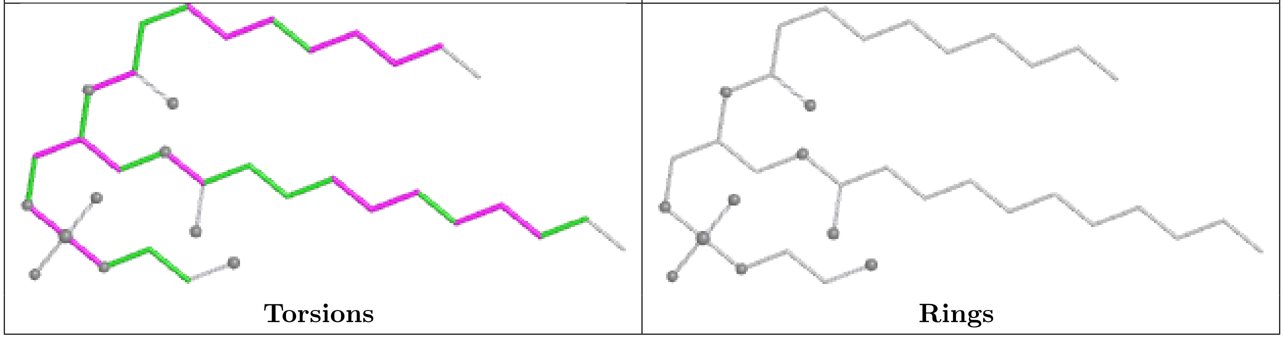


Torsions **Rings**

Ligand 3PE A 1903

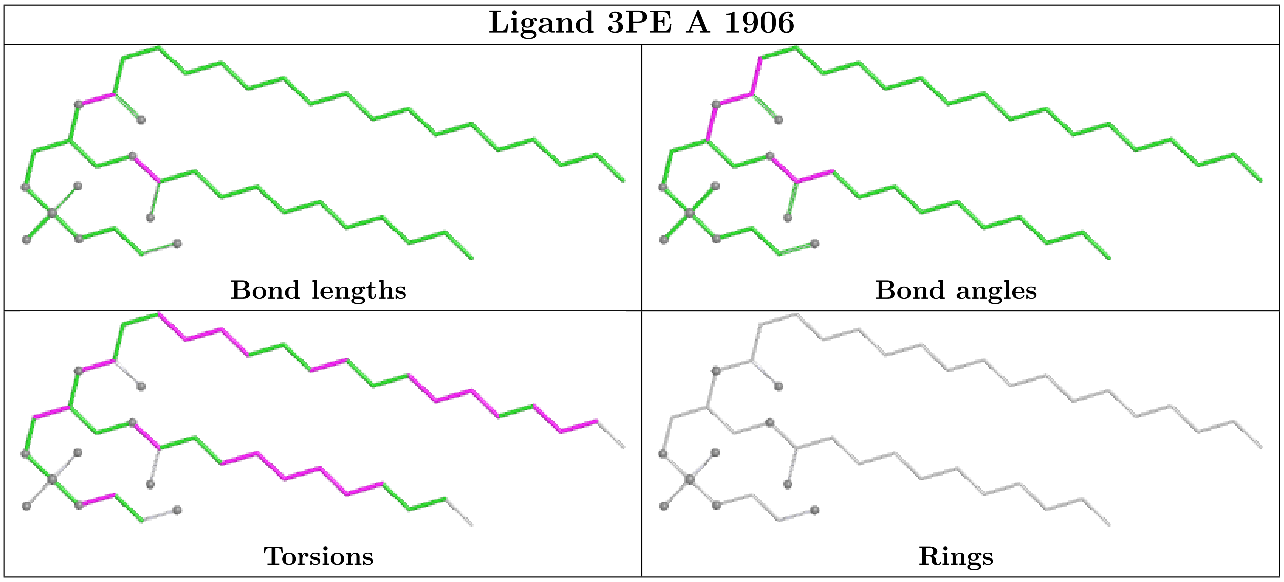


Bond lengths **Bond angles**



Torsions **Rings**

Ligand 3PE A 1906



