



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:35 PM UTC

PDB ID : 5SUQ / pdb_00005suq
Title : Crystal structure of the THO-Sub2 complex
Authors : Ren, Y.; Blobel, G.
Deposited on : 2016-08-03
Resolution : 6.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

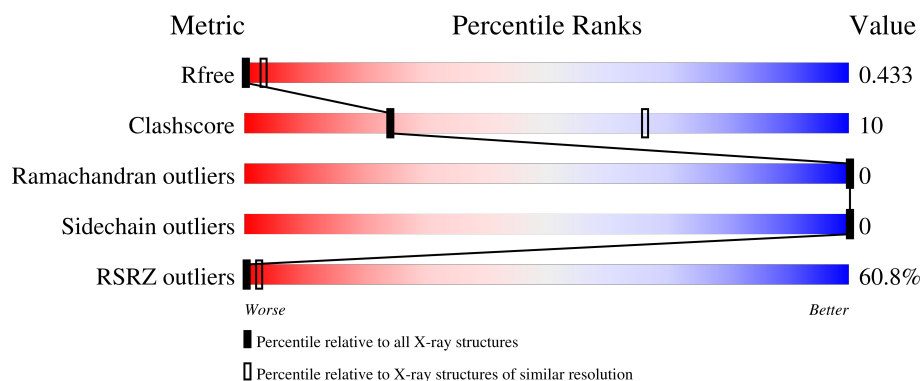
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	446	53% 65% 18% 16%
1	C	446	49% 64% 19% 16%
2	B	400	44% 53%
2	D	400	44% 53%
3	M	2300	93%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	N	2300	 93%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	KEG	A	501	-	-	X	-
4	KEG	A	503	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30788 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP-dependent RNA helicase SUB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			3010	1916	523	560	11			
1	C	374	Total	C	N	O	S	0	0	0
			3010	1916	523	560	11			

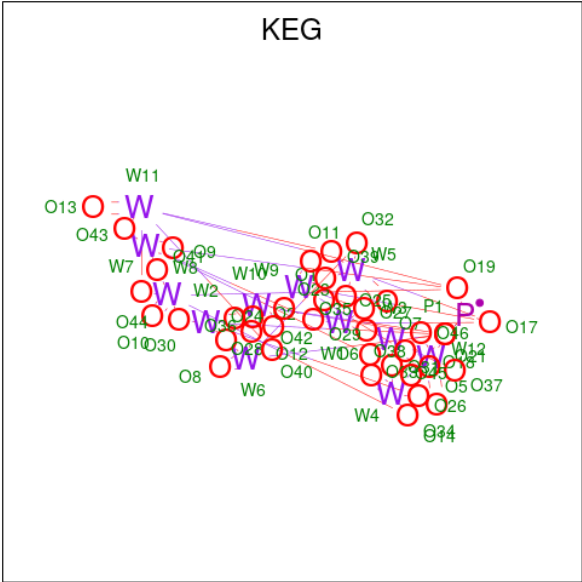
- Molecule 2 is a protein called Tex1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	0	0	0
			940	564	188	188			
2	D	188	Total	C	N	O	0	0	0
			940	564	188	188			

- Molecule 3 is a protein called Tho2, Hpr1, Mft1, and Thp2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	2231	Total	C	N	O	0	0	0
			11155	6693	2231	2231			
3	N	2230	Total	C	N	O	0	0	0
			11150	6690	2230	2230			

- Molecule 4 is 12-TUNGSTOPHOSPHATE (CCD ID: KEG) (formula: O₄₀PW₁₂).

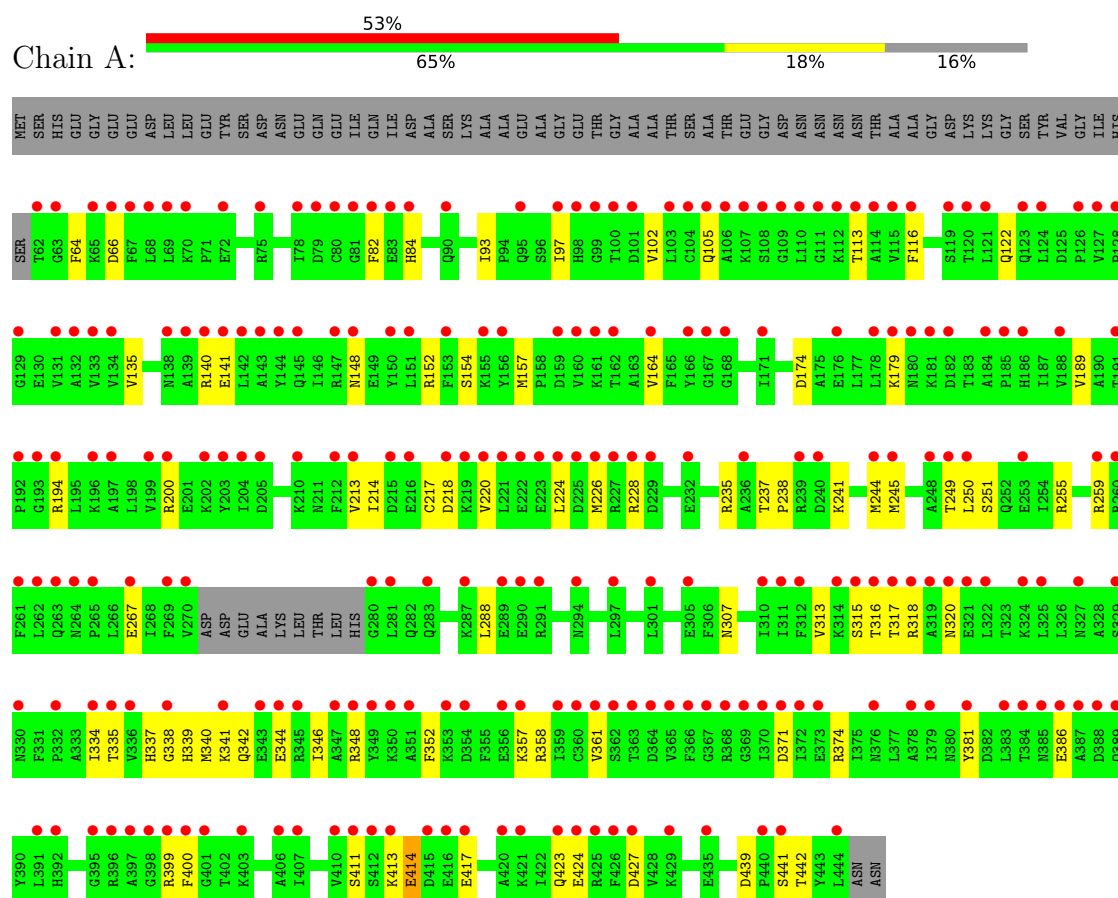


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P W 53 40 1 12	0	0
4	A	1	Total O P W 53 40 1 12	0	0
4	A	1	Total O P W 53 40 1 12	0	0
4	M	1	Total O P W 53 40 1 12	0	0
4	M	1	Total O P W 53 40 1 12	0	0
4	M	1	Total O P W 53 40 1 12	0	0
4	N	1	Total O P W 53 40 1 12	0	0
4	N	1	Total O P W 53 40 1 12	0	0
4	N	1	Total O P W 53 40 1 12	0	0
4	N	1	Total O P W 53 40 1 12	0	0
4	N	1	Total O P W 53 40 1 12	0	0

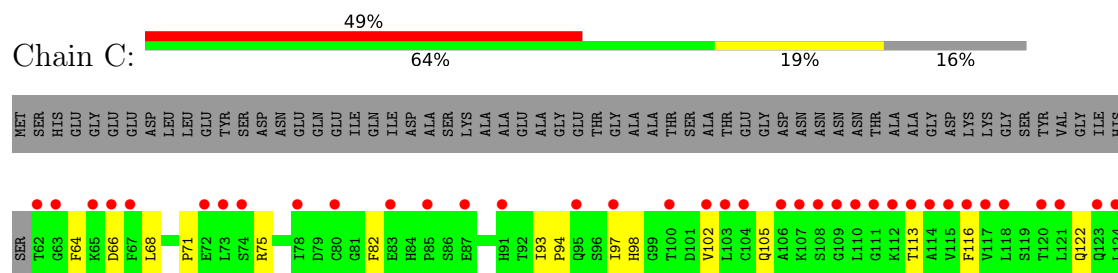
3 Residue-property plots

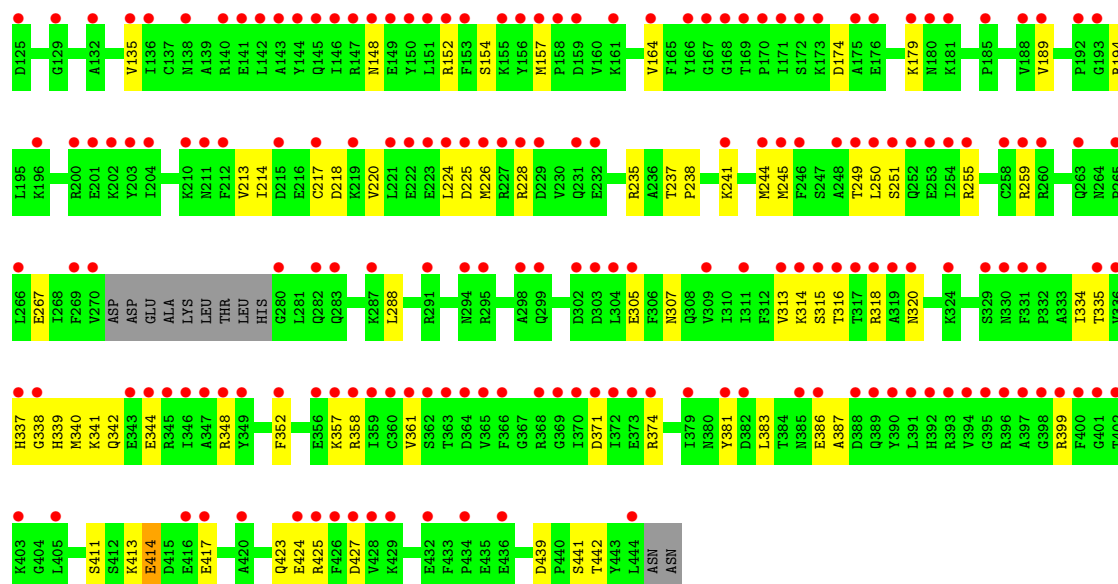
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: ATP-dependent RNA helicase SUB2



• Molecule 1: ATP-dependent RNA helicase SUB2





• Molecule 2: Tex1

Chain B:  44% 53%

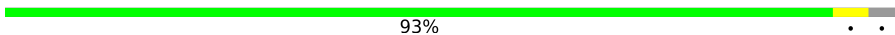


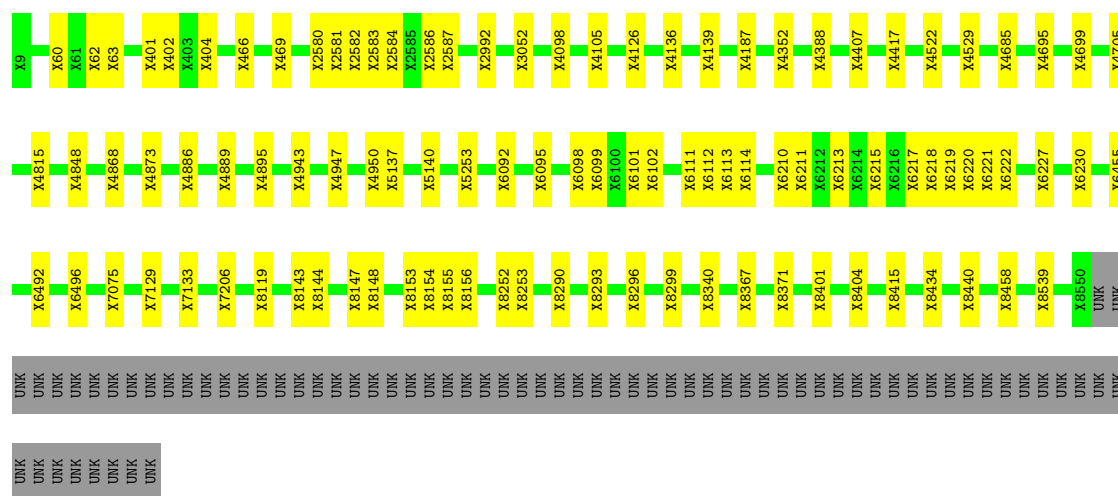
• Molecule 2: Tex1

Chain D:  44% 53%



• Molecule 3: Tho2, Hpr1, Mft1, and Thp2

Chain M:  93%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	153.34Å 319.53Å 176.44Å 90.00° 100.96° 90.00°	Depositor
Resolution (Å)	49.57 – 6.00 49.57 – 6.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.57-6.00) 98.4 (49.57-6.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 6.15Å)	Xtriage
Refinement program	PHENIX (1.10_2155)	Depositor
R, R_{free}	0.436 , 0.434 0.436 , 0.433	Depositor DCC
R_{free} test set	2100 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	293.8	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 385.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	30788	wwPDB-VP
Average B, all atoms (Å ²)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KEG

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	0.30	0/3063	0.62	10/4131 (0.2%)
1	C	0.30	0/3063	0.62	10/4131 (0.2%)
All	All	0.30	0/6126	0.62	20/8262 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	427	ASP	CB-CA-C	-8.79	92.94	110.42
1	A	427	ASP	CB-CA-C	-8.75	93.00	110.42
1	A	424	GLU	CB-CG-CD	7.60	125.52	112.60
1	C	424	GLU	CB-CG-CD	7.59	125.51	112.60
1	C	427	ASP	N-CA-CB	6.53	121.53	110.49
1	A	427	ASP	N-CA-CB	6.50	121.47	110.49
1	C	414	GLU	CB-CA-C	-6.36	97.02	110.31
1	A	414	GLU	CB-CA-C	-6.33	97.07	110.31
1	C	417	GLU	CA-CB-CG	6.10	126.31	114.10
1	A	417	GLU	CA-CB-CG	6.10	126.30	114.10
1	A	417	GLU	CG-CD-OE2	5.79	131.72	118.40
1	C	417	GLU	CG-CD-OE2	5.77	131.68	118.40
1	A	424	GLU	CG-CD-OE1	5.57	131.22	118.40
1	C	424	GLU	CG-CD-OE1	5.56	131.18	118.40
1	C	423	GLN	CA-C-N	-5.08	113.07	120.29
1	C	423	GLN	C-N-CA	-5.08	113.07	120.29
1	A	423	GLN	CA-C-N	-5.08	113.07	120.29
1	A	423	GLN	C-N-CA	-5.08	113.07	120.29
1	A	414	GLU	N-CA-CB	5.06	118.79	110.39
1	C	414	GLU	N-CA-CB	5.01	118.70	110.39

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	3010	0	3043	162	0
1	C	3010	0	3043	159	0
2	B	940	0	262	6	0
2	D	940	0	262	5	0
3	M	11155	0	2489	100	0
3	N	11150	0	2488	103	0
4	A	159	0	0	35	0
4	M	159	0	0	0	0
4	N	265	0	0	0	0
All	All	30788	0	11587	425	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 10.

All (425) 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:339:HIS:CB	1:C:341:LYS:CA	1.85	1.53
1:A:339:HIS:CB	1:C:341:LYS:HA	1.36	1.51
1:A:316:THR:C	1:C:341:LYS:HZ2	1.14	1.48
1:A:316:THR:C	1:C:341:LYS:NZ	1.70	1.46
1:C:98:HIS:CG	3:N:4695:UNK:CB	1.99	1.45
3:N:4815:UNK:CB	3:N:4873:UNK:CB	2.03	1.36
1:A:339:HIS:HB3	1:C:341:LYS:CA	1.43	1.36
3:M:4815:UNK:CB	3:M:4873:UNK:CB	2.02	1.34
4:A:501:KEG:O45	1:C:341:LYS:HG2	1.19	1.32
1:C:98:HIS:ND1	3:N:4695:UNK:CB	1.85	1.31
3:M:401:UNK:O	3:M:404:UNK:CB	1.83	1.27
3:N:401:UNK:O	3:N:404:UNK:CB	1.83	1.25
3:M:4098:UNK:CB	3:M:4126:UNK:HA	1.69	1.23
3:N:4098:UNK:CB	3:N:4126:UNK:HA	1.69	1.23
3:M:466:UNK:HA	3:M:5253:UNK:CB	1.69	1.23

