Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 04:46 AM EDT

PDB ID	:	5SUQ
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 (i) 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 (i)) were used in the production of this report:

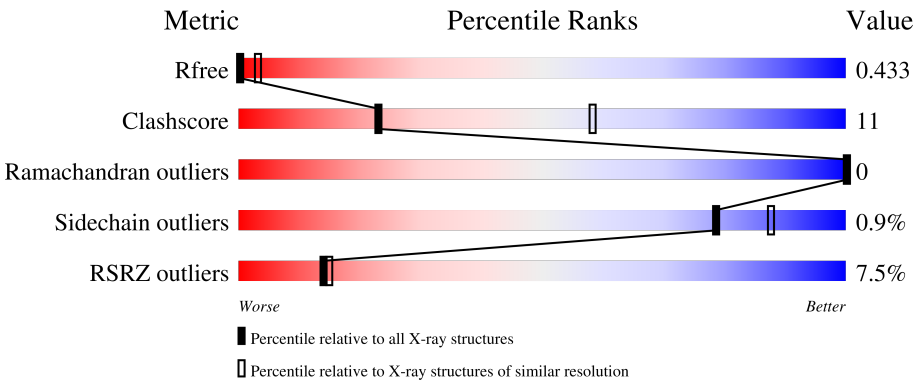
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1000 (8.00-3.88)
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)
RSRZ outliers	127900	1015 (8.20-3.78)

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 <=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	7%, 67%, 16%, •, 16%
1	C	446	5%, 66%, 17%, •, 16%
2	B	400	44%, •, 53%
2	D	400	44%, •, 53%
3	M	2300	93%, •, •

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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	502	-	-	X	-
4	KEG	A	503	-	-	X	-

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	374	3010	1916	523	560	11	0	0	0
1	C	374	3010	1916	523	560	11	0	0	0

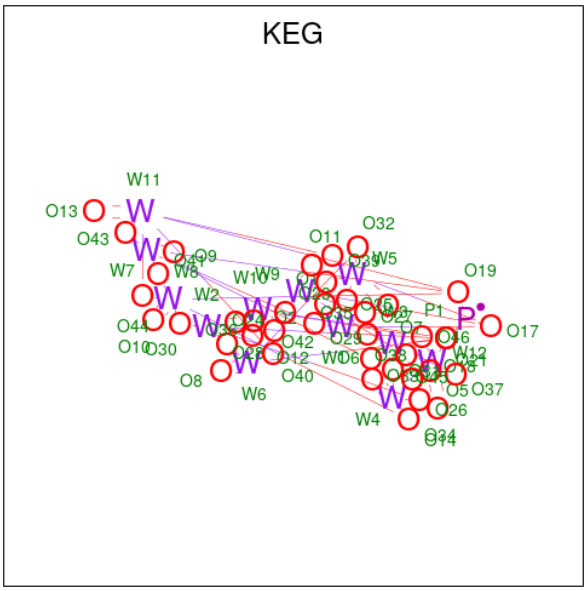
- Molecule 2 is a protein called Tex1.

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

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

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

- Molecule 4 is 12-TUNGSTOPHOSPHATE (three-letter code: KEG) (formula: $O_{40}PW_{12}$).



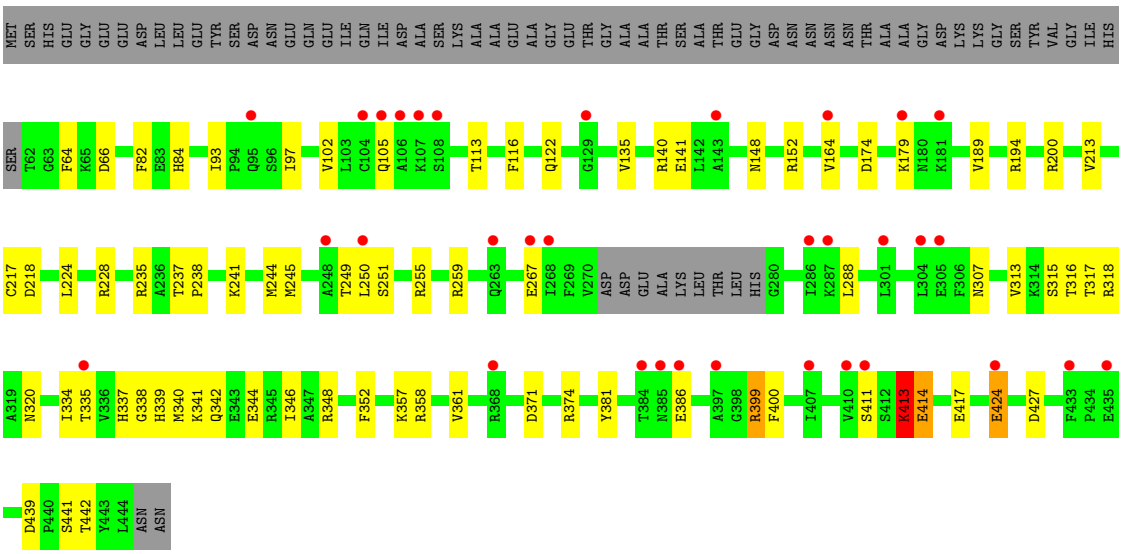
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	O	P	W	0	0
			53	40	1	12		
4	A	1	Total	O	P	W	0	0
			53	40	1	12		
4	A	1	Total	O	P	W	0	0
			53	40	1	12		
4	M	1	Total	O	P	W	0	0
			53	40	1	12		
4	M	1	Total	O	P	W	0	0
			53	40	1	12		
4	M	1	Total	O	P	W	0	0
			53	40	1	12		
4	N	1	Total	O	P	W	0	0
			53	40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

3 Residue-property plots (i)

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.

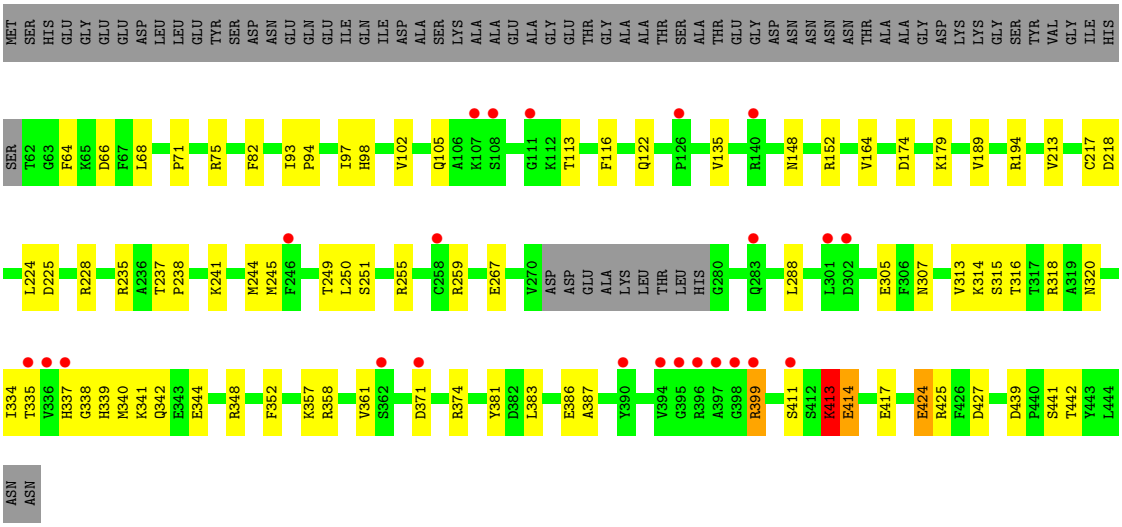
• Molecule 1: ATP-dependent RNA helicase SUB2

Chain A:



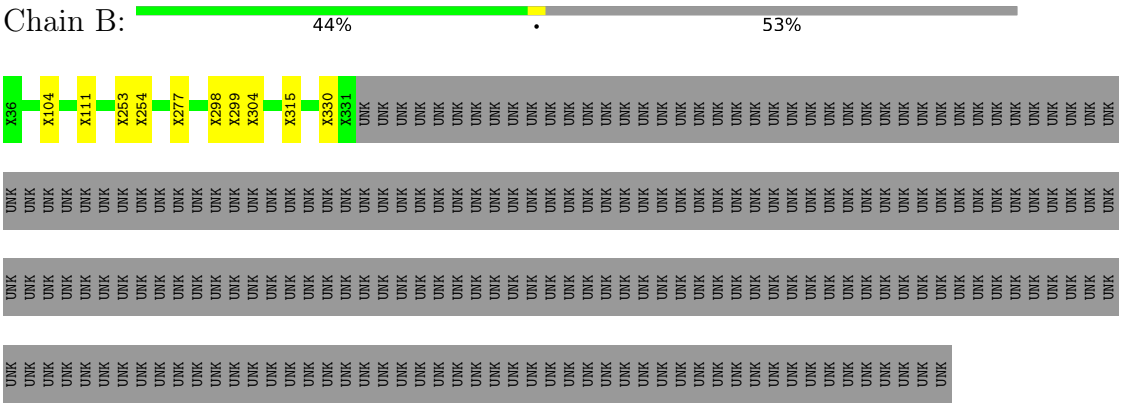
• Molecule 1: ATP-dependent RNA helicase SUB2

Chain C:



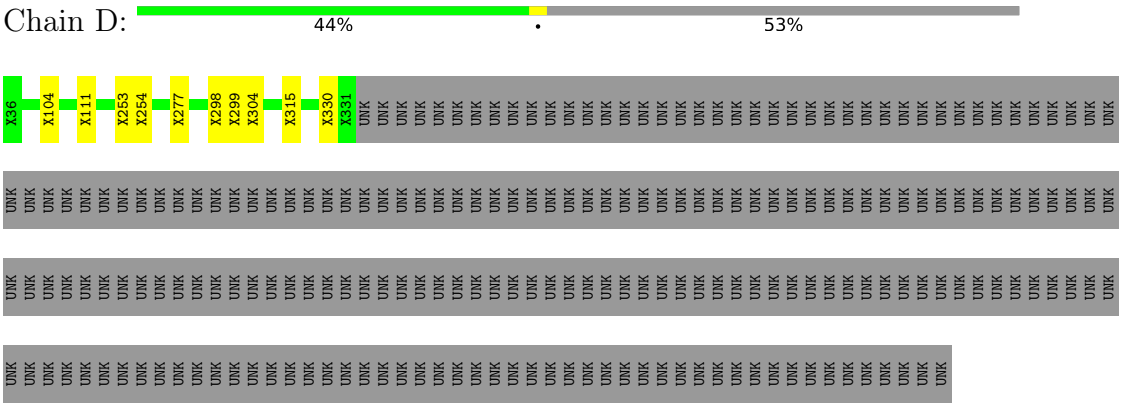
- Molecule 2: Tex1

Chain B:



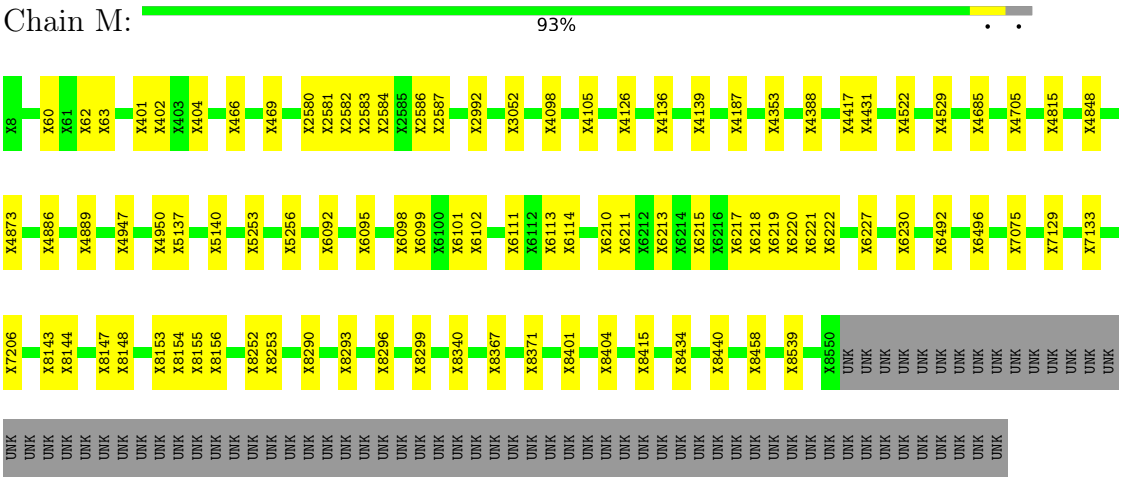
- Molecule 2: Tex1

Chain D:



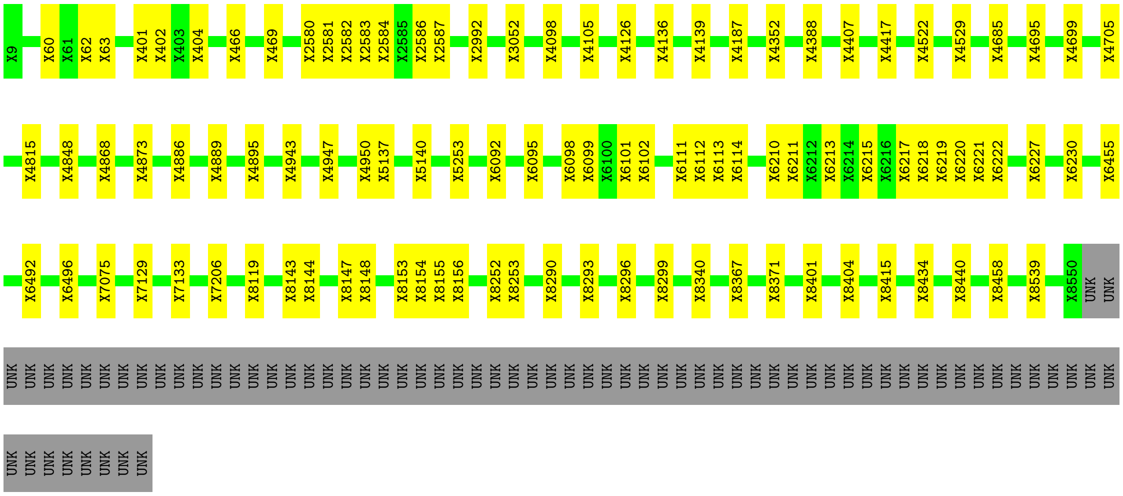
- Molecule 3: Tho2, Hpr1, Mft1, and Thp2

Chain M:



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

Chain N:


X9 X60 X61 X62 X63 X401 X402 X403 X404 X466 X469 X2580 X2581 X2582 X2583 X2584 X2585 X2586 X2587 X2992 X3052 X4098 X4105 X4126 X4136 X4139 X4187 X4352 X4388 X4407 X4417 X4522 X4529 X4685 X4695 X4699 X4705
X4815 X4848 X4868 X4873 X4886 X4889 X4895 X4943 X4947 X4950 X5137 X5140 X5253 X6092 X6095 X6098 X6099 X6100 X6101 X6102 X6111 X6112 X6113 X6114 X6210 X6211 X6212 X6213 X6214 X6215 X6216 X6217 X6218 X6219 X6220 X6221 X6222 X6227 X6230 X6455
X6492 X6496 X7075 X7129 X7133 X7206 X8119 X8143 X8144 X8147 X8148 X8153 X8154 X8155 X8156 X8252 X8253 X8290 X8293 X8296 X8299 X8340 X8367 X8371 X8401 X8404 X8415 X8434 X8440 X8458 X8539 X8550 UNK UNK
UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
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4 Data and refinement statistics (i)

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 50.18 – 5.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.57-6.00) 96.9 (50.18-5.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.07%)	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 , 320.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: 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	0.41	1/3063 (0.0%)	0.66	9/4131 (0.2%)
1	C	0.41	1/3063 (0.0%)	0.66	9/4131 (0.2%)
All	All	0.41	2/6126 (0.0%)	0.66	18/8262 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	GLU	CD-OE1	-5.23	1.19	1.25
1	C	414	GLU	CD-OE1	-5.22	1.20	1.25

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	427	ASP	CB-CA-C	-8.73	92.94	110.40
1	A	427	ASP	CB-CA-C	-8.70	93.00	110.40
1	C	427	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	427	ASP	CB-CG-OD2	8.40	125.86	118.30
1	A	427	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	C	427	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	A	417	GLU	CG-CD-OE2	6.71	131.72	118.30
1	C	417	GLU	CG-CD-OE2	6.69	131.68	118.30
1	C	414	GLU	CB-CA-C	-6.69	97.02	110.40
1	A	414	GLU	CB-CA-C	-6.66	97.07	110.40
1	A	424	GLU	CG-CD-OE1	6.46	131.22	118.30
1	C	424	GLU	CG-CD-OE1	6.44	131.18	118.30
1	C	427	ASP	N-CA-CB	6.07	121.53	110.60
1	A	427	ASP	N-CA-CB	6.04	121.47	110.60
1	C	417	GLU	CA-CB-CG	5.87	126.31	113.40
1	A	417	GLU	CA-CB-CG	5.87	126.30	113.40
1	C	413	LYS	CD-CE-NZ	5.43	124.20	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	413	LYS	CD-CE-NZ	5.42	124.17	111.70

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	3010	0	3043	158	0
1	C	3010	0	3043	155	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	53	0
4	M	159	0	0	18	0
4	N	265	0	0	30	0
All	All	30788	0	11587	484	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 11.