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

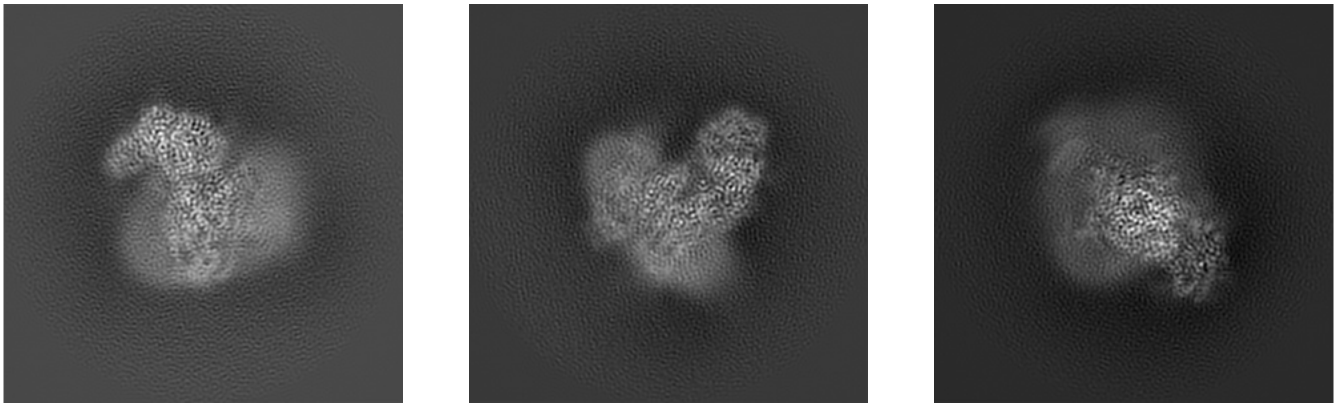
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-22415. 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 ⓘ

