



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 02:58 AM UTC

PDB ID : 7JPW / pdb_00007jpw
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

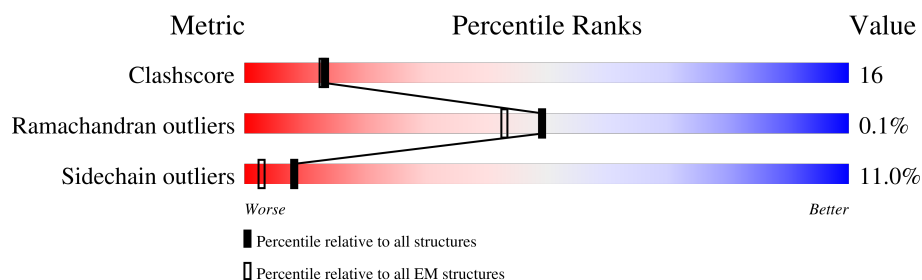
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	A	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		

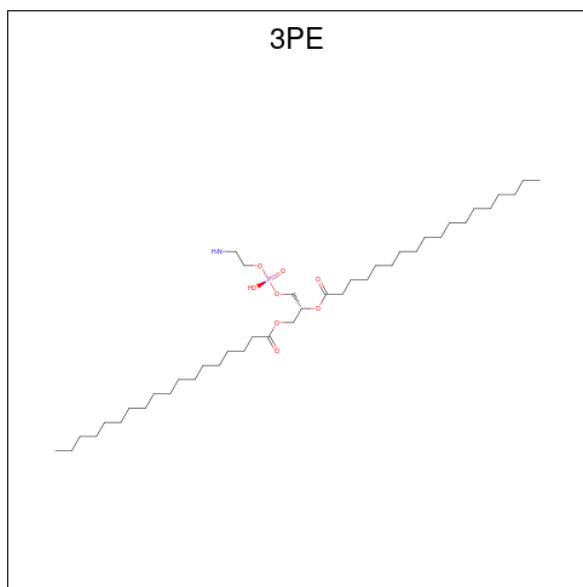
- Molecule 3 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

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 (CCD ID: CA) (formula: Ca).

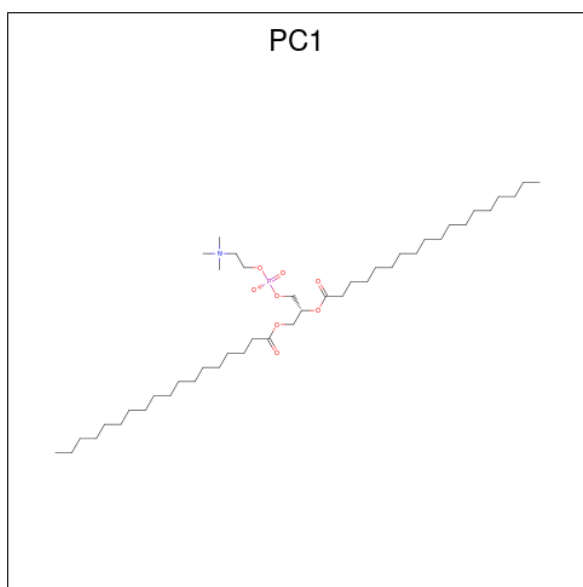
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	

- Molecule 5 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



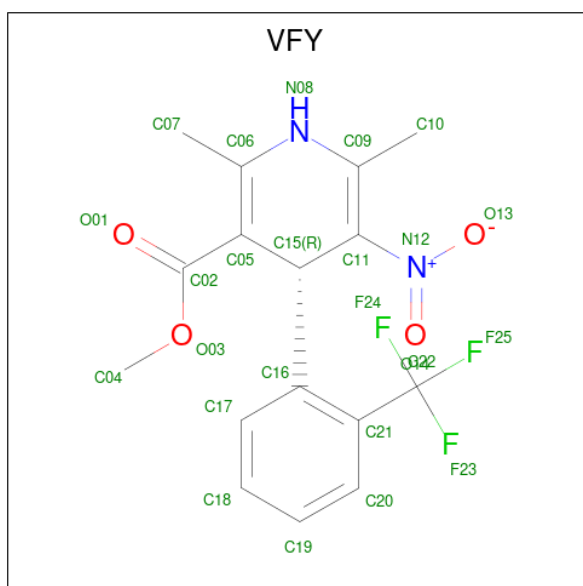
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			33	23	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
5	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
5	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
5	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
5	A	1	Total	C	N	O	P	0
			21	13	1	6	1	
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 (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