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503:KEG:O10	1:C:314:LYS:O	1.54	1.22
1:A:200:ARG:NH1	4:A:502:KEG:O2	1.72	1.21
1:A:141:GLU:OE2	1:A:342:GLN:HG2	1.42	1.20
4:A:501:KEG:O5	1:C:344:GLU:HG2	1.42	1.20
2:D:277:UNK:CB	2:D:304:UNK:O	1.90	1.20
1:A:340:MET:HA	4:A:501:KEG:O35	1.27	1.19
2:B:277:UNK:CB	2:B:304:UNK:O	1.90	1.18
1:A:340:MET:O	1:C:339:HIS:HA	1.40	1.17
1:A:339:HIS:CG	1:C:341:LYS:CA	1.92	1.17
1:C:71:PRO:HG2	3:N:4895:UNK:O	1.43	1.16
4:A:501:KEG:O27	1:C:341:LYS:N	1.70	1.16
1:A:339:HIS:CB	1:C:341:LYS:N	1.86	1.16
4:A:502:KEG:O5	1:C:387:ALA:HB3	1.44	1.16
1:A:141:GLU:HG2	1:A:342:GLN:HE21	1.11	1.13
1:A:339:HIS:HB3	1:C:341:LYS:N	1.01	1.11
1:A:342:GLN:HB2	1:C:339:HIS:CE1	1.85	1.10
4:A:501:KEG:O5	1:C:344:GLU:CG	2.00	1.10
4:A:503:KEG:O10	1:C:315:SER:CA	2.00	1.10
1:A:339:HIS:HB2	1:C:341:LYS:HA	1.28	1.09
1:A:342:GLN:CB	1:C:339:HIS:CE1	2.36	1.09
3:M:6098:UNK:O	3:M:6101:UNK:CB	2.02	1.08
3:N:6098:UNK:O	3:N:6101:UNK:CB	2.02	1.08
3:N:4886:UNK:HA	3:N:4950:UNK:C	1.84	1.07
1:A:340:MET:CA	4:A:501:KEG:O35	2.01	1.07
4:A:501:KEG:O45	1:C:341:LYS:CG	2.01	1.07
3:M:4886:UNK:HA	3:M:4950:UNK:C	1.84	1.07
3:N:2992:UNK:O	3:N:3052:UNK:O	1.72	1.06
1:C:413:LYS:HD2	1:C:414:GLU:H	1.19	1.06
1:A:339:HIS:CG	1:C:341:LYS:HA	1.70	1.06
3:M:2992:UNK:O	3:M:3052:UNK:O	1.72	1.05
3:N:4886:UNK:CB	3:N:4950:UNK:O	2.05	1.05
1:A:413:LYS:HD2	1:A:414:GLU:H	1.19	1.04
1:A:358:ARG:NH1	3:M:4353:UNK:HA	1.73	1.04
1:A:340:MET:C	1:C:339:HIS:HA	1.83	1.03
3:M:4886:UNK:CB	3:M:4950:UNK:O	2.05	1.03
1:C:98:HIS:CD2	3:N:4695:UNK:CB	2.41	1.03
3:N:6219:UNK:O	3:N:6222:UNK:N	1.93	1.02
1:A:358:ARG:NH1	3:M:4353:UNK:CA	2.21	1.01
1:A:141:GLU:CG	1:A:342:GLN:HE21	1.73	1.01
3:M:6219:UNK:O	3:M:6222:UNK:N	1.93	1.01
4:A:503:KEG:O10	1:C:315:SER:HA	1.55	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:8143:UNK:O	3:N:8147:UNK:N	1.94	1.00
3:M:8143:UNK:O	3:M:8147:UNK:N	1.94	0.99
1:A:342:GLN:HB2	1:C:339:HIS:HE1	1.23	0.98
3:N:7129:UNK:O	3:N:7133:UNK:N	1.98	0.96
1:A:339:HIS:O	1:C:340:MET:CA	2.13	0.96
1:C:75:ARG:HH12	3:N:4943:UNK:CB	1.79	0.95
1:A:340:MET:C	1:C:339:HIS:CA	2.39	0.94
3:M:7129:UNK:O	3:M:7133:UNK:N	1.98	0.94
3:M:4388:UNK:CB	3:M:4417:UNK:CB	2.46	0.94
3:N:4388:UNK:CB	3:N:4417:UNK:CB	2.46	0.93
1:A:339:HIS:C	1:C:340:MET:N	2.27	0.93
3:M:466:UNK:CA	3:M:5253:UNK:CB	2.47	0.93
1:A:358:ARG:HH11	3:M:4353:UNK:CA	1.82	0.93
3:N:4886:UNK:CA	3:N:4950:UNK:C	2.46	0.93
1:A:374:ARG:NE	3:M:4431:UNK:H2	1.67	0.92
3:M:4886:UNK:CA	3:M:4950:UNK:C	2.46	0.92
1:A:317:THR:N	1:C:341:LYS:NZ	2.17	0.92
1:A:341:LYS:N	1:C:339:HIS:HB3	1.85	0.91
3:N:466:UNK:HA	3:N:5253:UNK:CB	2.01	0.91
3:M:8153:UNK:O	3:M:8156:UNK:CB	2.19	0.90
4:A:503:KEG:O10	1:C:315:SER:CB	2.20	0.90
1:A:337:HIS:CE1	1:C:341:LYS:HD3	2.06	0.90
1:A:339:HIS:O	1:C:340:MET:HA	1.72	0.90
3:N:8153:UNK:O	3:N:8156:UNK:CB	2.19	0.90
1:A:141:GLU:CD	1:A:342:GLN:HG2	1.96	0.89
3:M:2583:UNK:O	3:M:2587:UNK:N	2.07	0.88
3:M:4105:UNK:C	3:M:4187:UNK:O	2.22	0.88
3:N:2583:UNK:O	3:N:2587:UNK:N	2.07	0.87
3:N:4105:UNK:C	3:N:4187:UNK:O	2.22	0.87
3:M:401:UNK:O	3:M:404:UNK:N	2.07	0.87
1:C:413:LYS:HD2	1:C:414:GLU:N	1.91	0.86
1:A:316:THR:CB	1:C:341:LYS:NZ	2.37	0.86
1:A:316:THR:HB	1:C:341:LYS:CE	2.06	0.85
1:A:340:MET:O	1:C:339:HIS:CA	2.24	0.85
2:B:253:UNK:O	2:B:254:UNK:CB	2.25	0.85
3:N:401:UNK:O	3:N:404:UNK:N	2.08	0.85
1:A:337:HIS:HE1	4:A:501:KEG:O11	1.59	0.84
1:A:235:ARG:HH12	3:M:6215:UNK:CB	1.89	0.84
3:M:4889:UNK:CB	3:M:4950:UNK:CB	2.54	0.84
3:N:4889:UNK:CB	3:N:4950:UNK:CB	2.55	0.84
1:A:141:GLU:OE2	1:A:342:GLN:CG	2.23	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:UNK:O	2:D:254:UNK:CB	2.25	0.84
1:A:140:ARG:HD2	4:A:503:KEG:O36	1.76	0.84
1:A:337:HIS:CE1	4:A:501:KEG:O11	2.31	0.83
1:A:413:LYS:HD2	1:A:414:GLU:N	1.91	0.83
4:A:503:KEG:O10	1:C:314:LYS:C	2.20	0.83
1:A:339:HIS:HE1	1:C:342:GLN:OE1	1.61	0.82
3:N:4886:UNK:HA	3:N:4950:UNK:CB	2.09	0.82
3:M:8415:UNK:CB	3:M:8440:UNK:CB	2.57	0.82
3:M:4886:UNK:HA	3:M:4950:UNK:CB	2.10	0.81
3:M:6210:UNK:O	3:M:6213:UNK:N	2.13	0.81
3:N:8415:UNK:CB	3:N:8440:UNK:CB	2.57	0.81
3:M:4522:UNK:CB	3:M:4529:UNK:N	2.43	0.81
3:N:4522:UNK:CB	3:N:4529:UNK:N	2.43	0.81
4:A:501:KEG:O11	1:C:341:LYS:HD3	1.81	0.81
3:M:4886:UNK:CA	3:M:4950:UNK:O	2.29	0.81
3:M:6111:UNK:O	3:M:6114:UNK:HA	1.81	0.80
3:N:6210:UNK:O	3:N:6213:UNK:N	2.13	0.80
1:A:374:ARG:HE	3:M:4431:UNK:H2	1.29	0.80
3:N:6111:UNK:O	3:N:6114:UNK:HA	1.82	0.79
4:A:501:KEG:O5	1:C:344:GLU:CD	2.24	0.79
3:N:8252:UNK:O	3:N:8253:UNK:C	2.30	0.79
1:A:339:HIS:C	1:C:339:HIS:C	2.49	0.79
3:N:2580:UNK:O	3:N:2584:UNK:N	2.16	0.79
1:A:84:HIS:HB2	1:A:400:PHE:HZ	1.47	0.78
3:M:8252:UNK:O	3:M:8253:UNK:C	2.31	0.78
3:N:4886:UNK:CA	3:N:4950:UNK:O	2.28	0.78
1:A:316:THR:CA	1:C:341:LYS:NZ	2.47	0.78
3:N:4889:UNK:CB	3:N:4947:UNK:HA	2.14	0.78
4:A:501:KEG:O1	1:C:341:LYS:N	2.15	0.78
3:M:4889:UNK:CB	3:M:4947:UNK:HA	2.14	0.78
1:A:339:HIS:C	1:C:340:MET:CA	2.53	0.78
3:M:2580:UNK:O	3:M:2584:UNK:N	2.16	0.78
1:C:358:ARG:NH1	3:N:4352:UNK:O	2.16	0.77
1:A:200:ARG:NH1	4:A:502:KEG:O30	2.18	0.76
1:A:341:LYS:N	1:C:339:HIS:CB	2.43	0.76
1:A:141:GLU:HG2	1:A:342:GLN:NE2	1.96	0.76
1:A:339:HIS:O	1:C:340:MET:C	2.29	0.76
1:A:340:MET:C	1:C:339:HIS:CB	2.59	0.75
3:M:4886:UNK:CB	3:M:4950:UNK:C	2.64	0.75
3:N:4098:UNK:CB	3:N:4126:UNK:CA	2.59	0.75
3:N:4886:UNK:CB	3:N:4950:UNK:C	2.64	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:HIS:CE1	1:C:342:GLN:OE1	2.39	0.75
3:N:4522:UNK:CB	3:N:4529:UNK:H2	2.00	0.75
3:M:4522:UNK:CB	3:M:4529:UNK:H2	2.00	0.75
3:N:401:UNK:O	3:N:404:UNK:CA	2.35	0.75
1:A:316:THR:HB	1:C:341:LYS:NZ	2.02	0.74
3:M:401:UNK:O	3:M:404:UNK:CA	2.35	0.74
3:M:466:UNK:CB	3:M:5253:UNK:CB	2.66	0.74
3:N:8144:UNK:HA	3:N:8147:UNK:CB	2.18	0.74
3:M:8144:UNK:HA	3:M:8147:UNK:CB	2.18	0.74
3:N:62:UNK:O	3:N:63:UNK:C	2.34	0.74
1:A:358:ARG:HH12	3:M:4353:UNK:HA	1.49	0.74
3:M:62:UNK:O	3:M:63:UNK:C	2.34	0.74
3:M:2582:UNK:O	3:M:2586:UNK:N	2.21	0.73
1:C:71:PRO:HG2	3:N:4895:UNK:C	2.18	0.73
1:A:340:MET:O	1:C:339:HIS:CG	2.42	0.72
3:N:6219:UNK:O	3:N:6220:UNK:C	2.36	0.72
1:A:141:GLU:CD	1:A:342:GLN:CG	2.63	0.72
1:A:337:HIS:CE1	1:C:341:LYS:HE2	2.24	0.72
3:N:2582:UNK:O	3:N:2586:UNK:N	2.21	0.72
3:N:6219:UNK:C	3:N:6221:UNK:N	2.51	0.71
3:M:4098:UNK:CB	3:M:4126:UNK:CA	2.59	0.71
1:C:66:ASP:OD1	3:N:4705:UNK:CB	2.38	0.71
1:A:84:HIS:HB2	1:A:400:PHE:CZ	2.26	0.71
1:A:339:HIS:CG	1:C:341:LYS:N	2.43	0.71
3:M:6219:UNK:O	3:M:6220:UNK:C	2.36	0.71
1:A:337:HIS:HE1	1:C:341:LYS:HD3	1.53	0.70
4:A:502:KEG:O5	1:C:387:ALA:CB	2.33	0.70
1:A:340:MET:N	1:C:339:HIS:C	2.50	0.69
4:A:503:KEG:O41	1:C:314:LYS:O	2.10	0.69
3:N:8340:UNK:CB	3:N:8539:UNK:HA	2.22	0.69
1:A:316:THR:O	1:C:341:LYS:NZ	1.92	0.69
3:M:8340:UNK:CB	3:M:8539:UNK:HA	2.22	0.68
1:A:374:ARG:CZ	3:M:4431:UNK:H2	2.05	0.68
1:C:94:PRO:HB3	3:N:4699:UNK:HA	1.76	0.68
3:N:6492:UNK:O	3:N:6496:UNK:CB	2.42	0.67
1:A:337:HIS:CE1	1:C:341:LYS:CD	2.79	0.66
3:M:6219:UNK:C	3:M:6221:UNK:N	2.51	0.66
3:M:6492:UNK:O	3:M:6496:UNK:CB	2.42	0.66
1:A:317:THR:N	1:C:341:LYS:HZ2	1.80	0.66
1:C:75:ARG:NH1	3:N:4943:UNK:CB	2.56	0.66
1:A:342:GLN:CA	1:C:339:HIS:CE1	2.55	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:HIS:ND1	1:A:338:GLY:O	2.29	0.66
1:A:341:LYS:HE2	1:C:316:THR:HB	1.77	0.65
1:C:337:HIS:ND1	1:C:338:GLY:O	2.29	0.65
1:C:154:SER:HA	1:C:157:MET:HE3	1.77	0.65
1:A:154:SER:HA	1:A:157:MET:HE3	1.77	0.65
1:A:358:ARG:HH11	3:M:4353:UNK:C	2.10	0.64
1:C:174:ASP:OD1	1:C:194:ARG:NH1	2.30	0.64
1:A:141:GLU:CD	1:A:342:GLN:HE21	2.05	0.64
1:A:174:ASP:OD1	1:A:194:ARG:NH1	2.30	0.64
1:C:235:ARG:HH12	3:N:6215:UNK:CB	2.10	0.64
1:A:341:LYS:HE2	1:C:316:THR:CB	2.28	0.64
1:A:358:ARG:NH1	3:M:4353:UNK:N	2.17	0.64
2:B:298:UNK:O	2:B:299:UNK:CB	2.46	0.64
1:A:141:GLU:CG	1:A:342:GLN:NE2	2.56	0.63
3:N:7129:UNK:O	3:N:7133:UNK:CB	2.47	0.63
1:A:224:LEU:O	1:A:228:ARG:HG3	1.99	0.63
3:M:7129:UNK:O	3:M:7133:UNK:CB	2.47	0.63
1:A:316:THR:HB	1:C:341:LYS:CD	2.28	0.62
1:A:339:HIS:HA	1:C:340:MET:N	2.14	0.62
1:A:214:ILE:HD12	1:A:245:MET:HE2	1.81	0.62
4:A:502:KEG:O31	1:C:386:GLU:HG3	2.00	0.62
1:C:224:LEU:O	1:C:228:ARG:HG3	1.99	0.62
1:C:318:ARG:NH2	1:C:381:TYR:HE2	1.99	0.61
1:A:141:GLU:CD	1:A:342:GLN:NE2	2.59	0.61
1:C:214:ILE:HD12	1:C:245:MET:HE2	1.81	0.61
3:N:8434:UNK:CB	3:N:8458:UNK:CB	2.79	0.61
1:A:318:ARG:NH2	1:A:381:TYR:HE2	1.99	0.60
3:N:8155:UNK:C	3:N:8156:UNK:O	2.49	0.60
1:A:339:HIS:CA	1:C:340:MET:N	2.64	0.60
3:M:8434:UNK:CB	3:M:8458:UNK:CB	2.79	0.60
1:A:341:LYS:NZ	1:C:316:THR:OG1	2.34	0.60
1:C:68:LEU:HD21	3:N:4868:UNK:CB	2.31	0.60
3:M:2580:UNK:O	3:M:2584:UNK:CB	2.50	0.60
1:A:337:HIS:CE1	1:C:341:LYS:CE	2.85	0.60
2:D:298:UNK:O	2:D:299:UNK:CB	2.46	0.60
3:M:8155:UNK:O	3:M:8156:UNK:C	2.49	0.60
3:N:2580:UNK:O	3:N:2584:UNK:CB	2.50	0.60
3:N:8155:UNK:O	3:N:8156:UNK:C	2.49	0.59
1:A:340:MET:HA	1:C:339:HIS:O	2.01	0.59
1:A:341:LYS:CD	1:C:339:HIS:CB	2.81	0.58
1:A:439:ASP:OD2	1:A:441:SER:OG	2.15	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:6218:UNK:O	3:M:6221:UNK:CB	2.51	0.58
3:N:6218:UNK:O	3:N:6221:UNK:CB	2.52	0.58
3:M:8155:UNK:C	3:M:8156:UNK:O	2.49	0.58
1:A:339:HIS:CG	1:C:340:MET:C	2.30	0.57
3:N:4685:UNK:CB	3:N:4848:UNK:HA	2.35	0.57
3:N:8367:UNK:CB	3:N:8404:UNK:O	2.53	0.57
1:C:439:ASP:OD2	1:C:441:SER:OG	2.15	0.57
1:A:313:VAL:HG12	1:A:315:SER:H	1.70	0.56
1:A:316:THR:HB	1:C:341:LYS:HD2	1.86	0.56
1:A:340:MET:CA	1:C:339:HIS:O	2.53	0.56
1:C:334:ILE:HG23	1:C:357:LYS:HD2	1.87	0.56
3:M:4685:UNK:CB	3:M:4848:UNK:HA	2.35	0.56
1:A:339:HIS:HB3	4:A:501:KEG:O27	2.04	0.56
1:C:313:VAL:HG12	1:C:315:SER:H	1.70	0.56
3:M:6210:UNK:H	3:M:6213:UNK:CB	2.19	0.56
3:M:8367:UNK:CB	3:M:8404:UNK:O	2.53	0.56
1:A:334:ILE:HG23	1:A:357:LYS:HD2	1.87	0.56
3:N:4886:UNK:HA	3:N:4950:UNK:CA	2.36	0.56
1:A:340:MET:CA	1:C:339:HIS:C	2.78	0.56
1:C:237:THR:OG1	1:C:241:LYS:NZ	2.29	0.55
3:N:6210:UNK:H	3:N:6213:UNK:CB	2.19	0.55
2:B:104:UNK:O	2:B:111:UNK:HA	2.06	0.55
1:A:337:HIS:NE2	1:C:341:LYS:HE2	2.22	0.55
1:A:341:LYS:CE	1:C:316:THR:OG1	2.55	0.55
1:A:340:MET:C	1:C:339:HIS:CG	2.81	0.54
3:M:4886:UNK:HA	3:M:4950:UNK:CA	2.36	0.54
1:A:374:ARG:NE	3:M:4431:UNK:N	2.44	0.54
2:D:104:UNK:O	2:D:111:UNK:HA	2.06	0.54
3:N:6227:UNK:O	3:N:6230:UNK:CB	2.56	0.54
3:M:6227:UNK:O	3:M:6230:UNK:CB	2.56	0.53
4:A:502:KEG:O25	1:C:425:ARG:NE	2.35	0.53
4:A:503:KEG:O10	1:C:315:SER:N	2.39	0.53
3:M:60:UNK:O	3:M:63:UNK:CB	2.57	0.53
3:M:6099:UNK:O	3:M:6102:UNK:N	2.42	0.53
3:M:6210:UNK:O	3:M:6211:UNK:C	2.57	0.53
3:N:6210:UNK:O	3:N:6211:UNK:C	2.57	0.53
1:A:342:GLN:CB	1:C:339:HIS:HE1	1.95	0.52
4:A:501:KEG:O13	1:C:320:ASN:ND2	2.42	0.52
1:A:386:GLU:OE2	1:C:225:ASP:OD2	2.27	0.52
3:N:6219:UNK:O	3:N:6221:UNK:N	2.43	0.52
1:A:316:THR:O	1:C:341:LYS:CE	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:MET:HA	4:A:501:KEG:O32	2.10	0.52
3:N:6455:UNK:CB	3:N:8119:UNK:CB	2.87	0.52
3:M:5137:UNK:N	3:M:5140:UNK:CB	2.73	0.52
3:M:6219:UNK:O	3:M:6221:UNK:N	2.43	0.52
3:N:6092:UNK:N	3:N:6095:UNK:CB	2.73	0.52
3:N:6099:UNK:O	3:N:6102:UNK:N	2.42	0.52
1:A:413:LYS:CD	1:A:414:GLU:N	2.69	0.52
1:C:344:GLU:O	1:C:348:ARG:HG3	2.10	0.52
3:N:60:UNK:O	3:N:63:UNK:CB	2.57	0.52
3:N:469:UNK:CB	3:N:5253:UNK:HA	2.40	0.52
3:N:5137:UNK:N	3:N:5140:UNK:CB	2.73	0.52
1:A:237:THR:OG1	1:A:241:LYS:NZ	2.29	0.51
1:A:339:HIS:CD2	1:C:340:MET:C	2.78	0.51
1:A:141:GLU:HG2	1:A:346:ILE:CG1	2.40	0.51
1:A:344:GLU:O	1:A:348:ARG:HG3	2.10	0.51
1:A:341:LYS:HD2	1:C:339:HIS:CG	2.44	0.51
3:M:469:UNK:CB	3:M:5256:UNK:CB	2.88	0.51
3:M:6092:UNK:N	3:M:6095:UNK:CB	2.73	0.51
1:A:255:ARG:O	1:A:259:ARG:HG3	2.10	0.51
4:A:503:KEG:O10	1:C:315:SER:HB3	2.09	0.51
1:C:255:ARG:O	1:C:259:ARG:HG3	2.10	0.51
1:C:220:VAL:HA	1:C:226:MET:HE3	1.93	0.50
3:N:6099:UNK:C	3:N:6101:UNK:N	2.73	0.50
1:C:413:LYS:CD	1:C:414:GLU:N	2.69	0.50
3:M:62:UNK:O	3:M:63:UNK:O	2.30	0.50
3:M:8290:UNK:O	3:M:8293:UNK:CB	2.60	0.50
3:M:8296:UNK:O	3:M:8299:UNK:O	2.30	0.50
3:N:8340:UNK:CB	3:N:8539:UNK:CA	2.90	0.50
1:A:220:VAL:HA	1:A:226:MET:HE3	1.93	0.50
3:M:8252:UNK:O	3:M:8253:UNK:O	2.30	0.50
1:A:288:LEU:O	1:A:411:SER:HA	2.12	0.50
3:N:8155:UNK:O	3:N:8156:UNK:O	2.30	0.50
3:N:8371:UNK:CB	3:N:8401:UNK:HA	2.42	0.50
1:C:71:PRO:CG	3:N:4895:UNK:O	2.37	0.49
3:M:8155:UNK:O	3:M:8156:UNK:O	2.30	0.49
4:A:503:KEG:O34	1:C:315:SER:HA	2.11	0.49
1:C:288:LEU:O	1:C:411:SER:HA	2.12	0.49
3:M:8154:UNK:O	3:M:8156:UNK:O	2.30	0.49
3:M:8371:UNK:CB	3:M:8401:UNK:HA	2.42	0.49
1:C:305:GLU:OE1	3:N:4407:UNK:CB	2.60	0.49
3:N:62:UNK:O	3:N:63:UNK:O	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:8252:UNK:O	3:N:8253:UNK:O	2.30	0.49
3:N:8290:UNK:O	3:N:8293:UNK:CB	2.60	0.49
3:N:8296:UNK:O	3:N:8299:UNK:O	2.30	0.49
1:A:340:MET:C	4:A:501:KEG:O7	2.56	0.49
3:N:8154:UNK:O	3:N:8156:UNK:O	2.30	0.49
1:A:340:MET:C	1:C:339:HIS:C	2.80	0.49
1:A:93:ILE:O	1:A:97:ILE:HG12	2.12	0.49
3:M:469:UNK:CB	3:M:5253:UNK:HA	2.43	0.49
3:N:4886:UNK:N	3:N:4950:UNK:O	2.46	0.49
1:C:93:ILE:O	1:C:97:ILE:HG12	2.12	0.48
1:A:358:ARG:HH11	3:M:4353:UNK:HA	1.50	0.48
1:A:341:LYS:HD3	1:C:339:HIS:CB	2.43	0.48
3:N:401:UNK:C	3:N:404:UNK:CB	2.83	0.48
1:A:358:ARG:HH12	3:M:4353:UNK:CA	2.12	0.48
1:A:316:THR:HB	1:C:341:LYS:HE2	1.95	0.48
3:M:4136:UNK:O	3:M:4139:UNK:N	2.47	0.48
3:N:7075:UNK:CB	3:N:7206:UNK:CB	2.92	0.48
3:M:4886:UNK:N	3:M:4950:UNK:O	2.47	0.47
1:C:164:VAL:HA	1:C:189:VAL:O	2.14	0.47
3:N:4136:UNK:O	3:N:4139:UNK:N	2.47	0.47
3:M:6098:UNK:O	3:M:6101:UNK:N	2.48	0.47
3:M:7075:UNK:CB	3:M:7206:UNK:CB	2.92	0.47
1:C:305:GLU:OE2	3:N:4407:UNK:CB	2.62	0.47
1:A:341:LYS:HD3	1:C:339:HIS:HB2	1.96	0.47
1:A:164:VAL:HA	1:A:189:VAL:O	2.14	0.47
3:M:8340:UNK:CB	3:M:8539:UNK:CA	2.90	0.47
1:A:371:ASP:OD2	1:A:399:ARG:HD3	2.15	0.47
1:C:439:ASP:HB3	1:C:442:THR:HG23	1.97	0.47
1:C:307:ASN:HB3	1:C:374:ARG:O	2.15	0.47
3:N:6098:UNK:O	3:N:6101:UNK:N	2.48	0.47
3:N:6112:UNK:HA	3:N:6113:UNK:HA	1.71	0.46
1:A:307:ASN:HB3	1:A:374:ARG:O	2.16	0.46
1:C:238:PRO:O	1:C:241:LYS:HD3	2.16	0.46
3:M:6099:UNK:C	3:M:6101:UNK:N	2.73	0.46
3:M:8340:UNK:CB	3:M:8539:UNK:N	2.79	0.46
3:N:8340:UNK:CB	3:N:8539:UNK:N	2.79	0.46
1:A:341:LYS:CD	1:C:339:HIS:HB3	2.45	0.46
1:A:179:LYS:HE3	1:A:179:LYS:HB2	1.57	0.46
3:M:402:UNK:C	3:M:404:UNK:N	2.76	0.46
1:A:339:HIS:HA	1:C:340:MET:H	1.81	0.46
1:A:374:ARG:NH2	3:M:4431:UNK:H2	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:ASP:OD2	1:C:399:ARG:HD3	2.15	0.45
1:C:383:LEU:HD12	1:C:383:LEU:HA	1.85	0.45
1:A:238:PRO:O	1:A:241:LYS:HD3	2.15	0.45
3:N:466:UNK:CA	3:N:5253:UNK:CB	2.86	0.45
3:N:401:UNK:C	3:N:404:UNK:N	2.79	0.45
1:A:64:PHE:CE2	1:A:82:PHE:HB3	2.51	0.45
1:A:439:ASP:HB3	1:A:442:THR:HG23	1.97	0.45
1:C:64:PHE:CE2	1:C:82:PHE:HB3	2.51	0.45
3:N:402:UNK:C	3:N:404:UNK:N	2.75	0.45
1:C:251:SER:O	1:C:255:ARG:HG3	2.16	0.45
3:M:401:UNK:C	3:M:404:UNK:N	2.78	0.45
3:M:6113:UNK:CB	3:M:6114:UNK:CB	2.95	0.45
1:A:141:GLU:HB3	1:A:346:ILE:HD11	1.98	0.45
1:A:251:SER:O	1:A:255:ARG:HG3	2.16	0.45
1:A:339:HIS:O	1:C:341:LYS:N	2.48	0.45
3:N:6113:UNK:CB	3:N:6114:UNK:CB	2.95	0.45
1:A:66:ASP:HB3	3:M:4705:UNK:CB	2.47	0.44
1:C:179:LYS:HB2	1:C:179:LYS:HE3	1.57	0.44
3:M:6217:UNK:O	3:M:6220:UNK:CB	2.66	0.44
3:N:4886:UNK:CA	3:N:4950:UNK:CB	2.91	0.44
1:A:341:LYS:HE2	1:C:316:THR:OG1	2.18	0.44
1:A:341:LYS:HD2	1:C:339:HIS:CB	2.47	0.44
1:A:342:GLN:CB	1:C:339:HIS:NE2	2.39	0.44
1:C:97:ILE:HD12	1:C:122:GLN:HG2	1.99	0.44
3:N:2582:UNK:O	3:N:2586:UNK:CB	2.65	0.44
1:A:97:ILE:HD12	1:A:122:GLN:HG2	1.99	0.44
1:A:340:MET:O	1:C:339:HIS:CB	2.61	0.44
3:M:401:UNK:C	3:M:404:UNK:CB	2.83	0.44
3:M:2582:UNK:O	3:M:2586:UNK:CB	2.65	0.44
3:M:6492:UNK:O	3:M:6496:UNK:N	2.51	0.44
1:C:334:ILE:HD11	1:C:352:PHE:HB2	2.00	0.44
3:N:6492:UNK:O	3:N:6496:UNK:N	2.51	0.44
1:A:320:ASN:ND2	1:C:341:LYS:HE3	2.34	0.43
3:N:8144:UNK:O	3:N:8148:UNK:N	2.52	0.43
1:A:102:VAL:HB	1:A:244:MET:HG2	2.00	0.43
1:A:135:VAL:HG22	1:A:213:VAL:HB	2.01	0.43
3:N:6217:UNK:O	3:N:6220:UNK:CB	2.66	0.43
3:N:7129:UNK:O	3:N:7133:UNK:CA	2.66	0.43
3:M:7129:UNK:O	3:M:7133:UNK:CA	2.66	0.42
3:M:8144:UNK:O	3:M:8148:UNK:N	2.52	0.42
1:A:113:THR:HA	1:A:116:PHE:CE2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:HD2	1:C:339:HIS:CD2	2.54	0.42
2:B:277:UNK:CB	2:B:304:UNK:C	2.86	0.42
1:C:113:THR:HA	1:C:116:PHE:CE2	2.54	0.42
1:A:141:GLU:CG	1:A:346:ILE:HG13	2.49	0.42
1:A:341:LYS:N	4:A:501:KEG:O32	2.47	0.42
1:A:141:GLU:HG3	1:A:346:ILE:HG13	2.01	0.42
1:A:334:ILE:HD11	1:A:352:PHE:HB2	2.00	0.42
1:C:102:VAL:HB	1:C:244:MET:HG2	2.00	0.42
1:C:135:VAL:HG22	1:C:213:VAL:HB	2.01	0.42
3:N:2581:UNK:HA	3:N:2584:UNK:CB	2.50	0.42
1:A:313:VAL:HG11	1:A:318:ARG:HB2	2.02	0.42
4:A:502:KEG:O6	1:C:386:GLU:HA	2.19	0.42
1:C:105:GLN:HB2	1:C:250:LEU:HD12	2.02	0.41
3:N:62:UNK:C	3:N:63:UNK:O	2.65	0.41
1:A:235:ARG:NH1	3:M:6215:UNK:CB	2.70	0.41
1:C:218:ASP:OD2	1:C:249:THR:OG1	2.38	0.41
3:M:2581:UNK:HA	3:M:2584:UNK:CB	2.50	0.41
1:A:105:GLN:HB2	1:A:250:LEU:HD12	2.02	0.41
1:A:259:ARG:NH1	1:A:267:GLU:OE1	2.53	0.41
1:C:148:ASN:O	1:C:152:ARG:HG3	2.20	0.41
3:N:6098:UNK:O	3:N:6101:UNK:CA	2.67	0.41
1:A:313:VAL:CG1	1:A:318:ARG:HB2	2.51	0.41
1:A:341:LYS:CD	1:C:339:HIS:HB2	2.49	0.41
1:C:313:VAL:HG11	1:C:318:ARG:HB2	2.02	0.41
1:A:148:ASN:O	1:A:152:ARG:HG3	2.20	0.41
1:C:316:THR:HG22	1:C:337:HIS:HB2	2.02	0.41
1:A:316:THR:HG22	1:A:337:HIS:HB2	2.02	0.41
1:A:316:THR:OG1	1:C:341:LYS:NZ	2.54	0.41
1:A:335:THR:HA	1:A:361:VAL:O	2.21	0.41
4:A:501:KEG:O27	1:C:341:LYS:HG2	2.20	0.41
1:C:259:ARG:NH1	1:C:267:GLU:OE1	2.53	0.41
3:N:6092:UNK:N	3:N:6095:UNK:N	2.60	0.41
1:C:313:VAL:CG1	1:C:318:ARG:HB2	2.51	0.41
1:A:218:ASP:OD2	1:A:249:THR:OG1	2.38	0.40
2:B:315:UNK:HA	2:B:330:UNK:O	2.22	0.40
1:C:335:THR:HA	1:C:361:VAL:O	2.21	0.40
2:D:315:UNK:HA	2:D:330:UNK:O	2.22	0.40
1:C:217:CYS:SG	1:C:245:MET:HB3	2.62	0.40
3:N:6099:UNK:O	3:N:6102:UNK:CB	2.69	0.40
1:A:217:CYS:SG	1:A:245:MET:HB3	2.61	0.40
3:M:6099:UNK:O	3:M:6102:UNK:CB	2.69	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	370/446 (83%)	362 (98%)	8 (2%)	0	100	100
1	C	370/446 (83%)	362 (98%)	8 (2%)	0	100	100
All	All	740/892 (83%)	724 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/386 (86%)	331 (100%)	0	100	100
1	C	331/386 (86%)	331 (100%)	0	100	100
All	All	662/772 (86%)	662 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	123	GLN
1	A	211	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	299	GLN
1	A	342	GLN
1	C	90	GLN
1	C	98	HIS
1	C	123	GLN
1	C	208	HIS
1	C	211	ASN
1	C	299	GLN
1	C	307	ASN
1	C	339	HIS