6.1.1 Primary map

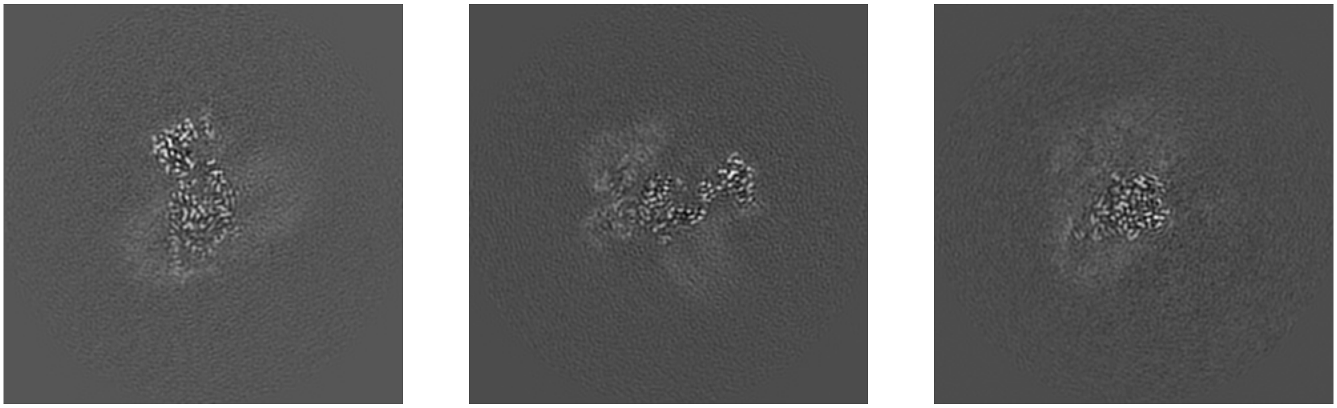


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

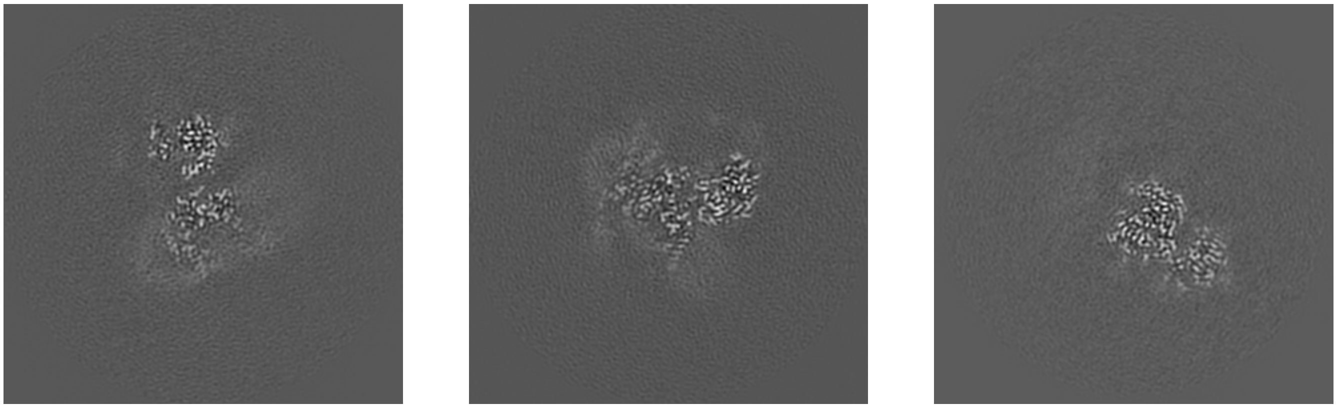


X Index: 140 Y Index: 140 Z Index: 140

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

6.3 Largest variance slices

6.3.1 Primary map

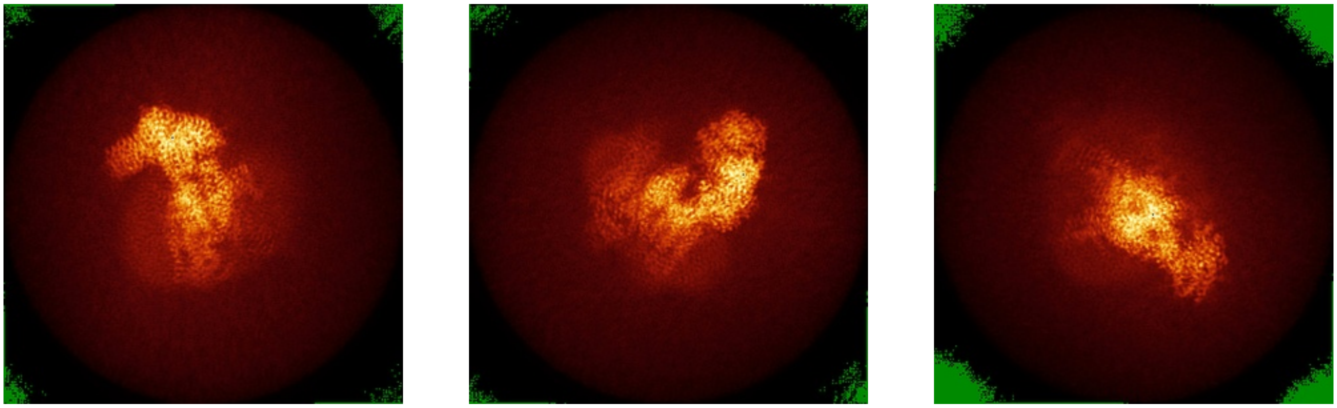


X Index: 151 Y Index: 130 Z Index: 184

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

6.4 Orthogonal standard-deviation projections (False-color)

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 ⓘ

6.5.1 Primary map

X

Y

Z

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.