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

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

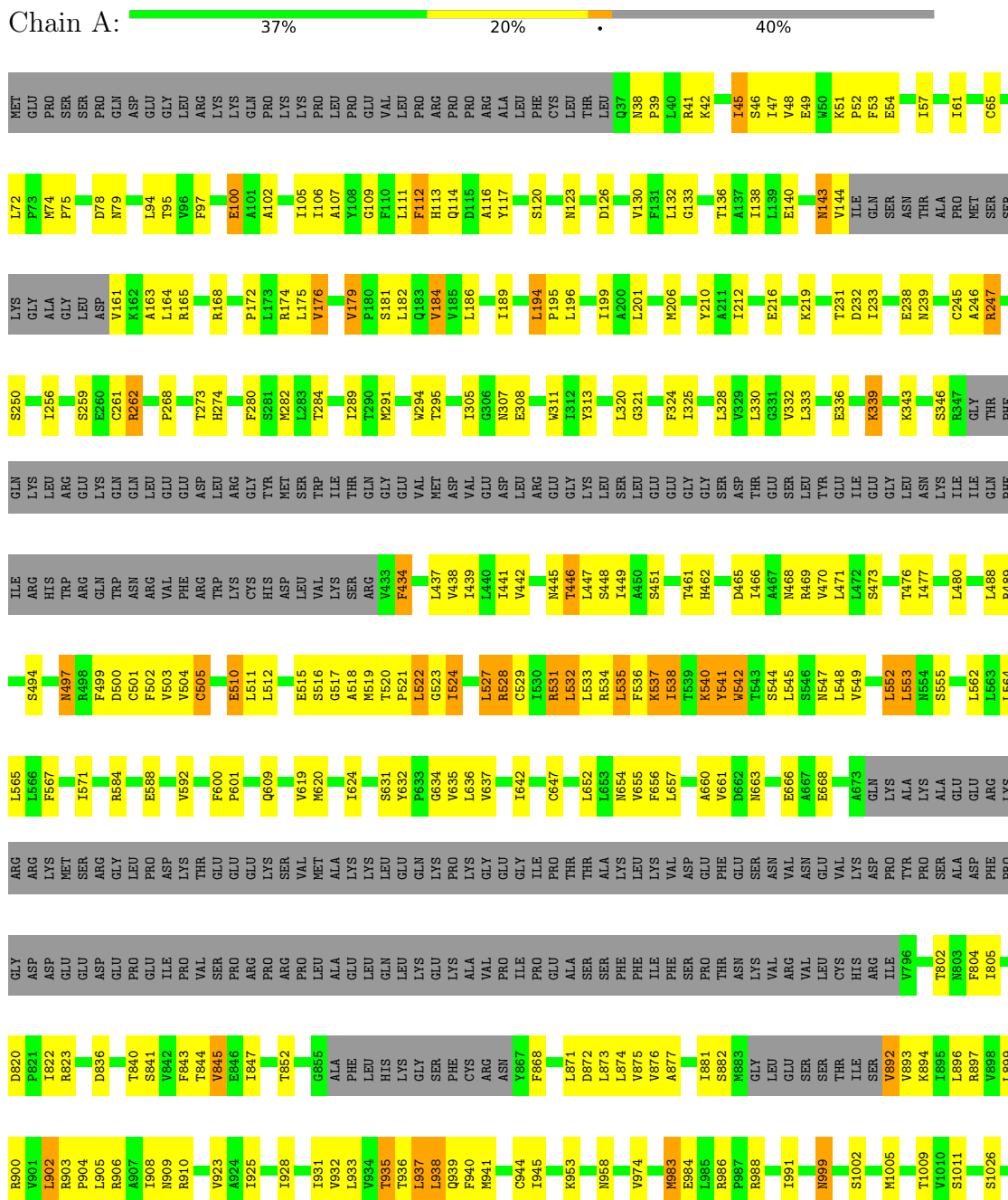


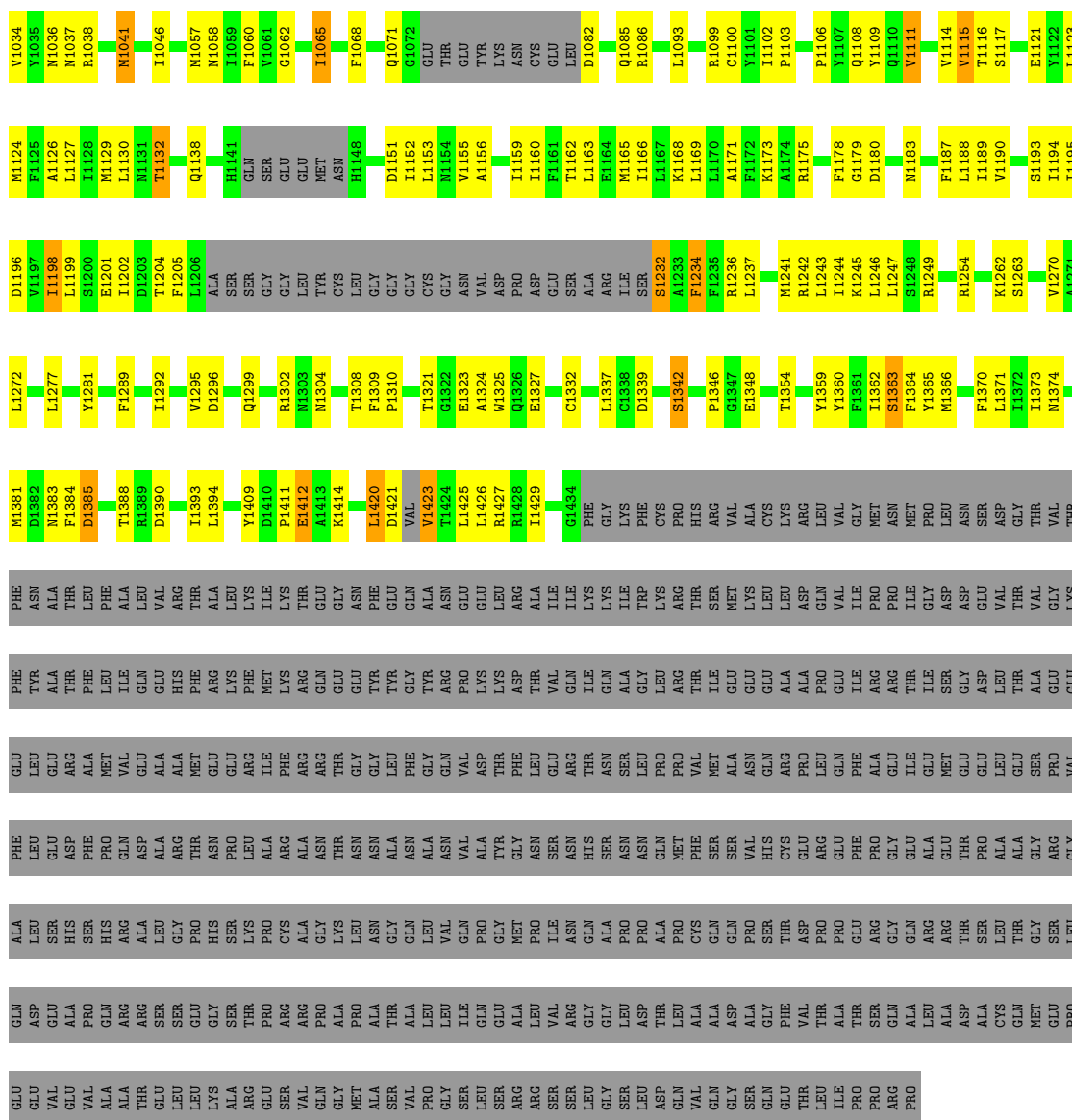
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	F	N	O	0
			25	16	3	2	4	

3 Residue-property plots

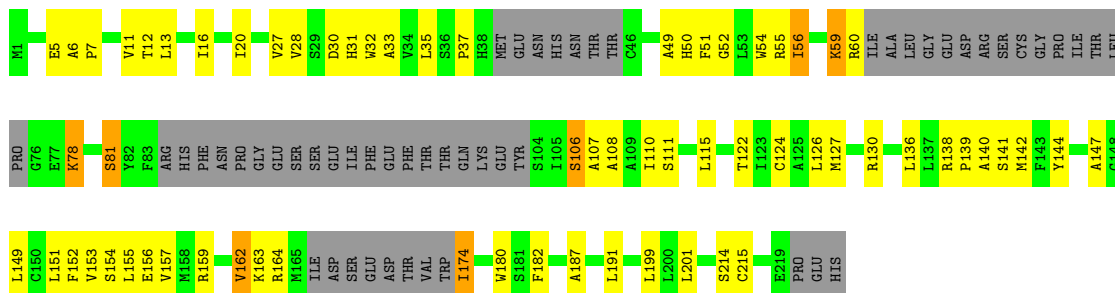
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: 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



ILE	N988	SER	THR	T715	Y629	S495	D365	A217	S91	MET
ILE	D989	ALA	SER	Q720	S630	T503	G366	Y226	E103	ALA
GLY	S990	TYR	ILE	N721	I638	T508	G367	E107	V107	GLY
GLN	K991	VAL	ARG	Y722	T641	L508	E368	K234	H111	ARG
PHE	S994	SER	ASP	W723	T642	Y513	E373	I235	Q112	PRO
VAL	G995	ILE	PRO	S724	T643	V523	I374	D236	W113	LEU
LEU	V996	ALA	CYS	K733	Q644	Y647	K380	L237	R114	ALA
LEU	L997	ASP	GLY	F736	T644	Q530	D381	V240	THR	TRP
TRP	D998	ILE	PRO	Y737	S648	Q531	V386	R243	LEU	LEU
LEU	C999	VAL	VAL	W738	E649	K532	P244	E121	THR	THR
VAL	I1005	GLN	CYS	T739	T650	F533	F389	V124	LEU	LEU
SER	F1006	ILE	D843	D740	L651	I534	R398	V125	TRP	GLN
GLY	H1007	GLY	R846	G741	F656	P539	Q402	A129	ALA	ALA
SER	V1008	TRP	N847	T744	E657	T540	C406	K254	TRP	TRP
ARG	V1009	THR	D857	T745	E658	I541	E407	D255	LEU	LEU
HIS	E1010	ALA	L863	R746	S659	R544	N408	D131	ILE	ILE
CYS	K1010	ALA	R867	Y747	F660	K545	K409	D132	LEU	LEU
LEU	L1011	ALA	D868	T748	Y661	R546	G410	L133	GLY	GLY
LEU	M1012	ALA	D869	K749	F663	R547	C410	D134	PRO	PRO
LEU	M1013	ALA	Y870	E750	F663	R547	G410	L135	SER	SER
LEU	M1014	ALA	T871	A751	D672	Q551	I423	K137	GLU	GLU
LEU	M1015	ALA	N872	G752	L673	Q556	M436	M281	PRO	PRO
LEU	T1016	TRP	Q873	S765	S676	L561	K442	D287	LEU	LEU
LEU	E1022	TRP	N874	F766	D677	D562	A443	D288	LEU	LEU
LEU	S1023	LEU	G875	S770	M678	F563	K444	D289	LEU	LEU
LEU	K1024	SER	R876	N773	T680	E567	Q445	S295	LEU	LEU
LEU	T1031	LEU	I881	N775	F686	D571	Q447	F296	LEU	LEU
LEU	R1032	THR	H888	N776	F687	I573	Y452	N297	LEU	LEU
LEU	D1042	PHE	L889	F783	F688	K573	L458	N299	LEU	LEU
LEU	D1048	GLY	I892	N784	F689	D691	V461	V303	LEU	LEU
LEU	D1060	ALA	S893	K785	I690	R591	T462	Q311	LEU	LEU
LEU	V1061	ALA	V894	E792	F692	L593	T463	L181	LEU	LEU
LEU	D1064	ASP	S900	S793	T694	S596	G464	N183	LEU	LEU
LEU	V1067	GLY	Y901	S798	F695	Q597	T465	E184	LEU	LEU
LEU	L1068	ASP	D902	T799	N696	K604	L466	V324	LEU	LEU
LEU	C1074	ASP	S905	I805	N697	G605	P467	I327	LEU	LEU
LEU	GLY	ASP	V906	T805	F698	M606	N470	T328	LEU	LEU
LEU	GLY	PHE	C907	V814	S699	T701	I471	A329	LEU	LEU
LEU	VAL	THR	E908	V815	T702	Y609	T472	K330	LEU	LEU
LEU	SER	ALA	P909	C816	D703	T610	T479	F195	LEU	LEU
LEU	SER	ALA	A912	T817	T704	W611	N480	K196	LEU	LEU
LEU	SER	ALA	PRO	V821	T705	T612	T481	K197	LEU	LEU
LEU	SER	ALA	LYS	V825	N706	T617	K482	L206	LEU	LEU
LEU	SER	ALA	GLY	E826	V708	L626	N483	S212	LEU	LEU
LEU	SER	ALA	ALA	T829	D711	P627	G491	L216	LEU	LEU
LEU	SER	ALA	GLY	K830						LEU
LEU	SER	ALA	ARG							LEU