All (484) 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:C:98:HIS:CG	3:N:4695:UNK:CB	1.99	1.45
1:A:316:THR:C	1:C:341:LYS:HZ2	1.14	1.43
1:A:316:THR:C	1:C:341:LYS:NZ	1.70	1.42
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:340:MET:C	1:C:339:HIS:HA	1.83	0.98
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
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
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:340:MET:C	1:C:339:HIS:CA	2.39	0.90
1:A:339:HIS:C	1:C:340:MET:N	2.27	0.88
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:A:316:THR:CB	1:C:341:LYS:NZ	2.37	0.87
1:C:413:LYS:HD2	1:C:414:GLU:N	1.91	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:141:GLU:CD	1:A:342:GLN:HG2	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:N:8252:UNK:O	3:N:8253:UNK:C	2.30	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
4:A:503:KEG:O10	1:C:314:LYS:C	2.20	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
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
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

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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
4:A:501:KEG:O5	1:C:344:GLU:CD	2.24	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:339:HIS:C	1:C:340:MET:CA	2.53	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: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
1:A:339:HIS:O	1:C:340:MET:C	2.29	0.71
3:M:6219:UNK:O	3:M:6220:UNK:C	2.36	0.71
1:A:340:MET:C	1:C:339:HIS:CB	2.59	0.71
1:A:339:HIS:C	1:C:339:HIS:C	2.49	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
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:A:141:GLU:CD	1:A:342:GLN:CG	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:340:MET:N	1:C:339:HIS:C	2.50	0.65
1:C:439:ASP:OD2	1:C:441:SER:OG	2.15	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: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:439:ASP:OD2	1:A:441:SER:OG	2.15	0.62
4:A:502:KEG:O31	1:C:386:GLU:HG3	2.00	0.62
1:C:237:THR:OG1	1:C:241:LYS:NZ	2.29	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
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
1:A:141:GLU:CD	1:A:342:GLN:HE21	2.05	0.60
3:N:8155:UNK:O	3:N:8156:UNK:C	2.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:A:141:GLU:CD	1:A:342:GLN:NE2	2.59	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
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
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
1:A:339:HIS:CG	1:C:340:MET:C	2.30	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
1:A:340:MET:HA	4:A:501:KEG:O32	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:340:MET:CA	1:C:339:HIS:C	2.78	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
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
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
1:A:340:MET:C	1:C:339:HIS:CG	2.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:8296:UNK:O	3:N:8299:UNK:O	2.30	0.49
1:A:340:MET:O	1:C:339:HIS:CB	2.61	0.49
3:N:8154:UNK:O	3:N:8156:UNK:O	2.30	0.49
1:A:339:HIS:CD2	1:C:340:MET:C	2.78	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
4:A:503:KEG:O41	4:A:503:KEG:O19	2.32	0.48
4:N:8705:KEG:O41	4:N:8705:KEG:O19	2.32	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
4:M:8701:KEG:O41	4:M:8701:KEG:O19	2.32	0.47
4:N:8701:KEG:O41	4:N:8701:KEG:O19	2.32	0.47
4:A:501:KEG:O41	4:A:501:KEG:O19	2.32	0.47
3:N:4136:UNK:O	3:N:4139:UNK:N	2.47	0.47
4:N:8702:KEG:O41	4:N:8702:KEG:O19	2.32	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
4:N:8703:KEG:O41	4:N:8703:KEG:O19	2.33	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
4:M:8703:KEG:O17	4:M:8703:KEG:O35	2.33	0.47
4:N:8704:KEG:O41	4:N:8704:KEG:O19	2.32	0.47
4:A:501:KEG:O35	4:A:501:KEG:O17	2.33	0.47
1:C:307:ASN:HB3	1:C:374:ARG:O	2.15	0.47
4:M:8702:KEG:O41	4:M:8702:KEG:O19	2.32	0.47
3:N:6098:UNK:O	3:N:6101:UNK:N	2.48	0.47
4:M:8703:KEG:O41	4:M:8703:KEG:O19	2.32	0.47
4:A:502:KEG:O43	4:A:502:KEG:O19	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:M:8701:KEG:O17	4:M:8701:KEG:O35	2.33	0.46
4:N:8702:KEG:O19	4:N:8702:KEG:O43	2.34	0.46
1:C:238:PRO:O	1:C:241:LYS:HD3	2.16	0.46
4:A:501:KEG:O38	4:A:501:KEG:O21	2.34	0.46
3:M:6099:UNK:C	3:M:6101:UNK:N	2.73	0.46
4:M:8702:KEG:O17	4:M:8702:KEG:O35	2.33	0.46
4:N:8702:KEG:O17	4:N:8702:KEG:O35	2.33	0.46
4:A:501:KEG:O19	4:A:501:KEG:O43	2.34	0.46
4:A:502:KEG:O19	4:A:502:KEG:O41	2.32	0.46
3:M:8340:UNK:CB	3:M:8539:UNK:N	2.79	0.46
4:M:8702:KEG:O19	4:M:8702:KEG:O43	2.33	0.46
4:N:8701:KEG:O38	4:N:8701:KEG:O21	2.34	0.46
4:M:8703:KEG:O19	4:M:8703:KEG:O43	2.33	0.46
4:M:8703:KEG:O38	4:M:8703:KEG:O21	2.34	0.46
4:N:8701:KEG:O19	4:N:8701:KEG:O43	2.34	0.46
4:N:8702:KEG:O38	4:N:8702:KEG:O21	2.34	0.46
4:M:8701:KEG:O21	4:M:8701:KEG:O38	2.34	0.46
4:M:8702:KEG:O38	4:M:8702:KEG:O21	2.34	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
4:N:8705:KEG:O19	4:N:8705:KEG:O43	2.34	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
4:N:8703:KEG:O17	4:N:8703:KEG:O35	2.33	0.46
4:N:8705:KEG:O38	4:N:8705:KEG:O21	2.34	0.46
1:A:339:HIS:HA	1:C:340:MET:H	1.81	0.46
4:A:502:KEG:O17	4:A:502:KEG:O35	2.33	0.46
4:N:8704:KEG:O19	4:N:8704:KEG:O43	2.33	0.46
1:A:374:ARG:NH2	3:M:4431:UNK:H2	2.14	0.45
1:C:371:ASP:OD2	1:C:399:ARG:HD3	2.15	0.45
4:N:8704:KEG:O17	4:N:8704:KEG:O35	2.33	0.45
1:C:383:LEU:HD12	1:C:383:LEU:HA	1.85	0.45
4:N:8703:KEG:O38	4:N:8703:KEG:O21	2.34	0.45
4:N:8705:KEG:O17	4:N:8705:KEG:O35	2.33	0.45
1:A:238:PRO:O	1:A:241:LYS:HD3	2.15	0.45
4:A:502:KEG:O38	4:A:502:KEG:O21	2.34	0.45
3:N:466:UNK:CA	3:N:5253:UNK:CB	2.86	0.45
4:A:503:KEG:O17	4:A:503:KEG:O35	2.33	0.45
4:M:8701:KEG:O19	4:M:8701:KEG:O43	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:401:UNK:C	3:N:404:UNK:N	2.79	0.45
4:N:8701:KEG:O17	4:N:8701:KEG:O35	2.33	0.45
4:N:8703:KEG:O19	4:N:8703:KEG:O43	2.33	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
4:A:503:KEG:O21	4:A:503:KEG:O38	2.34	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
4:A:503:KEG:O19	4:A:503:KEG:O43	2.34	0.45
1:C:251:SER:O	1:C:255:ARG:HG3	2.16	0.45
4:N:8704:KEG:O38	4:N:8704:KEG:O21	2.34	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:340:MET:C	4:A:501:KEG:O7	2.56	0.44
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
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
4:N:8702:KEG:O21	4:N:8702:KEG:O37	2.36	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
4:A:502:KEG:O19	4:A:502:KEG:O44	2.37	0.43
4:N:8701:KEG:O21	4:N:8701:KEG:O37	2.37	0.43
1:A:320:ASN:ND2	1:C:341:LYS:HE3	2.34	0.43
4:N:8704:KEG:O19	4:N:8704:KEG:O44	2.37	0.43
4:A:501:KEG:O21	4:A:501:KEG:O37	2.36	0.43
4:M:8703:KEG:O21	4:M:8703:KEG:O37	2.36	0.43
3:N:8144:UNK:O	3:N:8148:UNK:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:8701:KEG:O19	4:N:8701:KEG:O44	2.37	0.43
1:A:102:VAL:HB	1:A:244:MET:HG2	2.00	0.43
4:M:8702:KEG:O21	4:M:8702:KEG:O37	2.36	0.43
4:N:8704:KEG:O21	4:N:8704:KEG:O37	2.36	0.43
4:N:8705:KEG:O19	4:N:8705:KEG:O44	2.37	0.43
4:A:501:KEG:O19	4:A:501:KEG:O44	2.37	0.43
4:N:8705:KEG:O21	4:N:8705:KEG:O37	2.36	0.43
1:A:135:VAL:HG22	1:A:213:VAL:HB	2.01	0.43
4:A:502:KEG:O21	4:A:502:KEG:O37	2.37	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
1:A:341:LYS:HD2	1:C:339:HIS:CD2	2.54	0.42
4:A:503:KEG:O21	4:A:503:KEG:O37	2.37	0.42
4:N:8703:KEG:O21	4:N:8703:KEG:O37	2.36	0.42
4:M:8701:KEG:O19	4:M:8701:KEG:O44	2.37	0.42
4:M:8701:KEG:O21	4:M:8701:KEG:O37	2.37	0.42
4:M:8702:KEG:O19	4:M:8702:KEG:O44	2.37	0.42
4:M:8703:KEG:O19	4:M:8703:KEG:O44	2.36	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
4:N:8702:KEG:O19	4:N:8702:KEG:O44	2.37	0.42
1:A:341:LYS:N	4:A:501:KEG:O32	2.47	0.42
4:A:503:KEG:O19	4:A:503:KEG:O44	2.37	0.42
4:N:8703:KEG:O19	4:N:8703:KEG:O44	2.37	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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	328 (99%)	3 (1%)	78 88
1	C	331/386 (86%)	328 (99%)	3 (1%)	78 88
All	All	662/772 (86%)	656 (99%)	6 (1%)	78 88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	399	ARG
1	A	413	LYS
1	A	424	GLU
1	C	399	ARG
1	C	413	LYS
1	C	424	GLU

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

Mol	Chain	Res	Type
1	A	299	GLN
1	A	342	GLN
1	C	98	HIS
1	C	299	GLN
1	C	339	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	501	-	76,76,76	3.16	42 (55%)	6,234,234	1.37	2 (33%)
4	KEG	A	502	-	76,76,76	3.16	42 (55%)	6,234,234	1.38	2 (33%)
4	KEG	M	8701	-	76,76,76	3.16	42 (55%)	6,234,234	1.40	2 (33%)
4	KEG	M	8702	-	76,76,76	3.16	42 (55%)	6,234,234	1.37	2 (33%)
4	KEG	N	8701	-	76,76,76	3.16	42 (55%)	6,234,234	1.37	2 (33%)
4	KEG	N	8702	-	76,76,76	3.16	42 (55%)	6,234,234	1.38	2 (33%)
4	KEG	N	8703	-	76,76,76	3.16	42 (55%)	6,234,234	1.38	2 (33%)
4	KEG	N	8704	-	76,76,76	3.16	42 (55%)	6,234,234	1.38	2 (33%)
4	KEG	N	8705	-	76,76,76	3.16	42 (55%)	6,234,234	1.39	2 (33%)
4	KEG	M	8703	-	76,76,76	3.16	43 (56%)	6,234,234	1.39	2 (33%)
4	KEG	A	503	-	76,76,76	3.16	42 (55%)	6,234,234	1.37	2 (33%)