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 ⓘ

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	KEG	N	8701	-	76,76,76	3.13	42 (55%)	6,234,234	1.37	2 (33%)
4	KEG	N	8702	-	76,76,76	3.12	42 (55%)	6,234,234	1.38	2 (33%)
4	KEG	A	501	-	76,76,76	3.13	42 (55%)	6,234,234	1.37	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	KEG	N	8703	-	76,76,76	3.13	42 (55%)	6,234,234	1.38	2 (33%)
4	KEG	N	8705	-	76,76,76	3.13	42 (55%)	6,234,234	1.39	2 (33%)
4	KEG	M	8702	-	76,76,76	3.13	42 (55%)	6,234,234	1.37	2 (33%)
4	KEG	A	502	-	76,76,76	3.13	42 (55%)	6,234,234	1.38	2 (33%)
4	KEG	N	8704	-	76,76,76	3.13	42 (55%)	6,234,234	1.38	2 (33%)
4	KEG	M	8701	-	76,76,76	3.13	42 (55%)	6,234,234	1.40	2 (33%)
4	KEG	A	503	-	76,76,76	3.13	42 (55%)	6,234,234	1.37	2 (33%)
4	KEG	M	8703	-	76,76,76	3.12	42 (55%)	6,234,234	1.39	2 (33%)

All (462) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8704	KEG	P1-O18	-7.90	1.27	1.54
4	A	503	KEG	P1-O18	-7.89	1.27	1.54
4	M	8701	KEG	P1-O18	-7.89	1.27	1.54
4	N	8701	KEG	P1-O18	-7.88	1.27	1.54
4	A	501	KEG	P1-O18	-7.88	1.27	1.54
4	M	8702	KEG	P1-O18	-7.88	1.27	1.54
4	A	502	KEG	P1-O18	-7.87	1.27	1.54
4	N	8705	KEG	P1-O18	-7.87	1.27	1.54
4	N	8703	KEG	P1-O18	-7.87	1.27	1.54
4	M	8703	KEG	P1-O18	-7.86	1.27	1.54
4	N	8702	KEG	P1-O18	-7.84	1.27	1.54
4	M	8702	KEG	W2-O28	-7.53	1.55	1.93
4	N	8704	KEG	W2-O28	-7.51	1.55	1.93
4	A	503	KEG	W2-O28	-7.50	1.55	1.93
4	M	8703	KEG	W2-O28	-7.50	1.55	1.93
4	M	8701	KEG	W2-O28	-7.50	1.55	1.93
4	N	8705	KEG	W2-O28	-7.50	1.55	1.93
4	A	501	KEG	W2-O28	-7.50	1.55	1.93
4	N	8701	KEG	W2-O28	-7.50	1.55	1.93
4	N	8702	KEG	W2-O28	-7.49	1.55	1.93
4	A	502	KEG	W2-O28	-7.49	1.55	1.93
4	N	8703	KEG	W2-O28	-7.48	1.55	1.93
4	N	8704	KEG	W1-O29	-7.20	1.60	1.91
4	A	502	KEG	W1-O29	-7.20	1.60	1.91
4	N	8702	KEG	W1-O29	-7.19	1.60	1.91
4	N	8701	KEG	W1-O29	-7.19	1.60	1.91
4	M	8703	KEG	W1-O29	-7.19	1.60	1.91
4	M	8702	KEG	W1-O29	-7.19	1.60	1.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8701	KEG	W1-O29	-7.19	1.60	1.91
4	A	503	KEG	W1-O29	-7.19	1.60	1.91
4	A	501	KEG	W1-O29	-7.19	1.60	1.91
4	N	8703	KEG	W1-O29	-7.17	1.60	1.91
4	N	8705	KEG	W1-O29	-7.17	1.60	1.91
4	A	502	KEG	W3-O33	-7.09	1.61	1.91
4	M	8702	KEG	W3-O33	-7.07	1.61	1.91
4	A	501	KEG	W3-O33	-7.07	1.61	1.91
4	M	8701	KEG	W3-O33	-7.07	1.61	1.91
4	N	8703	KEG	W3-O33	-7.05	1.61	1.91
4	A	503	KEG	W3-O33	-7.05	1.61	1.91
4	N	8701	KEG	W3-O33	-7.04	1.61	1.91
4	M	8703	KEG	W3-O33	-7.04	1.61	1.91
4	N	8705	KEG	W3-O33	-7.04	1.61	1.91
4	N	8704	KEG	W3-O33	-7.03	1.61	1.91
4	A	501	KEG	W6-O36	-7.03	1.58	1.93
4	N	8702	KEG	W3-O33	-7.03	1.61	1.91
4	M	8701	KEG	W6-O36	-7.02	1.58	1.93
4	M	8702	KEG	W6-O36	-7.02	1.58	1.93
4	A	503	KEG	W6-O36	-7.02	1.58	1.93
4	N	8705	KEG	W6-O36	-7.02	1.58	1.93
4	N	8701	KEG	W6-O36	-7.01	1.58	1.93
4	M	8703	KEG	W6-O36	-7.01	1.58	1.93
4	N	8703	KEG	W6-O36	-7.01	1.58	1.93
4	A	502	KEG	W6-O36	-7.00	1.58	1.93
4	N	8704	KEG	W6-O36	-7.00	1.58	1.93
4	N	8702	KEG	W6-O36	-7.00	1.58	1.93
4	N	8703	KEG	W10-O28	-5.46	1.66	1.93
4	A	501	KEG	W10-O28	-5.45	1.66	1.93
4	A	502	KEG	W10-O28	-5.45	1.66	1.93
4	N	8701	KEG	W10-O28	-5.45	1.66	1.93
4	M	8703	KEG	W10-O28	-5.45	1.66	1.93
4	M	8702	KEG	W10-O28	-5.45	1.66	1.93
4	N	8702	KEG	W10-O28	-5.45	1.66	1.93
4	M	8701	KEG	W10-O28	-5.45	1.66	1.93
4	N	8705	KEG	W10-O28	-5.44	1.66	1.93
4	A	503	KEG	W10-O28	-5.44	1.66	1.93
4	N	8704	KEG	W10-O28	-5.43	1.66	1.93
4	A	502	KEG	W5-O23	-5.05	1.68	1.93
4	M	8703	KEG	W5-O23	-5.04	1.68	1.93
4	A	503	KEG	W5-O23	-5.03	1.68	1.93
4	A	501	KEG	W5-O23	-5.03	1.68	1.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8701	KEG	W5-O23	-5.03	1.68	1.93
4	M	8702	KEG	W5-O23	-5.03	1.68	1.93
4	N	8703	KEG	W5-O23	-5.03	1.68	1.93
4	N	8701	KEG	W5-O23	-5.03	1.68	1.93
4	N	8705	KEG	W5-O23	-5.03	1.68	1.93
4	N	8702	KEG	W5-O23	-5.02	1.68	1.93
4	N	8704	KEG	W5-O23	-5.01	1.68	1.93
4	M	8702	KEG	W7-O29	-4.81	1.70	1.91
4	N	8705	KEG	W7-O29	-4.80	1.70	1.91
4	A	503	KEG	W7-O29	-4.80	1.70	1.91
4	M	8701	KEG	W7-O29	-4.80	1.70	1.91
4	N	8704	KEG	W7-O29	-4.80	1.70	1.91
4	A	501	KEG	W7-O29	-4.80	1.70	1.91
4	A	502	KEG	W7-O29	-4.80	1.70	1.91
4	N	8701	KEG	W7-O29	-4.79	1.70	1.91
4	N	8703	KEG	W7-O29	-4.78	1.70	1.91
4	M	8703	KEG	W7-O29	-4.77	1.70	1.91
4	N	8702	KEG	W7-O29	-4.77	1.70	1.91
4	N	8703	KEG	P1-O19	-4.75	1.38	1.54
4	A	503	KEG	P1-O19	-4.73	1.38	1.54
4	A	501	KEG	P1-O19	-4.72	1.38	1.54
4	N	8702	KEG	P1-O19	-4.72	1.38	1.54
4	N	8701	KEG	P1-O19	-4.71	1.38	1.54
4	M	8701	KEG	P1-O19	-4.71	1.38	1.54
4	M	8703	KEG	P1-O19	-4.71	1.38	1.54
4	N	8705	KEG	P1-O19	-4.71	1.38	1.54
4	M	8702	KEG	P1-O19	-4.70	1.38	1.54
4	N	8704	KEG	P1-O19	-4.70	1.38	1.54
4	A	503	KEG	W2-O2	-4.68	1.58	1.71
4	A	502	KEG	P1-O19	-4.67	1.38	1.54
4	N	8702	KEG	W2-O2	-4.67	1.58	1.71
4	A	502	KEG	W2-O2	-4.66	1.58	1.71
4	N	8704	KEG	W2-O2	-4.66	1.58	1.71
4	N	8701	KEG	W2-O2	-4.64	1.58	1.71
4	M	8701	KEG	W2-O2	-4.64	1.58	1.71
4	M	8702	KEG	W2-O2	-4.63	1.58	1.71
4	N	8703	KEG	W2-O2	-4.63	1.58	1.71
4	N	8705	KEG	W2-O2	-4.62	1.58	1.71
4	A	501	KEG	W2-O2	-4.62	1.58	1.71
4	M	8703	KEG	W2-O2	-4.60	1.58	1.71
4	A	502	KEG	W10-O18	-4.41	2.19	2.43
4	A	501	KEG	W10-O18	-4.39	2.19	2.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8702	KEG	W10-O18	-4.39	2.19	2.43
4	M	8703	KEG	W10-O18	-4.38	2.19	2.43
4	A	503	KEG	W10-O18	-4.38	2.19	2.43
4	N	8703	KEG	W10-O18	-4.38	2.19	2.43
4	N	8704	KEG	W10-O18	-4.37	2.19	2.43
4	M	8701	KEG	W10-O18	-4.37	2.19	2.43
4	N	8701	KEG	W10-O18	-4.37	2.19	2.43
4	N	8705	KEG	W10-O18	-4.36	2.19	2.43
4	N	8702	KEG	W10-O18	-4.36	2.19	2.43
4	A	502	KEG	W1-O23	-4.35	1.71	1.93
4	A	503	KEG	W1-O23	-4.34	1.71	1.93
4	M	8701	KEG	W1-O23	-4.33	1.71	1.93
4	N	8701	KEG	W1-O23	-4.33	1.71	1.93
4	N	8704	KEG	W1-O23	-4.33	1.71	1.93
4	A	501	KEG	W1-O23	-4.33	1.71	1.93
4	M	8703	KEG	W1-O23	-4.32	1.71	1.93
4	N	8702	KEG	W1-O23	-4.32	1.71	1.93
4	N	8705	KEG	W1-O23	-4.32	1.71	1.93
4	N	8703	KEG	W1-O23	-4.31	1.71	1.93
4	M	8702	KEG	W1-O23	-4.31	1.71	1.93
4	N	8701	KEG	W2-O18	-4.30	2.19	2.43
4	M	8702	KEG	W2-O18	-4.30	2.19	2.43
4	N	8705	KEG	W2-O18	-4.30	2.19	2.43
4	M	8703	KEG	W2-O18	-4.29	2.19	2.43
4	N	8702	KEG	W2-O18	-4.29	2.19	2.43
4	A	502	KEG	W2-O18	-4.29	2.19	2.43
4	N	8703	KEG	W2-O18	-4.28	2.19	2.43
4	A	501	KEG	W2-O18	-4.28	2.19	2.43
4	A	503	KEG	W2-O18	-4.27	2.19	2.43
4	N	8704	KEG	W2-O18	-4.27	2.19	2.43
4	M	8701	KEG	W2-O18	-4.27	2.19	2.43
4	A	503	KEG	W11-O13	-4.13	1.60	1.71
4	A	501	KEG	W11-O13	-4.13	1.60	1.71
4	N	8705	KEG	W11-O13	-4.13	1.60	1.71
4	N	8704	KEG	W11-O13	-4.12	1.60	1.71
4	N	8703	KEG	W11-O13	-4.12	1.60	1.71
4	M	8703	KEG	W11-O13	-4.12	1.60	1.71
4	N	8701	KEG	W11-O13	-4.12	1.60	1.71
4	M	8701	KEG	W11-O13	-4.11	1.60	1.71
4	N	8702	KEG	W11-O13	-4.11	1.60	1.71
4	M	8702	KEG	W11-O13	-4.10	1.60	1.71
4	A	502	KEG	W11-O13	-4.10	1.60	1.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8702	KEG	W9-O42	-4.08	1.73	1.91
4	A	503	KEG	W9-O42	-4.08	1.73	1.91
4	N	8705	KEG	W9-O42	-4.08	1.73	1.91
4	N	8701	KEG	W9-O42	-4.07	1.73	1.91
4	M	8701	KEG	W9-O42	-4.07	1.73	1.91
4	N	8702	KEG	W9-O42	-4.07	1.73	1.91
4	A	501	KEG	W9-O42	-4.07	1.73	1.91
4	N	8704	KEG	W9-O42	-4.06	1.73	1.91
4	A	502	KEG	W9-O42	-4.06	1.73	1.91
4	N	8703	KEG	W9-O42	-4.05	1.73	1.91
4	M	8703	KEG	W9-O42	-4.04	1.74	1.91
4	A	502	KEG	W12-O14	-4.01	1.60	1.71
4	A	501	KEG	W12-O14	-3.98	1.60	1.71
4	M	8701	KEG	W12-O14	-3.98	1.60	1.71
4	N	8702	KEG	W12-O14	-3.98	1.60	1.71
4	A	503	KEG	W12-O14	-3.97	1.60	1.71
4	M	8702	KEG	W12-O14	-3.97	1.60	1.71
4	N	8705	KEG	W12-O14	-3.97	1.60	1.71
4	M	8703	KEG	W12-O14	-3.96	1.60	1.71
4	N	8704	KEG	W12-O14	-3.95	1.60	1.71
4	N	8701	KEG	W12-O14	-3.93	1.60	1.71
4	N	8703	KEG	W12-O14	-3.93	1.60	1.71
4	M	8703	KEG	W1-O17	-3.78	2.22	2.43
4	A	502	KEG	W1-O17	-3.78	2.22	2.43
4	N	8705	KEG	W1-O17	-3.78	2.22	2.43
4	M	8702	KEG	W1-O17	-3.78	2.22	2.43
4	N	8703	KEG	W1-O17	-3.78	2.22	2.43
4	M	8701	KEG	W1-O17	-3.78	2.22	2.43
4	A	501	KEG	W1-O17	-3.77	2.22	2.43
4	N	8701	KEG	W1-O17	-3.77	2.22	2.43
4	A	503	KEG	W1-O17	-3.76	2.22	2.43
4	N	8704	KEG	W1-O17	-3.76	2.22	2.43
4	N	8702	KEG	W1-O17	-3.75	2.22	2.43
4	A	502	KEG	W10-O36	-3.74	1.74	1.93
4	N	8702	KEG	W10-O36	-3.73	1.74	1.93
4	M	8701	KEG	W10-O36	-3.73	1.74	1.93
4	N	8704	KEG	W10-O36	-3.73	1.74	1.93
4	M	8703	KEG	W10-O36	-3.72	1.74	1.93
4	A	501	KEG	W10-O36	-3.72	1.74	1.93
4	N	8701	KEG	W10-O36	-3.72	1.74	1.93
4	M	8702	KEG	W10-O36	-3.72	1.74	1.93
4	N	8705	KEG	W10-O36	-3.72	1.74	1.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8703	KEG	W10-O36	-3.72	1.74	1.93
4	A	503	KEG	W10-O36	-3.71	1.74	1.93
4	A	502	KEG	W8-O10	-3.65	1.61	1.71
4	N	8704	KEG	W8-O10	-3.62	1.61	1.71
4	N	8701	KEG	W8-O10	-3.62	1.61	1.71
4	M	8701	KEG	W8-O10	-3.61	1.61	1.71
4	N	8702	KEG	W8-O10	-3.61	1.61	1.71
4	A	503	KEG	W8-O10	-3.59	1.61	1.71
4	N	8705	KEG	W8-O10	-3.59	1.61	1.71
4	M	8702	KEG	W8-O10	-3.58	1.61	1.71
4	N	8703	KEG	W8-O10	-3.58	1.61	1.71
4	A	501	KEG	W8-O10	-3.57	1.61	1.71
4	M	8703	KEG	W8-O10	-3.57	1.61	1.71
4	A	502	KEG	W3-O21	3.35	2.61	2.43
4	N	8705	KEG	W3-O21	3.34	2.61	2.43
4	A	503	KEG	W3-O21	3.34	2.61	2.43
4	M	8701	KEG	W3-O21	3.33	2.61	2.43
4	N	8704	KEG	W3-O21	3.33	2.61	2.43
4	N	8701	KEG	W3-O21	3.33	2.61	2.43
4	A	501	KEG	W3-O21	3.33	2.61	2.43
4	N	8703	KEG	W3-O21	3.33	2.61	2.43
4	M	8703	KEG	W3-O21	3.31	2.61	2.43
4	M	8702	KEG	W3-O21	3.31	2.61	2.43
4	N	8702	KEG	W3-O21	3.31	2.61	2.43
4	A	501	KEG	W6-O24	-3.30	1.76	1.93
4	M	8701	KEG	W6-O24	-3.30	1.76	1.93
4	A	502	KEG	W6-O24	-3.28	1.77	1.93
4	N	8704	KEG	W6-O24	-3.28	1.77	1.93
4	M	8702	KEG	W6-O24	-3.28	1.77	1.93
4	A	503	KEG	W6-O24	-3.27	1.77	1.93
4	M	8703	KEG	W6-O24	-3.27	1.77	1.93
4	N	8703	KEG	W6-O24	-3.26	1.77	1.93
4	N	8705	KEG	W6-O24	-3.26	1.77	1.93
4	N	8701	KEG	W6-O24	-3.26	1.77	1.93
4	N	8702	KEG	W6-O24	-3.25	1.77	1.93
4	N	8701	KEG	W9-O11	-3.11	1.62	1.71
4	N	8704	KEG	W9-O11	-3.10	1.62	1.71
4	M	8703	KEG	W9-O11	-3.10	1.63	1.71
4	A	501	KEG	W9-O11	-3.09	1.63	1.71
4	M	8702	KEG	W9-O11	-3.08	1.63	1.71
4	A	502	KEG	W9-O11	-3.07	1.63	1.71
4	N	8703	KEG	W9-O11	-3.07	1.63	1.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	KEG	W9-O11	-3.07	1.63	1.71
4	N	8703	KEG	W3-O25	-3.06	1.78	1.91
4	N	8705	KEG	W9-O11	-3.06	1.63	1.71
4	N	8705	KEG	W3-O25	-3.06	1.78	1.91
4	N	8703	KEG	W2-O24	-3.05	1.78	1.93
4	M	8703	KEG	W3-O25	-3.05	1.78	1.91
4	M	8701	KEG	W3-O25	-3.05	1.78	1.91
4	N	8704	KEG	W3-O25	-3.05	1.78	1.91
4	N	8701	KEG	W3-O25	-3.05	1.78	1.91
4	A	501	KEG	W3-O25	-3.05	1.78	1.91
4	A	503	KEG	W3-O25	-3.05	1.78	1.91
4	M	8701	KEG	W9-O11	-3.05	1.63	1.71
4	M	8702	KEG	W3-O25	-3.05	1.78	1.91
4	N	8702	KEG	W3-O25	-3.04	1.78	1.91
4	N	8701	KEG	W2-O24	-3.04	1.78	1.93
4	A	502	KEG	W3-O25	-3.04	1.78	1.91
4	N	8702	KEG	W2-O24	-3.03	1.78	1.93
4	N	8702	KEG	W9-O11	-3.03	1.63	1.71
4	N	8704	KEG	W2-O24	-3.03	1.78	1.93
4	N	8705	KEG	W2-O24	-3.03	1.78	1.93
4	A	503	KEG	W2-O24	-3.03	1.78	1.93
4	M	8703	KEG	W2-O24	-3.03	1.78	1.93
4	M	8701	KEG	W2-O24	-3.02	1.78	1.93
4	A	501	KEG	W2-O24	-3.02	1.78	1.93
4	A	502	KEG	W2-O24	-3.02	1.78	1.93
4	M	8702	KEG	W2-O24	-3.01	1.78	1.93
4	N	8705	KEG	W10-O12	-2.91	1.63	1.71
4	N	8702	KEG	W10-O12	-2.91	1.63	1.71
4	N	8703	KEG	W10-O12	-2.91	1.63	1.71
4	N	8701	KEG	W10-O12	-2.90	1.63	1.71
4	M	8701	KEG	W10-O12	-2.89	1.63	1.71
4	M	8703	KEG	W10-O12	-2.87	1.63	1.71
4	N	8704	KEG	W10-O12	-2.87	1.63	1.71
4	A	501	KEG	W10-O12	-2.86	1.63	1.71
4	M	8702	KEG	W10-O12	-2.86	1.63	1.71
4	A	503	KEG	W10-O12	-2.84	1.63	1.71
4	N	8702	KEG	W8-O44	-2.84	1.79	1.93
4	M	8703	KEG	W6-O8	-2.83	1.63	1.71
4	N	8703	KEG	W8-O44	-2.83	1.79	1.93
4	N	8704	KEG	W8-O44	-2.83	1.79	1.93
4	A	502	KEG	W10-O12	-2.83	1.63	1.71
4	N	8704	KEG	W6-O8	-2.83	1.63	1.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8701	KEG	W8-O44	-2.83	1.79	1.93
4	A	502	KEG	W8-O44	-2.82	1.79	1.93
4	M	8703	KEG	W8-O44	-2.82	1.79	1.93
4	N	8702	KEG	W6-O8	-2.82	1.63	1.71
4	A	501	KEG	W8-O44	-2.82	1.79	1.93
4	N	8703	KEG	W6-O8	-2.81	1.63	1.71
4	M	8701	KEG	W6-O8	-2.81	1.63	1.71
4	A	502	KEG	W6-O8	-2.81	1.63	1.71
4	N	8705	KEG	W6-O8	-2.81	1.63	1.71
4	N	8701	KEG	W8-O44	-2.81	1.79	1.93
4	A	503	KEG	W8-O44	-2.80	1.79	1.93
4	A	501	KEG	W6-O8	-2.80	1.63	1.71
4	M	8702	KEG	W6-O8	-2.80	1.63	1.71
4	M	8702	KEG	W8-O44	-2.80	1.79	1.93
4	N	8701	KEG	W6-O8	-2.80	1.63	1.71
4	N	8705	KEG	W8-O44	-2.79	1.79	1.93
4	A	503	KEG	W6-O8	-2.78	1.63	1.71
4	N	8704	KEG	W5-O7	-2.73	1.64	1.71
4	A	502	KEG	W5-O7	-2.71	1.64	1.71
4	M	8703	KEG	W5-O7	-2.70	1.64	1.71
4	M	8701	KEG	W5-O7	-2.70	1.64	1.71
4	A	503	KEG	W5-O7	-2.69	1.64	1.71
4	M	8702	KEG	W5-O7	-2.69	1.64	1.71
4	A	501	KEG	W3-O37	2.69	2.07	1.93
4	N	8703	KEG	W5-O7	-2.68	1.64	1.71
4	N	8704	KEG	W3-O37	2.68	2.07	1.93
4	N	8705	KEG	W5-O7	-2.68	1.64	1.71
4	N	8703	KEG	W3-O37	2.68	2.07	1.93
4	N	8705	KEG	W3-O37	2.67	2.07	1.93
4	M	8701	KEG	W3-O37	2.67	2.07	1.93
4	A	502	KEG	W3-O37	2.67	2.07	1.93
4	M	8703	KEG	W3-O37	2.67	2.07	1.93
4	N	8701	KEG	W5-O7	-2.66	1.64	1.71
4	N	8702	KEG	W5-O7	-2.66	1.64	1.71
4	A	503	KEG	W3-O37	2.66	2.07	1.93
4	N	8701	KEG	W3-O37	2.66	2.07	1.93
4	A	501	KEG	W5-O7	-2.66	1.64	1.71
4	M	8702	KEG	W3-O37	2.66	2.07	1.93
4	N	8702	KEG	W3-O37	2.65	2.07	1.93
4	N	8704	KEG	P1-O21	2.59	1.63	1.54
4	N	8703	KEG	P1-O21	2.58	1.63	1.54
4	M	8702	KEG	P1-O21	2.57	1.63	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8702	KEG	P1-O21	2.57	1.63	1.54
4	N	8701	KEG	P1-O21	2.56	1.63	1.54
4	A	503	KEG	P1-O21	2.56	1.63	1.54
4	M	8703	KEG	P1-O21	2.56	1.63	1.54
4	A	503	KEG	W1-O1	-2.55	1.64	1.71
4	N	8705	KEG	P1-O21	2.55	1.63	1.54
4	A	501	KEG	P1-O21	2.55	1.63	1.54
4	M	8703	KEG	W11-O40	-2.54	1.80	1.91
4	N	8701	KEG	W1-O1	-2.54	1.64	1.71
4	A	502	KEG	W11-O40	-2.54	1.80	1.91
4	M	8701	KEG	P1-O21	2.54	1.63	1.54
4	M	8702	KEG	W11-O40	-2.54	1.80	1.91
4	A	502	KEG	P1-O21	2.54	1.63	1.54
4	N	8703	KEG	W11-O40	-2.54	1.80	1.91
4	M	8701	KEG	W11-O40	-2.53	1.80	1.91
4	N	8703	KEG	W1-O1	-2.53	1.64	1.71
4	A	503	KEG	W11-O40	-2.53	1.80	1.91
4	N	8701	KEG	W11-O40	-2.53	1.80	1.91
4	A	501	KEG	W11-O40	-2.53	1.80	1.91
4	N	8704	KEG	W11-O40	-2.53	1.80	1.91
4	N	8705	KEG	W1-O1	-2.53	1.64	1.71
4	N	8702	KEG	W11-O40	-2.53	1.80	1.91
4	M	8701	KEG	W1-O1	-2.52	1.64	1.71
4	N	8705	KEG	W11-O40	-2.52	1.80	1.91
4	N	8702	KEG	W1-O1	-2.51	1.64	1.71
4	A	502	KEG	W1-O1	-2.51	1.64	1.71
4	M	8702	KEG	W1-O1	-2.51	1.64	1.71
4	A	501	KEG	W1-O1	-2.50	1.64	1.71
4	M	8703	KEG	W1-O1	-2.50	1.64	1.71
4	A	502	KEG	W5-O32	2.49	2.01	1.91
4	A	503	KEG	W5-O32	2.49	2.01	1.91
4	N	8704	KEG	W1-O1	-2.48	1.64	1.71
4	M	8703	KEG	W5-O32	2.48	2.01	1.91
4	N	8703	KEG	W5-O32	2.48	2.01	1.91
4	M	8701	KEG	W5-O32	2.48	2.01	1.91
4	M	8702	KEG	W5-O32	2.48	2.01	1.91
4	N	8701	KEG	W5-O32	2.47	2.01	1.91
4	N	8702	KEG	W5-O32	2.47	2.01	1.91
4	A	501	KEG	W5-O32	2.47	2.01	1.91
4	N	8704	KEG	W5-O32	2.46	2.01	1.91
4	N	8705	KEG	W5-O32	2.45	2.01	1.91
4	M	8702	KEG	W4-O6	-2.38	1.64	1.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8701	KEG	W6-O32	2.37	2.01	1.91
4	A	501	KEG	W6-O32	2.36	2.01	1.91
4	A	501	KEG	W4-O6	-2.36	1.65	1.71
4	N	8704	KEG	W6-O32	2.36	2.01	1.91
4	A	502	KEG	W6-O32	2.36	2.01	1.91
4	N	8702	KEG	W4-O21	2.35	2.55	2.43
4	N	8702	KEG	W4-O6	-2.35	1.65	1.71
4	N	8703	KEG	W6-O32	2.35	2.01	1.91
4	A	501	KEG	W4-O21	2.35	2.55	2.43
4	N	8705	KEG	W4-O6	-2.34	1.65	1.71
4	A	502	KEG	W4-O6	-2.34	1.65	1.71
4	M	8702	KEG	W4-O21	2.34	2.55	2.43
4	M	8703	KEG	W4-O21	2.34	2.55	2.43
4	N	8703	KEG	W4-O21	2.33	2.55	2.43
4	N	8705	KEG	W6-O32	2.33	2.01	1.91
4	M	8702	KEG	W6-O32	2.33	2.01	1.91
4	N	8701	KEG	W4-O6	-2.33	1.65	1.71
4	A	503	KEG	W4-O6	-2.33	1.65	1.71
4	A	502	KEG	W4-O21	2.33	2.55	2.43
4	M	8703	KEG	W6-O32	2.33	2.01	1.91
4	M	8701	KEG	W4-O21	2.33	2.55	2.43
4	N	8701	KEG	W4-O21	2.33	2.55	2.43
4	N	8704	KEG	W4-O6	-2.33	1.65	1.71
4	N	8702	KEG	W6-O32	2.33	2.01	1.91
4	A	503	KEG	W6-O32	2.32	2.01	1.91
4	A	503	KEG	W4-O21	2.32	2.55	2.43
4	N	8704	KEG	W4-O21	2.32	2.55	2.43
4	M	8701	KEG	W4-O6	-2.32	1.65	1.71
4	N	8701	KEG	W6-O32	2.32	2.00	1.91
4	N	8703	KEG	W4-O6	-2.32	1.65	1.71
4	N	8702	KEG	W1-O25	-2.32	1.81	1.91
4	M	8702	KEG	W1-O25	-2.31	1.81	1.91
4	N	8705	KEG	W4-O21	2.31	2.55	2.43
4	M	8701	KEG	W1-O25	-2.30	1.81	1.91
4	M	8703	KEG	W1-O25	-2.30	1.81	1.91
4	N	8705	KEG	W1-O25	-2.30	1.81	1.91
4	M	8703	KEG	W4-O6	-2.30	1.65	1.71
4	N	8701	KEG	W7-O33	-2.30	1.81	1.91
4	N	8704	KEG	W1-O25	-2.30	1.81	1.91
4	N	8703	KEG	W1-O25	-2.29	1.81	1.91
4	N	8702	KEG	W7-O33	-2.29	1.81	1.91
4	N	8701	KEG	W1-O25	-2.29	1.81	1.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	KEG	W1-O25	-2.29	1.81	1.91
4	N	8703	KEG	W7-O33	-2.29	1.81	1.91
4	A	502	KEG	W4-O26	-2.29	1.81	1.91
4	N	8704	KEG	W7-O33	-2.28	1.81	1.91
4	M	8703	KEG	W7-O33	-2.28	1.81	1.91
4	N	8705	KEG	W7-O33	-2.28	1.81	1.91
4	N	8701	KEG	W4-O26	-2.28	1.81	1.91
4	M	8701	KEG	W4-O26	-2.28	1.81	1.91
4	M	8702	KEG	W4-O26	-2.28	1.81	1.91
4	A	503	KEG	W7-O33	-2.27	1.81	1.91
4	M	8703	KEG	W4-O26	-2.27	1.81	1.91
4	N	8705	KEG	W4-O26	-2.27	1.81	1.91
4	A	501	KEG	W1-O25	-2.27	1.81	1.91
4	A	502	KEG	W7-O33	-2.26	1.81	1.91
4	A	501	KEG	W7-O33	-2.26	1.81	1.91
4	N	8704	KEG	W4-O26	-2.26	1.81	1.91
4	A	503	KEG	W1-O25	-2.26	1.81	1.91
4	M	8701	KEG	W7-O33	-2.26	1.81	1.91
4	N	8703	KEG	W4-O26	-2.26	1.81	1.91
4	A	501	KEG	W4-O26	-2.26	1.81	1.91
4	N	8702	KEG	W4-O26	-2.25	1.81	1.91
4	A	503	KEG	W4-O26	-2.25	1.81	1.91
4	A	502	KEG	W2-O26	-2.24	1.81	1.91
4	A	503	KEG	W2-O26	-2.24	1.81	1.91
4	N	8704	KEG	W2-O26	-2.24	1.81	1.91
4	M	8702	KEG	W7-O33	-2.24	1.81	1.91
4	A	501	KEG	W2-O26	-2.23	1.81	1.91
4	M	8702	KEG	W2-O26	-2.23	1.81	1.91
4	N	8701	KEG	W2-O26	-2.22	1.81	1.91
4	N	8702	KEG	W2-O26	-2.22	1.81	1.91
4	N	8705	KEG	W2-O26	-2.22	1.81	1.91
4	M	8701	KEG	W2-O26	-2.21	1.81	1.91
4	M	8703	KEG	W2-O26	-2.21	1.81	1.91
4	N	8703	KEG	W2-O26	-2.20	1.81	1.91
4	M	8702	KEG	W11-O44	-2.13	1.82	1.93
4	N	8704	KEG	W8-O41	-2.13	1.82	1.93
4	N	8702	KEG	W8-O41	-2.12	1.82	1.93
4	M	8701	KEG	W8-O41	-2.11	1.82	1.93
4	N	8705	KEG	W8-O41	-2.11	1.83	1.93
4	N	8702	KEG	W11-O44	-2.11	1.83	1.93
4	A	501	KEG	W8-O41	-2.11	1.83	1.93
4	N	8705	KEG	W11-O44	-2.11	1.83	1.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	KEG	W11-O44	-2.10	1.83	1.93
4	M	8703	KEG	W11-O44	-2.10	1.83	1.93
4	M	8702	KEG	W8-O41	-2.10	1.83	1.93
4	N	8703	KEG	W8-O41	-2.10	1.83	1.93
4	N	8701	KEG	W11-O44	-2.10	1.83	1.93
4	M	8703	KEG	W8-O41	-2.10	1.83	1.93
4	A	503	KEG	W8-O41	-2.09	1.83	1.93
4	N	8701	KEG	W8-O41	-2.09	1.83	1.93
4	N	8703	KEG	W11-O44	-2.09	1.83	1.93
4	N	8704	KEG	W11-O44	-2.09	1.83	1.93
4	A	502	KEG	W11-O44	-2.09	1.83	1.93
4	A	501	KEG	W11-O44	-2.09	1.83	1.93
4	A	502	KEG	W8-O41	-2.09	1.83	1.93
4	M	8701	KEG	W11-O44	-2.08	1.83	1.93