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

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: PC1, CA, VFY, 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	0.55	0/9233	0.56	4/12534 (0.0%)
2	E	0.30	0/1358	0.54	2/1832 (0.1%)
3	F	0.70	0/7974	0.57	0/10816
All	All	0.60	0/18565	0.56	6/25182 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	81	SER	CA-C-N	6.28	132.21	121.29
2	E	81	SER	C-N-CA	6.28	132.21	121.29
1	A	661	VAL	N-CA-C	-6.16	107.85	113.71
1	A	541	TYR	CA-C-N	5.30	131.66	121.54
1	A	541	TYR	C-N-CA	5.30	131.66	121.54
1	A	522	LEU	N-CA-C	-5.27	105.62	111.36

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	322	0
2	E	1326	0	1345	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	7804	0	7617	181	0
4	A	1	0	0	0	0
5	A	364	0	524	87	0
6	A	54	0	88	20	0
7	A	25	0	0	5	0
All	All	18583	0	18719	603	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 (603) 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: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:1366:MET:HE3	5:A:1904:3PE:H2D1	1.39	1.03
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
1:A:1366:MET:HE3	5:A:1904:3PE:H2A1	1.41	0.97
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:501:CYS:C	1:A:505:CYS:HG	1.76	0.93
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:CG	1:A:537:LYS:HE3	1.98	0.89
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
5:A:1907:3PE:C2C	5:A:1907:3PE:H272	2.03	0.88
5:A:1906:3PE:O11	5:A:1906:3PE:N	2.08	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:693:LYS:HE3	3:F:698:PRO:HD2	1.58	0.85
1:A:502:PHE:C	1:A:505:CYS:SG	2.58	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
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:1129:MET:HE1	5:A:1903:3PE:H2C2	1.61	0.81
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
1:A:1366:MET:HE3	5:A:1904:3PE:C2A	2.09	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: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
1:A:500:ASP:CG	1:A:537:LYS:CE	2.59	0.76
1:A:1366:MET:HE2	5:A:1904:3PE:H2A1	1.65	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1178:PHE:O	2:E:138:ARG:NH1	2.22	0.72
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
1:A:206:MET:HG3	6:A:1909:PC1:H3F2	1.75	0.69
5:A:1906:3PE:HN1	5:A:1906:3PE:C1	2.05	0.69
1:A:1241:MET:HE1	6:A:1909:PC1:H3B2	1.74	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: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
2:E:139:PRO:HA	2:E:142:MET:HE2	1.79	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:711:ASP:OD1	3:F:739:THR:OG1	2.07	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1129:MET:HE1	5:A:1903:3PE:H2F2	1.80	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
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
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
3:F:1023:SER:OG	3:F:1024:LYS:N	2.30	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:1366:MET:CE	5:A:1904:3PE:H2D1	2.24	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:CYS:SG	1:A:246:ALA:N	2.76	0.59
1:A:501:CYS:C	1:A:505:CYS:SG	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:867:HIS:C	3:F:869:ASP:H	2.11	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
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
5:A:1906:3PE:N	5:A:1906:3PE:O22	2.39	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
5:A:1906:3PE:HN1	5:A:1906:3PE:P	2.29	0.55
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:1241:MET:HE1	6:A:1909:PC1:C3B	2.35	0.55
3:F:481:LEU:HG	3:F:482:LYS:N	2.21	0.55
2:E:31:HIS:HD1	2:E:180:TRP:CD1	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
3:F:64:TYR:O	3:F:66:ASP:N	2.43	0.52
1:A:1156:ALA:O	1:A:1160:ILE:HG13	2.10	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:1129:MET:HE1	5:A:1903:3PE:C2C	2.34	0.52
3:F:715:THR:HG21	3:F:745:ARG:HG3	1.92	0.52
3:F:1042:ASP:OD1	3:F:1042:ASP:N	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:LEU:HD21	1:A:133:GLY:C	2.37	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
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
3:F:64:TYR:C	3:F:66:ASP:H	2.20	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:516:SER:OG	1:A:517:GLY:N	2.44	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:537:LYS:HZ2	1:A:538:ILE:HA	1.78	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:715:THR:HG22	3:F:745:ARG:HH21	1.77	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
1:A:542:TRP:CD1	1:A:544:SER:HB3	2.49	0.47
3:F:750:GLU:H	3:F:750:GLU:CD	2.22	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
5:A:1906:3PE:N	5:A:1906:3PE:C1	2.73	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: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
3:F:1048:ASP:OD1	3:F:1048:ASP:N	2.47	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:676:SER:C	3:F:678:ASN:H	2.23	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
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
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
3:F:1031:THR:OG1	3:F:1032:ARG:N	2.47	0.45
1:A:519:MET:O	1:A:520:THR:OG1	2.28	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: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:155:ALA:C	3:F:157:PHE:H	2.24	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1129:MET:CE	5:A:1903:3PE:H2F2	2.45	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
1:A:238:GLU:HG2	1:A:239:ASN:N	2.31	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:867:HIS:C	3:F:869:ASP:N	2.75	0.44
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
3:F:36:TRP:CZ3	3:F:1020:MET:HE1	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:436:MET:HB3	3:F:436:MET:HE2	1.75	0.44
3:F:783:PHE:CE2	3:F:876:ARG:HD2	2.52	0.44
1:A:74:MET:HE3	1:A:74:MET:HB3	1.81	0.43
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:210:TYR:O	1:A:313:TYR:OH	2.35	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:544:ARG:C	3:F:545:LYS:HD3	2.43	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
2:E:59:LYS:HD2	2:E:59:LYS:HA	1.34	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
2:E:55:ARG:HB3	2:E:81:SER:C	2.44	0.43
1:A:903:ARG:N	1:A:904:PRO:HD2	2.33	0.43
1:A:1173:LYS:C	1:A:1175:ARG:H	2.26	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:281:MET:HE1	3:F:389:PHE:CZ	2.54	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:274:HIS:CD2	1:A:274:HIS:C	2.97	0.42
1:A:941:MET:HE2	1:A:941:MET:HB3	1.94	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
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
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
1:A:1165:MET:HB3	1:A:1165:MET:HE3	1.83	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1187:PHE:CD2	2:E:142:MET:HE1	2.55	0.42
1:A:1346:PRO:C	1:A:1348:GLU:H	2.28	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:161:VAL:N	1:A:164:LEU:HD23	2.36	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:29:SER:OG	3:F:30:ALA:N	2.51	0.41
3:F:642:ILE:H	3:F:642:ILE:HG12	1.73	0.41
3:F:785:LYS:HB2	3:F:785:LYS:HE2	1.87	0.41
1:A:500:ASP:CG	1:A:537:LYS:HD2	2.41	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
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
2:E:142:MET:HE3	2:E:142:MET:HB2	1.70	0.41
3:F:297:ASN:C	3:F:299:ASN:H	2.29	0.41
3:F:348:ASN:C	3:F:350:ASN:H	2.29	0.41
3:F:508:LEU:H	3:F:508:LEU:HG	1.73	0.41
1:A:282:MET:HE2	5:A:1903:3PE:H371	2.03	0.41
1:A:1245:LYS:C	1:A:1247:LEU:H	2.29	0.41
1:A:1364:PHE:O	1:A:1365:TYR:C	2.62	0.41
3:F:64:TYR:C	3:F:66:ASP:N	2.78	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:373:GLU:H	3:F:373:GLU:CD	2.28	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
1:A:1065:ILE:HG23	1:A:1381:MET:HE3	2.02	0.41
5:A:1907:3PE:O22	5:A:1907:3PE:H11	2.21	0.41
2:E:78:LYS:HZ3	2:E:78:LYS:HG3	1.74	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:773:ASN:OD1	3:F:773:ASN:N	2.51	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
3:F:1064:ASP:OD1	3:F:1064:ASP:N	2.51	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
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
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
3:F:1006:PHE:CD1	3:F:1006:PHE:C	2.99	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	79
2	E	159/222 (72%)	142 (89%)	17 (11%)	0	100	100
3	F	968/1105 (88%)	871 (90%)	96 (10%)	1 (0%)	48	79
All	All	2222/3200 (69%)	2006 (90%)	214 (10%)	2 (0%)	49	79