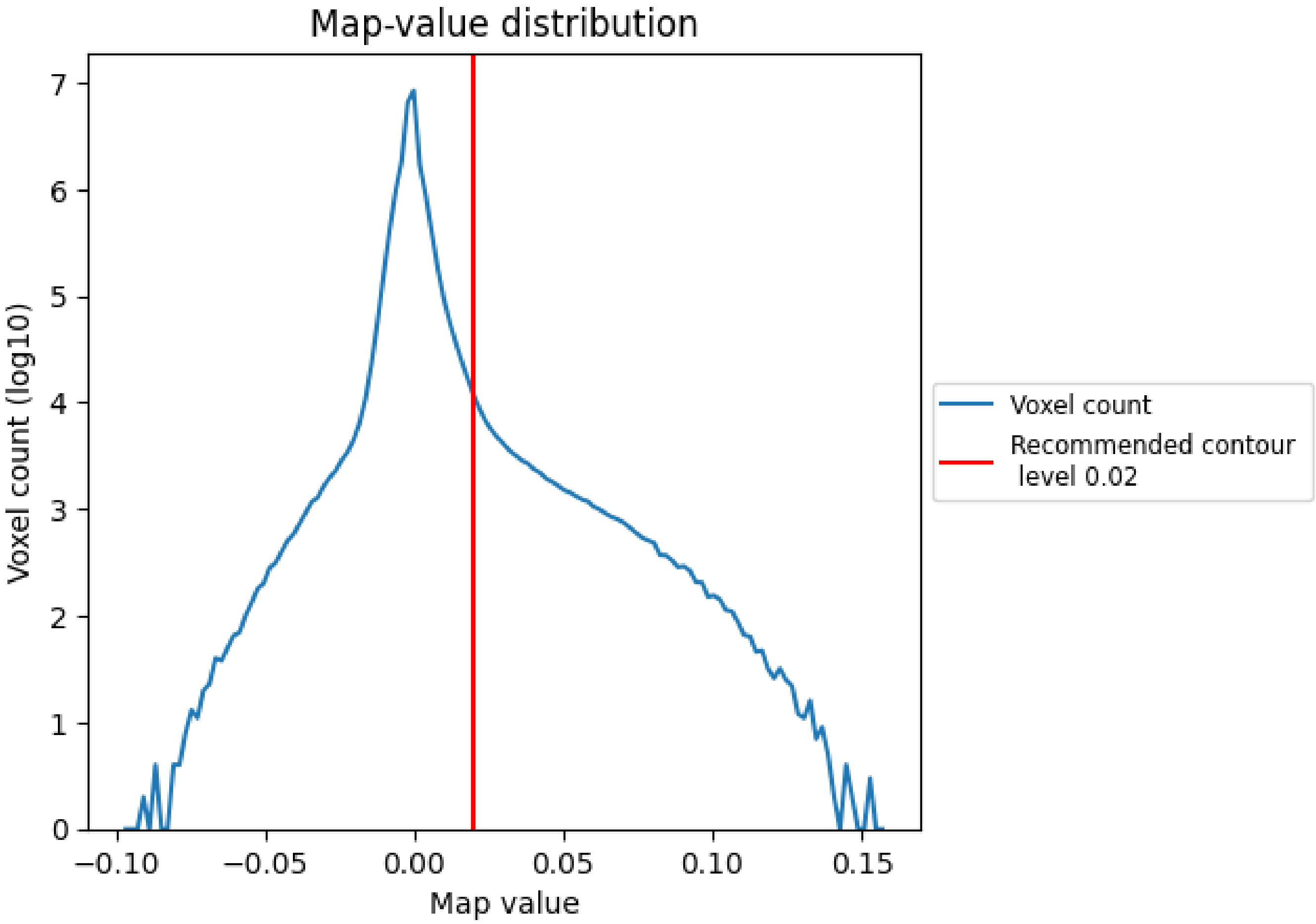
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