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	8701	KEG	O19-P1-O18	-2.23	104.65	108.92
4	N	8705	KEG	O19-P1-O18	-2.23	104.65	108.92
4	N	8702	KEG	O19-P1-O18	-2.22	104.68	108.92
4	A	502	KEG	O19-P1-O18	-2.20	104.71	108.92
4	M	8703	KEG	O19-P1-O18	-2.19	104.74	108.92
4	N	8704	KEG	O19-P1-O18	-2.18	104.74	108.92
4	A	501	KEG	O19-P1-O18	-2.18	104.74	108.92
4	M	8702	KEG	O19-P1-O18	-2.18	104.75	108.92
4	N	8703	KEG	O19-P1-O18	-2.18	104.75	108.92
4	N	8701	KEG	O19-P1-O18	-2.17	104.77	108.92
4	A	503	KEG	O19-P1-O18	-2.16	104.79	108.92
4	M	8701	KEG	O21-P1-O18	2.12	112.97	108.92
4	M	8703	KEG	O21-P1-O18	2.10	112.95	108.92
4	N	8705	KEG	O21-P1-O18	2.10	112.94	108.92
4	N	8704	KEG	O21-P1-O18	2.10	112.93	108.92
4	A	501	KEG	O21-P1-O18	2.09	112.93	108.92
4	N	8701	KEG	O21-P1-O18	2.09	112.92	108.92
4	N	8703	KEG	O21-P1-O18	2.08	112.91	108.92
4	A	503	KEG	O21-P1-O18	2.08	112.90	108.92
4	M	8702	KEG	O21-P1-O18	2.08	112.90	108.92
4	A	502	KEG	O21-P1-O18	2.07	112.89	108.92
4	N	8702	KEG	O21-P1-O18	2.07	112.89	108.92

There are no chirality outliers.

There are no torsion outliers.

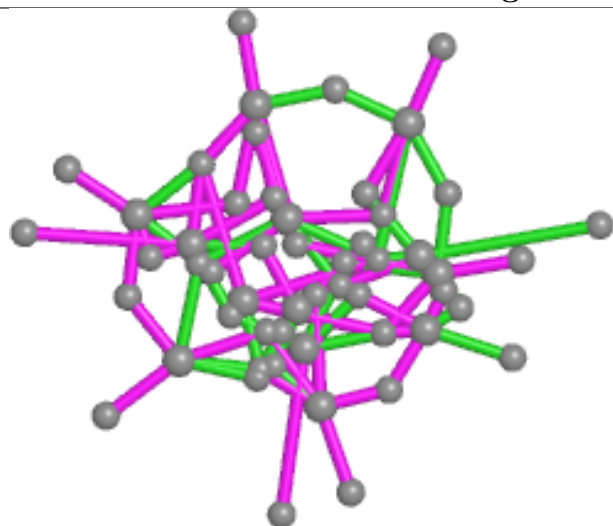
There are no ring outliers.

3 monomers are involved in 35 short contacts:

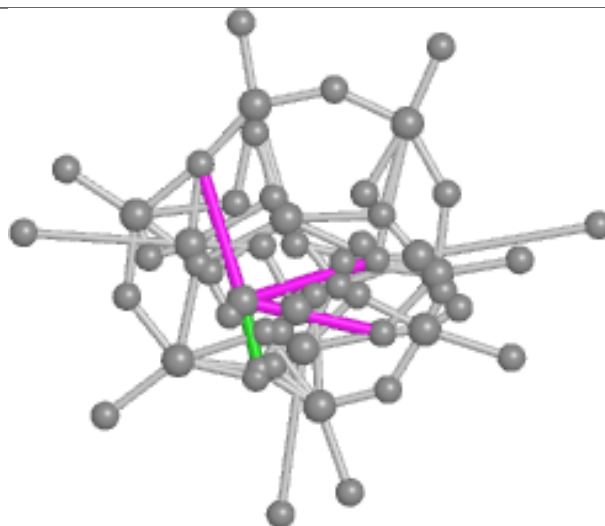
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	KEG	18	0
4	A	502	KEG	7	0
4	A	503	KEG	10	0

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.