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%)	853 (87%)	128 (13%)	4	20
2	E	143/192 (74%)	128 (90%)	15 (10%)	6	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	868/973 (89%)	791 (91%)	77 (9%)	9	34
All	All	1992/2793 (71%)	1772 (89%)	220 (11%)	8	26

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	49	GLU
1	A	54	GLU
1	A	72	LEU
1	A	95	THR
1	A	100	GLU
1	A	112	PHE
1	A	132	LEU
1	A	140	GLU
1	A	143	ASN
1	A	144	VAL
1	A	175	LEU
1	A	176	VAL
1	A	179	VAL
1	A	184	VAL
1	A	189	ILE
1	A	194	LEU
1	A	201	LEU
1	A	247	ARG
1	A	250	SER
1	A	262	ARG
1	A	289	ILE
1	A	295	THR
1	A	330	LEU
1	A	332	VAL
1	A	339	LYS
1	A	434	PHE
1	A	439	ILE
1	A	446	THR
1	A	447	LEU
1	A	448	SER
1	A	449	ILE
1	A	451	SER
1	A	461	THR
1	A	468	ASN
1	A	494	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	497	ASN
1	A	505	CYS
1	A	510	GLU
1	A	511	LEU
1	A	512	LEU
1	A	515	GLU
1	A	524	ILE
1	A	527	LEU
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	545	LEU
1	A	552	LEU
1	A	553	LEU
1	A	571	ILE
1	A	592	VAL
1	A	609	GLN
1	A	619	VAL
1	A	636	LEU
1	A	657	LEU
1	A	666	GLU
1	A	668	GLU
1	A	802	THR
1	A	804	PHE
1	A	822	ILE
1	A	845	VAL
1	A	852	THR
1	A	872	ASP
1	A	874	LEU
1	A	876	VAL
1	A	892	VAL
1	A	899	LEU
1	A	902	LEU
1	A	923	VAL
1	A	925	ILE
1	A	933	LEU
1	A	935	THR
1	A	936	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	937	LEU
1	A	938	LEU
1	A	974	VAL
1	A	983	MET
1	A	991	ILE
1	A	999	ASN
1	A	1011	SER
1	A	1036	ASN
1	A	1041	MET
1	A	1065	ILE
1	A	1093	LEU
1	A	1100	CYS
1	A	1111	VAL
1	A	1114	VAL
1	A	1115	VAL
1	A	1117	SER
1	A	1123	LEU
1	A	1124	MET
1	A	1127	LEU
1	A	1132	THR
1	A	1153	LEU
1	A	1188	LEU
1	A	1193	SER
1	A	1198	ILE
1	A	1202	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	1246	LEU
1	A	1262	LYS
1	A	1270	VAL
1	A	1272	LEU
1	A	1289	PHE
1	A	1292	ILE
1	A	1295	VAL
1	A	1308	THR
1	A	1332	CYS
1	A	1337	LEU
1	A	1342	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1354	THR
1	A	1363	SER
1	A	1385	ASP
1	A	1412	GLU
1	A	1420	LEU
1	A	1421	ASP
1	A	1423	VAL
1	A	1427	ARG
2	E	5	GLU
2	E	11	VAL
2	E	12	THR
2	E	13	LEU
2	E	56	ILE
2	E	59	LYS
2	E	60	ARG
2	E	78	LYS
2	E	106	SER
2	E	162	VAL
2	E	164	ARG
2	E	174	ILE
2	E	201	LEU
2	E	214	SER
2	E	215	CYS
3	F	31	VAL
3	F	37	VAL
3	F	45	VAL
3	F	65	GLN
3	F	88	LYS
3	F	91	SER
3	F	112	GLN
3	F	125	VAL
3	F	132	ASP
3	F	139	ASP
3	F	212	SER
3	F	226	VAL
3	F	235	ILE
3	F	237	LEU
3	F	240	VAL
3	F	254	LYS
3	F	257	LEU
3	F	269	LEU
3	F	270	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	295	SER
3	F	314	VAL
3	F	324	VAL
3	F	327	ILE
3	F	328	THR
3	F	348	ASN
3	F	368	GLU
3	F	381	ASP
3	F	423	ILE
3	F	442	LYS
3	F	465	THR
3	F	472	THR
3	F	503	THR
3	F	508	LEU
3	F	523	VAL
3	F	532	LYS
3	F	571	ASP
3	F	596	SER
3	F	610	THR
3	F	612	THR
3	F	617	THR
3	F	630	SER
3	F	641	THR
3	F	642	ILE
3	F	649	GLU
3	F	651	LEU
3	F	672	ASP
3	F	673	LEU
3	F	678	ASN
3	F	680	THR
3	F	704	LEU
3	F	705	ILE
3	F	711	ASP
3	F	739	THR
3	F	770	SER
3	F	775	ASN
3	F	793	SER
3	F	798	SER
3	F	814	VAL
3	F	817	ILE
3	F	871	THR
3	F	874	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	881	ILE
3	F	894	VAL
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	997	LEU
3	F	999	CYS
3	F	1005	ILE
3	F	1008	VAL
3	F	1014	THR
3	F	1061	VAL
3	F	1067	VAL
3	F	1068	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	445	ASN
1	A	453	HIS
1	A	797	ASN
1	A	803	ASN
1	A	869	ASN
1	A	909	ASN
1	A	939	GLN
1	A	958	ASN
1	A	996	HIS
1	A	999	ASN
1	A	1058	ASN
1	A	1069	GLN
1	A	1084	ASN
1	A	1138	GLN
1	A	1183	ASN
1	A	1287	GLN
1	A	1374	ASN
1	A	1383	ASN
1	A	1398	HIS
1	A	1419	HIS
2	E	209	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	56	GLN
3	F	164	GLN
3	F	165	HIS
3	F	169	HIS
3	F	308	HIS
3	F	316	ASN
3	F	348	ASN
3	F	470	ASN
3	F	542	ASN
3	F	551	GLN
3	F	556	GLN
3	F	679	ASN
3	F	685	ASN
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
5	3PE	A	1905	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
5	3PE	A	1908	-	20,20,50	1.05	1 (5%)	22,23,55	1.00	1 (4%)
6	PC1	A	1909	-	53,53,53	0.94	2 (3%)	59,61,61	1.02	3 (5%)
5	3PE	A	1910	-	31,31,50	1.17	2 (6%)	34,36,55	1.17	2 (5%)
5	3PE	A	1902	-	32,32,50	1.15	2 (6%)	35,37,55	1.20	4 (11%)
5	3PE	A	1907	-	37,37,50	1.07	2 (5%)	40,42,55	1.11	3 (7%)
5	3PE	A	1911	-	50,50,50	0.92	2 (4%)	53,55,55	1.06	3 (5%)
5	3PE	A	1903	-	50,50,50	0.92	2 (4%)	53,55,55	1.07	3 (5%)
5	3PE	A	1904	-	42,42,50	1.00	2 (4%)	45,47,55	1.12	3 (6%)
7	VFY	A	1912	-	24,26,26	3.75	7 (29%)	32,39,39	2.63	8 (25%)
5	3PE	A	1906	-	43,43,50	1.00	2 (4%)	46,48,55	1.10	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	1905	-	-	29/54/54/54	-
5	3PE	A	1908	-	-	11/21/21/54	-
6	PC1	A	1909	-	-	35/57/57/57	-
5	3PE	A	1910	-	-	18/35/35/54	-
5	3PE	A	1902	-	-	12/36/36/54	-
5	3PE	A	1907	-	-	25/41/41/54	-
5	3PE	A	1911	-	-	25/54/54/54	-
5	3PE	A	1903	-	-	22/54/54/54	-
5	3PE	A	1904	-	-	25/46/46/54	-
7	VFY	A	1912	-	-	6/18/40/40	0/2/2/2
5	3PE	A	1906	-	-	31/47/47/54	-