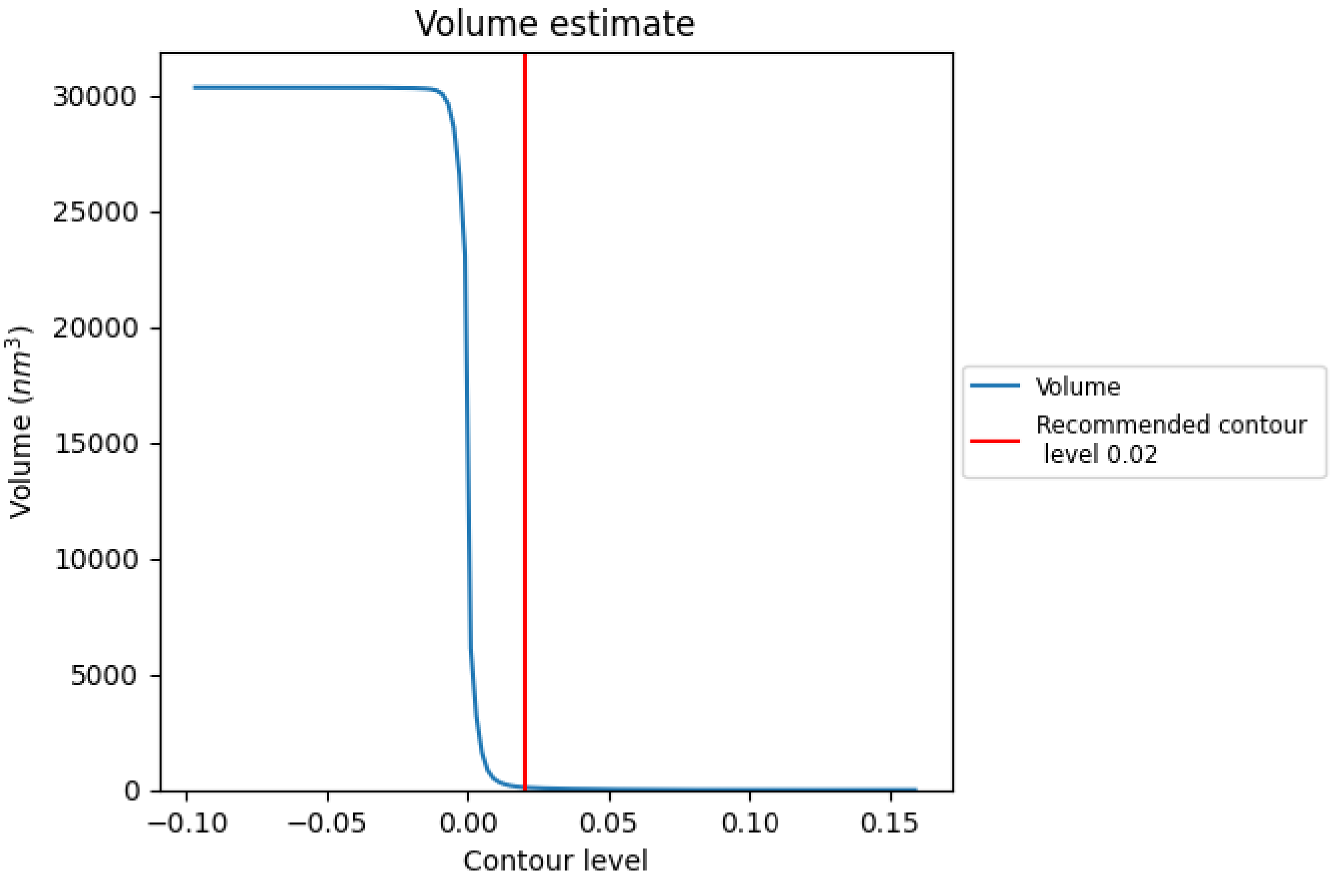
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