All (463) 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	-7.79	1.55	1.93
4	N	8704	KEG	W2-O28	-7.76	1.55	1.93
4	A	503	KEG	W2-O28	-7.75	1.55	1.93
4	M	8703	KEG	W2-O28	-7.75	1.55	1.93
4	M	8701	KEG	W2-O28	-7.75	1.55	1.93
4	N	8705	KEG	W2-O28	-7.75	1.55	1.93
4	A	501	KEG	W2-O28	-7.75	1.55	1.93
4	N	8701	KEG	W2-O28	-7.75	1.55	1.93
4	N	8702	KEG	W2-O28	-7.74	1.55	1.93
4	A	502	KEG	W2-O28	-7.74	1.55	1.93
4	N	8703	KEG	W2-O28	-7.73	1.55	1.93
4	A	501	KEG	W6-O36	-7.27	1.58	1.93
4	M	8701	KEG	W6-O36	-7.25	1.58	1.93
4	M	8702	KEG	W6-O36	-7.25	1.58	1.93
4	A	503	KEG	W6-O36	-7.25	1.58	1.93
4	N	8705	KEG	W6-O36	-7.25	1.58	1.93
4	N	8701	KEG	W6-O36	-7.25	1.58	1.93
4	M	8703	KEG	W6-O36	-7.24	1.58	1.93
4	N	8703	KEG	W6-O36	-7.24	1.58	1.93
4	A	502	KEG	W6-O36	-7.24	1.58	1.93
4	N	8704	KEG	W6-O36	-7.23	1.58	1.93
4	N	8702	KEG	W6-O36	-7.23	1.58	1.93
4	N	8704	KEG	W1-O29	-7.11	1.60	1.91
4	A	502	KEG	W1-O29	-7.11	1.60	1.91
4	N	8702	KEG	W1-O29	-7.10	1.60	1.91
4	N	8701	KEG	W1-O29	-7.10	1.60	1.91
4	M	8703	KEG	W1-O29	-7.10	1.60	1.91
4	M	8702	KEG	W1-O29	-7.10	1.60	1.91
4	M	8701	KEG	W1-O29	-7.10	1.60	1.91
4	A	503	KEG	W1-O29	-7.10	1.60	1.91
4	A	501	KEG	W1-O29	-7.09	1.60	1.91
4	N	8703	KEG	W1-O29	-7.08	1.60	1.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8705	KEG	W1-O29	-7.08	1.60	1.91
4	A	502	KEG	W3-O33	-7.00	1.61	1.91
4	M	8702	KEG	W3-O33	-6.98	1.61	1.91
4	A	501	KEG	W3-O33	-6.98	1.61	1.91
4	M	8701	KEG	W3-O33	-6.98	1.61	1.91
4	N	8703	KEG	W3-O33	-6.97	1.61	1.91
4	A	503	KEG	W3-O33	-6.96	1.61	1.91
4	N	8701	KEG	W3-O33	-6.96	1.61	1.91
4	M	8703	KEG	W3-O33	-6.95	1.61	1.91
4	N	8705	KEG	W3-O33	-6.95	1.61	1.91
4	N	8704	KEG	W3-O33	-6.95	1.61	1.91
4	N	8702	KEG	W3-O33	-6.94	1.61	1.91
4	N	8703	KEG	W10-O28	-5.64	1.66	1.93
4	A	501	KEG	W10-O28	-5.63	1.66	1.93
4	A	502	KEG	W10-O28	-5.63	1.66	1.93
4	N	8701	KEG	W10-O28	-5.63	1.66	1.93
4	M	8703	KEG	W10-O28	-5.63	1.66	1.93
4	M	8702	KEG	W10-O28	-5.63	1.66	1.93
4	N	8702	KEG	W10-O28	-5.63	1.66	1.93
4	M	8701	KEG	W10-O28	-5.62	1.66	1.93
4	N	8705	KEG	W10-O28	-5.62	1.66	1.93
4	A	503	KEG	W10-O28	-5.62	1.66	1.93
4	N	8704	KEG	W10-O28	-5.61	1.66	1.93
4	A	502	KEG	W5-O23	-5.22	1.68	1.93
4	M	8703	KEG	W5-O23	-5.21	1.68	1.93
4	A	503	KEG	W5-O23	-5.20	1.68	1.93
4	A	501	KEG	W5-O23	-5.20	1.68	1.93
4	M	8701	KEG	W5-O23	-5.20	1.68	1.93
4	M	8702	KEG	W5-O23	-5.19	1.68	1.93
4	N	8703	KEG	W5-O23	-5.19	1.68	1.93
4	N	8701	KEG	W5-O23	-5.19	1.68	1.93
4	N	8705	KEG	W5-O23	-5.19	1.68	1.93
4	N	8702	KEG	W5-O23	-5.19	1.68	1.93
4	N	8704	KEG	W5-O23	-5.17	1.68	1.93
4	N	8703	KEG	P1-O19	-4.75	1.38	1.54
4	M	8702	KEG	W7-O29	-4.75	1.70	1.91
4	N	8705	KEG	W7-O29	-4.75	1.70	1.91
4	A	503	KEG	W7-O29	-4.75	1.70	1.91
4	M	8701	KEG	W7-O29	-4.75	1.70	1.91
4	N	8704	KEG	W7-O29	-4.74	1.70	1.91
4	A	501	KEG	W7-O29	-4.74	1.70	1.91
4	A	502	KEG	W7-O29	-4.74	1.70	1.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8701	KEG	W7-O29	-4.74	1.70	1.91
4	A	503	KEG	P1-O19	-4.73	1.38	1.54
4	N	8703	KEG	W7-O29	-4.73	1.70	1.91
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	A	503	KEG	W2-O2	-4.72	1.58	1.71
4	M	8703	KEG	W7-O29	-4.72	1.70	1.91
4	N	8702	KEG	W7-O29	-4.71	1.70	1.91
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	8702	KEG	W2-O2	-4.70	1.58	1.71
4	A	502	KEG	W2-O2	-4.70	1.58	1.71
4	N	8704	KEG	P1-O19	-4.70	1.38	1.54
4	N	8704	KEG	W2-O2	-4.69	1.58	1.71
4	A	502	KEG	P1-O19	-4.67	1.38	1.54
4	N	8701	KEG	W2-O2	-4.67	1.58	1.71
4	M	8701	KEG	W2-O2	-4.67	1.58	1.71
4	M	8702	KEG	W2-O2	-4.67	1.58	1.71
4	N	8703	KEG	W2-O2	-4.67	1.58	1.71
4	N	8705	KEG	W2-O2	-4.66	1.58	1.71
4	A	501	KEG	W2-O2	-4.66	1.58	1.71
4	M	8703	KEG	W2-O2	-4.64	1.58	1.71
4	A	502	KEG	W1-O23	-4.49	1.71	1.93
4	A	503	KEG	W1-O23	-4.48	1.71	1.93
4	M	8701	KEG	W1-O23	-4.47	1.71	1.93
4	N	8701	KEG	W1-O23	-4.47	1.71	1.93
4	N	8704	KEG	W1-O23	-4.47	1.71	1.93
4	A	501	KEG	W1-O23	-4.47	1.71	1.93
4	M	8703	KEG	W1-O23	-4.46	1.71	1.93
4	A	502	KEG	W10-O18	-4.46	2.19	2.43
4	N	8702	KEG	W1-O23	-4.46	1.71	1.93
4	N	8705	KEG	W1-O23	-4.46	1.71	1.93
4	N	8703	KEG	W1-O23	-4.45	1.71	1.93
4	M	8702	KEG	W1-O23	-4.45	1.71	1.93
4	A	501	KEG	W10-O18	-4.44	2.19	2.43
4	M	8702	KEG	W10-O18	-4.44	2.19	2.43
4	M	8703	KEG	W10-O18	-4.43	2.19	2.43
4	A	503	KEG	W10-O18	-4.43	2.19	2.43
4	N	8703	KEG	W10-O18	-4.43	2.19	2.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8704	KEG	W10-O18	-4.42	2.19	2.43
4	M	8701	KEG	W10-O18	-4.42	2.19	2.43
4	N	8701	KEG	W10-O18	-4.42	2.19	2.43
4	N	8705	KEG	W10-O18	-4.41	2.19	2.43
4	N	8702	KEG	W10-O18	-4.41	2.19	2.43
4	N	8701	KEG	W2-O18	-4.35	2.19	2.43
4	M	8702	KEG	W2-O18	-4.35	2.19	2.43
4	N	8705	KEG	W2-O18	-4.34	2.19	2.43
4	M	8703	KEG	W2-O18	-4.34	2.19	2.43
4	N	8702	KEG	W2-O18	-4.34	2.19	2.43
4	A	502	KEG	W2-O18	-4.33	2.19	2.43
4	N	8703	KEG	W2-O18	-4.33	2.19	2.43
4	A	501	KEG	W2-O18	-4.33	2.19	2.43
4	A	503	KEG	W2-O18	-4.32	2.19	2.43
4	N	8704	KEG	W2-O18	-4.32	2.19	2.43
4	M	8701	KEG	W2-O18	-4.31	2.19	2.43
4	A	503	KEG	W11-O13	-4.16	1.60	1.71
4	A	501	KEG	W11-O13	-4.16	1.60	1.71
4	N	8705	KEG	W11-O13	-4.16	1.60	1.71
4	N	8704	KEG	W11-O13	-4.15	1.60	1.71
4	N	8703	KEG	W11-O13	-4.15	1.60	1.71
4	M	8703	KEG	W11-O13	-4.15	1.60	1.71
4	N	8701	KEG	W11-O13	-4.15	1.60	1.71
4	M	8701	KEG	W11-O13	-4.14	1.60	1.71
4	N	8702	KEG	W11-O13	-4.14	1.60	1.71
4	M	8702	KEG	W11-O13	-4.13	1.60	1.71
4	A	502	KEG	W11-O13	-4.13	1.60	1.71
4	A	502	KEG	W12-O14	-4.04	1.60	1.71
4	M	8702	KEG	W9-O42	-4.03	1.73	1.91
4	A	503	KEG	W9-O42	-4.03	1.73	1.91
4	N	8705	KEG	W9-O42	-4.03	1.73	1.91
4	N	8701	KEG	W9-O42	-4.03	1.73	1.91
4	M	8701	KEG	W9-O42	-4.02	1.73	1.91
4	N	8702	KEG	W9-O42	-4.02	1.73	1.91
4	A	501	KEG	W9-O42	-4.02	1.73	1.91
4	N	8704	KEG	W9-O42	-4.01	1.73	1.91
4	A	502	KEG	W9-O42	-4.01	1.73	1.91
4	N	8703	KEG	W9-O42	-4.01	1.73	1.91
4	A	501	KEG	W12-O14	-4.01	1.60	1.71
4	M	8701	KEG	W12-O14	-4.01	1.60	1.71
4	N	8702	KEG	W12-O14	-4.00	1.60	1.71
4	A	503	KEG	W12-O14	-4.00	1.60	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8702	KEG	W12-O14	-4.00	1.60	1.71
4	N	8705	KEG	W12-O14	-3.99	1.60	1.71
4	M	8703	KEG	W9-O42	-3.99	1.74	1.91
4	M	8703	KEG	W12-O14	-3.99	1.60	1.71
4	N	8704	KEG	W12-O14	-3.97	1.60	1.71
4	N	8701	KEG	W12-O14	-3.96	1.60	1.71
4	N	8703	KEG	W12-O14	-3.96	1.60	1.71
4	A	502	KEG	W10-O36	-3.86	1.74	1.93
4	N	8702	KEG	W10-O36	-3.85	1.74	1.93
4	M	8701	KEG	W10-O36	-3.85	1.74	1.93
4	N	8704	KEG	W10-O36	-3.85	1.74	1.93
4	M	8703	KEG	W10-O36	-3.84	1.74	1.93
4	A	501	KEG	W10-O36	-3.84	1.74	1.93
4	N	8701	KEG	W10-O36	-3.84	1.74	1.93
4	M	8702	KEG	W10-O36	-3.84	1.74	1.93
4	N	8705	KEG	W10-O36	-3.84	1.74	1.93
4	N	8703	KEG	W10-O36	-3.84	1.74	1.93
4	A	503	KEG	W10-O36	-3.83	1.74	1.93
4	M	8703	KEG	W1-O17	-3.83	2.22	2.43
4	A	502	KEG	W1-O17	-3.82	2.22	2.43
4	N	8705	KEG	W1-O17	-3.82	2.22	2.43
4	M	8702	KEG	W1-O17	-3.82	2.22	2.43
4	N	8703	KEG	W1-O17	-3.82	2.22	2.43
4	M	8701	KEG	W1-O17	-3.82	2.22	2.43
4	A	501	KEG	W1-O17	-3.82	2.22	2.43
4	N	8701	KEG	W1-O17	-3.81	2.22	2.43
4	A	503	KEG	W1-O17	-3.80	2.22	2.43
4	N	8704	KEG	W1-O17	-3.80	2.22	2.43
4	N	8702	KEG	W1-O17	-3.79	2.22	2.43
4	A	502	KEG	W8-O10	-3.68	1.61	1.71
4	N	8704	KEG	W8-O10	-3.65	1.61	1.71
4	N	8701	KEG	W8-O10	-3.65	1.61	1.71
4	M	8701	KEG	W8-O10	-3.64	1.61	1.71
4	N	8702	KEG	W8-O10	-3.63	1.61	1.71
4	A	503	KEG	W8-O10	-3.62	1.61	1.71
4	N	8705	KEG	W8-O10	-3.61	1.61	1.71
4	M	8702	KEG	W8-O10	-3.61	1.61	1.71
4	N	8703	KEG	W8-O10	-3.60	1.61	1.71
4	A	501	KEG	W8-O10	-3.60	1.61	1.71
4	M	8703	KEG	W8-O10	-3.60	1.61	1.71
4	A	501	KEG	W6-O24	-3.41	1.76	1.93
4	M	8701	KEG	W6-O24	-3.41	1.76	1.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	KEG	W6-O24	-3.39	1.77	1.93
4	N	8704	KEG	W6-O24	-3.38	1.77	1.93
4	M	8702	KEG	W6-O24	-3.38	1.77	1.93
4	A	503	KEG	W6-O24	-3.38	1.77	1.93
4	M	8703	KEG	W6-O24	-3.38	1.77	1.93
4	A	502	KEG	W3-O21	3.37	2.61	2.43
4	N	8703	KEG	W6-O24	-3.37	1.77	1.93
4	N	8705	KEG	W6-O24	-3.37	1.77	1.93
4	N	8701	KEG	W6-O24	-3.36	1.77	1.93
4	N	8702	KEG	W6-O24	-3.36	1.77	1.93
4	N	8705	KEG	W3-O21	3.35	2.61	2.43
4	A	503	KEG	W3-O21	3.35	2.61	2.43
4	M	8701	KEG	W3-O21	3.35	2.61	2.43
4	N	8704	KEG	W3-O21	3.35	2.61	2.43
4	N	8701	KEG	W3-O21	3.35	2.61	2.43
4	A	501	KEG	W3-O21	3.35	2.61	2.43
4	N	8703	KEG	W3-O21	3.34	2.61	2.43
4	M	8703	KEG	W3-O21	3.33	2.61	2.43
4	M	8702	KEG	W3-O21	3.33	2.61	2.43
4	N	8702	KEG	W3-O21	3.33	2.61	2.43
4	N	8703	KEG	W2-O24	-3.15	1.78	1.93
4	N	8701	KEG	W2-O24	-3.14	1.78	1.93
4	N	8702	KEG	W2-O24	-3.13	1.78	1.93
4	N	8704	KEG	W2-O24	-3.13	1.78	1.93
4	N	8701	KEG	W9-O11	-3.13	1.62	1.71
4	N	8704	KEG	W9-O11	-3.12	1.62	1.71
4	N	8705	KEG	W2-O24	-3.12	1.78	1.93
4	A	503	KEG	W2-O24	-3.12	1.78	1.93
4	M	8703	KEG	W2-O24	-3.12	1.78	1.93
4	M	8701	KEG	W2-O24	-3.12	1.78	1.93
4	M	8703	KEG	W9-O11	-3.12	1.63	1.71
4	A	501	KEG	W2-O24	-3.11	1.78	1.93
4	A	502	KEG	W2-O24	-3.11	1.78	1.93
4	A	501	KEG	W9-O11	-3.11	1.63	1.71
4	M	8702	KEG	W2-O24	-3.11	1.78	1.93
4	M	8702	KEG	W9-O11	-3.10	1.63	1.71
4	A	502	KEG	W9-O11	-3.09	1.63	1.71
4	N	8703	KEG	W9-O11	-3.09	1.63	1.71
4	A	503	KEG	W9-O11	-3.09	1.63	1.71
4	N	8705	KEG	W9-O11	-3.08	1.63	1.71
4	M	8701	KEG	W9-O11	-3.07	1.63	1.71
4	N	8702	KEG	W9-O11	-3.05	1.63	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8703	KEG	W3-O25	-3.03	1.78	1.91
4	N	8705	KEG	W3-O25	-3.03	1.78	1.91
4	M	8703	KEG	W3-O25	-3.02	1.78	1.91
4	M	8701	KEG	W3-O25	-3.02	1.78	1.91
4	N	8704	KEG	W3-O25	-3.02	1.78	1.91
4	N	8701	KEG	W3-O25	-3.02	1.78	1.91
4	A	501	KEG	W3-O25	-3.02	1.78	1.91
4	A	503	KEG	W3-O25	-3.02	1.78	1.91
4	M	8702	KEG	W3-O25	-3.02	1.78	1.91
4	N	8702	KEG	W3-O25	-3.01	1.78	1.91
4	A	502	KEG	W3-O25	-3.01	1.78	1.91
4	N	8705	KEG	W10-O12	-2.93	1.63	1.71
4	N	8702	KEG	W10-O12	-2.93	1.63	1.71
4	N	8702	KEG	W8-O44	-2.93	1.79	1.93
4	N	8703	KEG	W10-O12	-2.92	1.63	1.71
4	N	8701	KEG	W10-O12	-2.92	1.63	1.71
4	N	8703	KEG	W8-O44	-2.92	1.79	1.93
4	N	8704	KEG	W8-O44	-2.92	1.79	1.93
4	M	8701	KEG	W8-O44	-2.91	1.79	1.93
4	A	502	KEG	W8-O44	-2.91	1.79	1.93
4	M	8703	KEG	W8-O44	-2.91	1.79	1.93
4	A	501	KEG	W8-O44	-2.91	1.79	1.93
4	M	8701	KEG	W10-O12	-2.90	1.63	1.71
4	N	8701	KEG	W8-O44	-2.89	1.79	1.93
4	A	503	KEG	W8-O44	-2.89	1.79	1.93
4	M	8702	KEG	W8-O44	-2.89	1.79	1.93
4	M	8703	KEG	W10-O12	-2.89	1.63	1.71
4	N	8704	KEG	W10-O12	-2.89	1.63	1.71
4	A	501	KEG	W10-O12	-2.88	1.63	1.71
4	M	8702	KEG	W10-O12	-2.88	1.63	1.71
4	N	8705	KEG	W8-O44	-2.87	1.79	1.93
4	A	503	KEG	W10-O12	-2.86	1.63	1.71
4	M	8703	KEG	W6-O8	-2.85	1.63	1.71
4	A	502	KEG	W10-O12	-2.85	1.63	1.71
4	N	8704	KEG	W6-O8	-2.84	1.63	1.71
4	N	8702	KEG	W6-O8	-2.84	1.63	1.71
4	N	8703	KEG	W6-O8	-2.83	1.63	1.71
4	M	8701	KEG	W6-O8	-2.83	1.63	1.71
4	A	502	KEG	W6-O8	-2.83	1.63	1.71
4	N	8705	KEG	W6-O8	-2.82	1.63	1.71
4	A	501	KEG	W6-O8	-2.82	1.63	1.71
4	M	8702	KEG	W6-O8	-2.82	1.63	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8701	KEG	W6-O8	-2.82	1.63	1.71
4	A	503	KEG	W6-O8	-2.79	1.63	1.71
4	A	501	KEG	W3-O37	2.79	2.07	1.93
4	N	8704	KEG	W3-O37	2.78	2.07	1.93
4	N	8703	KEG	W3-O37	2.78	2.07	1.93
4	N	8705	KEG	W3-O37	2.78	2.07	1.93
4	M	8701	KEG	W3-O37	2.77	2.07	1.93
4	A	502	KEG	W3-O37	2.77	2.07	1.93
4	M	8703	KEG	W3-O37	2.77	2.07	1.93
4	A	503	KEG	W3-O37	2.76	2.07	1.93
4	N	8701	KEG	W3-O37	2.76	2.07	1.93
4	M	8702	KEG	W3-O37	2.76	2.07	1.93
4	N	8702	KEG	W3-O37	2.75	2.07	1.93
4	N	8704	KEG	W5-O7	-2.75	1.64	1.71
4	A	502	KEG	W5-O7	-2.73	1.64	1.71
4	M	8703	KEG	W5-O7	-2.72	1.64	1.71
4	M	8701	KEG	W5-O7	-2.71	1.64	1.71
4	A	503	KEG	W5-O7	-2.71	1.64	1.71
4	M	8702	KEG	W5-O7	-2.71	1.64	1.71
4	N	8703	KEG	W5-O7	-2.70	1.64	1.71
4	N	8705	KEG	W5-O7	-2.70	1.64	1.71
4	N	8701	KEG	W5-O7	-2.68	1.64	1.71
4	N	8702	KEG	W5-O7	-2.68	1.64	1.71
4	A	501	KEG	W5-O7	-2.67	1.64	1.71
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
4	N	8702	KEG	P1-O21	2.57	1.63	1.54
4	A	503	KEG	W1-O1	-2.57	1.64	1.71
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	N	8701	KEG	W1-O1	-2.56	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	N	8703	KEG	W1-O1	-2.55	1.64	1.71
4	N	8705	KEG	W1-O1	-2.54	1.64	1.71
4	M	8701	KEG	P1-O21	2.54	1.63	1.54
4	A	502	KEG	P1-O21	2.54	1.63	1.54
4	M	8701	KEG	W1-O1	-2.53	1.64	1.71
4	N	8702	KEG	W1-O1	-2.52	1.64	1.71
4	A	502	KEG	W1-O1	-2.52	1.64	1.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8703	KEG	W11-O40	-2.52	1.80	1.91
4	A	502	KEG	W11-O40	-2.52	1.80	1.91
4	M	8702	KEG	W1-O1	-2.52	1.64	1.71
4	M	8702	KEG	W11-O40	-2.52	1.80	1.91
4	N	8703	KEG	W11-O40	-2.51	1.80	1.91
4	A	501	KEG	W1-O1	-2.51	1.64	1.71
4	M	8701	KEG	W11-O40	-2.51	1.80	1.91
4	M	8703	KEG	W1-O1	-2.51	1.64	1.71
4	A	503	KEG	W11-O40	-2.51	1.80	1.91
4	N	8701	KEG	W11-O40	-2.51	1.80	1.91
4	A	501	KEG	W11-O40	-2.51	1.80	1.91
4	N	8704	KEG	W11-O40	-2.51	1.80	1.91
4	N	8702	KEG	W11-O40	-2.51	1.80	1.91
4	N	8704	KEG	W1-O1	-2.50	1.64	1.71
4	N	8705	KEG	W11-O40	-2.50	1.80	1.91
4	A	502	KEG	W5-O32	2.44	2.01	1.91
4	A	503	KEG	W5-O32	2.44	2.01	1.91
4	M	8703	KEG	W5-O32	2.43	2.01	1.91
4	N	8703	KEG	W5-O32	2.43	2.01	1.91
4	M	8701	KEG	W5-O32	2.43	2.01	1.91
4	M	8702	KEG	W5-O32	2.43	2.01	1.91
4	N	8701	KEG	W5-O32	2.42	2.01	1.91
4	N	8702	KEG	W5-O32	2.42	2.01	1.91
4	A	501	KEG	W5-O32	2.41	2.01	1.91
4	N	8704	KEG	W5-O32	2.41	2.01	1.91
4	N	8705	KEG	W5-O32	2.40	2.01	1.91
4	M	8702	KEG	W4-O6	-2.39	1.64	1.71
4	A	501	KEG	W4-O6	-2.37	1.65	1.71
4	N	8702	KEG	W4-O6	-2.37	1.65	1.71
4	N	8702	KEG	W4-O21	2.36	2.55	2.43
4	N	8705	KEG	W4-O6	-2.36	1.65	1.71
4	A	501	KEG	W4-O21	2.35	2.55	2.43
4	A	502	KEG	W4-O6	-2.35	1.65	1.71
4	N	8701	KEG	W4-O6	-2.35	1.65	1.71
4	M	8702	KEG	W4-O21	2.35	2.55	2.43
4	M	8703	KEG	W4-O21	2.34	2.55	2.43
4	A	503	KEG	W4-O6	-2.34	1.65	1.71
4	N	8703	KEG	W4-O21	2.34	2.55	2.43
4	N	8704	KEG	W4-O6	-2.34	1.65	1.71
4	A	502	KEG	W4-O21	2.34	2.55	2.43
4	M	8701	KEG	W4-O21	2.34	2.55	2.43
4	N	8701	KEG	W4-O21	2.34	2.55	2.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	8701	KEG	W4-O6	-2.33	1.65	1.71
4	N	8703	KEG	W4-O6	-2.33	1.65	1.71
4	A	503	KEG	W4-O21	2.33	2.55	2.43
4	N	8704	KEG	W4-O21	2.33	2.55	2.43
4	M	8701	KEG	W6-O32	2.32	2.01	1.91
4	N	8705	KEG	W4-O21	2.32	2.55	2.43
4	A	501	KEG	W6-O32	2.31	2.01	1.91
4	N	8704	KEG	W6-O32	2.31	2.01	1.91
4	M	8703	KEG	W4-O6	-2.31	1.65	1.71
4	A	502	KEG	W6-O32	2.31	2.01	1.91
4	N	8703	KEG	W6-O32	2.30	2.01	1.91
4	N	8702	KEG	W1-O25	-2.30	1.81	1.91
4	M	8702	KEG	W1-O25	-2.29	1.81	1.91
4	N	8705	KEG	W6-O32	2.29	2.01	1.91
4	M	8702	KEG	W6-O32	2.29	2.01	1.91
4	M	8701	KEG	W1-O25	-2.29	1.81	1.91
4	M	8703	KEG	W1-O25	-2.29	1.81	1.91
4	M	8703	KEG	W6-O32	2.28	2.01	1.91
4	N	8705	KEG	W1-O25	-2.28	1.81	1.91
4	N	8701	KEG	W7-O33	-2.28	1.81	1.91
4	N	8702	KEG	W6-O32	2.28	2.01	1.91
4	N	8704	KEG	W1-O25	-2.28	1.81	1.91
4	N	8703	KEG	W1-O25	-2.28	1.81	1.91
4	N	8702	KEG	W7-O33	-2.27	1.81	1.91
4	N	8701	KEG	W1-O25	-2.27	1.81	1.91
4	A	503	KEG	W6-O32	2.27	2.01	1.91
4	N	8701	KEG	W6-O32	2.27	2.00	1.91
4	A	502	KEG	W1-O25	-2.27	1.81	1.91
4	N	8703	KEG	W7-O33	-2.27	1.81	1.91
4	A	502	KEG	W4-O26	-2.27	1.81	1.91
4	N	8704	KEG	W7-O33	-2.27	1.81	1.91
4	M	8703	KEG	W7-O33	-2.26	1.81	1.91
4	N	8705	KEG	W7-O33	-2.26	1.81	1.91
4	N	8701	KEG	W4-O26	-2.26	1.81	1.91
4	M	8701	KEG	W4-O26	-2.26	1.81	1.91
4	M	8702	KEG	W4-O26	-2.26	1.81	1.91
4	A	503	KEG	W7-O33	-2.25	1.81	1.91
4	M	8703	KEG	W4-O26	-2.25	1.81	1.91
4	N	8705	KEG	W4-O26	-2.25	1.81	1.91
4	A	501	KEG	W1-O25	-2.25	1.81	1.91
4	A	502	KEG	W7-O33	-2.25	1.81	1.91
4	A	501	KEG	W7-O33	-2.24	1.81	1.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	8704	KEG	W4-O26	-2.24	1.81	1.91
4	A	503	KEG	W1-O25	-2.24	1.81	1.91
4	M	8701	KEG	W7-O33	-2.24	1.81	1.91
4	N	8703	KEG	W4-O26	-2.24	1.81	1.91
4	A	501	KEG	W4-O26	-2.24	1.81	1.91
4	N	8702	KEG	W4-O26	-2.24	1.81	1.91
4	A	503	KEG	W4-O26	-2.23	1.81	1.91
4	A	502	KEG	W2-O26	-2.23	1.81	1.91
4	A	503	KEG	W2-O26	-2.22	1.81	1.91
4	N	8704	KEG	W2-O26	-2.22	1.81	1.91
4	M	8702	KEG	W7-O33	-2.22	1.81	1.91
4	A	501	KEG	W2-O26	-2.22	1.81	1.91
4	M	8702	KEG	W2-O26	-2.21	1.81	1.91
4	N	8701	KEG	W2-O26	-2.21	1.81	1.91
4	N	8702	KEG	W2-O26	-2.21	1.81	1.91
4	N	8705	KEG	W2-O26	-2.21	1.81	1.91
4	M	8701	KEG	W2-O26	-2.20	1.81	1.91
4	M	8703	KEG	W2-O26	-2.20	1.81	1.91
4	M	8702	KEG	W11-O44	-2.19	1.82	1.93
4	N	8704	KEG	W8-O41	-2.19	1.82	1.93
4	N	8702	KEG	W8-O41	-2.18	1.82	1.93
4	N	8703	KEG	W2-O26	-2.18	1.81	1.91
4	M	8701	KEG	W8-O41	-2.17	1.82	1.93
4	N	8705	KEG	W8-O41	-2.17	1.83	1.93
4	N	8702	KEG	W11-O44	-2.17	1.83	1.93
4	A	501	KEG	W8-O41	-2.17	1.83	1.93
4	N	8705	KEG	W11-O44	-2.17	1.83	1.93
4	A	503	KEG	W11-O44	-2.17	1.83	1.93
4	M	8703	KEG	W11-O44	-2.17	1.83	1.93
4	M	8702	KEG	W8-O41	-2.16	1.83	1.93
4	N	8703	KEG	W8-O41	-2.16	1.83	1.93
4	N	8701	KEG	W11-O44	-2.16	1.83	1.93
4	M	8703	KEG	W8-O41	-2.16	1.83	1.93
4	A	503	KEG	W8-O41	-2.16	1.83	1.93
4	N	8701	KEG	W8-O41	-2.15	1.83	1.93
4	N	8703	KEG	W11-O44	-2.15	1.83	1.93
4	N	8704	KEG	W11-O44	-2.15	1.83	1.93
4	A	502	KEG	W11-O44	-2.15	1.83	1.93
4	A	501	KEG	W11-O44	-2.15	1.83	1.93
4	A	502	KEG	W8-O41	-2.15	1.83	1.93
4	M	8701	KEG	W11-O44	-2.15	1.83	1.93
4	M	8703	KEG	W3-O31	2.01	2.03	1.93