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	A	1906	3PE	C11-O13-P-O12
5	A	1906	3PE	C12-C11-O13-P
5	A	1907	3PE	C1-O11-P-O12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
5	A	1911	3PE	C31-C32-C33-C34
5	A	1904	3PE	O32-C31-O31-C3
5	A	1910	3PE	O32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
6	A	1909	PC1	C29-C2A-C2B-C2C
5	A	1906	3PE	C31-C32-C33-C34
5	A	1911	3PE	C28-C29-C2A-C2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
5	A	1906	3PE	C29-C2A-C2B-C2C
5	A	1906	3PE	O21-C2-C3-O31
5	A	1911	3PE	C39-C3A-C3B-C3C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
6	A	1909	PC1	C3F-C3G-C3H-C3I
5	A	1902	3PE	O11-C1-C2-C3
5	A	1903	3PE	C28-C29-C2A-C2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
5	A	1906	3PE	C33-C34-C35-C36
5	A	1910	3PE	C2-C1-O11-P
6	A	1909	PC1	O21-C21-C22-C23

Continued on next page...

Continued from previous page...

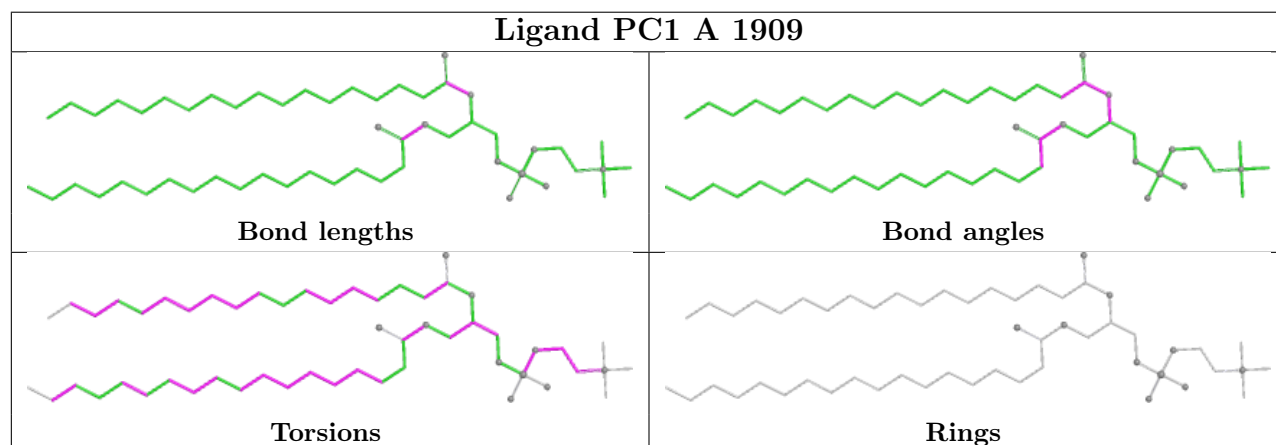
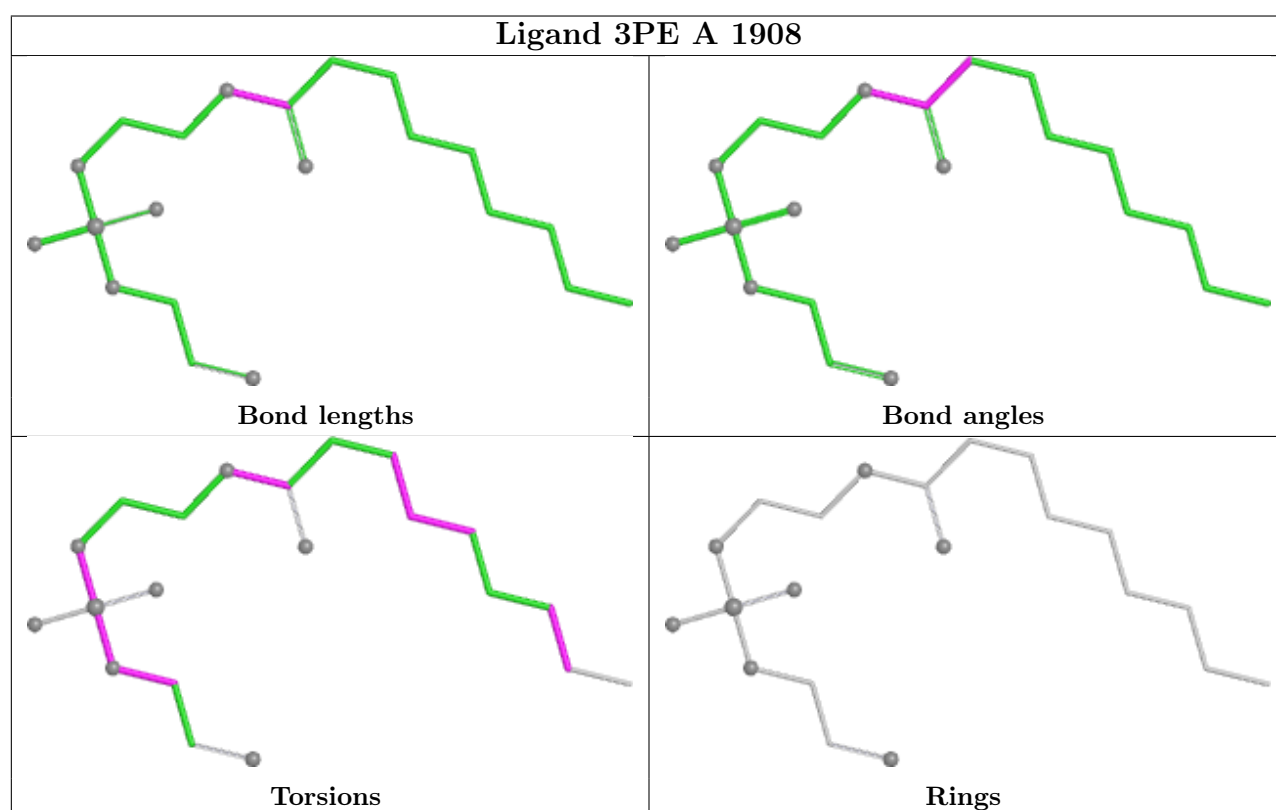
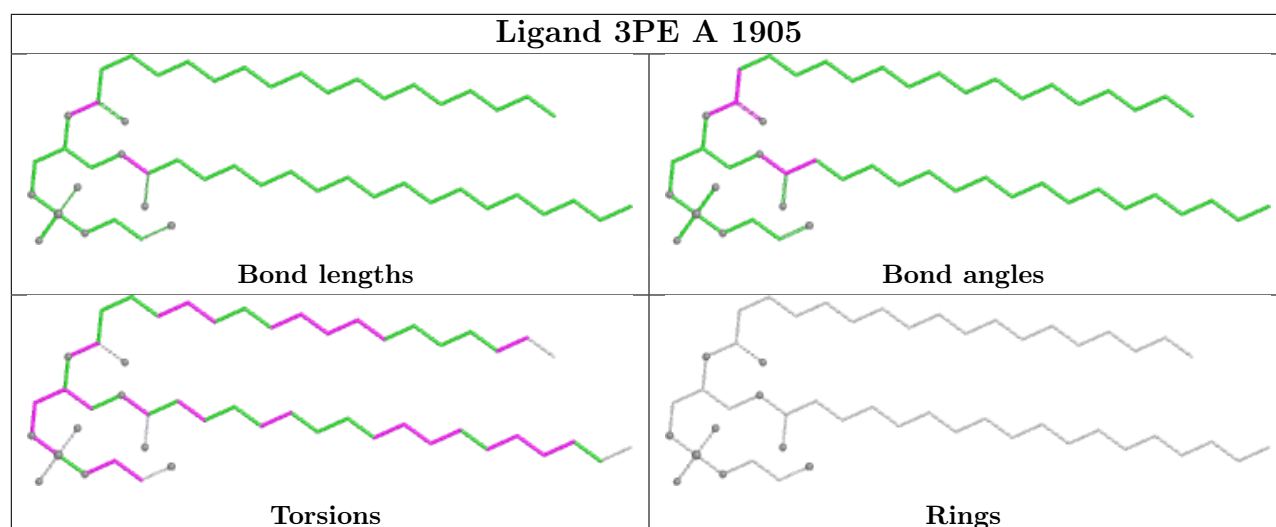
Mol	Chain	Res	Type	Atoms
5	A	1906	3PE	C23-C24-C25-C26
5	A	1906	3PE	C2D-C2E-C2F-C2G
5	A	1910	3PE	C32-C33-C34-C35
5	A	1911	3PE	C2B-C2C-C2D-C2E
5	A	1910	3PE	O31-C31-C32-C33
5	A	1911	3PE	O11-C1-C2-C3
5	A	1906	3PE	C1-C2-O21-C21
6	A	1909	PC1	C3C-C3D-C3E-C3F
6	A	1909	PC1	C35-C36-C37-C38
6	A	1909	PC1	O22-C21-C22-C23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