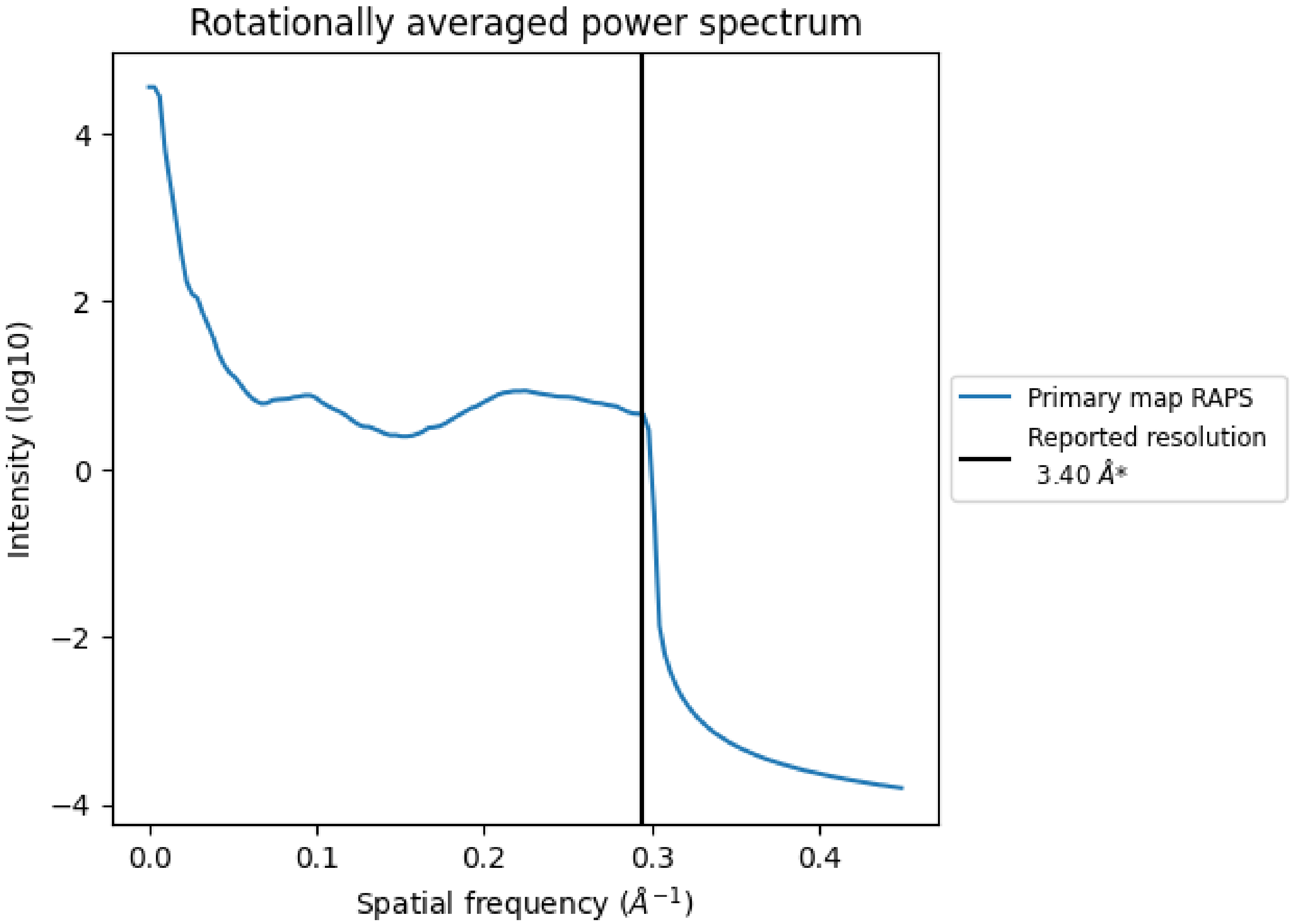
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 114 nm^3; this corresponds to an approximate mass of 103 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 0.294 Å^{-1}

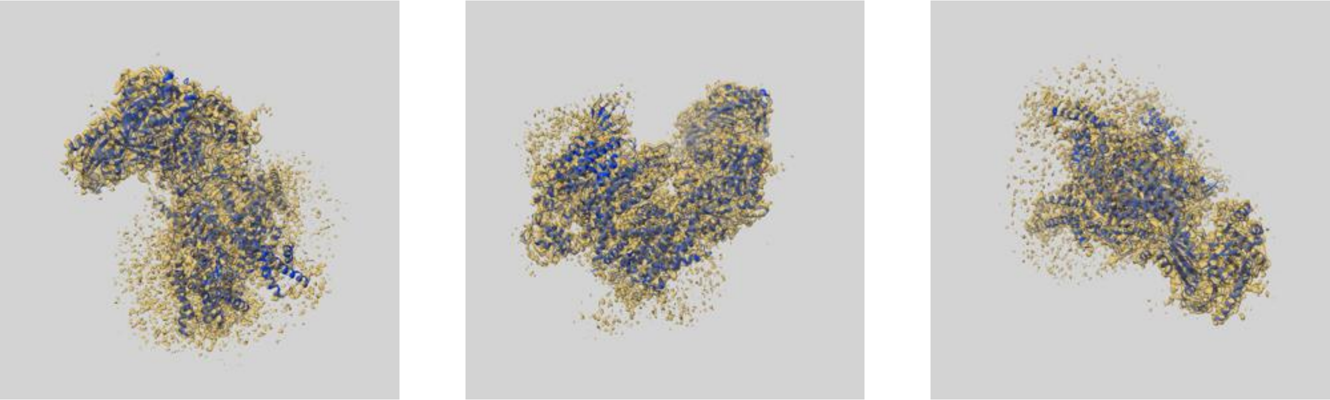
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