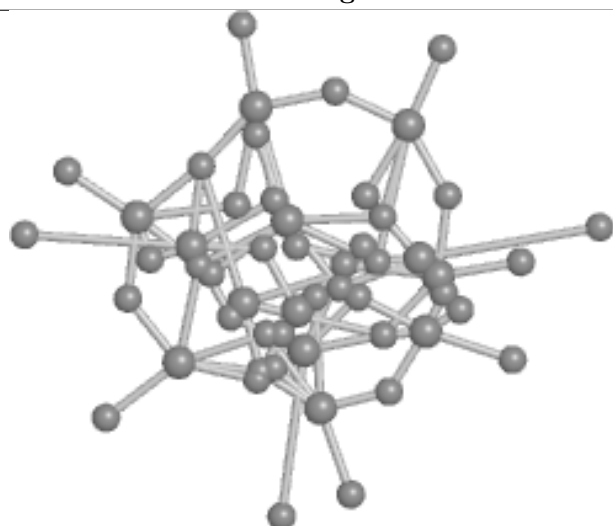
Ligand KEG N 8701



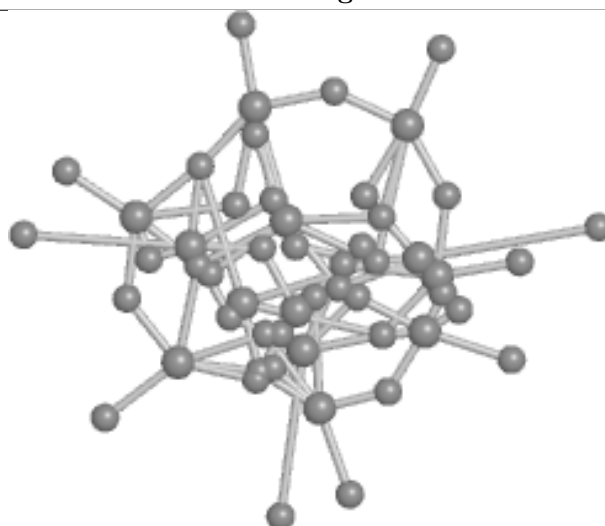
Bond lengths



Bond angles

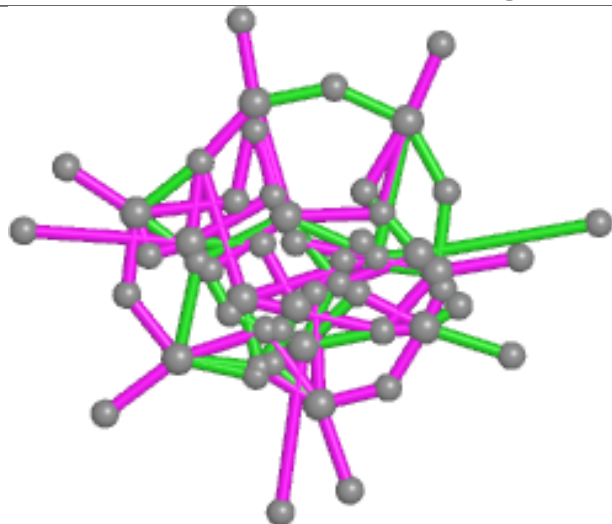


Torsions

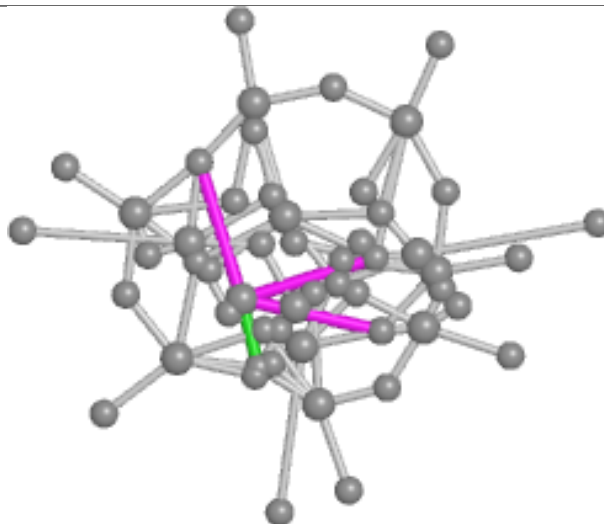


Rings

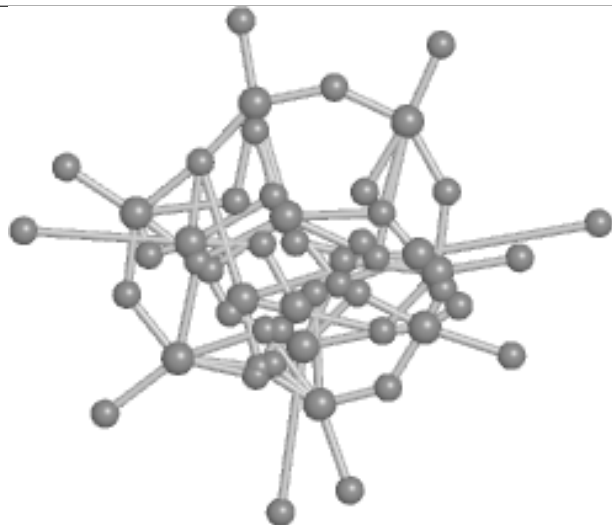
Ligand KEG N 8702



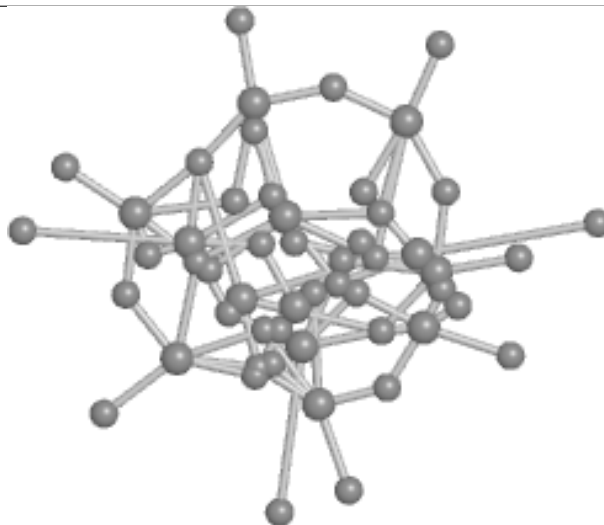
Bond lengths



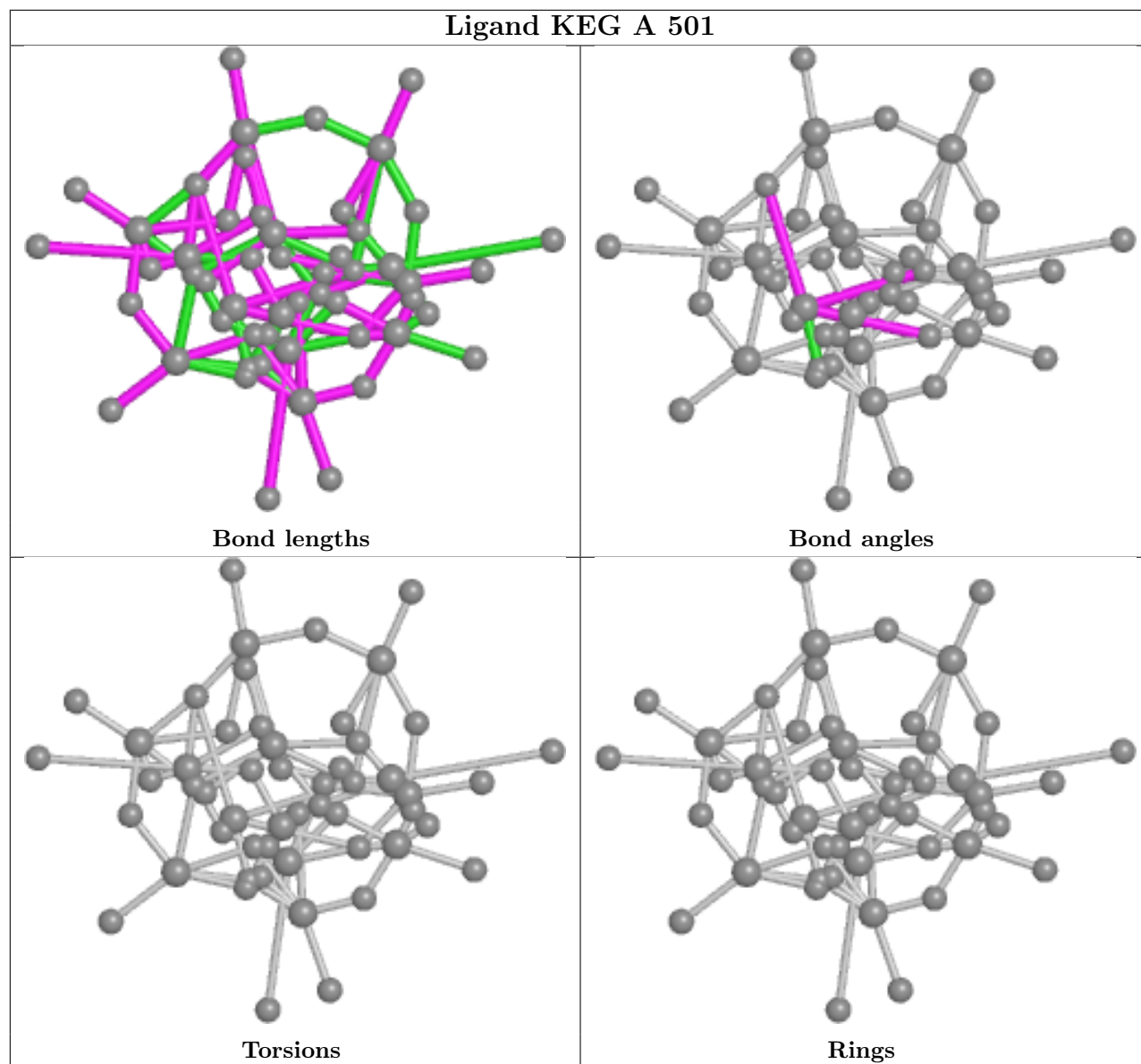
Bond angles



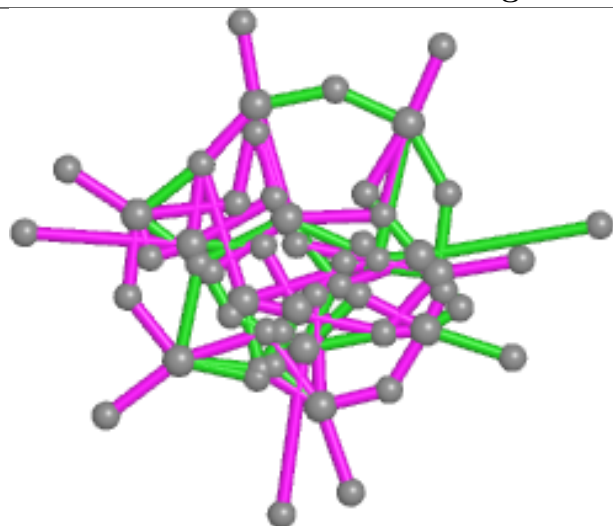
Torsions



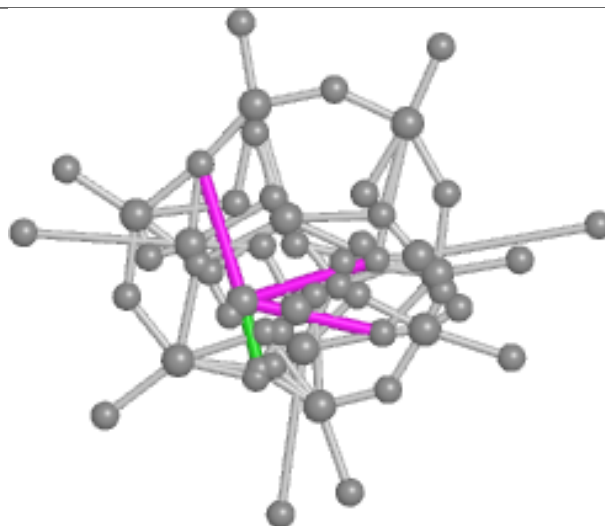
Rings



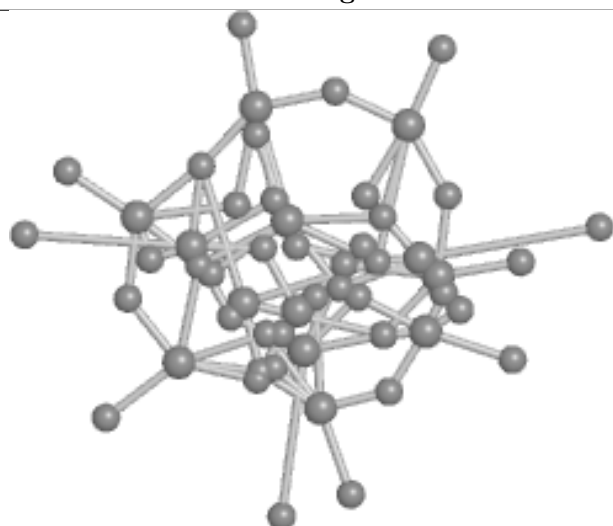
Ligand KEG N 8703



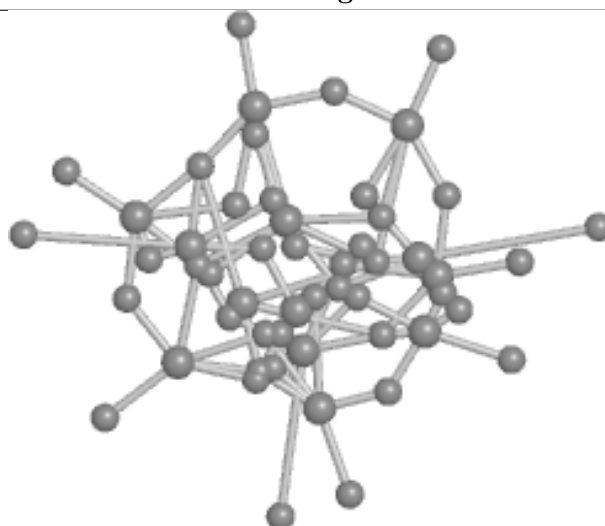
Bond lengths



Bond angles

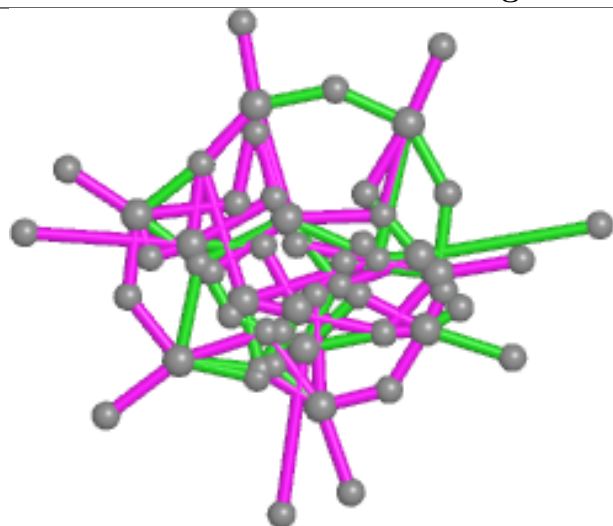


Torsions

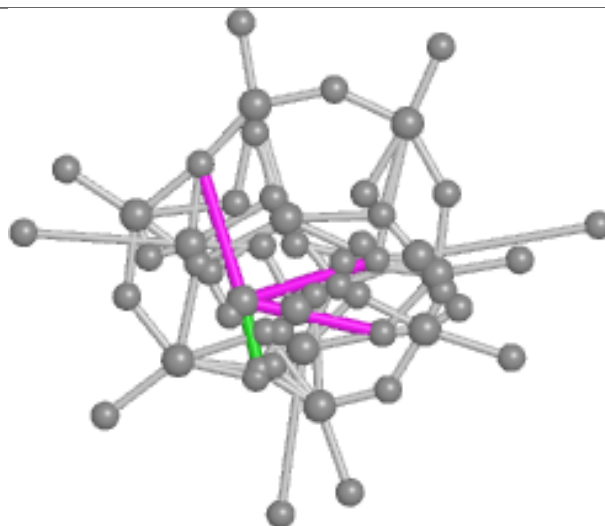


Rings

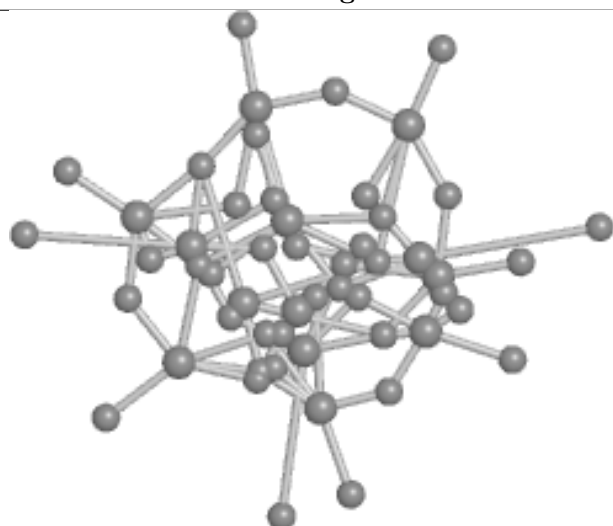
Ligand KEG N 8705



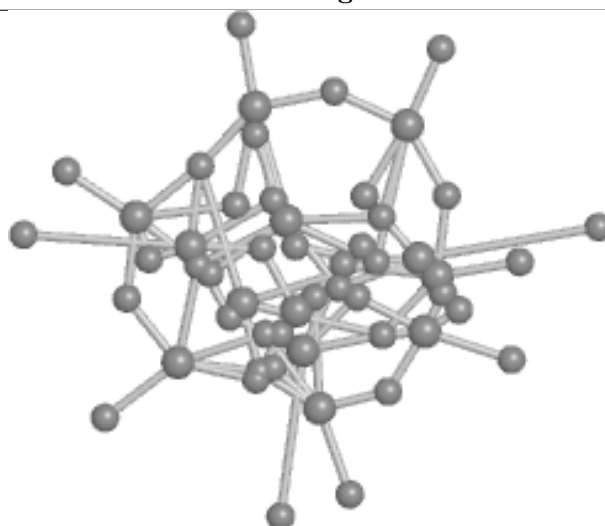
Bond lengths



Bond angles

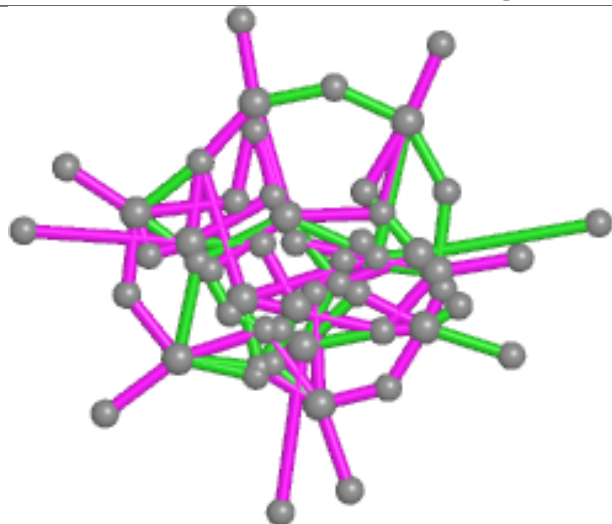


Torsions

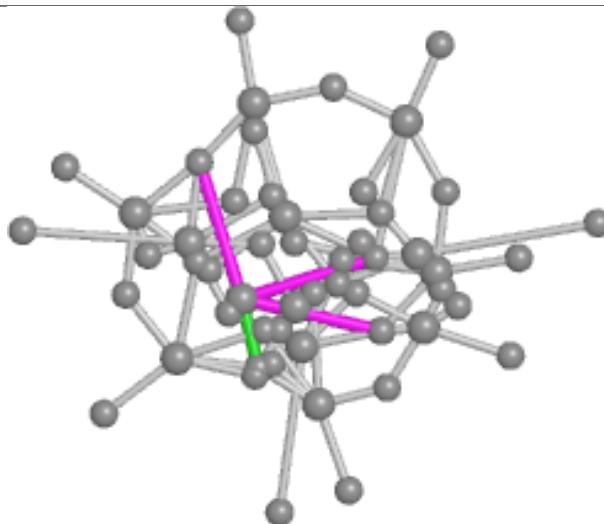


Rings

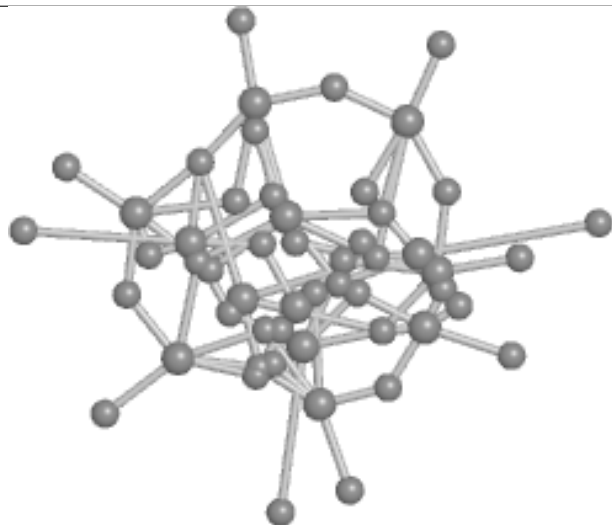
Ligand KEG M 8702



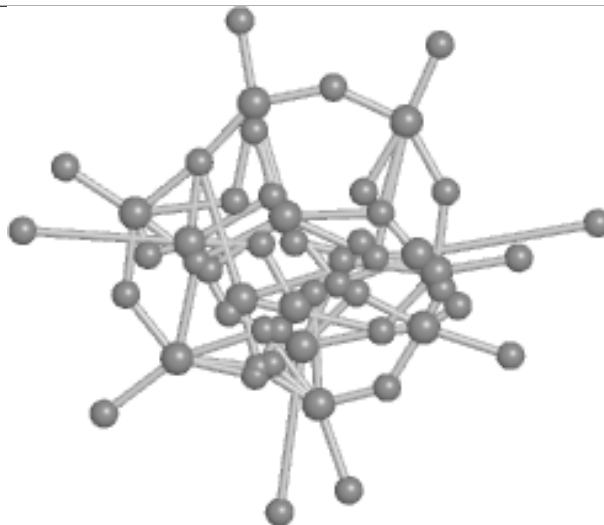
Bond lengths



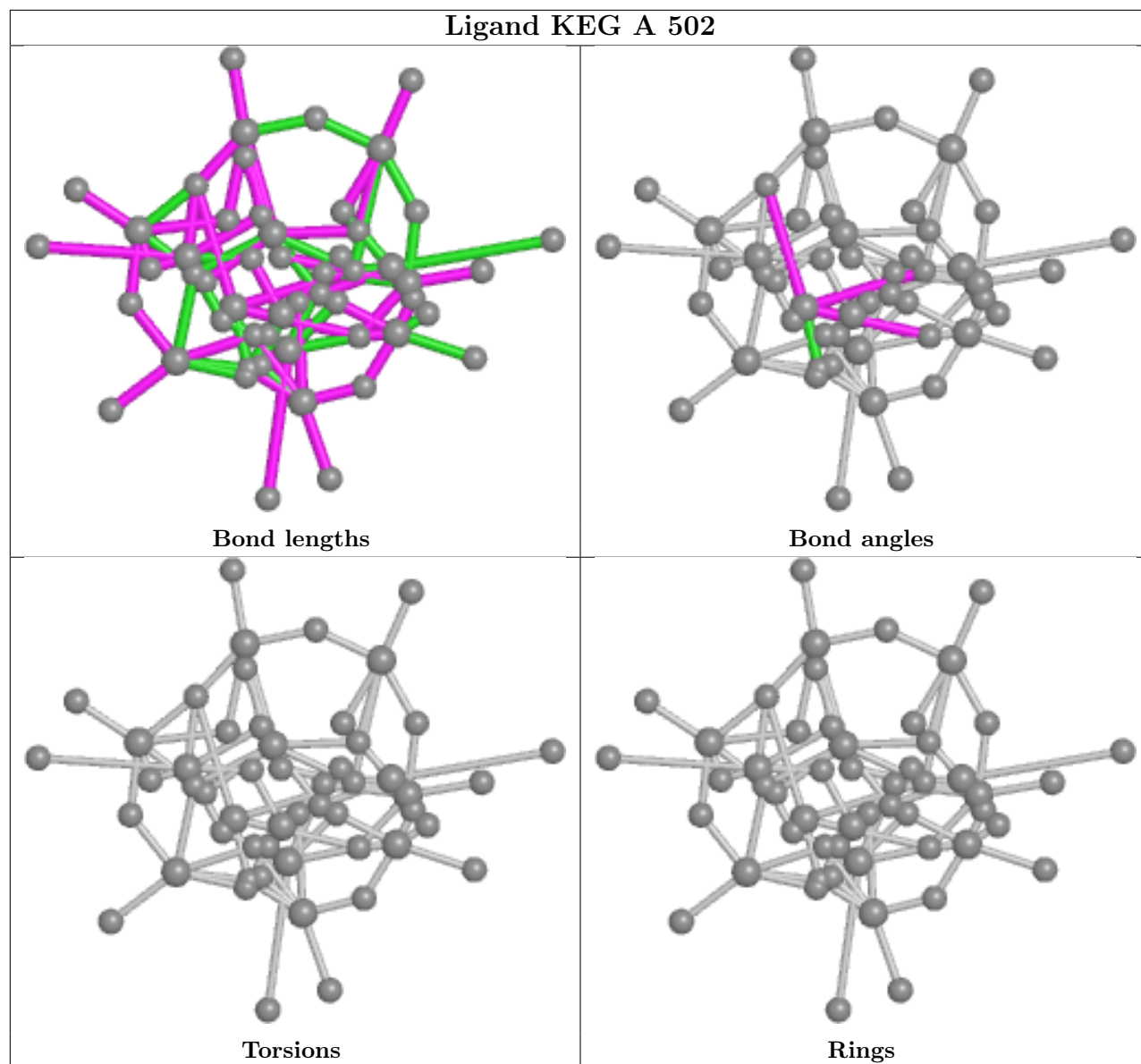
Bond angles



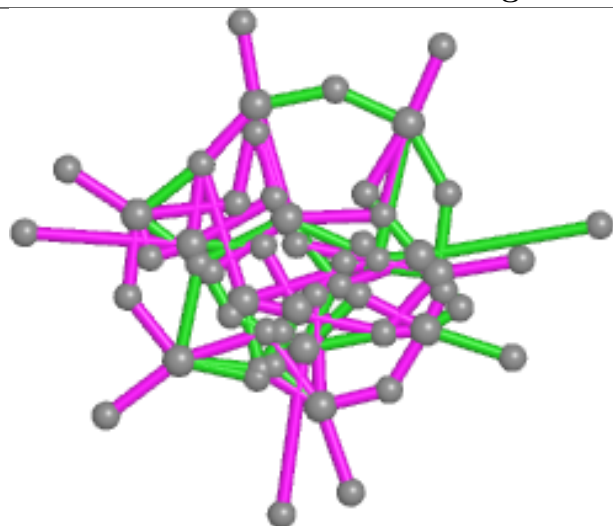
Torsions



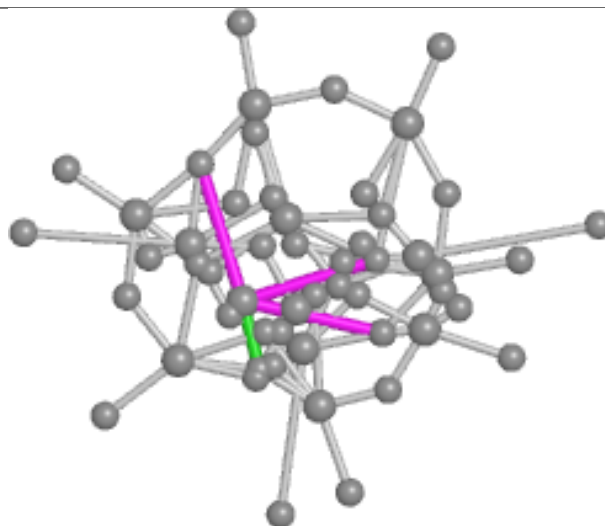
Rings



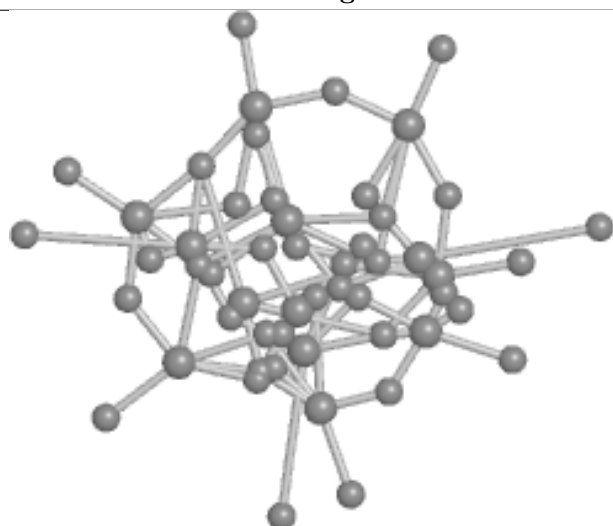
Ligand KEG N 8704



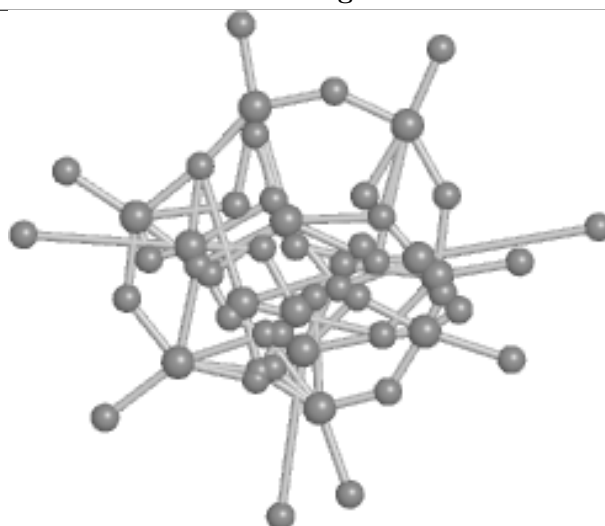
Bond lengths



Bond angles

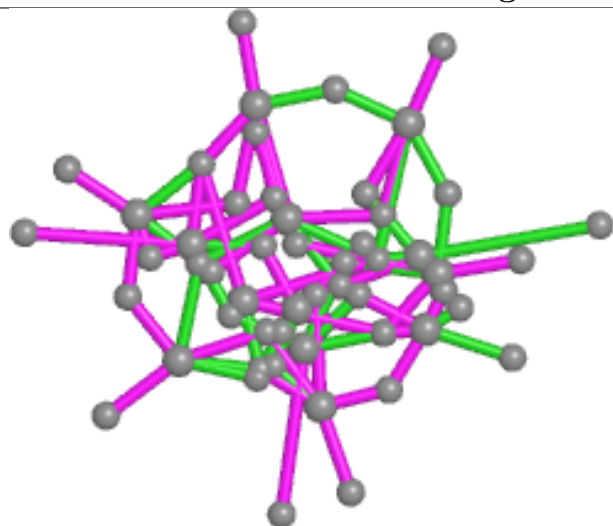


Torsions

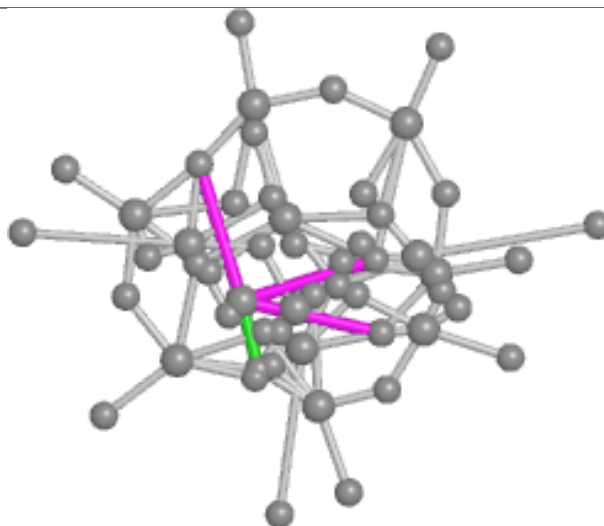


Rings

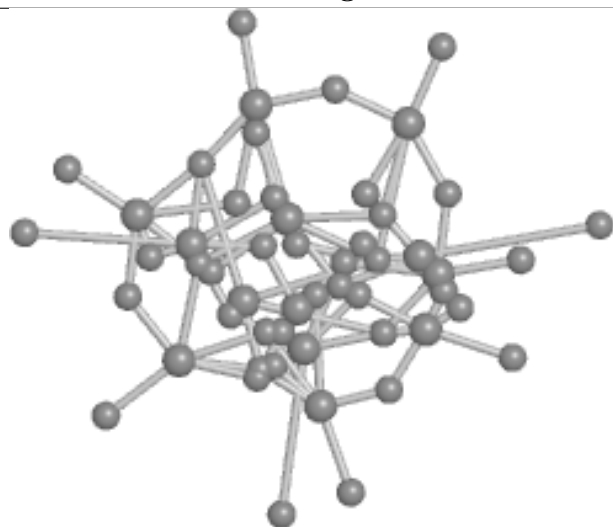
Ligand KEG M 8701



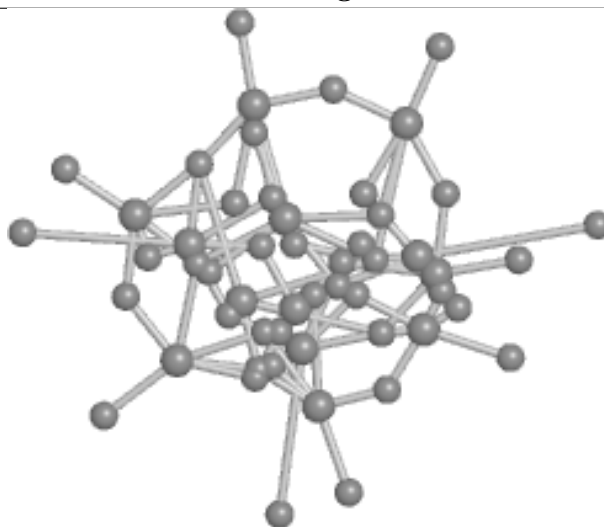
Bond lengths



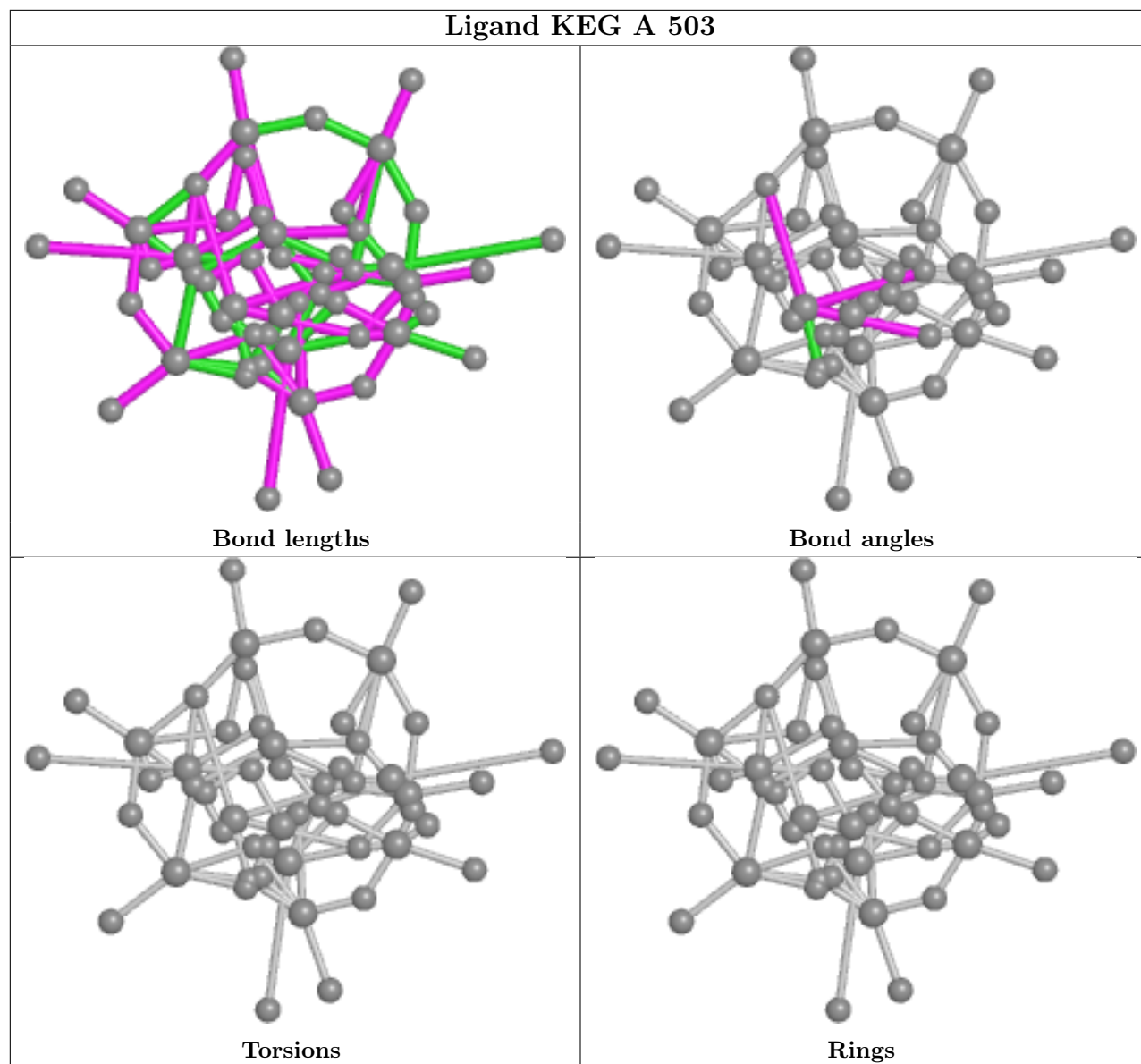
Bond angles

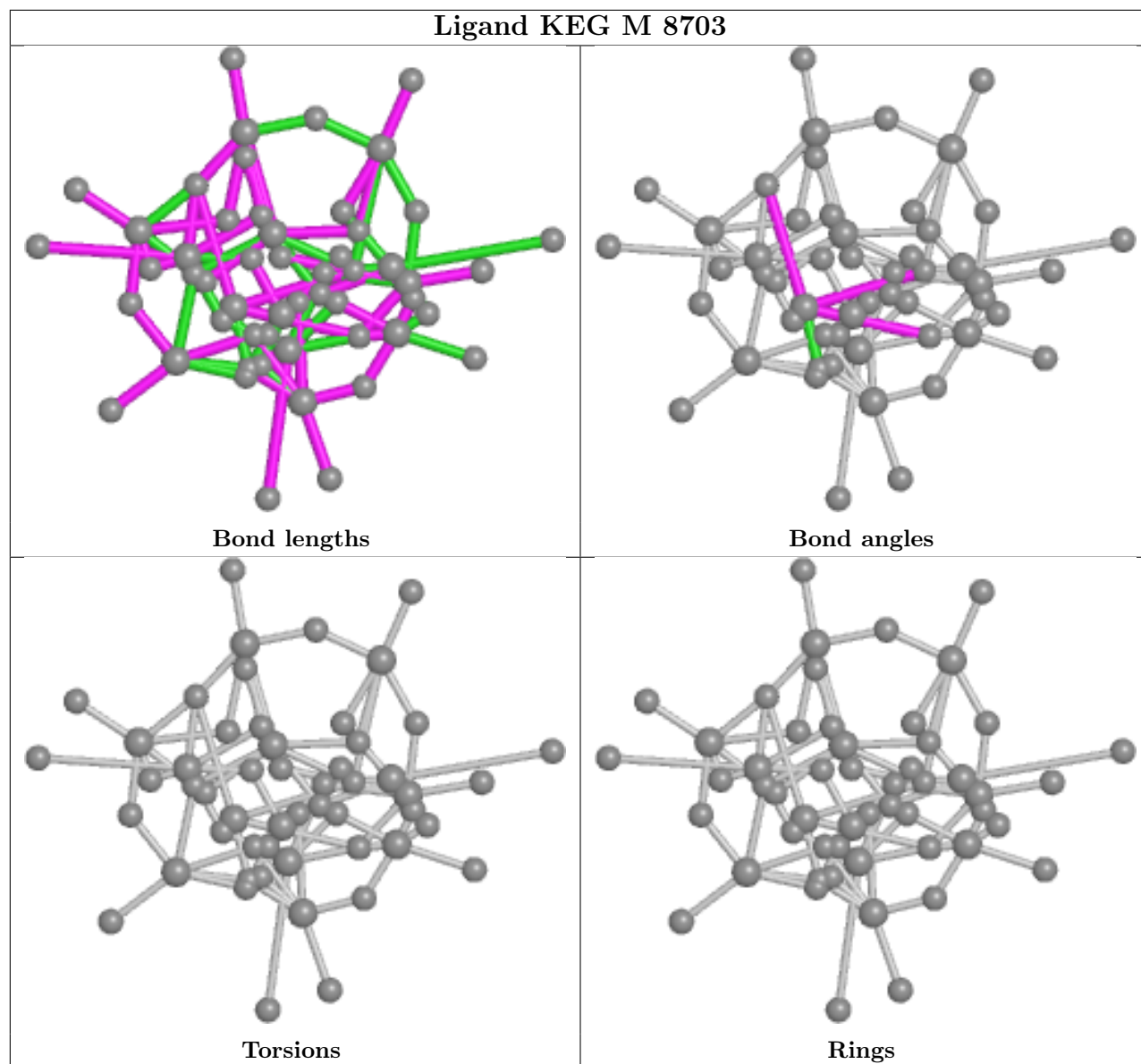


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	N	126
3	M	126
2	B	27
2	D	27