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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.

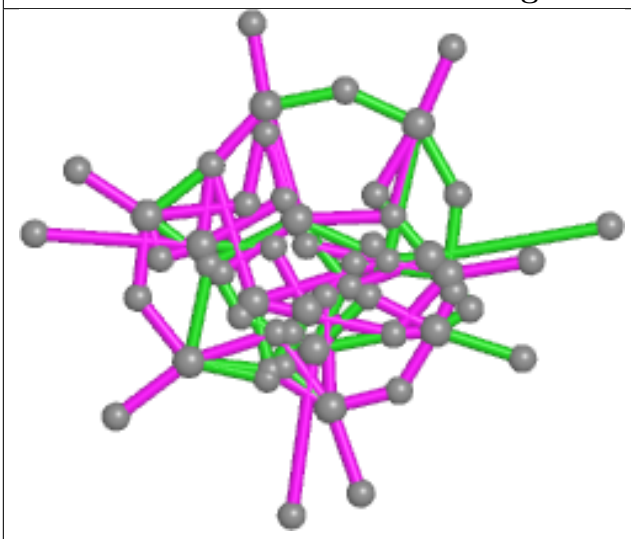
There are no ring outliers.

11 monomers are involved in 101 short contacts:

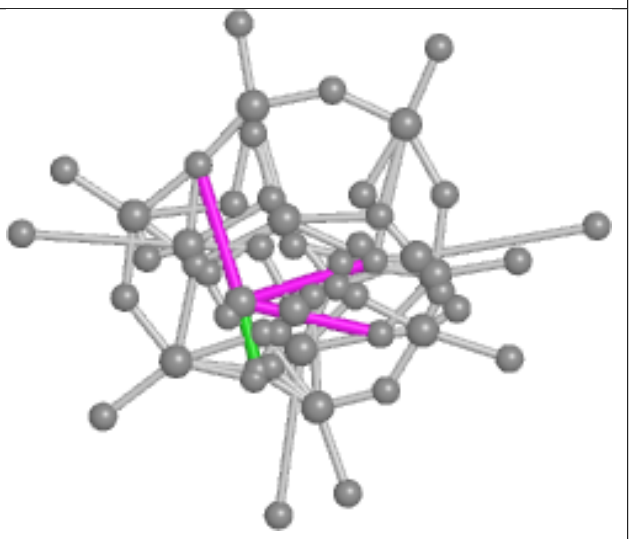
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	KEG	24	0
4	A	502	KEG	13	0
4	M	8701	KEG	6	0
4	M	8702	KEG	6	0
4	N	8701	KEG	6	0
4	N	8702	KEG	6	0
4	N	8703	KEG	6	0
4	N	8704	KEG	6	0
4	N	8705	KEG	6	0
4	M	8703	KEG	6	0
4	A	503	KEG	16	0