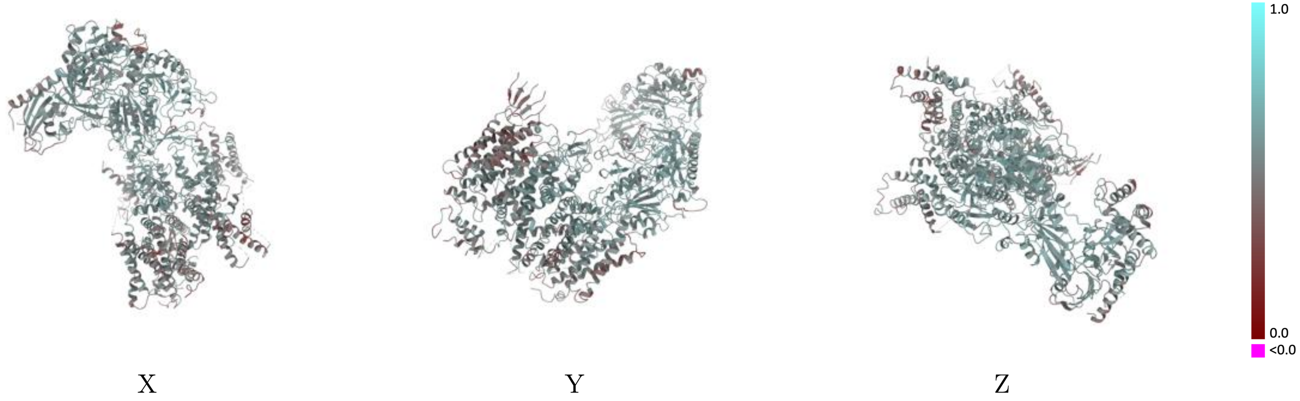
This section contains information regarding the fit between EMDB map EMD-22415 and PDB model 7JPL. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay


X Y Z

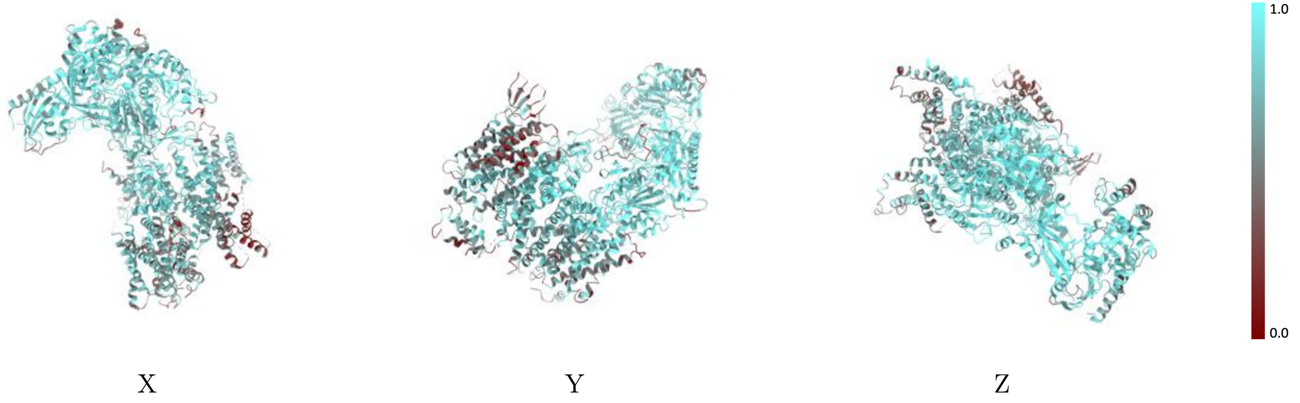
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