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	5289:UNK	C	6033:UNK	N	143.88
1	M	5289:UNK	C	6033:UNK	N	142.81
1	N	5148:UNK	C	5197:UNK	N	119.38
1	M	5148:UNK	C	5197:UNK	N	119.33
1	N	492:UNK	C	2104:UNK	N	118.52
1	M	492:UNK	C	2104:UNK	N	116.29
1	N	2121:UNK	C	2503:UNK	N	113.46
1	M	2121:UNK	C	2503:UNK	N	110.84
1	M	4017:UNK	C	4063:UNK	N	96.53
1	N	4017:UNK	C	4063:UNK	N	96.53
1	N	3052:UNK	C	3180:UNK	N	87.26
1	M	3052:UNK	C	3180:UNK	N	87.14
1	M	2992:UNK	C	3011:UNK	N	66.88
1	N	2992:UNK	C	3011:UNK	N	66.88
1	N	7362:UNK	C	8092:UNK	N	66.56
1	M	7362:UNK	C	8092:UNK	N	66.31
1	M	6744:UNK	C	6808:UNK	N	65.65
1	N	6744:UNK	C	6808:UNK	N	65.65
1	M	2846:UNK	C	2857:UNK	N	58.81
1	N	2846:UNK	C	2857:UNK	N	58.81
1	M	2958:UNK	C	2971:UNK	N	58.36
1	N	2958:UNK	C	2971:UNK	N	58.36
1	M	2927:UNK	C	2938:UNK	N	56.61
1	M	221:UNK	C	232:UNK	N	56.04
1	N	221:UNK	C	232:UNK	N	56.04
1	N	2927:UNK	C	2938:UNK	N	55.65
1	M	3200:UNK	C	4002:UNK	N	55.11
1	N	3200:UNK	C	4002:UNK	N	54.88
1	M	7079:UNK	C	7103:UNK	N	52.41
1	N	7079:UNK	C	7103:UNK	N	52.41
1	M	6081:UNK	C	6092:UNK	N	49.92
1	N	6081:UNK	C	6092:UNK	N	49.92
1	M	6871:UNK	C	6877:UNK	N	43.24
1	N	6871:UNK	C	6877:UNK	N	43.24
1	M	8498:UNK	C	8539:UNK	N	41.00
1	N	8498:UNK	C	8539:UNK	N	41.00
1	M	6502:UNK	C	6514:UNK	N	39.49
1	N	6502:UNK	C	6514:UNK	N	39.49
1	M	4105:UNK	C	4110:UNK	N	38.22
1	N	4105:UNK	C	4110:UNK	N	38.21
1	M	2681:UNK	C	2800:UNK	N	38.17
1	M	4618:UNK	C	4629:UNK	N	38.07

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	4618:UNK	C	4629:UNK	N	38.07
1	M	4734:UNK	C	4746:UNK	N	37.66
1	N	4734:UNK	C	4746:UNK	N	37.66
1	M	2523:UNK	C	2537:UNK	N	36.92
1	N	2523:UNK	C	2537:UNK	N	36.92
1	N	8253:UNK	C	8256:UNK	N	36.58
1	M	4688:UNK	C	4690:UNK	N	36.49
1	N	4688:UNK	C	4690:UNK	N	36.49
1	N	2681:UNK	C	2800:UNK	N	36.35
1	M	8253:UNK	C	8256:UNK	N	36.29
1	M	2895:UNK	C	2906:UNK	N	36.08
1	N	2895:UNK	C	2906:UNK	N	36.08
1	M	471:UNK	C	482:UNK	N	35.36
1	N	471:UNK	C	482:UNK	N	35.36
1	M	8126:UNK	C	8133:UNK	N	35.02
1	N	8126:UNK	C	8133:UNK	N	35.02
1	M	6114:UNK	C	6123:UNK	N	34.38
1	N	6114:UNK	C	6123:UNK	N	34.38
1	M	4353:UNK	C	4366:UNK	N	34.34
1	N	4353:UNK	C	4366:UNK	N	34.34
1	M	6826:UNK	C	6830:UNK	N	34.23
1	N	6826:UNK	C	6830:UNK	N	34.23
1	M	6680:UNK	C	6692:UNK	N	33.69
1	N	6680:UNK	C	6692:UNK	N	33.69
1	M	411:UNK	C	425:UNK	N	33.36
1	N	411:UNK	C	425:UNK	N	33.36
1	M	6053:UNK	C	6066:UNK	N	32.68
1	N	6053:UNK	C	6066:UNK	N	32.68
1	M	4567:UNK	C	4578:UNK	N	31.33
1	N	4567:UNK	C	4578:UNK	N	31.33
1	M	4895:UNK	C	4905:UNK	N	30.94
1	N	4895:UNK	C	4905:UNK	N	30.94
1	M	4709:UNK	C	4720:UNK	N	30.88
1	N	4709:UNK	C	4720:UNK	N	30.88
1	M	4217:UNK	C	4230:UNK	N	30.33
1	N	4217:UNK	C	4230:UNK	N	30.33
1	M	6647:UNK	C	6659:UNK	N	29.73
1	N	6647:UNK	C	6659:UNK	N	29.73
1	M	4273:UNK	C	4286:UNK	N	29.70
1	N	4273:UNK	C	4286:UNK	N	29.70
1	M	4187:UNK	C	4199:UNK	N	29.38
1	N	4187:UNK	C	4199:UNK	N	29.38

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	4443:UNK	C	4454:UNK	N	29.37
1	M	4763:UNK	C	4780:UNK	N	29.37
1	N	4443:UNK	C	4454:UNK	N	29.37
1	N	4763:UNK	C	4780:UNK	N	29.37
1	M	5238:UNK	C	5251:UNK	N	28.59
1	N	5238:UNK	C	5251:UNK	N	28.59
1	M	4244:UNK	C	4255:UNK	N	28.49
1	N	4244:UNK	C	4255:UNK	N	28.49
1	M	7222:UNK	C	7342:UNK	N	28.20
1	N	7222:UNK	C	7342:UNK	N	28.20
1	M	4472:UNK	C	4484:UNK	N	28.19
1	N	4472:UNK	C	4484:UNK	N	28.19
1	M	8299:UNK	C	8311:UNK	N	28.06
1	N	8299:UNK	C	8311:UNK	N	28.06
1	M	8226:UNK	C	8234:UNK	N	28.03
1	N	8226:UNK	C	8234:UNK	N	28.03
1	M	4076:UNK	C	4089:UNK	N	27.97
1	N	4076:UNK	C	4089:UNK	N	27.97
1	M	6468:UNK	C	6480:UNK	N	27.60
1	N	6468:UNK	C	6480:UNK	N	27.60
1	M	8442:UNK	C	8449:UNK	N	26.57
1	N	8442:UNK	C	8449:UNK	N	26.57
1	M	4325:UNK	C	4337:UNK	N	26.47
1	N	4325:UNK	C	4337:UNK	N	26.46
1	M	8106:UNK	C	8109:UNK	N	25.92
1	N	8106:UNK	C	8109:UNK	N	25.92
1	M	6283:UNK	C	6296:UNK	N	25.90
1	N	6283:UNK	C	6296:UNK	N	25.90
1	M	292:UNK	C	303:UNK	N	25.77
1	N	292:UNK	C	303:UNK	N	25.77
1	M	8483:UNK	C	8485:UNK	N	24.83
1	N	8483:UNK	C	8485:UNK	N	24.83
1	M	4875:UNK	C	4886:UNK	N	24.81
1	N	4875:UNK	C	4886:UNK	N	24.81
1	M	186:UNK	C	200:UNK	N	24.57
1	N	186:UNK	C	200:UNK	N	24.57
1	M	4540:UNK	C	4552:UNK	N	24.41
1	N	4540:UNK	C	4552:UNK	N	24.41
1	M	5211:UNK	C	5225:UNK	N	24.30
1	M	8325:UNK	C	8338:UNK	N	24.29
1	N	5211:UNK	C	5225:UNK	N	24.29
1	N	8325:UNK	C	8338:UNK	N	24.29

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	134:UNK	C	138:UNK	N	23.96
1	M	350:UNK	C	365:UNK	N	23.96
1	N	134:UNK	C	138:UNK	N	23.96
1	N	350:UNK	C	365:UNK	N	23.96
1	M	6711:UNK	C	6724:UNK	N	23.79
1	N	6711:UNK	C	6724:UNK	N	23.79
1	M	6845:UNK	C	6856:UNK	N	23.48
1	N	6845:UNK	C	6856:UNK	N	23.48
1	M	6935:UNK	C	7068:UNK	N	23.38
1	N	6935:UNK	C	7068:UNK	N	23.38
1	M	4931:UNK	C	4942:UNK	N	23.35
1	N	4931:UNK	C	4942:UNK	N	23.35
1	M	2558:UNK	C	2569:UNK	N	23.23
1	N	2558:UNK	C	2569:UNK	N	23.23
1	M	8156:UNK	C	8166:UNK	N	23.07
1	N	8156:UNK	C	8166:UNK	N	23.07
1	M	6350:UNK	C	6372:UNK	N	22.69
1	N	6350:UNK	C	6372:UNK	N	22.69
1	M	4417:UNK	C	4431:UNK	N	22.67
1	N	4417:UNK	C	4431:UNK	N	22.67
1	M	117:UNK	C	119:UNK	N	22.35
1	N	117:UNK	C	119:UNK	N	22.35
1	M	4380:UNK	C	4386:UNK	N	21.94
1	N	4380:UNK	C	4386:UNK	N	21.94
1	M	4644:UNK	C	4671:UNK	N	21.42
1	N	4644:UNK	C	4671:UNK	N	21.42
1	M	6888:UNK	C	6900:UNK	N	20.85
1	N	6888:UNK	C	6900:UNK	N	20.85
1	M	8427:UNK	C	8432:UNK	N	20.71
1	N	8427:UNK	C	8432:UNK	N	20.71
1	M	264:UNK	C	276:UNK	N	20.62
1	N	264:UNK	C	276:UNK	N	20.62
1	M	63:UNK	C	69:UNK	N	20.54
1	N	63:UNK	C	69:UNK	N	20.54
1	M	17:UNK	C	24:UNK	N	20.40
1	N	17:UNK	C	24:UNK	N	20.40
1	M	150:UNK	C	158:UNK	N	19.85
1	N	150:UNK	C	158:UNK	N	19.85
1	M	4950:UNK	C	5137:UNK	N	19.70
1	N	4950:UNK	C	5137:UNK	N	19.70
1	M	4794:UNK	C	4804:UNK	N	19.52
1	N	4794:UNK	C	4804:UNK	N	19.52

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	8204:UNK	C	8211:UNK	N	19.44
1	N	8204:UNK	C	8211:UNK	N	19.43
1	M	4399:UNK	C	4407:UNK	N	19.41
1	N	4399:UNK	C	4407:UNK	N	19.41
1	M	4163:UNK	C	4173:UNK	N	19.34
1	N	4163:UNK	C	4173:UNK	N	19.34
1	M	2647:UNK	C	2663:UNK	N	19.24
1	N	2647:UNK	C	2663:UNK	N	19.24
1	M	98:UNK	C	108:UNK	N	19.08
1	N	98:UNK	C	108:UNK	N	19.08
1	M	4854:UNK	C	4865:UNK	N	19.05
1	N	4854:UNK	C	4865:UNK	N	19.05
1	M	6557:UNK	C	6601:UNK	N	18.71
1	N	6557:UNK	C	6601:UNK	N	18.71
1	M	6911:UNK	C	6924:UNK	N	18.05
1	N	6911:UNK	C	6924:UNK	N	18.05
1	M	2809:UNK	C	2822:UNK	N	17.92
1	N	2809:UNK	C	2822:UNK	N	17.92
1	N	4828:UNK	C	4841:UNK	N	17.16
1	M	4828:UNK	C	4841:UNK	N	17.15
1	M	8179:UNK	C	8193:UNK	N	17.14
1	N	8179:UNK	C	8193:UNK	N	17.14
1	M	6194:UNK	C	6210:UNK	N	15.76
1	N	6194:UNK	C	6210:UNK	N	15.76
1	B	254:UNK	C	261:UNK	N	15.57
1	D	254:UNK	C	261:UNK	N	15.57
1	M	382:UNK	C	394:UNK	N	15.53
1	N	382:UNK	C	394:UNK	N	15.53
1	M	6161:UNK	C	6172:UNK	N	15.30
1	N	6161:UNK	C	6172:UNK	N	15.30
1	M	79:UNK	C	83:UNK	N	15.14
1	N	79:UNK	C	83:UNK	N	15.14
1	M	8355:UNK	C	8367:UNK	N	15.11
1	N	8355:UNK	C	8367:UNK	N	15.11
1	M	6416:UNK	C	6431:UNK	N	14.90
1	N	6416:UNK	C	6431:UNK	N	14.90
1	N	7167:UNK	C	7201:UNK	N	14.22
1	M	7167:UNK	C	7201:UNK	N	14.21
1	M	8269:UNK	C	8274:UNK	N	14.20
1	N	8269:UNK	C	8274:UNK	N	14.20
1	M	442:UNK	C	455:UNK	N	14.03
1	N	442:UNK	C	455:UNK	N	14.03

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	4128:UNK	C	4136:UNK	N	14.01
1	N	4128:UNK	C	4136:UNK	N	14.01
1	M	6316:UNK	C	6327:UNK	N	13.82
1	N	6316:UNK	C	6327:UNK	N	13.82
1	M	38:UNK	C	44:UNK	N	13.50
1	N	38:UNK	C	44:UNK	N	13.50
1	B	84:UNK	C	91:UNK	N	12.91
1	D	84:UNK	C	91:UNK	N	12.91
1	M	2608:UNK	C	2630:UNK	N	12.79
1	N	2608:UNK	C	2630:UNK	N	12.79
1	B	42:UNK	C	49:UNK	N	12.40
1	D	42:UNK	C	49:UNK	N	12.40
1	M	6532:UNK	C	6542:UNK	N	12.09
1	N	6532:UNK	C	6542:UNK	N	12.09
1	M	4588:UNK	C	4598:UNK	N	11.91
1	N	4588:UNK	C	4598:UNK	N	11.90
1	B	168:UNK	C	175:UNK	N	11.88
1	D	168:UNK	C	175:UNK	N	11.88
1	M	6622:UNK	C	6636:UNK	N	11.62
1	N	6622:UNK	C	6636:UNK	N	11.61
1	M	6242:UNK	C	6267:UNK	N	11.55
1	N	6242:UNK	C	6267:UNK	N	11.55
1	M	8407:UNK	C	8415:UNK	N	11.17
1	N	8407:UNK	C	8415:UNK	N	11.16
1	N	4303:UNK	C	4314:UNK	N	11.14
1	M	4303:UNK	C	4314:UNK	N	11.13
1	B	127:UNK	C	133:UNK	N	11.04
1	D	127:UNK	C	133:UNK	N	11.04
1	M	4499:UNK	C	4511:UNK	N	10.80
1	N	4499:UNK	C	4511:UNK	N	10.80
1	M	8379:UNK	C	8393:UNK	N	10.75
1	N	8379:UNK	C	8393:UNK	N	10.75
1	M	5262:UNK	C	5273:UNK	N	10.22
1	N	5262:UNK	C	5273:UNK	N	10.22
1	B	211:UNK	C	216:UNK	N	10.20
1	D	211:UNK	C	216:UNK	N	10.20
1	M	6389:UNK	C	6402:UNK	N	10.15
1	N	6389:UNK	C	6402:UNK	N	10.15
1	M	319:UNK	C	332:UNK	N	10.11
1	N	319:UNK	C	332:UNK	N	10.11
1	M	169:UNK	C	175:UNK	N	10.01
1	N	169:UNK	C	175:UNK	N	10.01

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	8460:UNK	C	8471:UNK	N	9.97
1	N	8460:UNK	C	8471:UNK	N	9.97
1	M	7143:UNK	C	7147:UNK	N	9.83
1	N	7143:UNK	C	7147:UNK	N	9.83
1	B	299:UNK	C	304:UNK	N	9.31
1	D	299:UNK	C	304:UNK	N	9.31
1	M	4145:UNK	C	4151:UNK	N	8.71
1	N	4145:UNK	C	4151:UNK	N	8.71
1	M	6442:UNK	C	6453:UNK	N	8.69
1	N	6442:UNK	C	6453:UNK	N	8.69
1	B	320:UNK	C	327:UNK	N	7.11
1	D	320:UNK	C	327:UNK	N	7.11
1	B	97:UNK	C	101:UNK	N	7.02
1	D	97:UNK	C	101:UNK	N	7.02
1	N	4525:UNK	C	4529:UNK	N	6.93
1	M	4525:UNK	C	4529:UNK	N	6.92
1	B	287:UNK	C	293:UNK	N	6.66
1	D	287:UNK	C	293:UNK	N	6.66
1	B	199:UNK	C	205:UNK	N	6.62
1	D	199:UNK	C	205:UNK	N	6.62
1	B	179:UNK	C	184:UNK	N	6.48
1	D	179:UNK	C	184:UNK	N	6.48
1	B	309:UNK	C	315:UNK	N	5.88
1	D	309:UNK	C	315:UNK	N	5.88
1	B	268:UNK	C	272:UNK	N	5.87
1	D	268:UNK	C	272:UNK	N	5.86
1	B	222:UNK	C	228:UNK	N	5.63
1	D	222:UNK	C	228:UNK	N	5.63
1	B	138:UNK	C	142:UNK	N	5.56
1	D	138:UNK	C	142:UNK	N	5.56
1	B	277:UNK	C	283:UNK	N	5.52
1	D	277:UNK	C	283:UNK	N	5.52
1	B	54:UNK	C	58:UNK	N	5.34
1	D	54:UNK	C	58:UNK	N	5.34
1	B	157:UNK	C	162:UNK	N	4.74
1	D	157:UNK	C	162:UNK	N	4.74
1	B	233:UNK	C	237:UNK	N	4.70
1	D	233:UNK	C	237:UNK	N	4.70
1	B	73:UNK	C	78:UNK	N	4.64
1	D	73:UNK	C	78:UNK	N	4.64
1	B	64:UNK	C	67:UNK	N	3.96
1	D	64:UNK	C	67:UNK	N	3.96

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	8287:UNK	C	8289:UNK	N	3.95
1	N	8287:UNK	C	8289:UNK	N	3.95
1	B	106:UNK	C	109:UNK	N	3.94
1	D	106:UNK	C	109:UNK	N	3.94
1	B	242:UNK	C	246:UNK	N	3.91
1	D	242:UNK	C	246:UNK	N	3.91
1	B	190:UNK	C	193:UNK	N	3.80
1	D	190:UNK	C	193:UNK	N	3.80
1	B	148:UNK	C	151:UNK	N	3.75
1	D	148:UNK	C	151:UNK	N	3.74
1	B	116:UNK	C	119:UNK	N	3.73
1	D	116:UNK	C	119:UNK	N	3.73

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	374/446 (83%)	3.10	237 (63%) 0 2	200, 200, 200, 200	0
1	C	374/446 (83%)	2.77	218 (58%) 0 2	200, 200, 200, 200	0
2	B	0/400	-	-	-	-
2	D	0/400	-	-	-	-
3	M	0/2300	-	-	-	-
3	N	0/2300	-	-	-	-
All	All	748/6292 (11%)	2.93	455 (60%) 0 2	200, 200, 200, 200	0