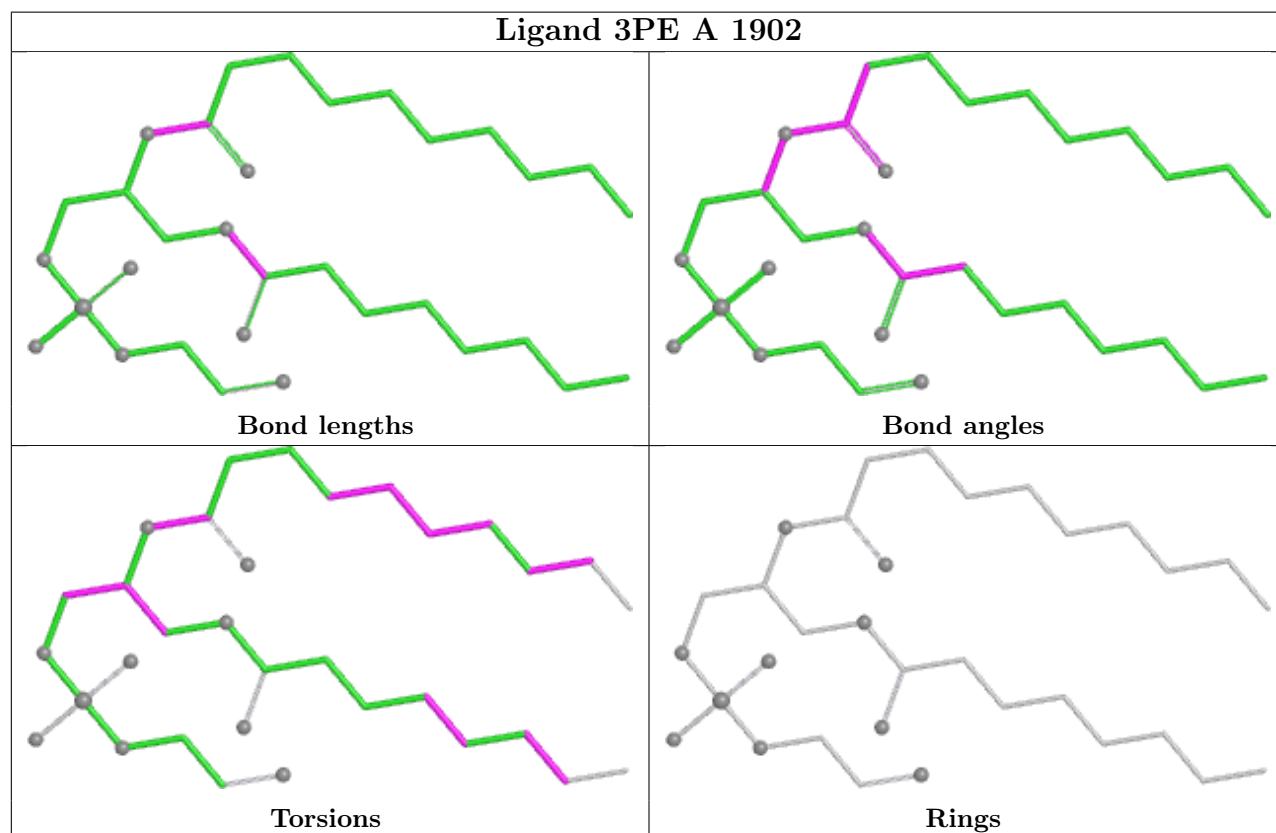
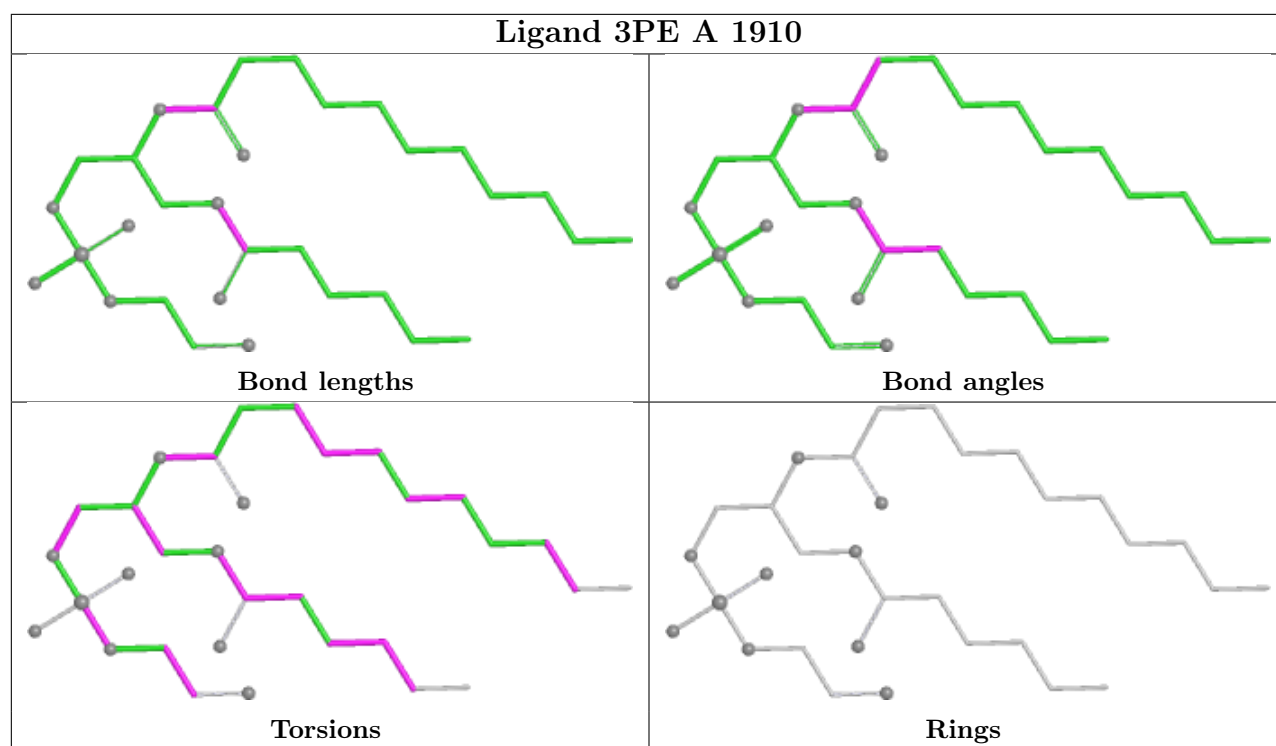
There are no ring outliers.