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

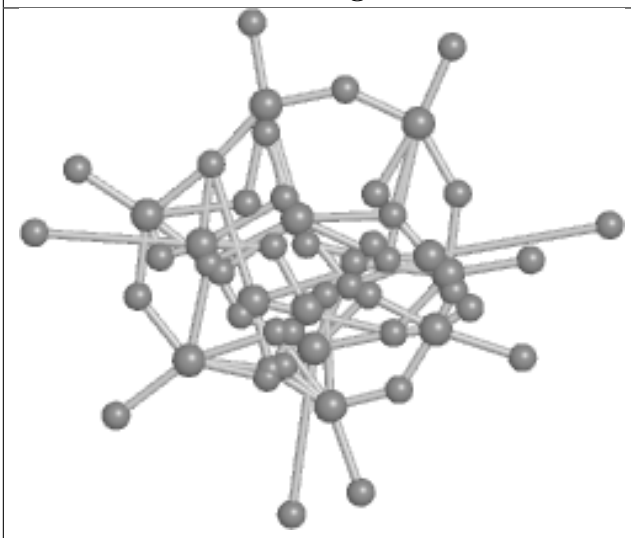
Ligand KEG A 501



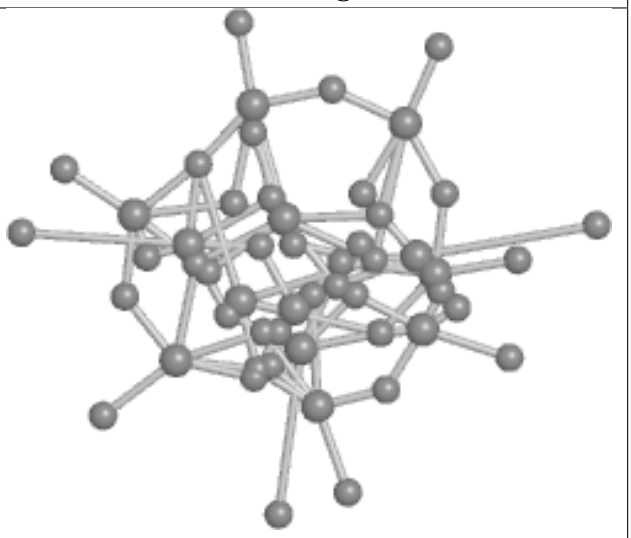
Bond lengths



Bond angles

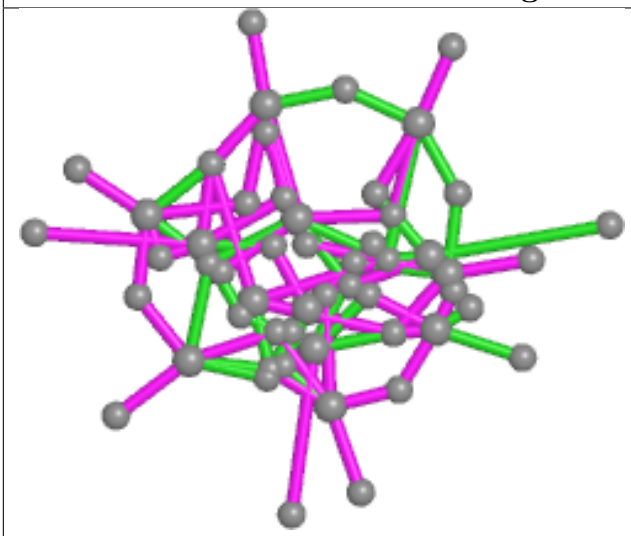


Torsions

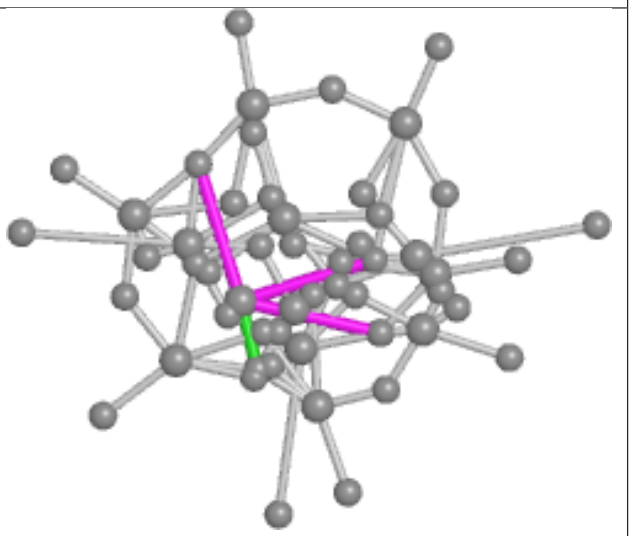


Rings

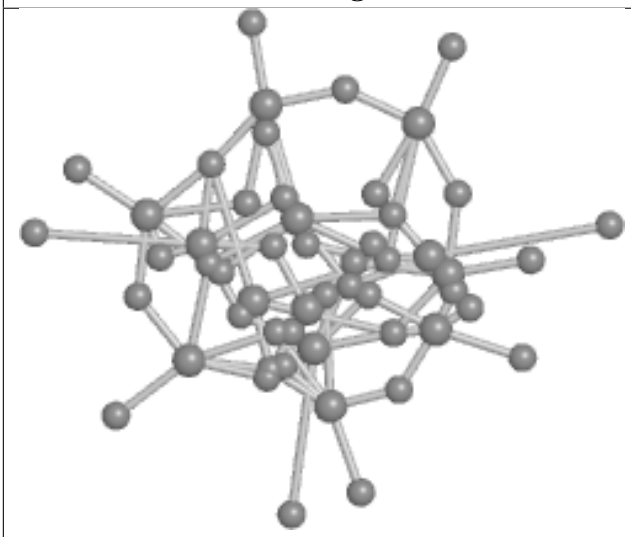
Ligand KEG A 502



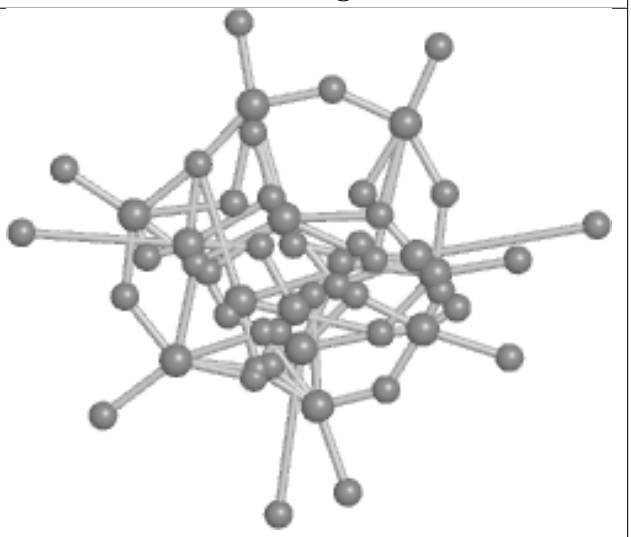
Bond lengths



Bond angles

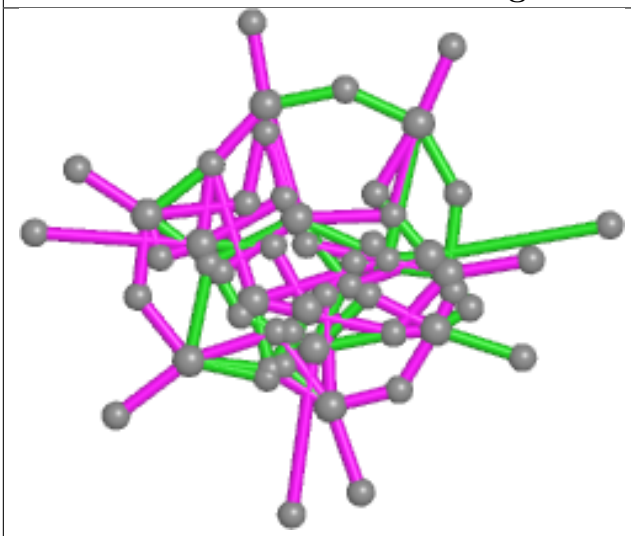


Torsions

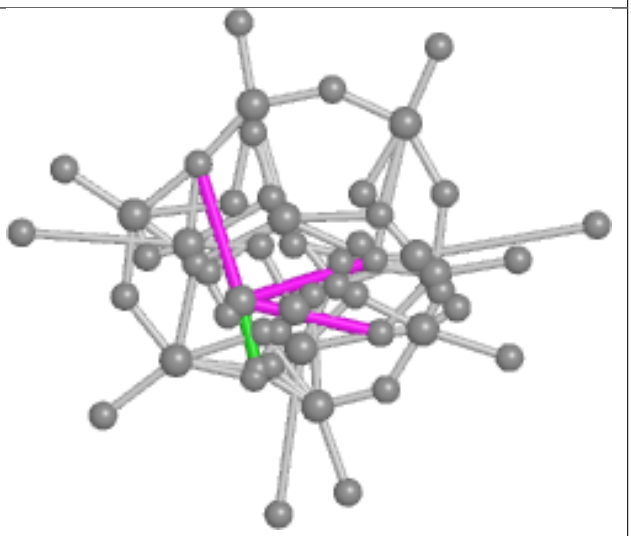


Rings

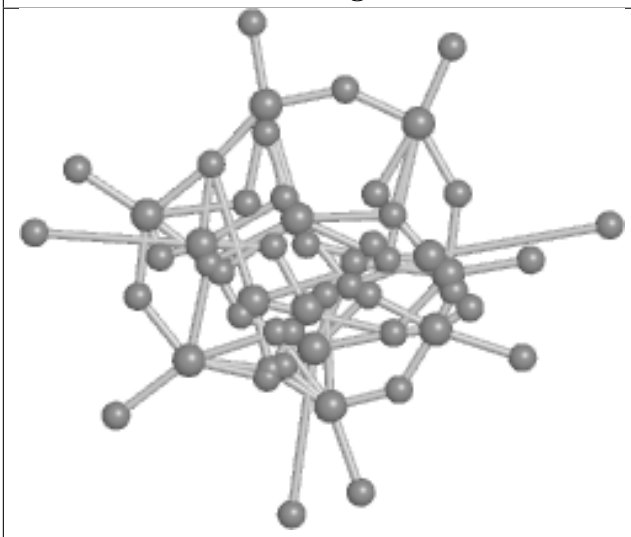
Ligand KEG M 8701



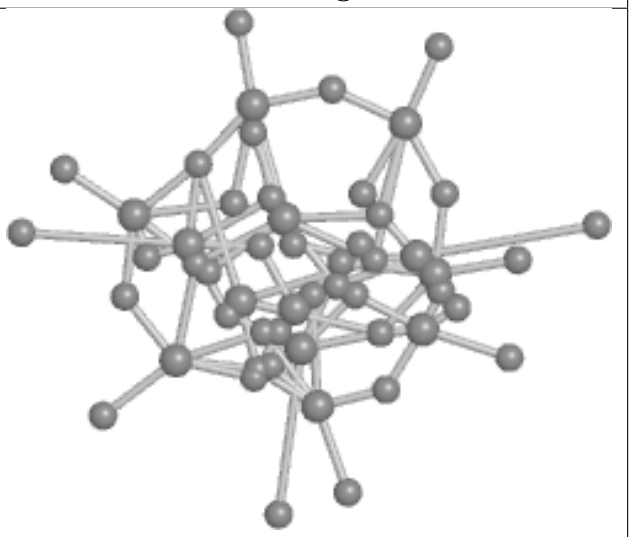
Bond lengths



Bond angles

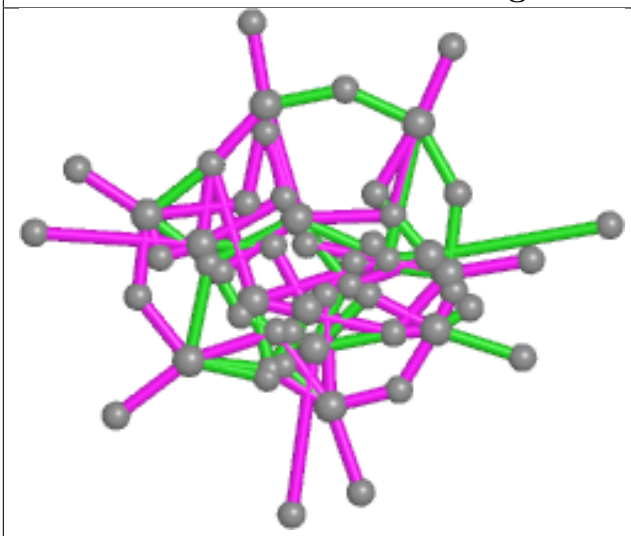


Torsions

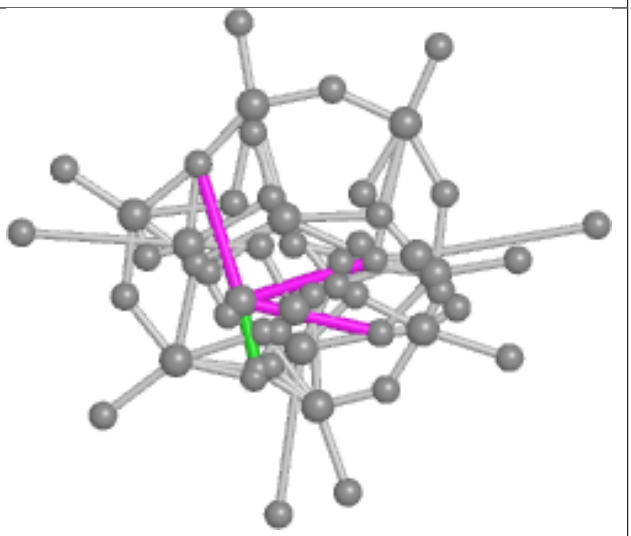


Rings

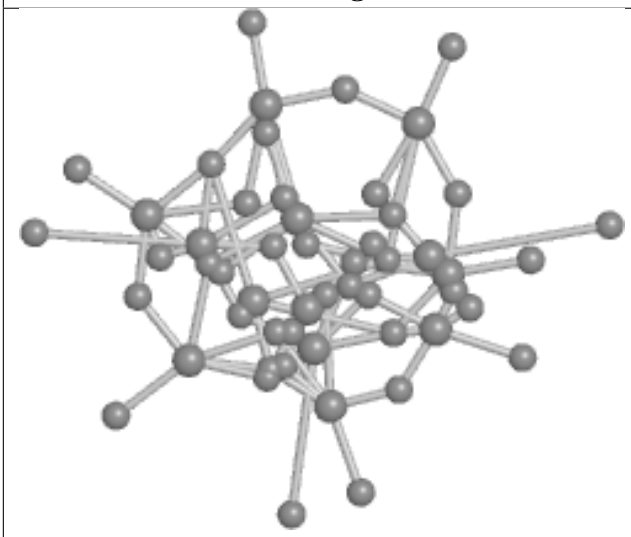
Ligand KEG M 8702



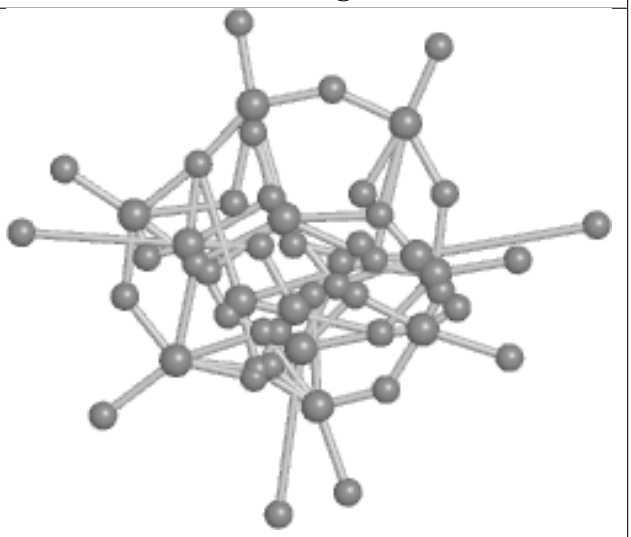
Bond lengths



Bond angles

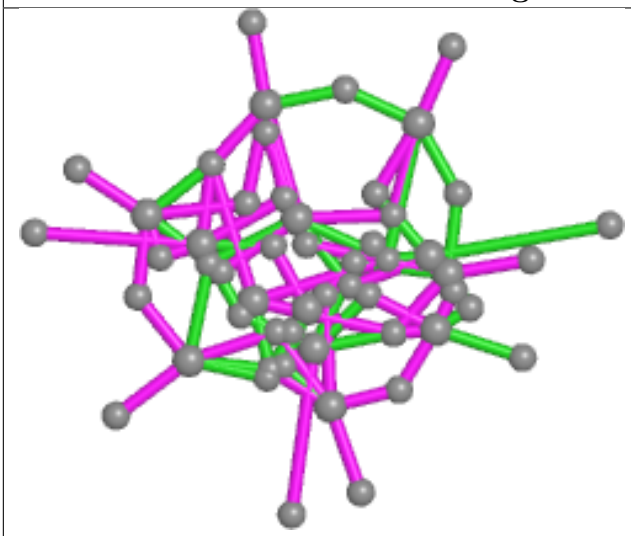


Torsions

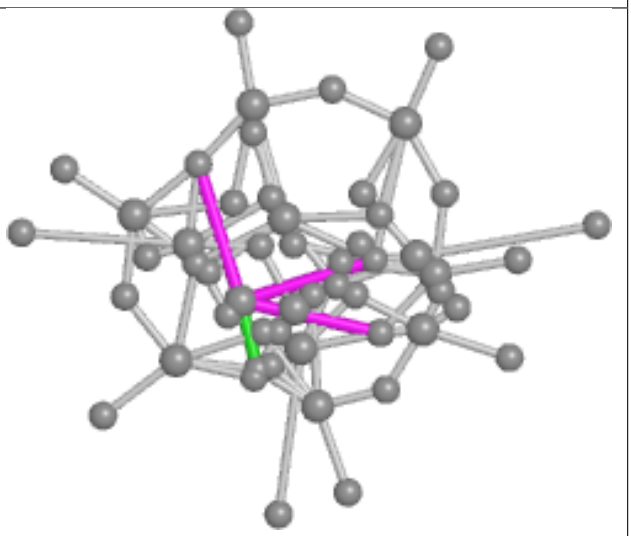


Rings

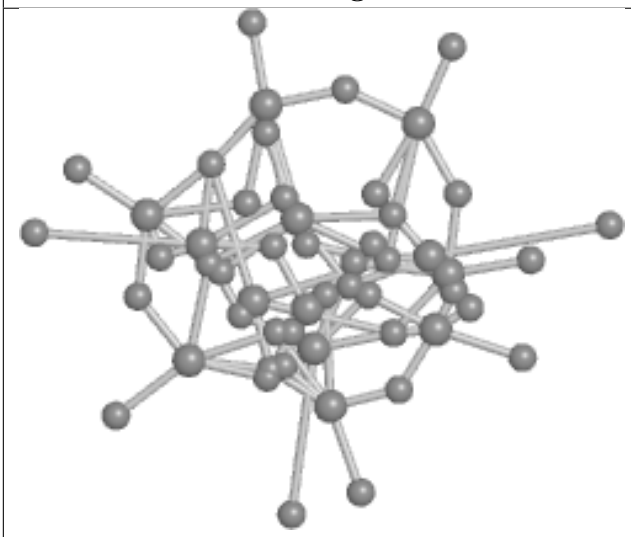
Ligand KEG N 8701



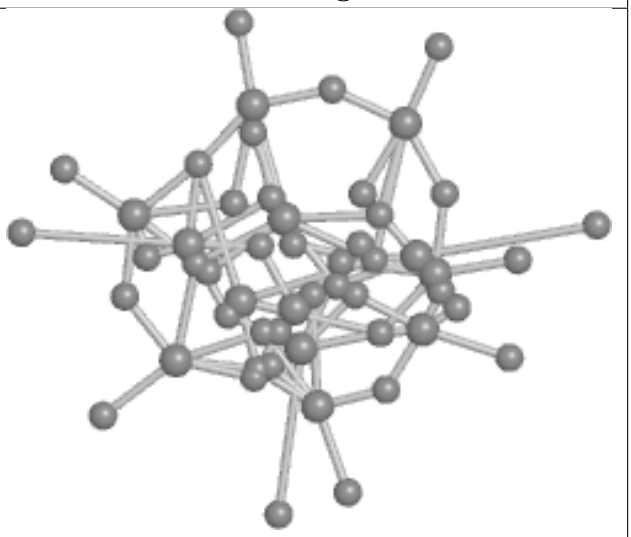
Bond lengths



Bond angles

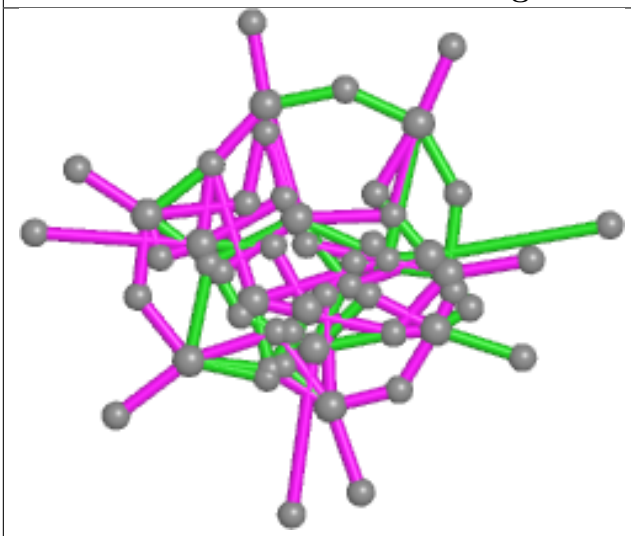


Torsions

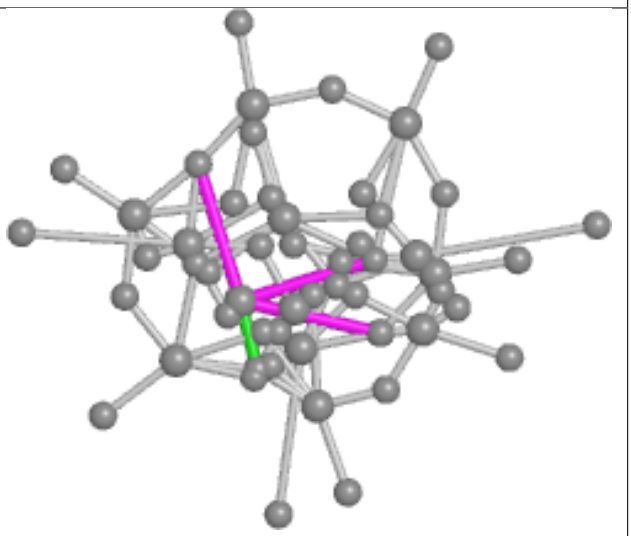


Rings

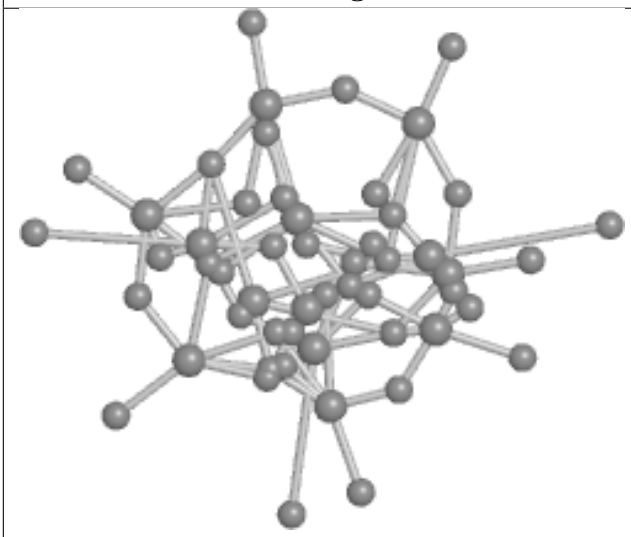
Ligand KEG N 8702



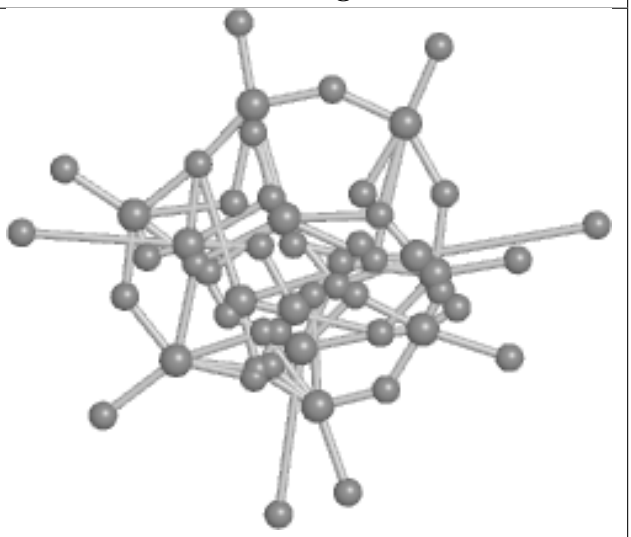
Bond lengths



Bond angles

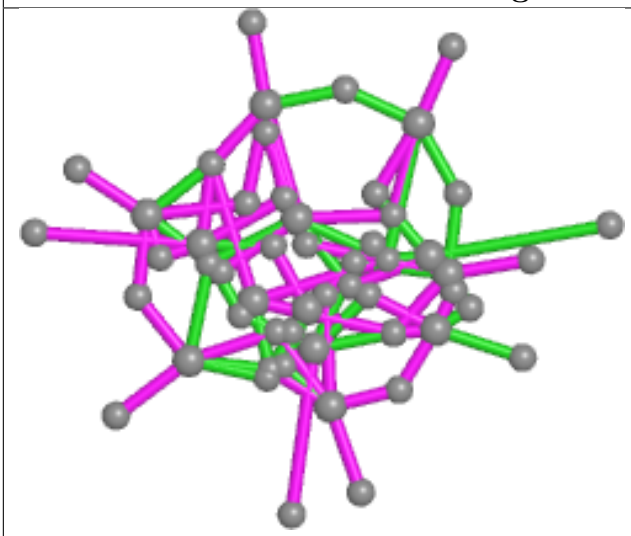


Torsions

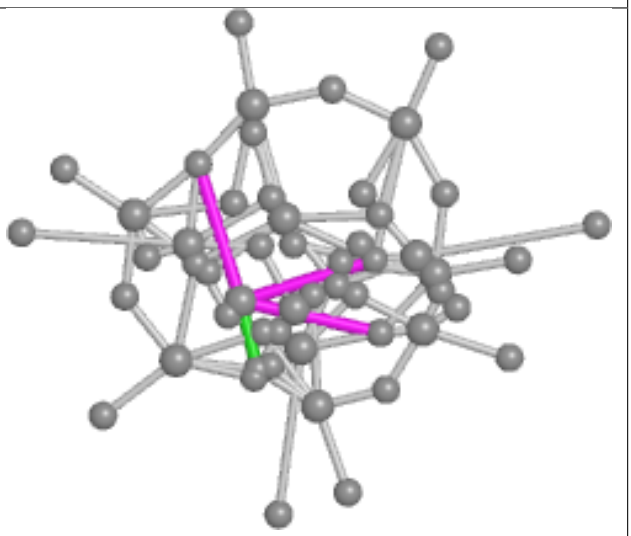


Rings

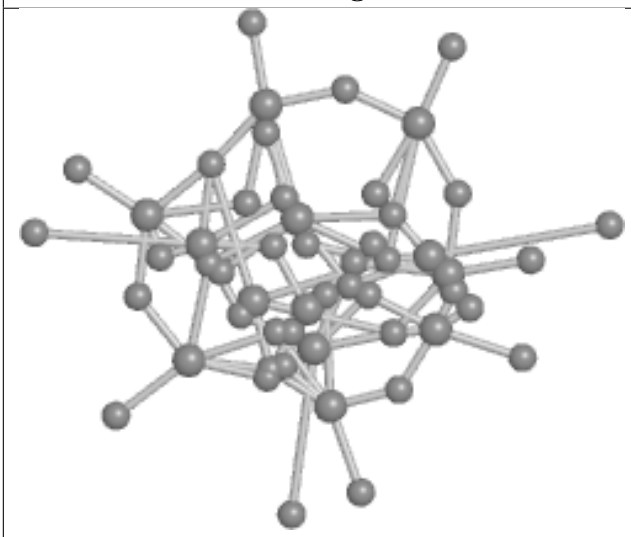
Ligand KEG N 8703



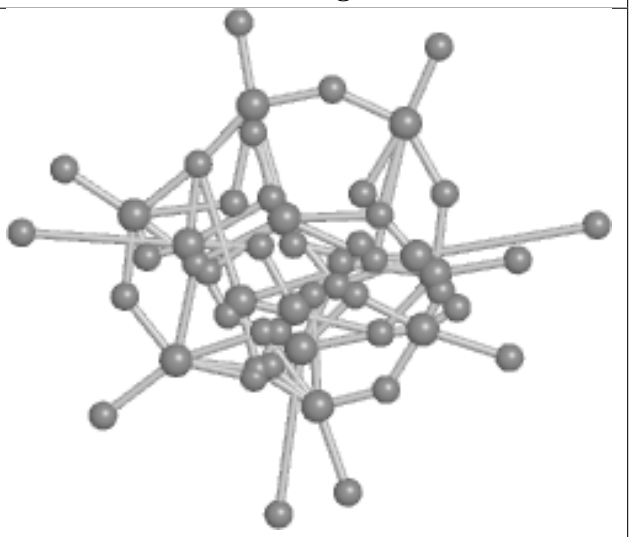
Bond lengths



Bond angles

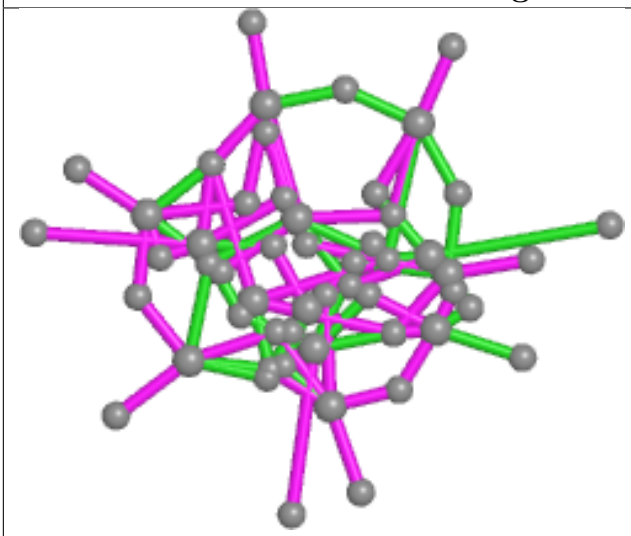


Torsions

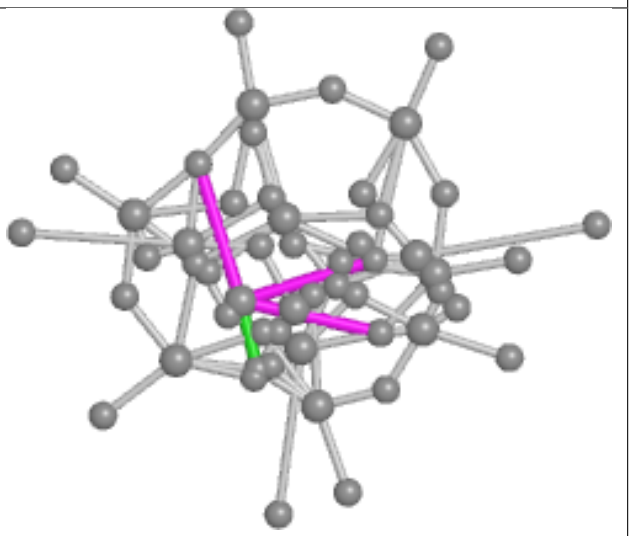


Rings

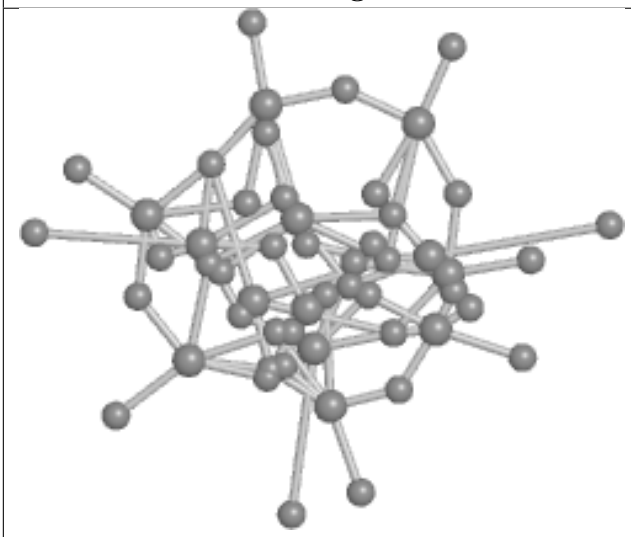