All (455) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	GLU	24.1
1	A	386	GLU	22.0
1	A	222	GLU	16.9
1	A	385	ASN	15.7
1	C	108	SER	14.3
1	A	384	THR	13.4
1	C	399	ARG	12.8
1	C	222	GLU	11.7
1	C	172	SER	11.7
1	A	62	THR	11.6
1	C	166	TYR	11.2
1	A	179	LYS	11.1
1	C	398	GLY	10.9
1	C	336	VAL	10.4
1	A	263	GLN	10.0
1	C	371	ASP	9.9
1	C	258	CYS	9.4
1	C	395	GLY	9.4
1	A	155	LYS	9.1
1	C	109	GLY	9.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	335	THR	9.0
1	A	181	LYS	9.0
1	C	225	ASP	8.9
1	C	107	LYS	8.8
1	A	425	ARG	8.8
1	C	255	ARG	8.7
1	C	140	ARG	8.7
1	A	219	LYS	8.6
1	A	335	THR	8.6
1	A	305	GLU	8.5
1	A	141	GLU	8.4
1	A	388	ASP	8.1
1	A	182	ASP	7.9
1	A	226	MET	7.8
1	C	343	GLU	7.8
1	A	225	ASP	7.7
1	C	200	ARG	7.7
1	C	396	ARG	7.6
1	C	424	GLU	7.4
1	A	107	LYS	7.3
1	A	364	ASP	7.3
1	C	390	TYR	7.2
1	A	191	THR	7.1
1	A	144	TYR	7.0
1	A	108	SER	7.0
1	C	391	LEU	6.8
1	A	129	GLY	6.8
1	A	348	ARG	6.8
1	C	283	GLN	6.8
1	A	229	ASP	6.7
1	C	110	LEU	6.7
1	A	184	ALA	6.6
1	A	84	HIS	6.6
1	A	106	ALA	6.4
1	A	347	ALA	6.3
1	A	417	GLU	6.3
1	A	109	GLY	6.2
1	C	397	ALA	6.2
1	A	426	PHE	6.1
1	A	370	ILE	6.0
1	A	249	THR	6.0
1	A	220	VAL	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	345	ARG	5.9
1	C	153	PHE	5.8
1	A	366	PHE	5.7
1	C	113	THR	5.7
1	C	392	HIS	5.6
1	A	291	ARG	5.6
1	A	280	GLY	5.6
1	A	151	LEU	5.5
1	C	228	ARG	5.5
1	C	168	GLY	5.4
1	A	411	SER	5.4
1	C	176	GLU	5.4
1	C	91	HIS	5.3
1	C	141	GLU	5.3
1	A	138	ASN	5.3
1	C	270	VAL	5.3
1	C	330	ASN	5.3
1	C	338	GLY	5.3
1	A	320	ASN	5.2
1	A	95	GLN	5.2
1	A	164	VAL	5.2
1	A	112	LYS	5.2
1	A	368	ARG	5.2
1	C	303	ASP	5.2
1	A	228	ARG	5.1
1	A	356	GLU	5.1
1	A	267	GLU	5.1
1	A	248	ALA	5.1
1	A	67	PHE	5.0
1	C	246	PHE	5.0
1	C	260	ARG	5.0
1	C	400	PHE	5.0
1	A	367	GLY	5.0
1	C	224	LEU	4.9
1	A	79	ASP	4.9
1	C	319	ALA	4.8
1	A	105	GLN	4.8
1	C	317	THR	4.8
1	C	329	SER	4.7
1	A	113	THR	4.7
1	C	344	GLU	4.7
1	C	250	LEU	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	226	MET	4.7
1	C	356	GLU	4.7
1	C	362	SER	4.6
1	A	332	PRO	4.6
1	A	351	ALA	4.6
1	A	319	ALA	4.6
1	C	155	LYS	4.6
1	A	166	TYR	4.6
1	C	346	ILE	4.6
1	A	369	GLY	4.6
1	A	80	CYS	4.6
1	A	383	LEU	4.6
1	C	291	ARG	4.5
1	A	199	VAL	4.5
1	C	357	LYS	4.5
1	A	193	GLY	4.5
1	C	144	TYR	4.5
1	C	347	ALA	4.5
1	A	330	ASN	4.5
1	C	145	GLN	4.5
1	C	370	ILE	4.5
1	A	387	ALA	4.5
1	A	253	GLU	4.4
1	C	385	ASN	4.4
1	A	444	LEU	4.4
1	A	395	GLY	4.4
1	A	223	GLU	4.4
1	A	397	ALA	4.4
1	A	111	GLY	4.4
1	C	348	ARG	4.3
1	A	216	GLU	4.3
1	C	294	ASN	4.3
1	C	269	PHE	4.3
1	A	110	LEU	4.3
1	C	149	GLU	4.3
1	C	123	GLN	4.3
1	A	301	LEU	4.3
1	A	343	GLU	4.2
1	C	148	ASN	4.2
1	A	336	VAL	4.2
1	A	410	VAL	4.2
1	A	147	ARG	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	83	GLU	4.2
1	C	394	VAL	4.2
1	C	217	CYS	4.1
1	A	128	PRO	4.1
1	C	223	GLU	4.1
1	A	353	LYS	4.1
1	A	318	ARG	4.1
1	A	159	ASP	4.1
1	C	416	GLU	4.1
1	A	416	GLU	4.0
1	C	87	GLU	4.0
1	A	440	PRO	4.0
1	A	90	GLN	4.0
1	A	116	PHE	4.0
1	A	227	ARG	4.0
1	C	221	LEU	4.0
1	A	373	GLU	3.9
1	A	401	GLY	3.9
1	A	75	ARG	3.9
1	A	224	LEU	3.9
1	A	290	GLU	3.9
1	A	360	CYS	3.9
1	A	334	ILE	3.9
1	A	194	ARG	3.9
1	C	427	ASP	3.9
1	C	401	GLY	3.9
1	A	148	ASN	3.9
1	A	103	LEU	3.9
1	A	392	HIS	3.8
1	A	176	GLU	3.8
1	C	364	ASP	3.8
1	A	324	LYS	3.8
1	C	112	LYS	3.8
1	A	270	VAL	3.8
1	C	417	GLU	3.8
1	A	396	ARG	3.8
1	C	231	GLN	3.8
1	C	202	LYS	3.8
1	A	142	LEU	3.8
1	A	287	LYS	3.7
1	C	74	SER	3.7
1	C	157	MET	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	167	GLY	3.7
1	C	444	LEU	3.7
1	C	138	ASN	3.6
1	A	363	THR	3.6
1	A	72	GLU	3.6
1	C	360	CYS	3.6
1	C	66	ASP	3.6
1	C	167	GLY	3.6
1	C	181	LYS	3.6
1	A	329	SER	3.6
1	A	317	THR	3.6
1	C	259	ARG	3.6
1	C	280	GLY	3.6
1	A	200	ARG	3.5
1	C	212	PHE	3.5
1	C	425	ARG	3.5
1	A	376	ASN	3.5
1	A	97	ILE	3.5
1	A	314	LYS	3.5
1	A	232	GLU	3.5
1	A	259	ARG	3.5
1	C	143	ALA	3.5
1	C	80	CYS	3.5
1	C	361	VAL	3.5
1	A	421	LYS	3.5
1	A	281	LEU	3.5
1	C	386	GLU	3.5
1	C	104	CYS	3.5
1	A	403	LYS	3.5
1	A	269	PHE	3.5
1	C	147	ARG	3.5
1	A	365	VAL	3.4
1	A	371	ASP	3.4
1	A	160	VAL	3.4
1	A	399	ARG	3.4
1	A	68	LEU	3.4
1	A	101	ASP	3.4
1	C	161	LYS	3.4
1	C	337	HIS	3.4
1	C	359	ILE	3.4
1	C	287	LYS	3.4
1	C	229	ASP	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	62	THR	3.4
1	C	192	PRO	3.3
1	A	115	VAL	3.3
1	C	193	GLY	3.3
1	C	215	ASP	3.3
1	C	252	GLN	3.3
1	C	251	SER	3.3
1	C	121	LEU	3.3
1	A	236	ALA	3.3
1	A	316	THR	3.3
1	A	240	ASP	3.3
1	A	427	ASP	3.3
1	A	321	GLU	3.3
1	C	164	VAL	3.3
1	C	368	ARG	3.2
1	A	192	PRO	3.2
1	A	186	HIS	3.2
1	C	332	PRO	3.2
1	A	315	SER	3.2
1	A	168	GLY	3.2
1	C	142	LEU	3.2
1	A	361	VAL	3.2
1	A	145	GLN	3.2
1	C	305	GLU	3.2
1	C	78	ILE	3.2
1	C	97	ILE	3.2
1	C	379	ILE	3.2
1	A	435	GLU	3.1
1	C	402	THR	3.1
1	C	111	GLY	3.1
1	A	202	LYS	3.1
1	A	400	PHE	3.1
1	A	338	GLY	3.1
1	C	179	LYS	3.1
1	A	132	ALA	3.1
1	C	73	LEU	3.1
1	A	126	PRO	3.1
1	C	120	THR	3.1
1	C	314	LYS	3.1
1	C	352	PHE	3.1
1	C	313	VAL	3.1
1	A	114	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	156	TYR	3.1
1	C	117	VAL	3.0
1	A	412	SER	3.0
1	A	312	PHE	3.0
1	A	205	ASP	3.0
1	A	162	THR	3.0
1	C	388	ASP	3.0
1	A	196	LYS	3.0
1	A	65	LYS	3.0
1	C	95	GLN	2.9
1	C	169	THR	2.9
1	A	127	VAL	2.9
1	A	171	ILE	2.9
1	C	106	ALA	2.9
1	C	152	ARG	2.9
1	A	260	ARG	2.9
1	A	350	LYS	2.9
1	A	178	LEU	2.9
1	A	391	LEU	2.9
1	C	369	GLY	2.9
1	A	140	ARG	2.9
1	A	415	ASP	2.9
1	C	302	ASP	2.9
1	A	378	ALA	2.8
1	C	363	THR	2.8
1	A	327	ASN	2.8
1	A	70	LYS	2.8
1	C	324	LYS	2.8
1	C	432	GLU	2.8
1	A	143	ALA	2.8
1	A	153	PHE	2.8
1	A	150	TYR	2.8
1	C	254	ILE	2.8
1	C	374	ARG	2.8
1	A	81	GLY	2.8
1	A	215	ASP	2.8
1	C	150	TYR	2.8
1	C	188	VAL	2.8
1	A	357	LYS	2.8
1	A	262	LEU	2.8
1	A	212	PHE	2.8
1	C	429	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	429	LYS	2.7
1	A	203	TYR	2.7
1	C	436	GLU	2.7
1	C	420	ALA	2.7
1	A	123	GLN	2.7
1	C	318	ARG	2.7
1	C	245	MET	2.7
1	C	403	LYS	2.7
1	C	103	LEU	2.7
1	A	185	PRO	2.7
1	A	344	GLU	2.7
1	A	104	CYS	2.7
1	A	180	ASN	2.7
1	A	188	VAL	2.7
1	C	173	LYS	2.7
1	A	245	MET	2.7
1	C	373	GLU	2.7
1	A	100	THR	2.7
1	A	362	SER	2.7
1	A	372	ILE	2.6
1	C	171	ILE	2.6
1	C	428	VAL	2.6
1	A	244	MET	2.6
1	A	389	GLN	2.6
1	C	210	LYS	2.6
1	A	345	ARG	2.6
1	C	151	LEU	2.6
1	A	289	GLU	2.6
1	A	82	PHE	2.6
1	A	413	LYS	2.6
1	C	241	LYS	2.6
1	C	129	GLY	2.6
1	A	124	LEU	2.6
1	C	282	GLN	2.6
1	C	349	TYR	2.6
1	A	265	PRO	2.6
1	C	185	PRO	2.5
1	A	161	LYS	2.5
1	C	426	PHE	2.5
1	C	358	ARG	2.5
1	A	311	ILE	2.5
1	C	266	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	72	GLU	2.5
1	A	406	ALA	2.5
1	A	66	ASP	2.5
1	A	294	ASN	2.5
1	C	365	VAL	2.5
1	C	315	SER	2.5
1	C	382	ASP	2.5
1	C	63	GLY	2.5
1	A	239	ARG	2.5
1	A	63	GLY	2.5
1	C	253	GLU	2.4
1	C	372	ILE	2.4
1	C	265	PRO	2.4
1	C	65	LYS	2.4
1	A	121	LEU	2.4
1	C	309	VAL	2.4
1	A	354	ASP	2.4
1	C	116	PHE	2.4
1	C	100	THR	2.4
1	C	249	THR	2.4
1	C	102	VAL	2.4
1	C	118	LEU	2.4
1	C	320	ASN	2.4
1	A	213	VAL	2.4
1	C	295	ARG	2.4
1	A	341	LYS	2.4
1	A	204	ILE	2.4
1	C	83	GLU	2.4
1	C	196	LYS	2.4
1	C	405	LEU	2.4
1	C	114	ALA	2.4
1	A	407	ILE	2.4
1	C	204	ILE	2.4
1	C	311	ILE	2.4
1	C	244	MET	2.4
1	C	381	TYR	2.4
1	C	389	GLN	2.4
1	A	379	ILE	2.4
1	A	349	TYR	2.4
1	C	248	ALA	2.3
1	A	261	PHE	2.3
1	A	98	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	232	GLU	2.3
1	A	210	LYS	2.3
1	A	423	GLN	2.3
1	C	331	PHE	2.3
1	A	218	ASP	2.3
1	C	211	ASN	2.3
1	A	381	TYR	2.3
1	A	441	SER	2.3
1	C	434	PRO	2.3
1	C	203	TYR	2.2
1	A	134	VAL	2.2
1	A	221	LEU	2.2
1	A	297	LEU	2.2
1	A	398	GLY	2.2
1	C	298	ALA	2.2
1	C	125	ASP	2.2
1	A	133	VAL	2.2
1	C	132	ALA	2.2
1	C	299	GLN	2.2
1	C	366	PHE	2.2
1	A	264	ASN	2.2
1	C	304	LEU	2.2
1	A	120	THR	2.2
1	C	316	THR	2.2
1	C	227	ARG	2.2
1	A	69	LEU	2.2
1	A	197	ALA	2.2
1	C	180	ASN	2.2
1	C	115	VAL	2.2
1	C	159	ASP	2.2
1	C	393	ARG	2.2
1	A	420	ALA	2.2
1	C	85	PRO	2.2
1	C	158	PRO	2.2
1	C	156	TYR	2.2
1	C	189	VAL	2.2
1	A	99	GLY	2.1
1	C	124	LEU	2.1
1	A	119	SER	2.1
1	C	135	VAL	2.1
1	A	139	ALA	2.1
1	A	78	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	146	ILE	2.1
1	A	131	VAL	2.1
1	A	283	GLN	2.1
1	C	175	ALA	2.1
1	C	170	PRO	2.1
1	A	322	LEU	2.1
1	C	219	LYS	2.1
1	C	263	GLN	2.1
1	A	310	ILE	2.1
1	C	67	PHE	2.1
1	C	201	GLU	2.1
1	A	325	LEU	2.0
1	C	136	ILE	2.0
1	A	359	ILE	2.0
1	A	250	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	KEG	N	8703	53/53	0.85	0.15	200,200,200,200	53
4	KEG	A	502	53/53	0.88	0.18	200,200,200,200	53
4	KEG	A	503	53/53	0.89	0.20	200,200,200,200	53
4	KEG	M	8703	53/53	0.91	0.14	200,200,200,200	53
4	KEG	N	8704	53/53	0.93	0.12	200,200,200,200	53
4	KEG	N	8702	53/53	0.94	0.12	200,200,200,200	53
4	KEG	N	8705	53/53	0.94	0.11	200,200,200,200	53
4	KEG	M	8701	53/53	0.96	0.08	200,200,200,200	53

Continued on next page...

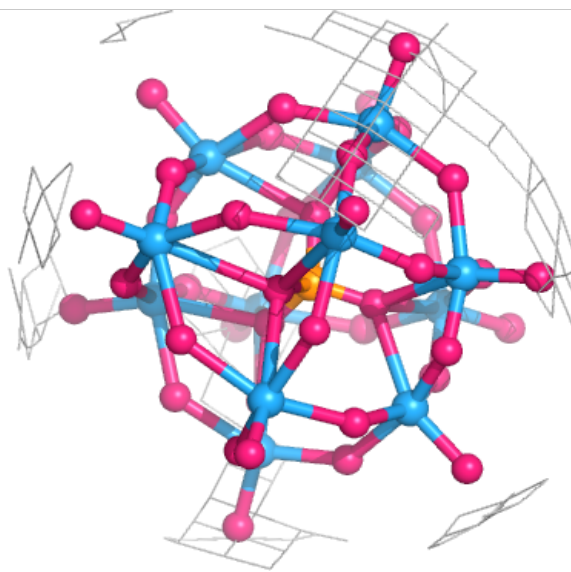
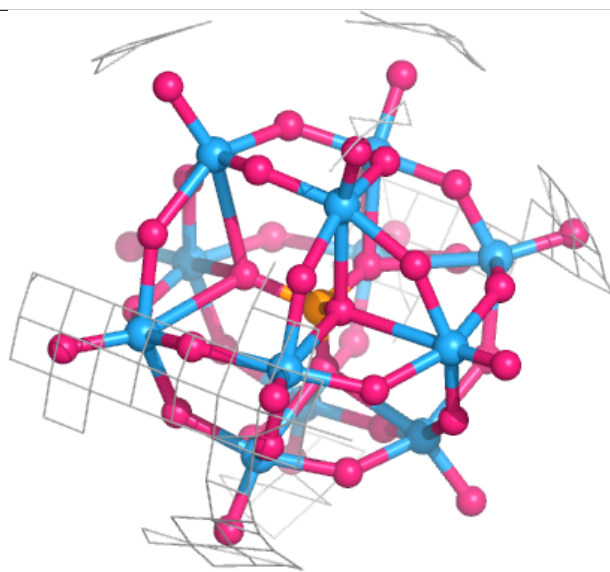
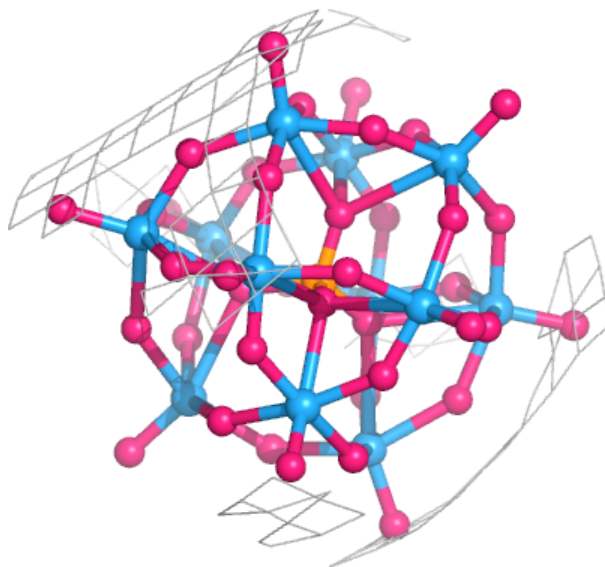
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	KEG	M	8702	53/53	0.96	0.09	200,200,200,200	53
4	KEG	A	501	53/53	0.96	0.11	200,200,200,200	53
4	KEG	N	8701	53/53	0.96	0.08	200,200,200,200	53

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

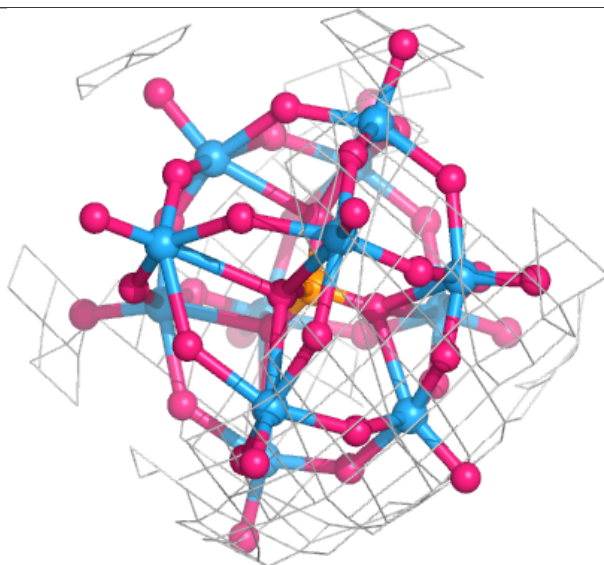
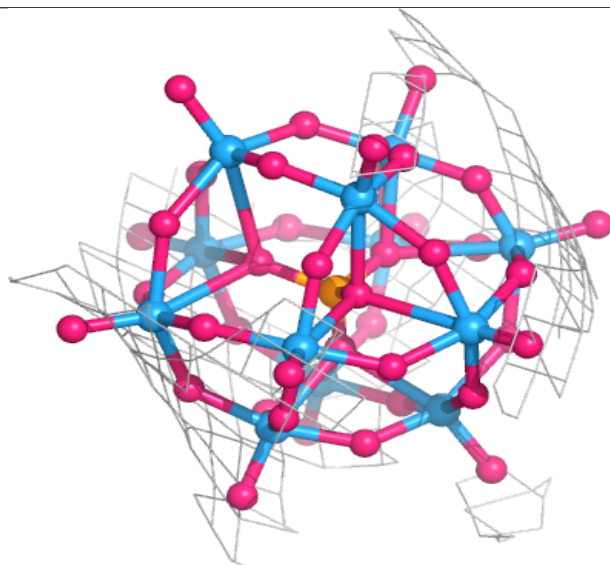
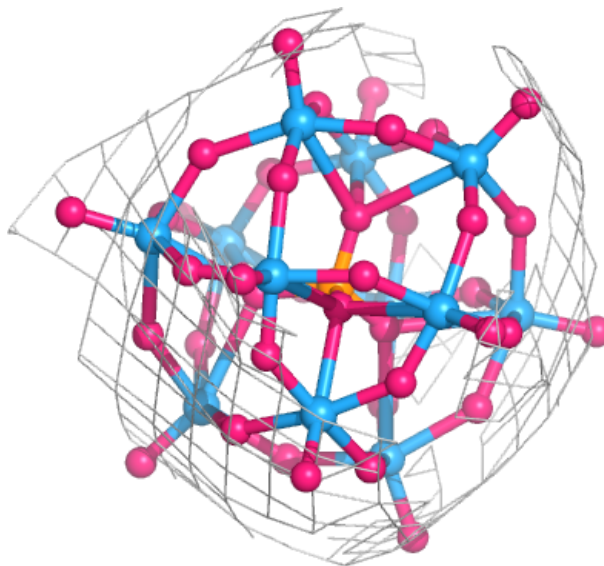
Electron density around KEG N 8703:

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



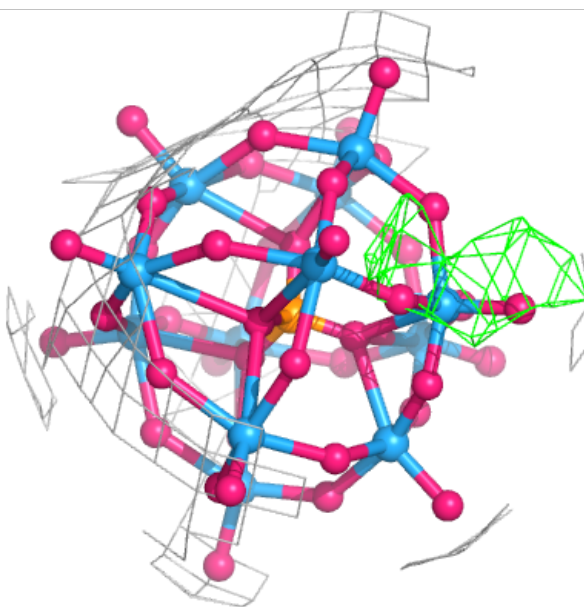
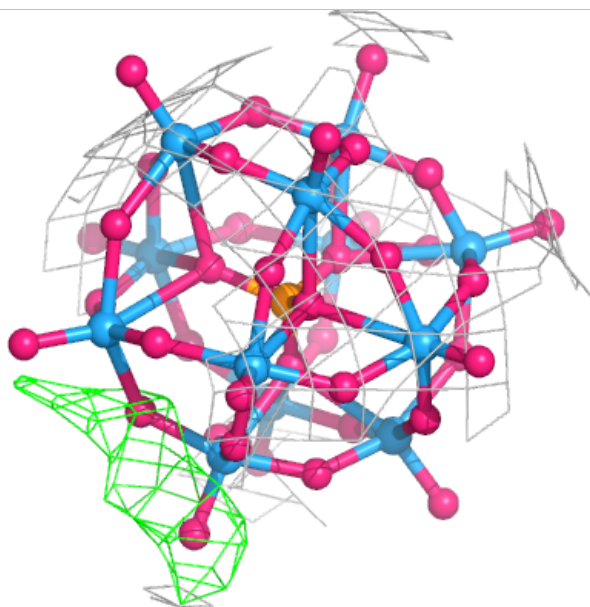
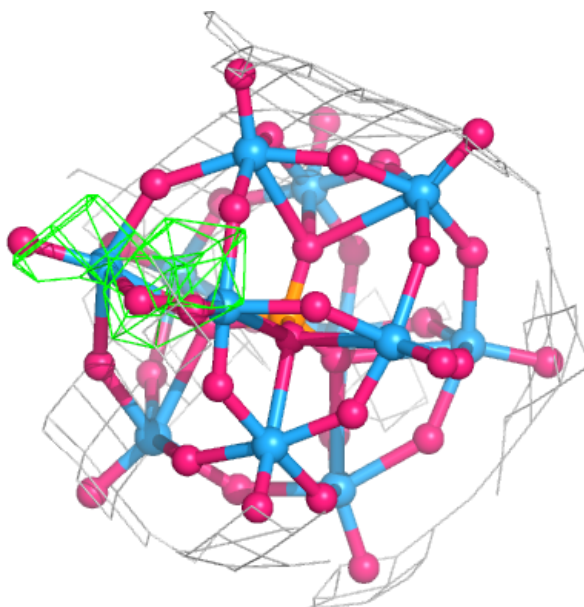
Electron density around KEG A 502:

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



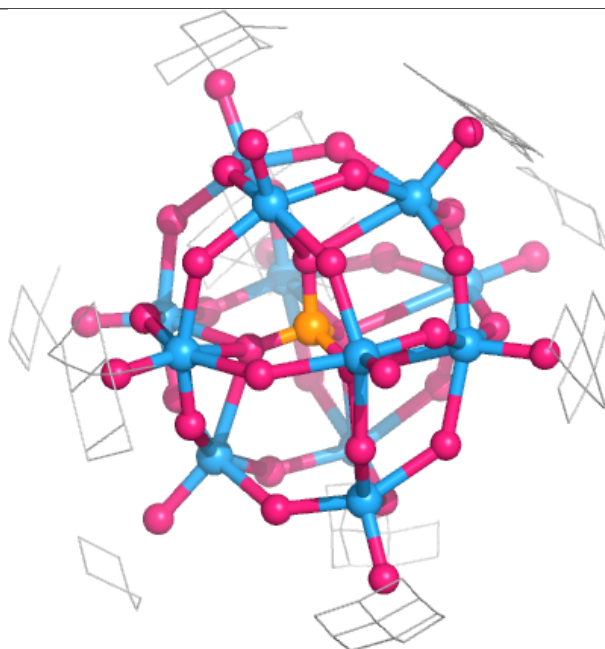
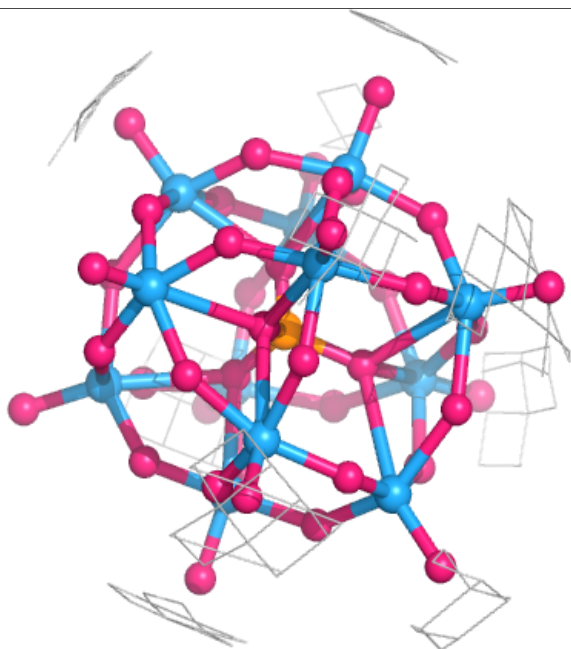
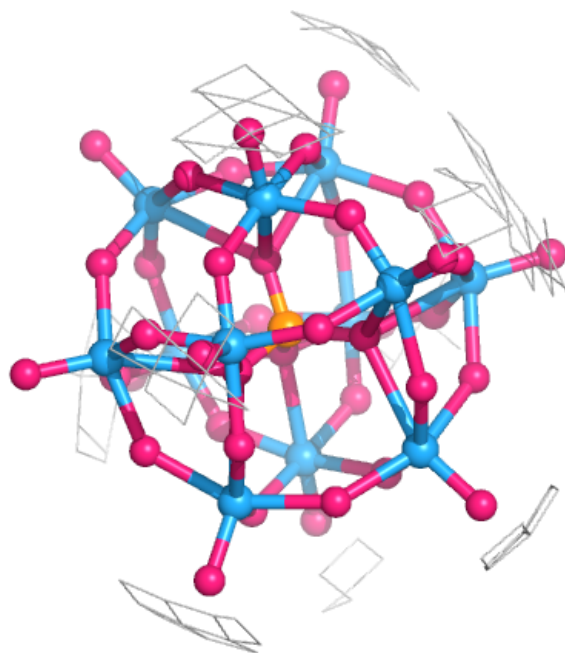
Electron density around KEG A 503:

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



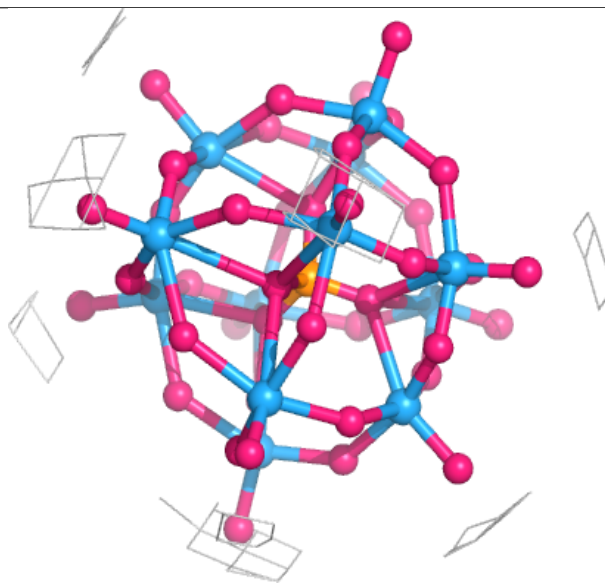
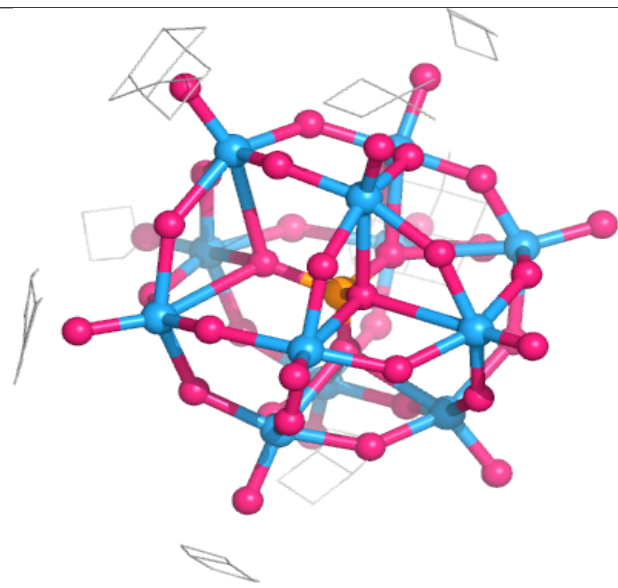
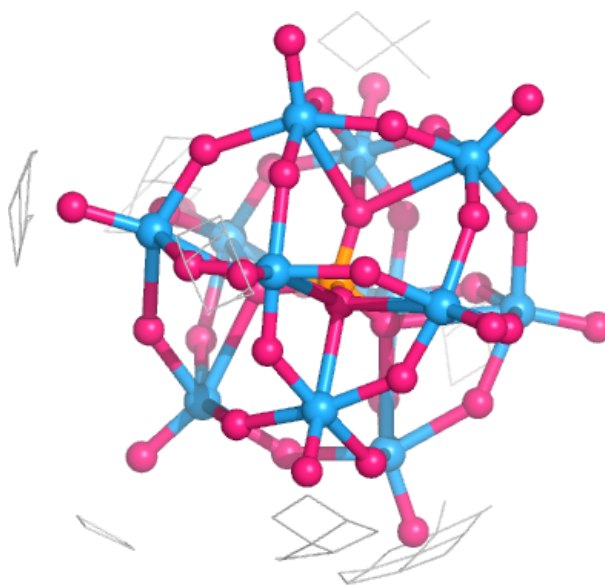
Electron density around KEG M 8703:

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



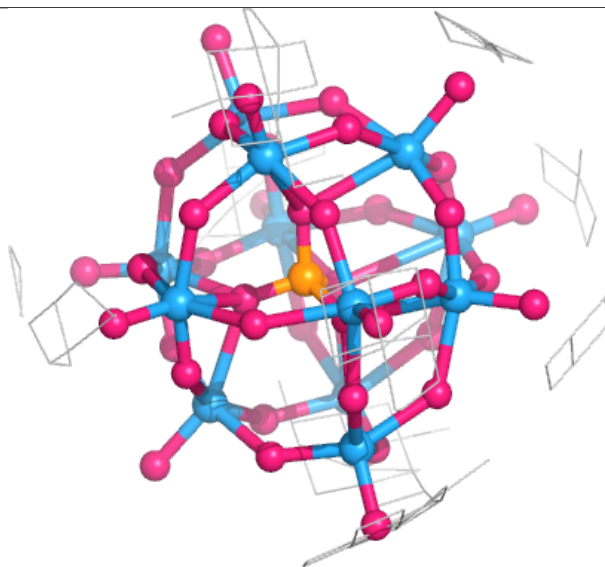
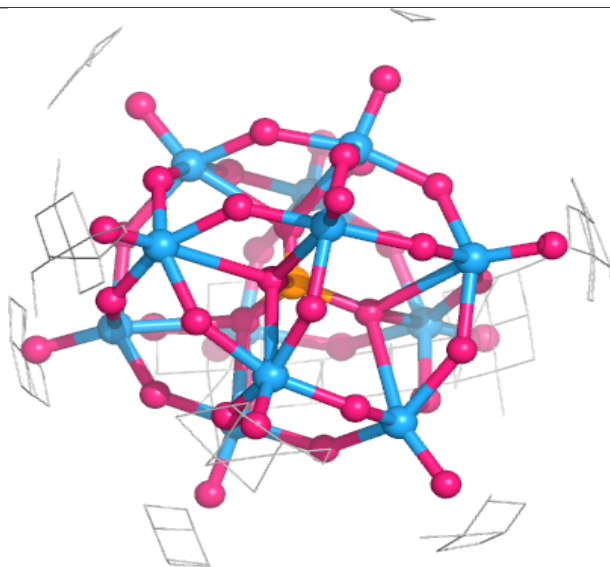
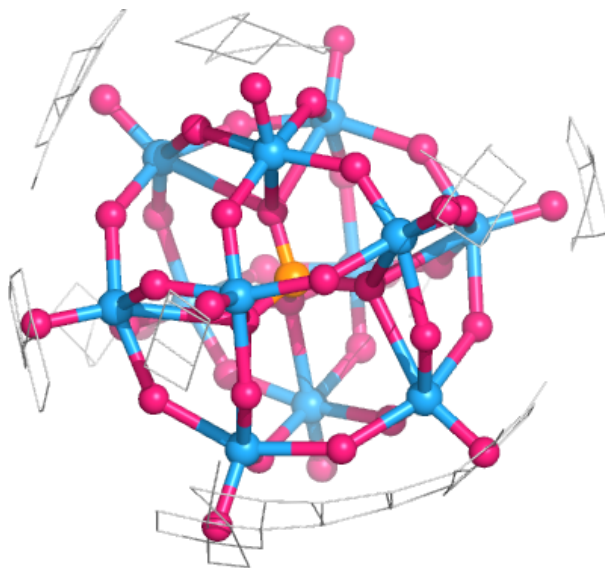
Electron density around KEG N 8704:

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



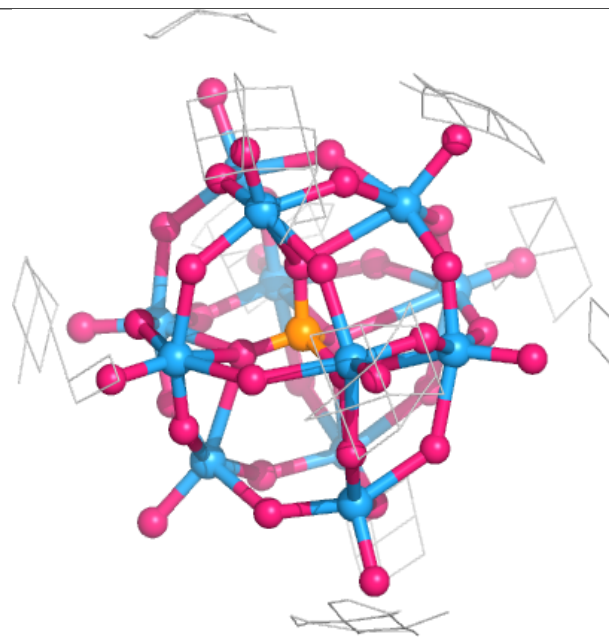
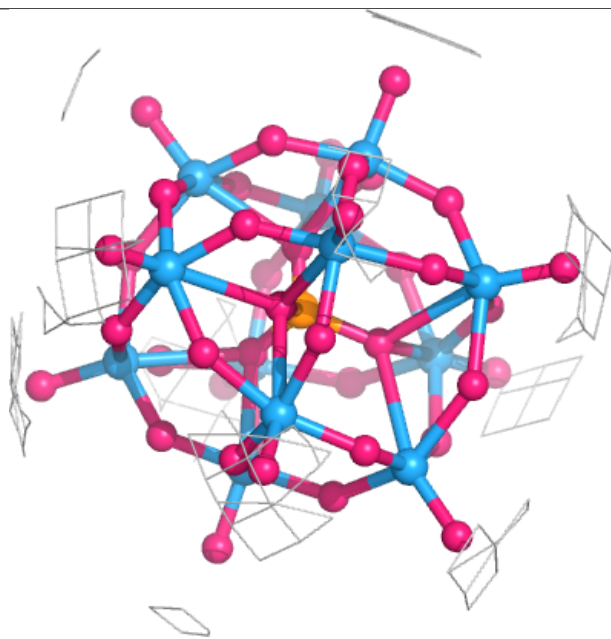
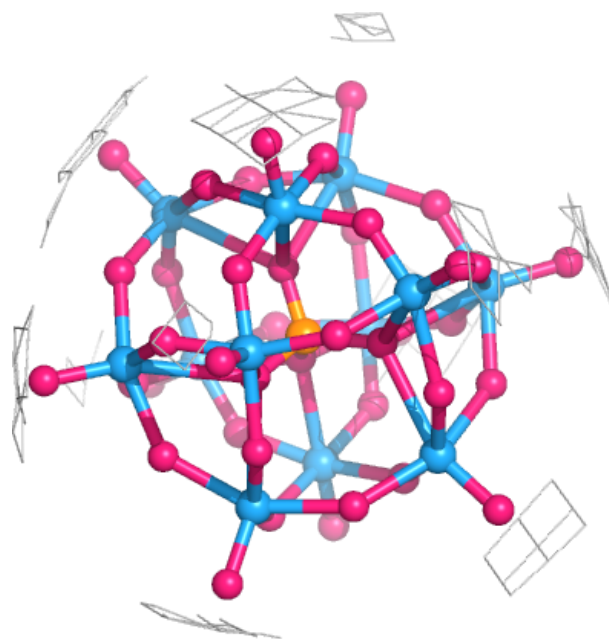
Electron density around KEG N 8702:

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



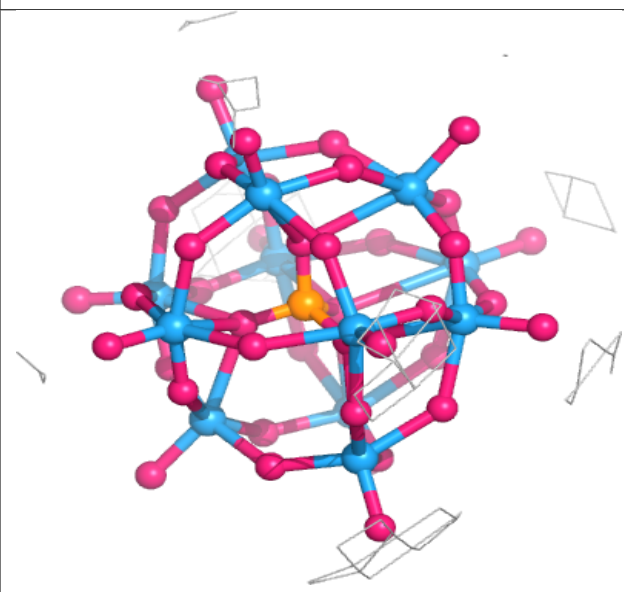
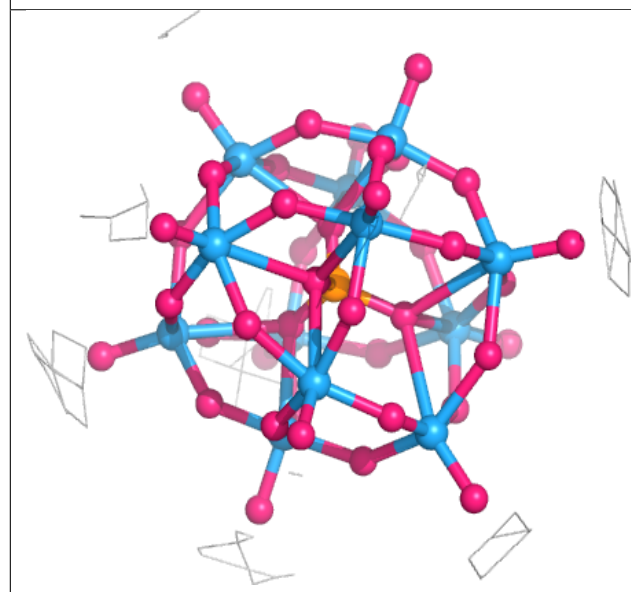
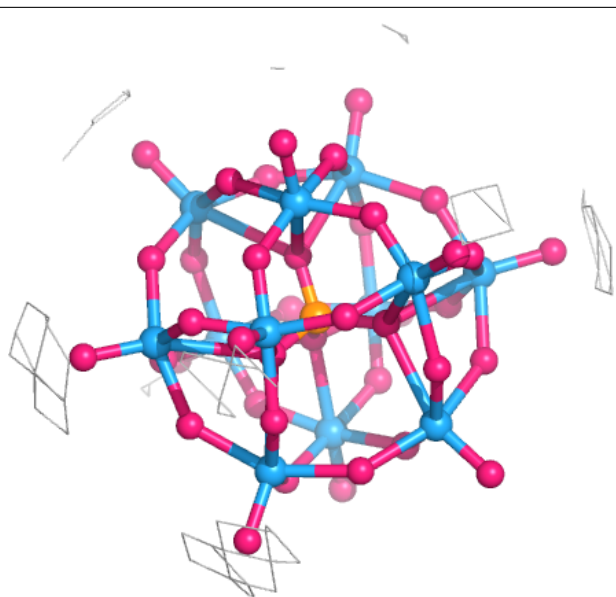
Electron density around KEG N 8705:

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



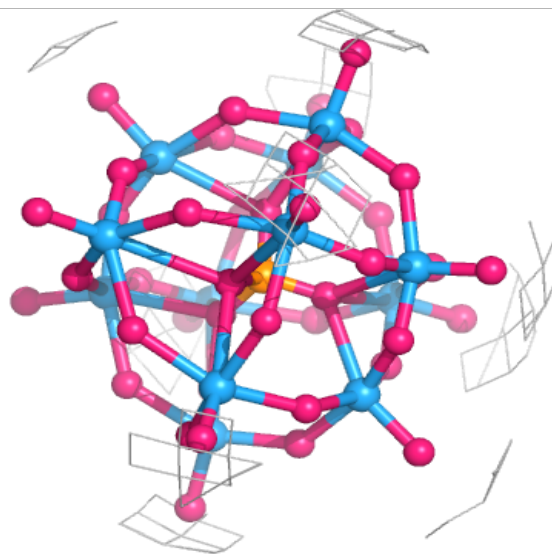
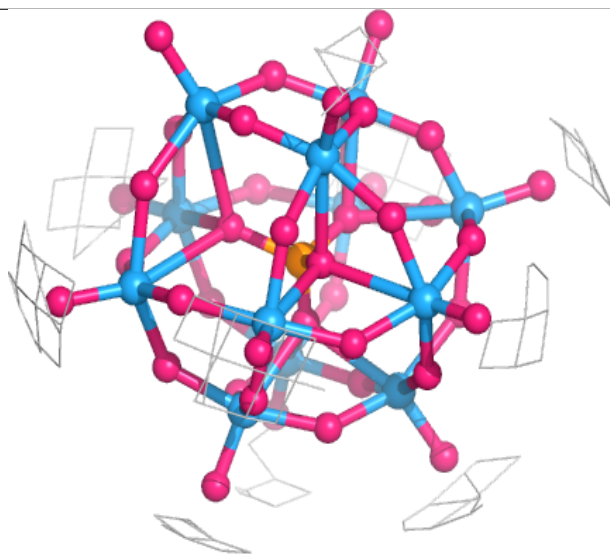
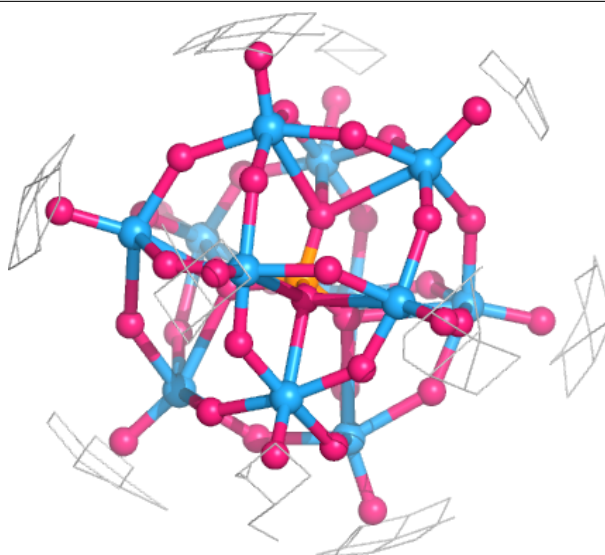
Electron density around KEG M 8701:

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



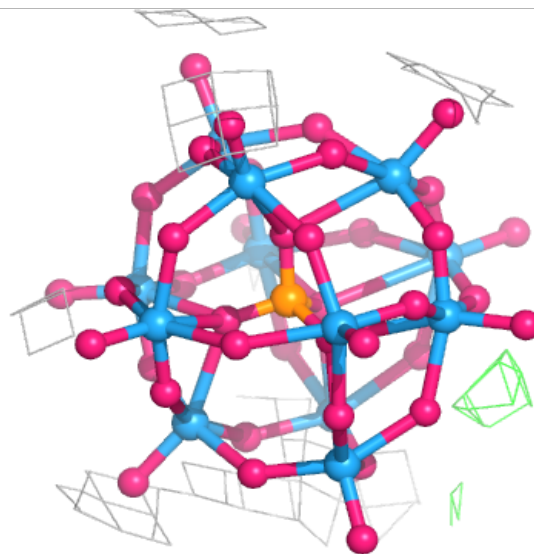
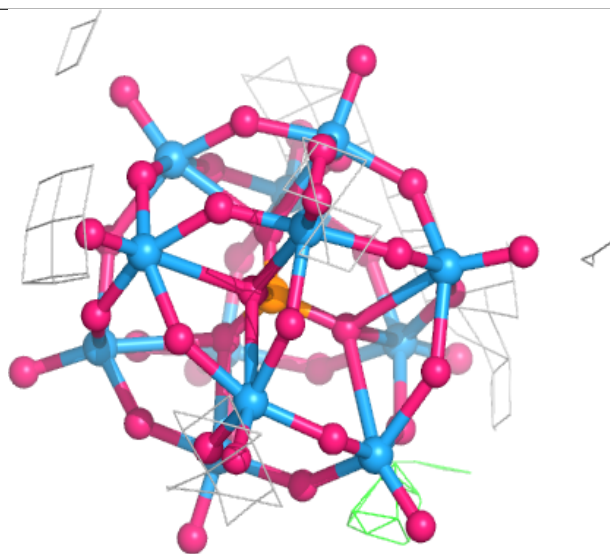
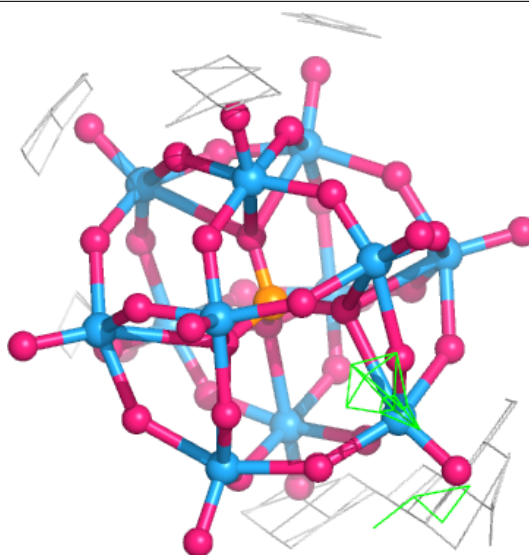
Electron density around KEG M 8702:

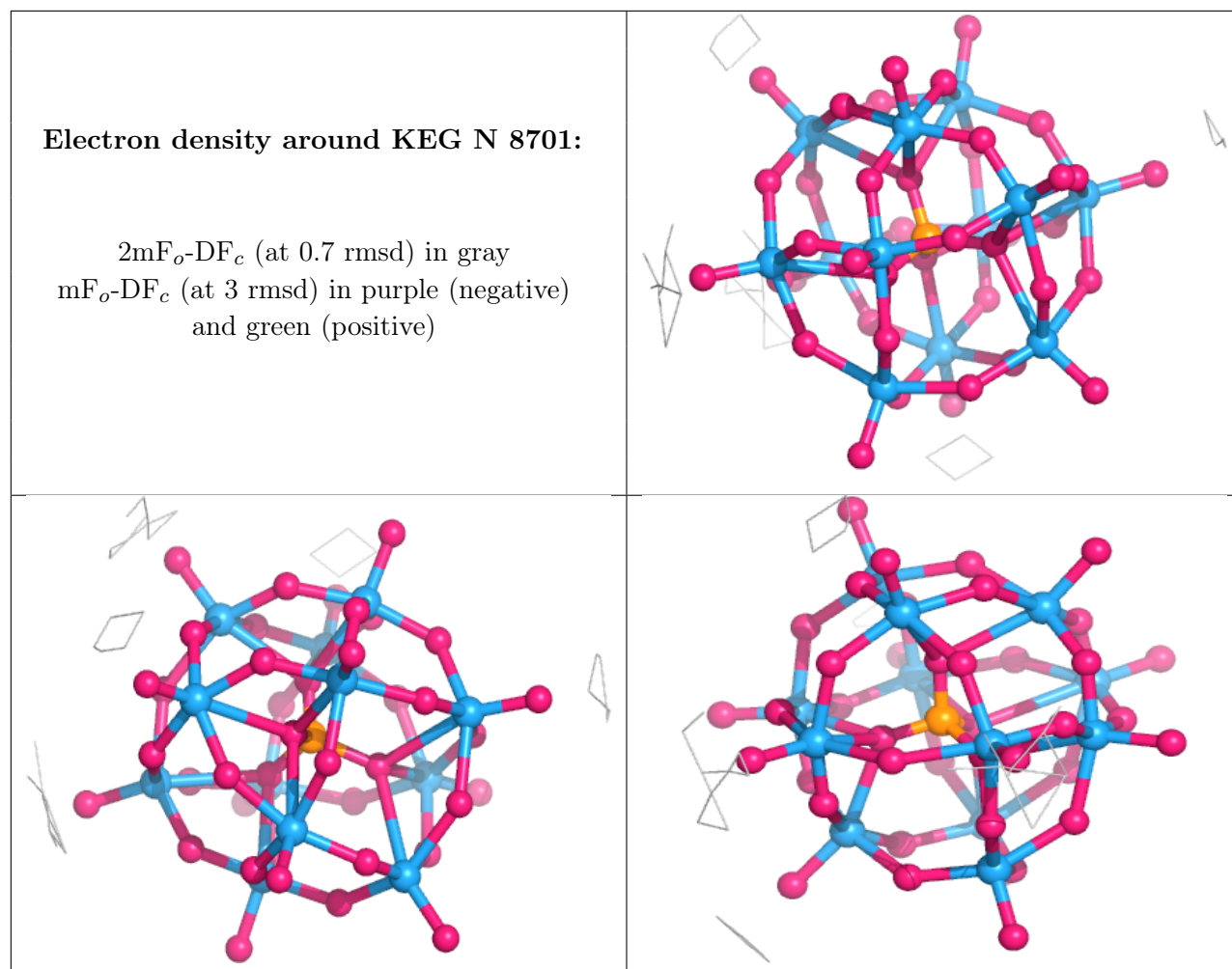
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around KEG A 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.