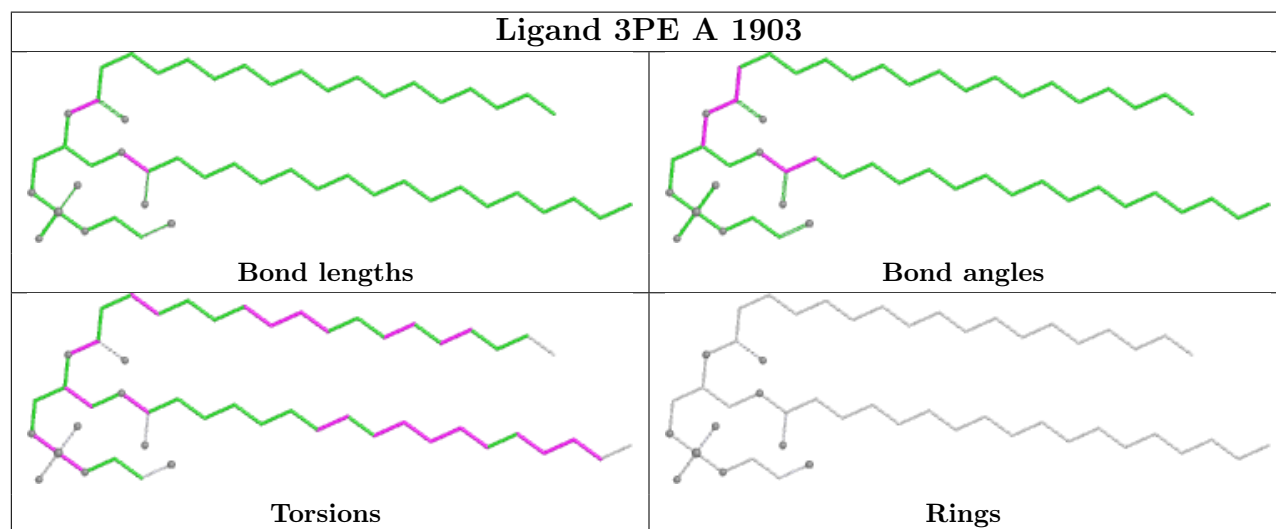
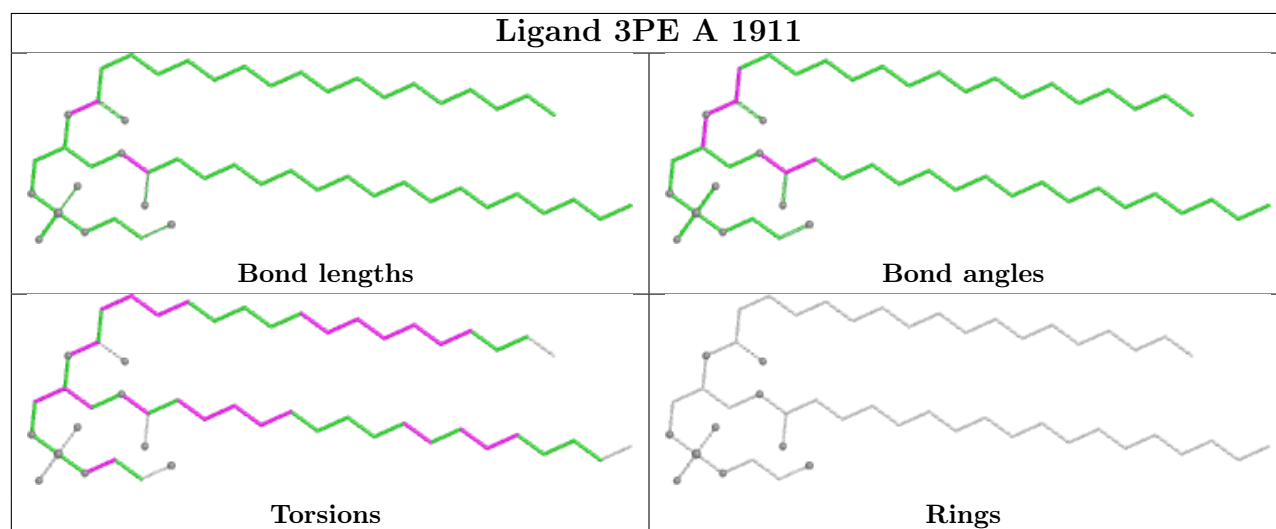
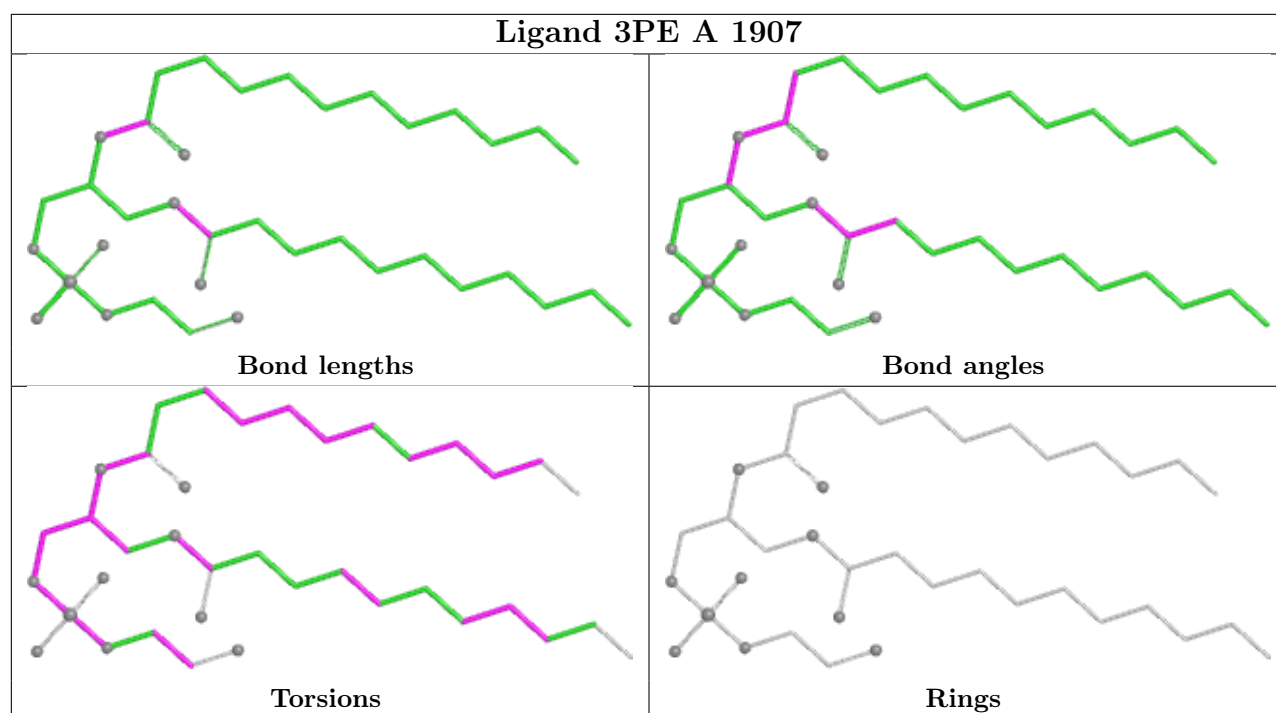
11 monomers are involved in 110 short contacts:

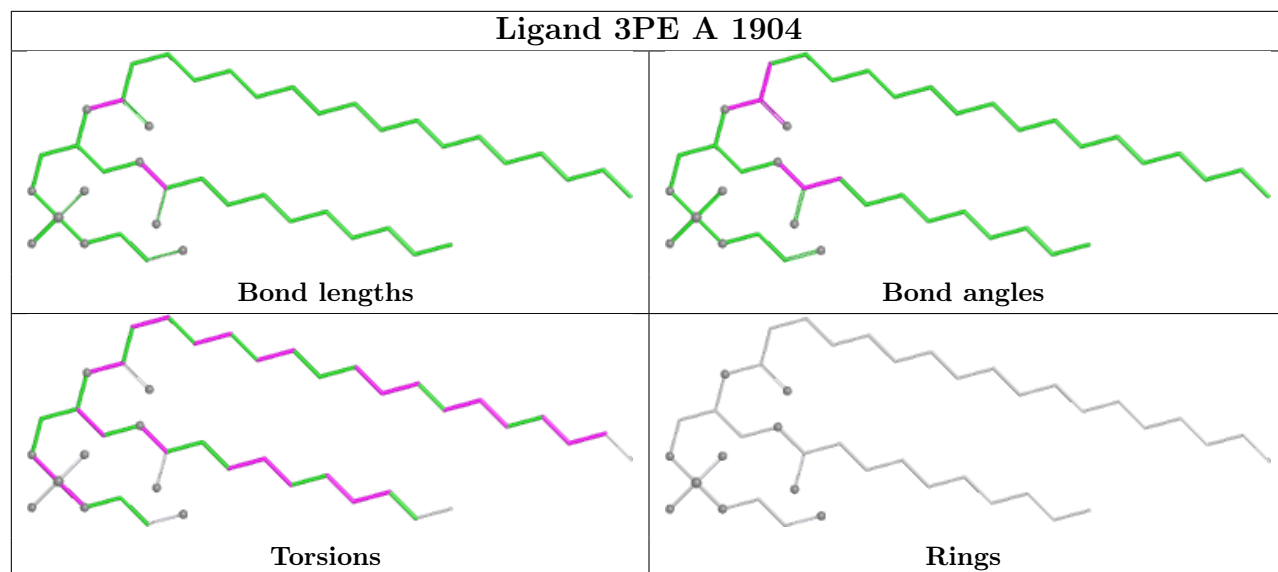
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1905	3PE	9	0
5	A	1908	3PE	10	0
6	A	1909	PC1	20	0
5	A	1910	3PE	4	0
5	A	1902	3PE	2	0
5	A	1907	3PE	11	0
5	A	1911	3PE	15	0
5	A	1903	3PE	12	0
5	A	1904	3PE	14	0
7	A	1912	VFY	5	0
5	A	1906	3PE	12	0

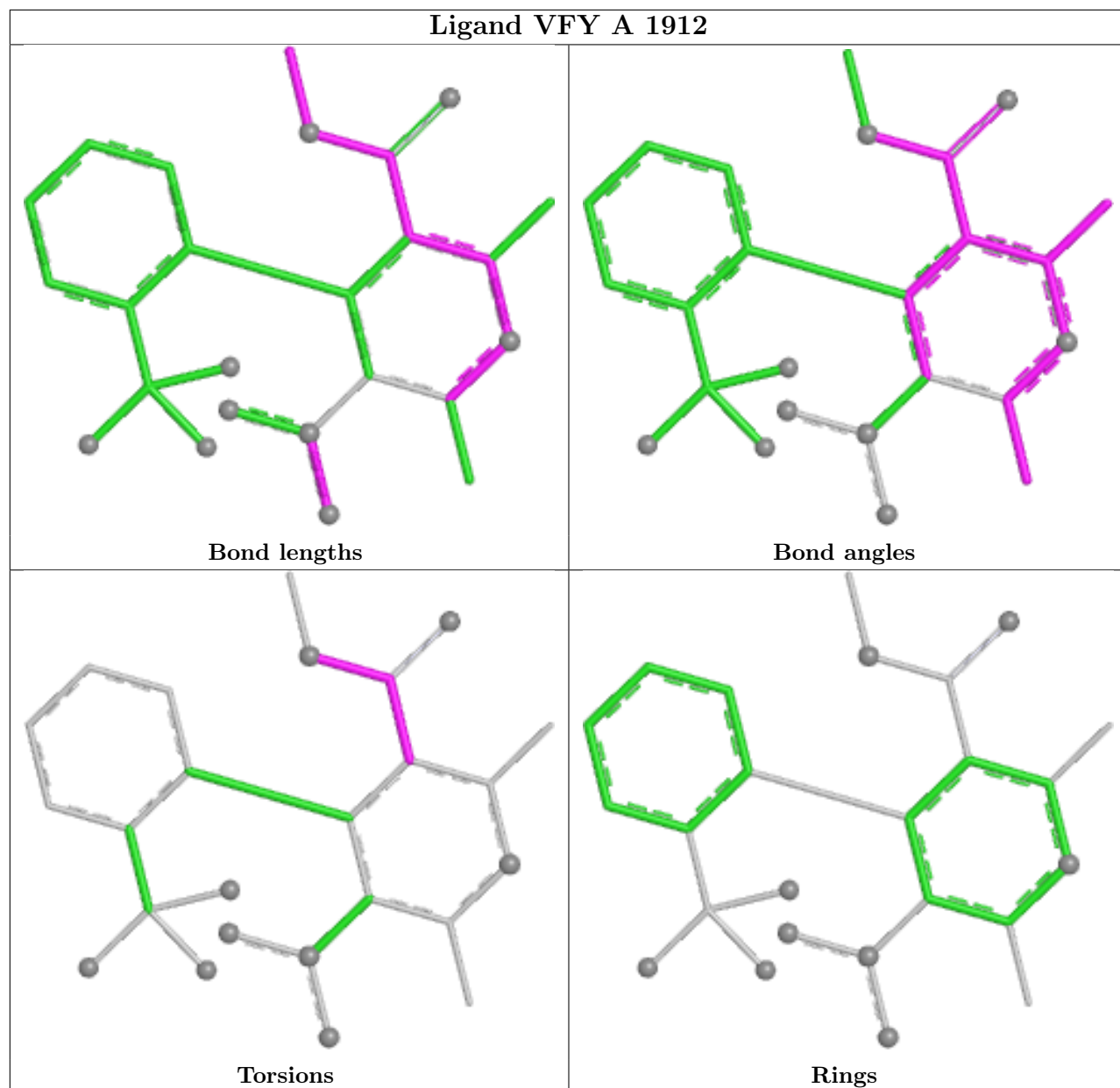
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

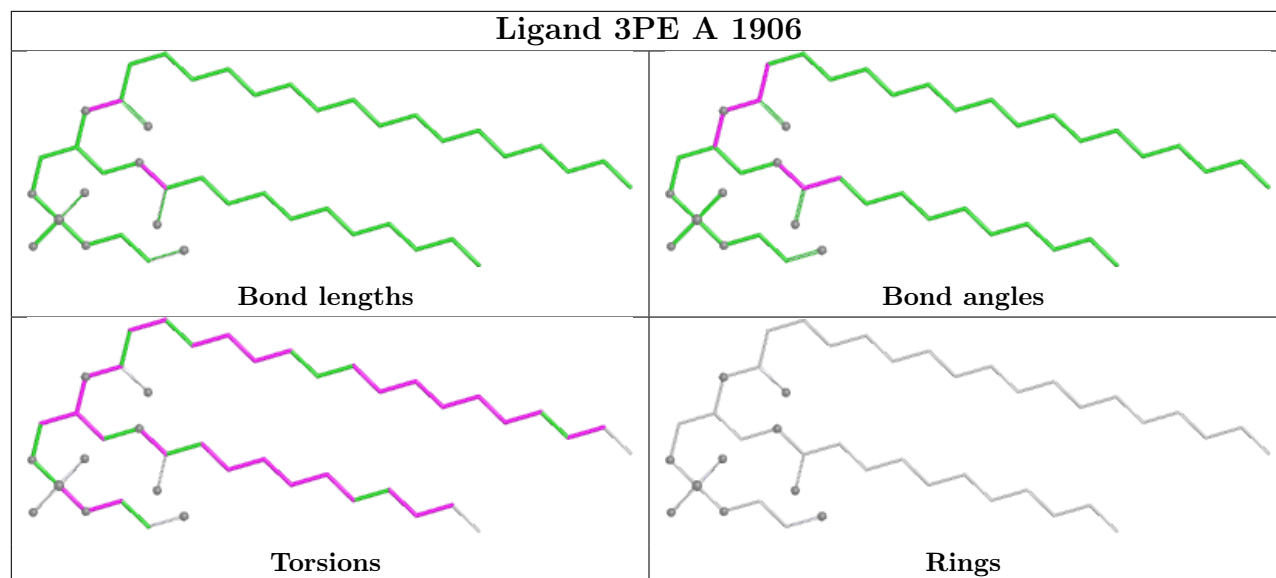












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.