Ligand KEG N 8704



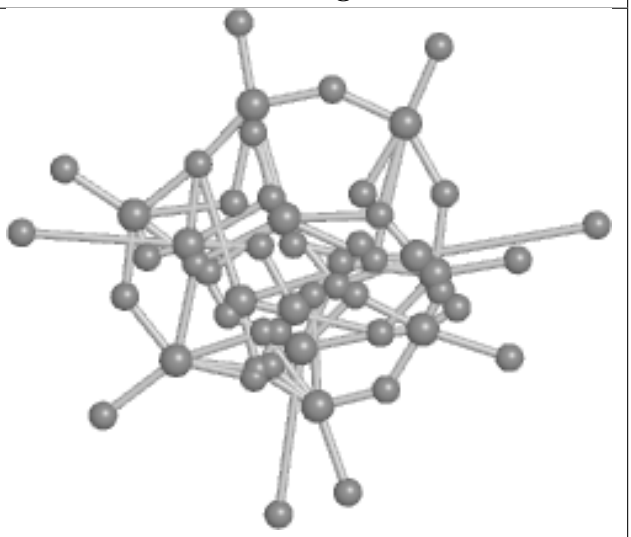
Bond lengths



Bond angles

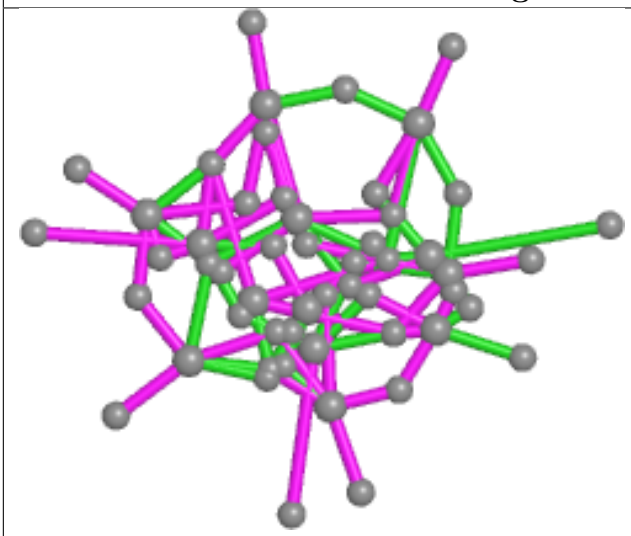


Torsions

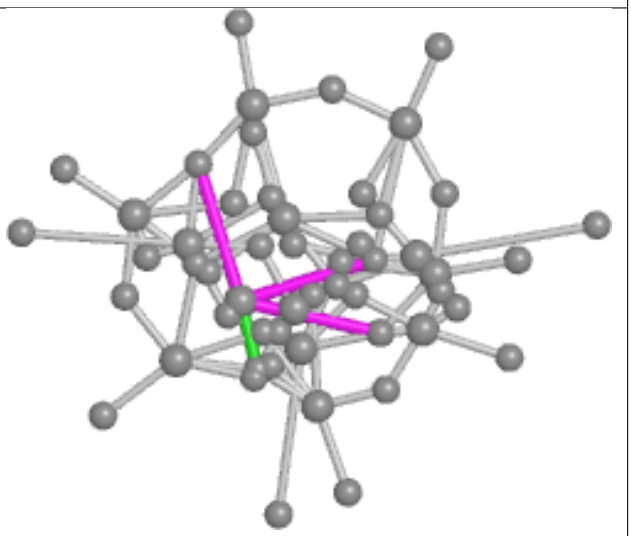


Rings

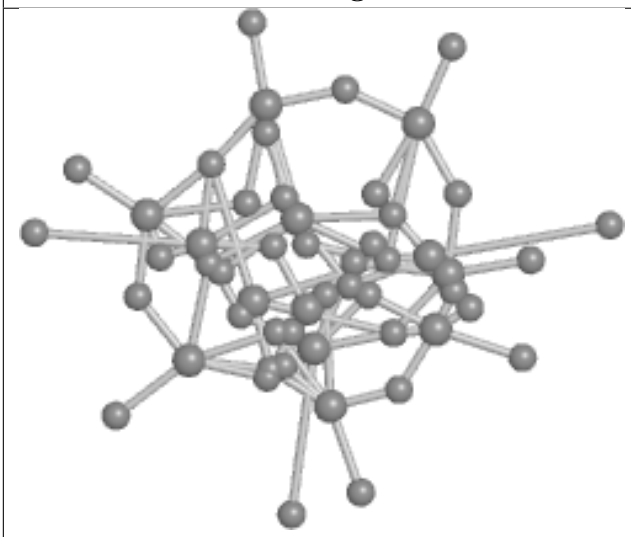
Ligand KEG N 8705



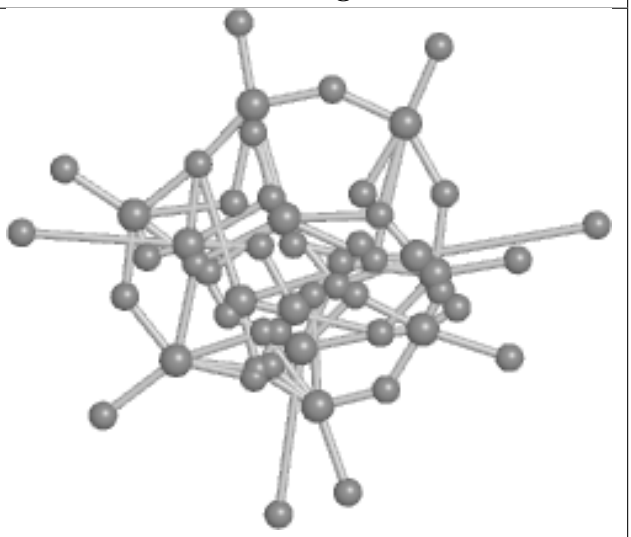
Bond lengths



Bond angles

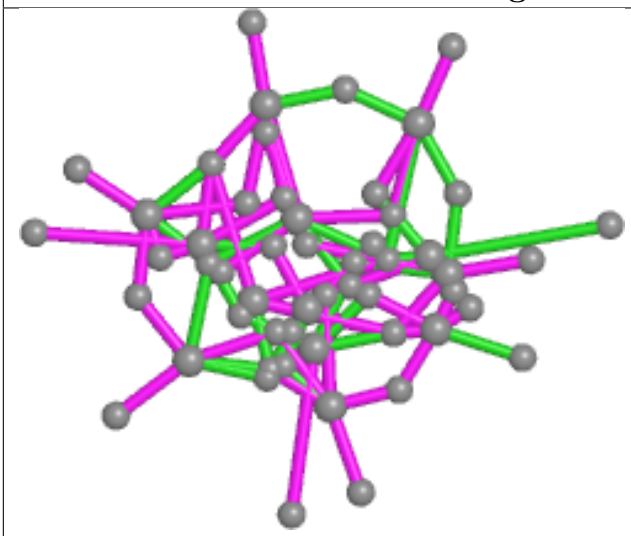


Torsions

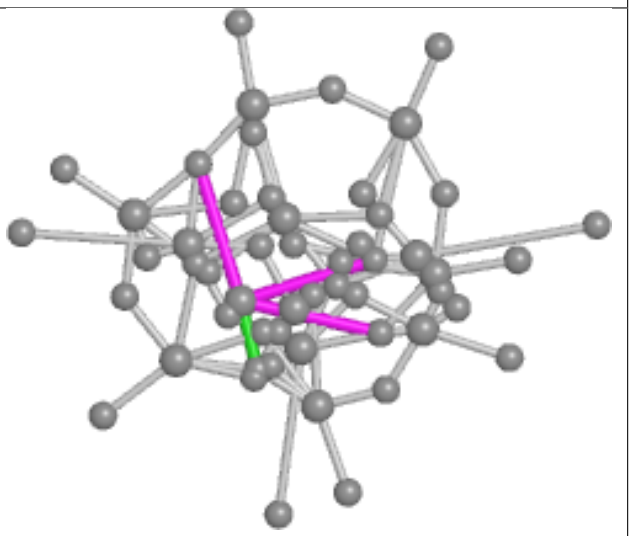


Rings

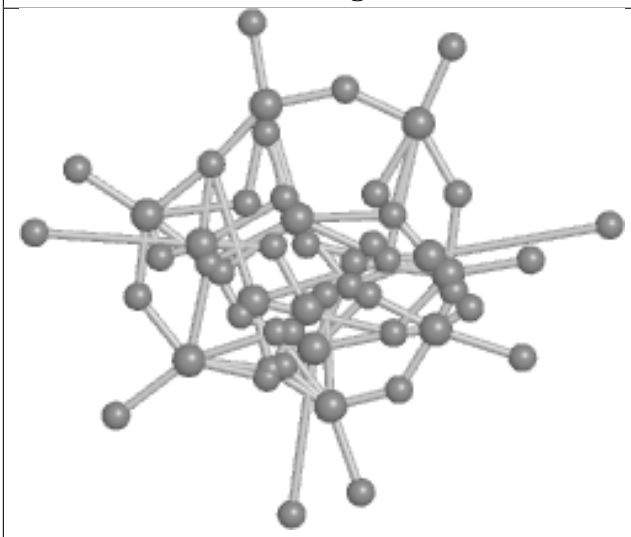
Ligand KEG M 8703



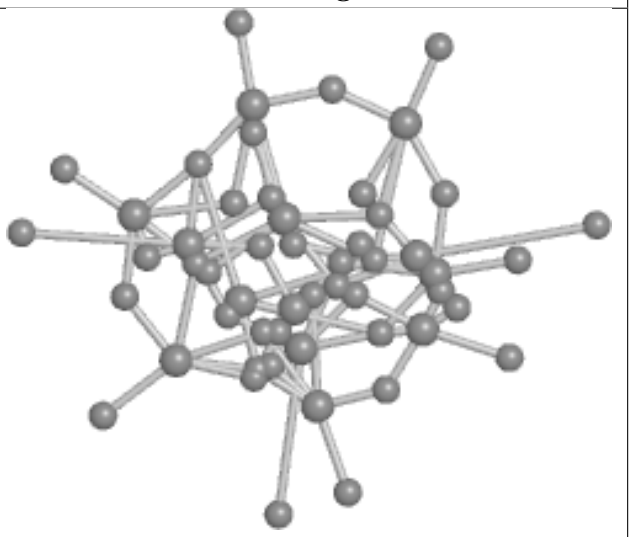
Bond lengths



Bond angles

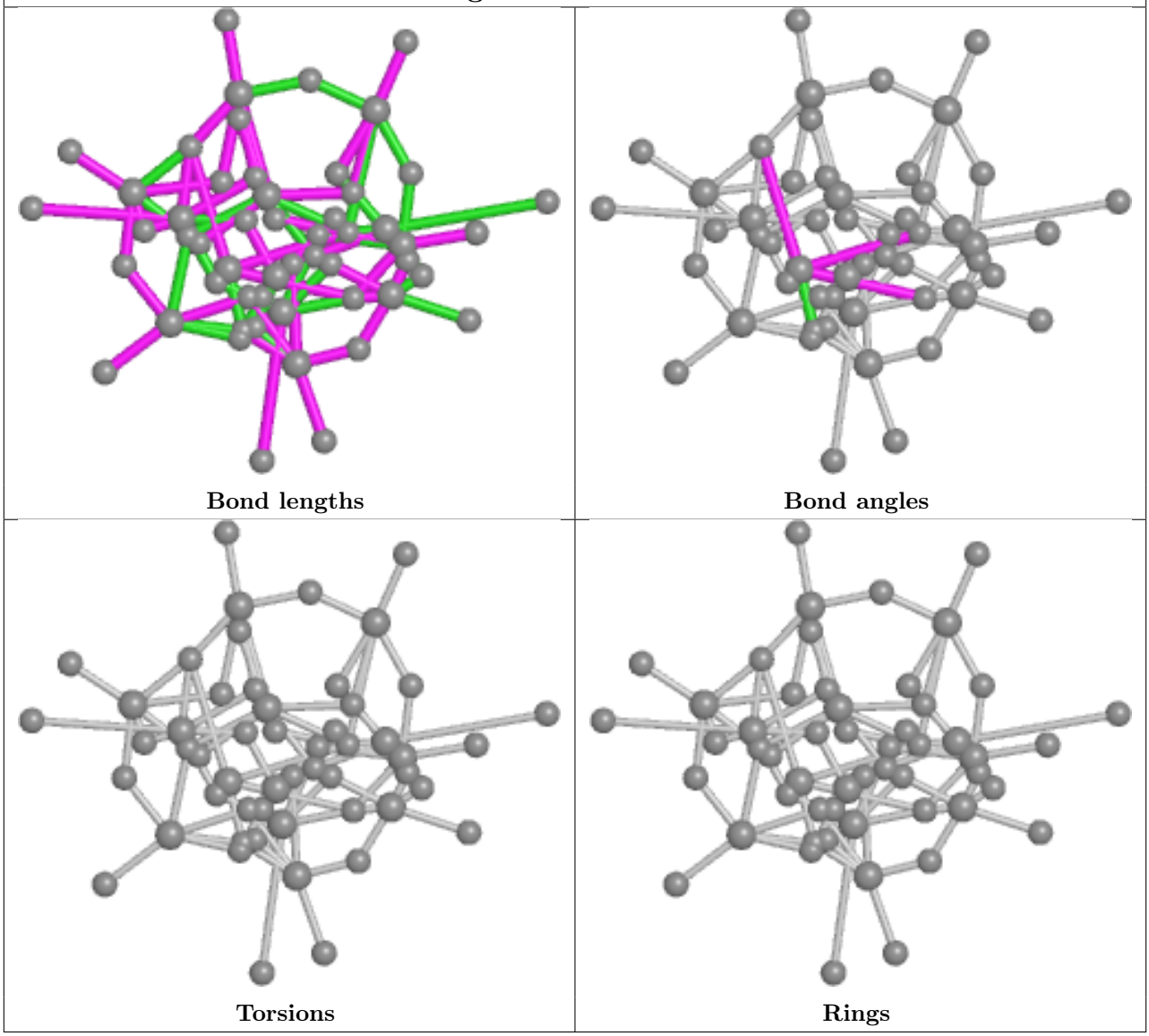


Torsions



Rings

Ligand KEG A 503



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

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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

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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

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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

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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

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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

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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

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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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	374/446 (83%)	0.57	33 (8%)	10	12	200, 200, 200, 200	0
1	C	374/446 (83%)	0.42	23 (6%)	21	20	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%)	0.49	56 (7%)	14	15	200, 200, 200, 200	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	108	SER	5.3