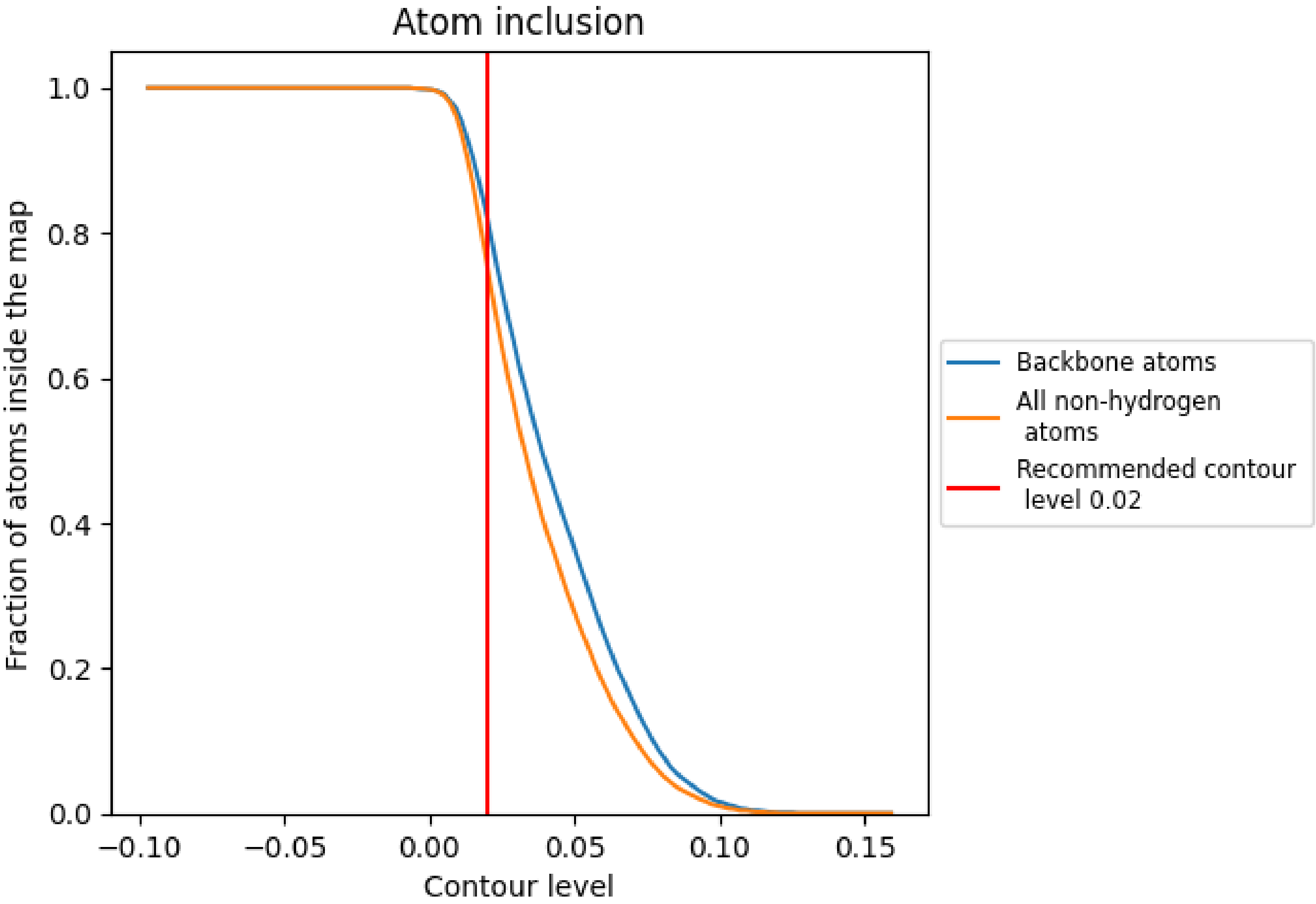
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 ⓘ



At the recommended contour level, 82% of all backbone atoms, 75% 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	0.7510	0.5300
A	0.7080	0.5230
E	0.5670	0.4570
F	0.8350	0.5510