1	A	384	THR	5.3
1	A	106	ALA	5.2
1	C	335	THR	4.7
1	A	104	CYS	4.5
1	A	424	GLU	4.3
1	C	390	TYR	4.1
1	C	283	GLN	4.0
1	A	267	GLU	3.9
1	A	305	GLU	3.9
1	C	399	ARG	3.6
1	A	435	GLU	3.6
1	A	386	GLU	3.5
1	A	411	SER	3.5
1	A	179	LYS	3.5
1	C	336	VAL	3.3
1	A	335	THR	3.3
1	A	105	GLN	3.1
1	A	304	LEU	3.1
1	C	394	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	362	SER	3.0
1	C	398	GLY	2.9
1	C	397	ALA	2.9
1	A	248	ALA	2.9
1	C	302	ASP	2.9
1	A	286	ILE	2.8
1	C	337	HIS	2.8
1	C	395	GLY	2.7
1	A	287	LYS	2.7
1	A	385	ASN	2.7
1	A	397	ALA	2.6
1	A	107	LYS	2.6
1	A	368	ARG	2.6
1	C	108	SER	2.5
1	C	107	LYS	2.5
1	A	164	VAL	2.5
1	C	126	PRO	2.5
1	C	258	CYS	2.4
1	C	246	PHE	2.4
1	A	407	ILE	2.4
1	C	371	ASP	2.4
1	A	129	GLY	2.3
1	C	301	LEU	2.3
1	A	263	GLN	2.3
1	A	95	GLN	2.3
1	A	301	LEU	2.3
1	A	181	LYS	2.2
1	A	143	ALA	2.1
1	A	268	ILE	2.1
1	C	411	SER	2.1
1	A	433	PHE	2.1
1	C	111	GLY	2.1
1	A	410	VAL	2.0
1	A	250	LEU	2.0
1	C	140	ARG	2.0
1	C	396	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

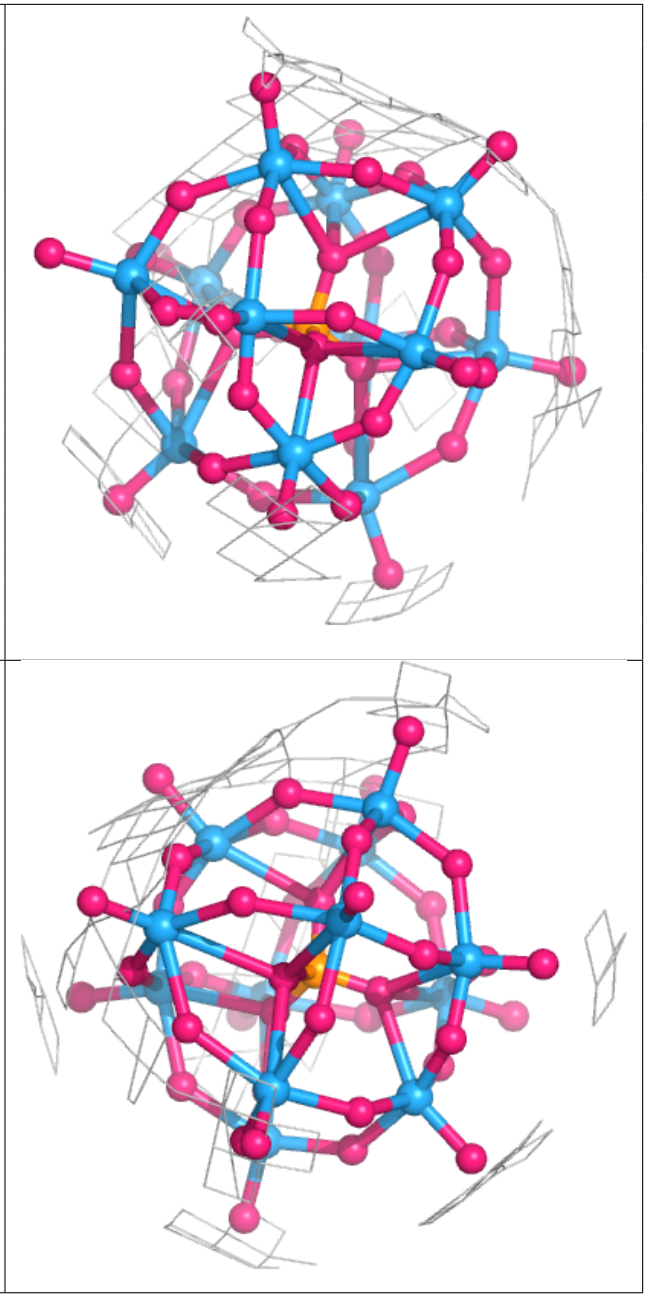
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	KEG	A	503	53/53	0.87	0.35	200,200,200,200	53
4	KEG	A	502	53/53	0.88	0.25	200,200,200,200	53
4	KEG	N	8703	53/53	0.90	0.17	200,200,200,200	53
4	KEG	A	501	53/53	0.92	0.18	200,200,200,200	53
4	KEG	N	8702	53/53	0.97	0.15	200,200,200,200	53
4	KEG	N	8701	53/53	0.98	0.09	200,200,200,200	53
4	KEG	M	8701	53/53	0.98	0.16	200,200,200,200	53
4	KEG	M	8703	53/53	0.98	0.20	200,200,200,200	53
4	KEG	N	8704	53/53	0.98	0.16	200,200,200,200	53
4	KEG	N	8705	53/53	0.98	0.12	200,200,200,200	53
4	KEG	M	8702	53/53	0.99	0.09	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.

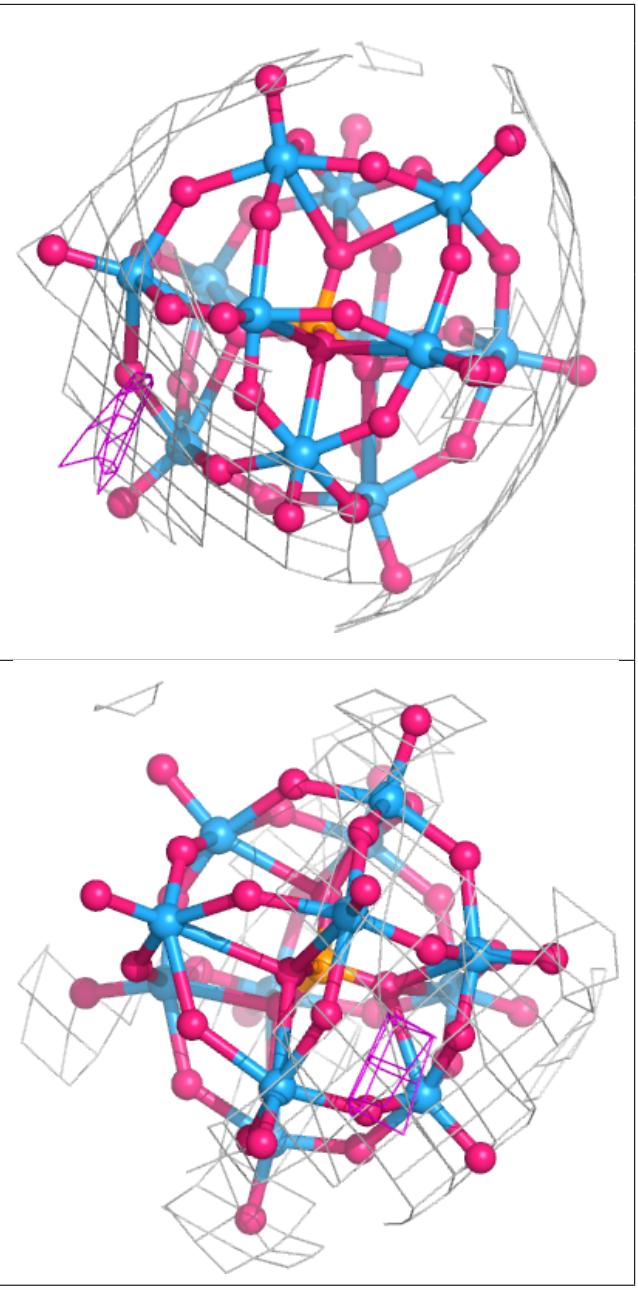
Electron density around KEG A 503:

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



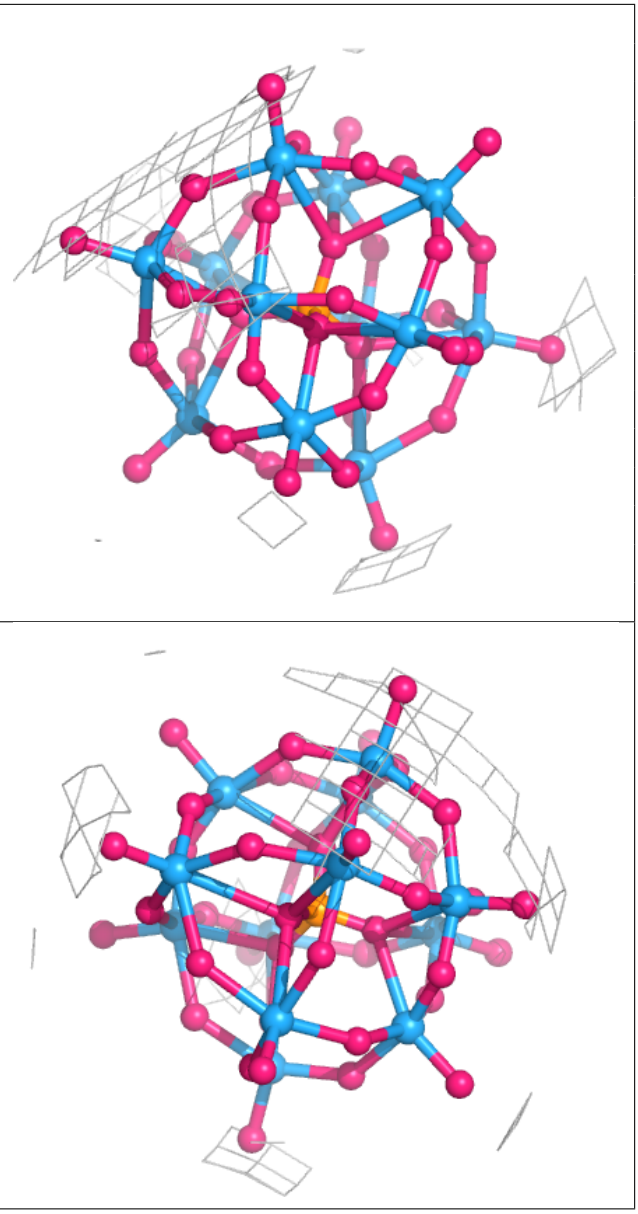
Electron density around KEG A 502:

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



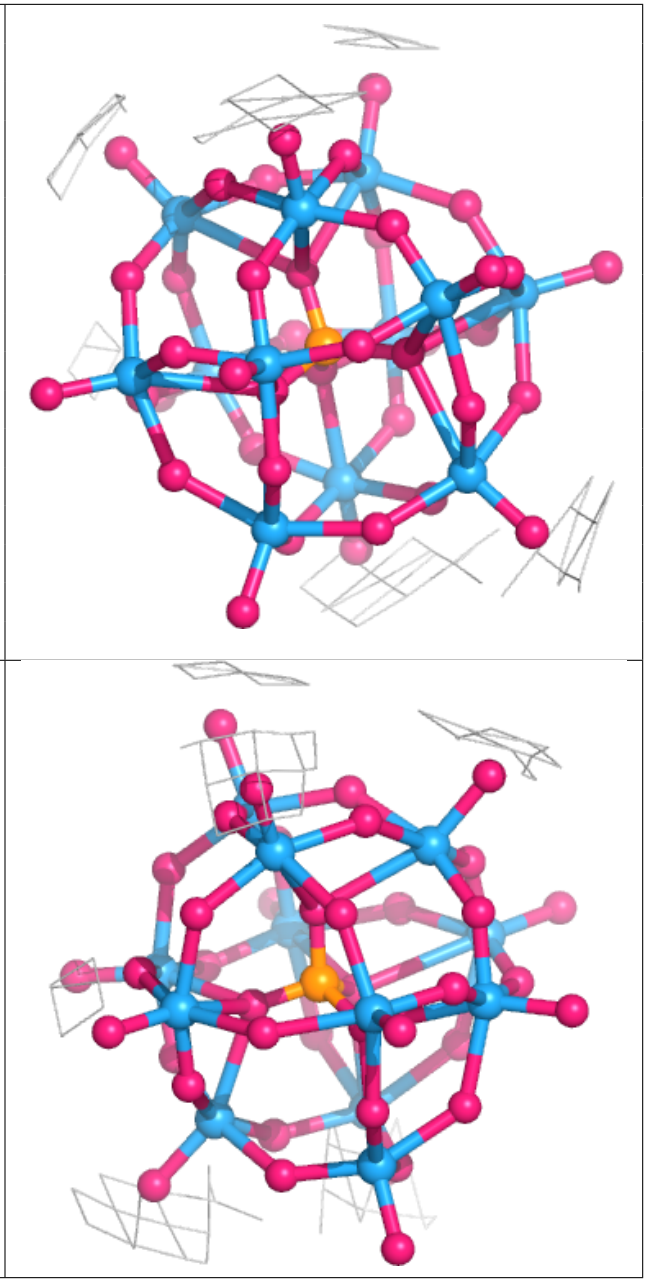
Electron density around KEG N 8703:

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



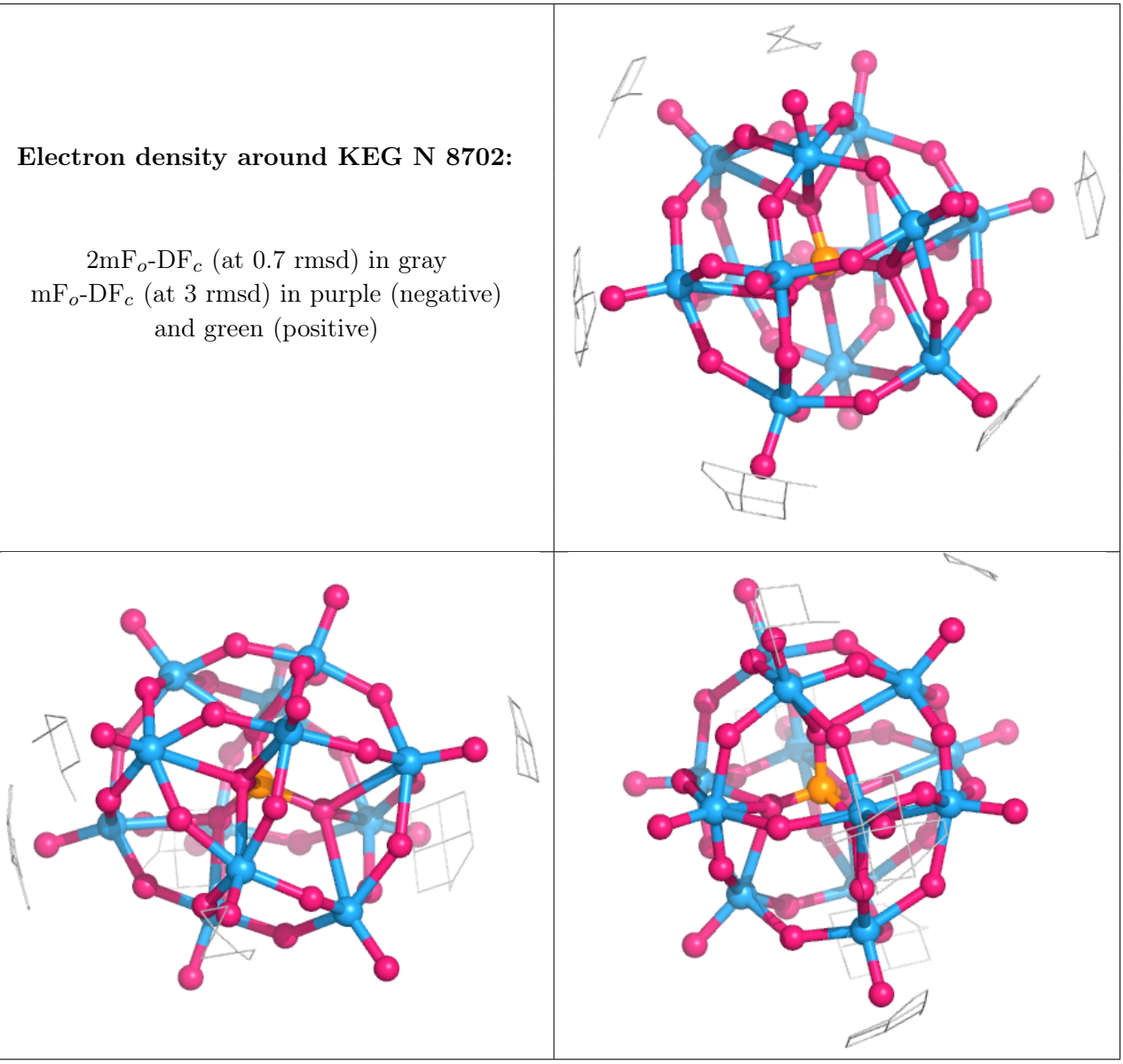
Electron density around KEG A 501:

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



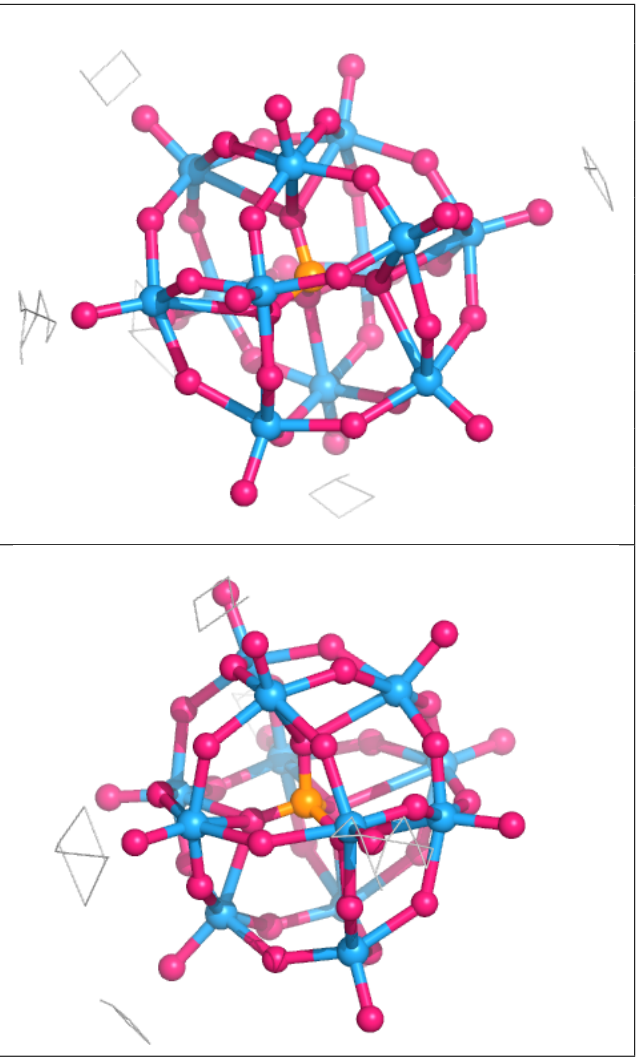
Electron density around KEG N 8702:

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



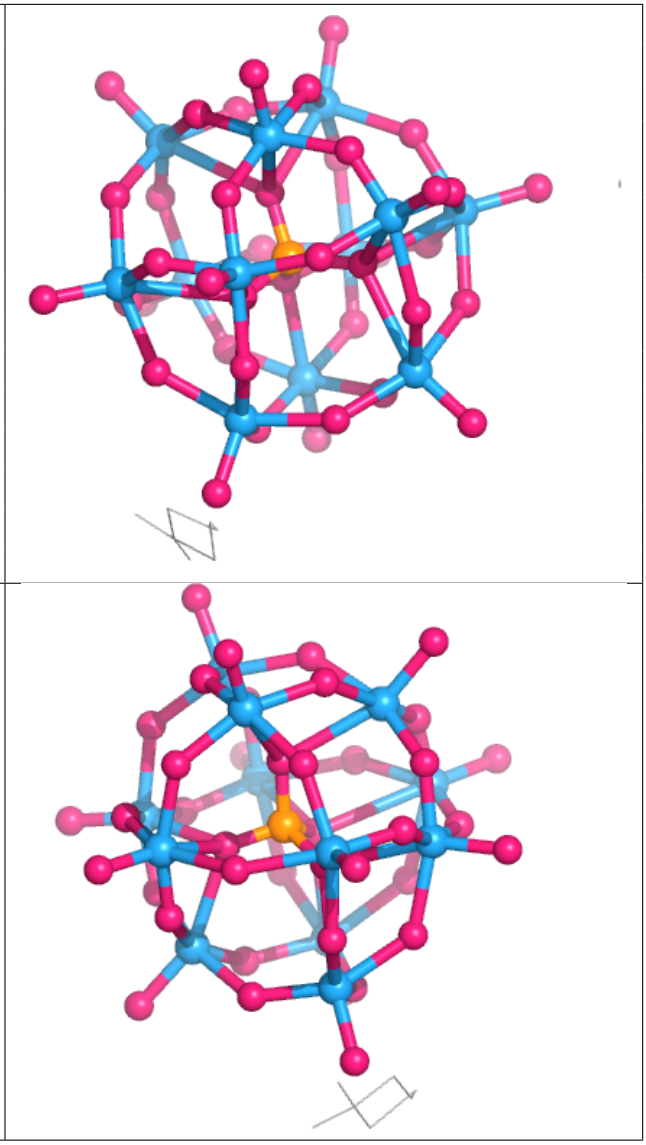
Electron density around KEG N 8701:

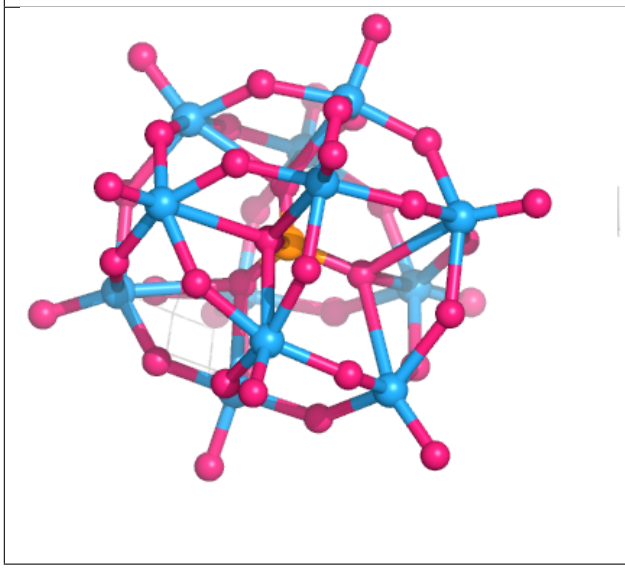
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around KEG M 8701:

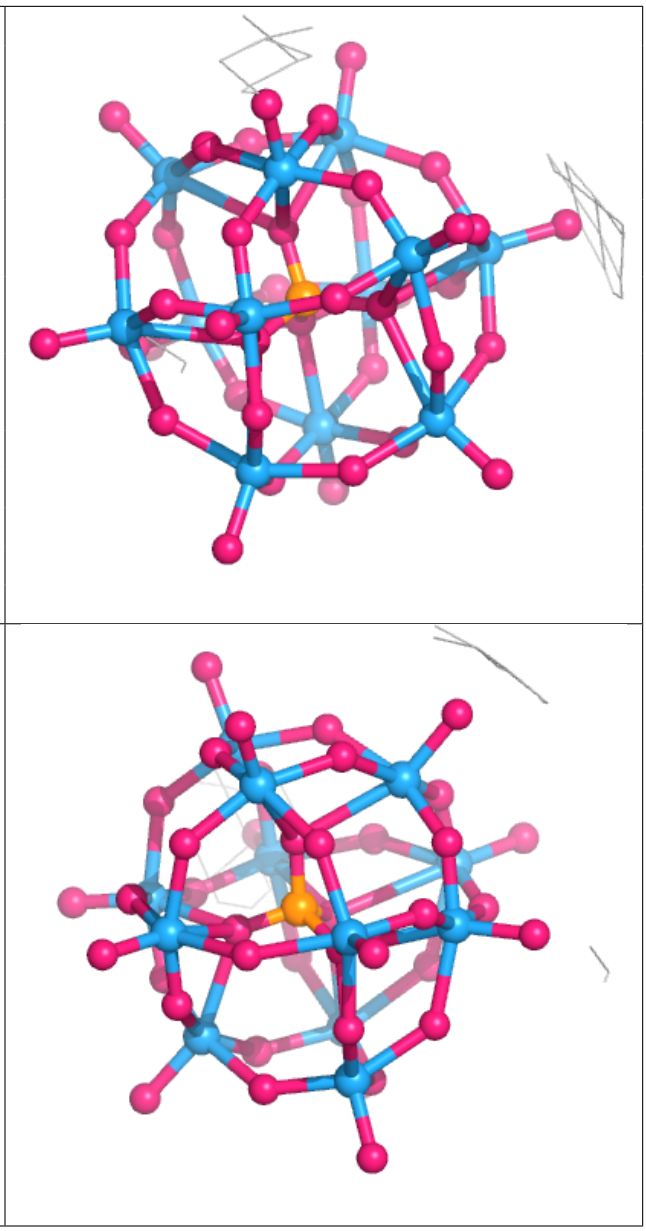
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





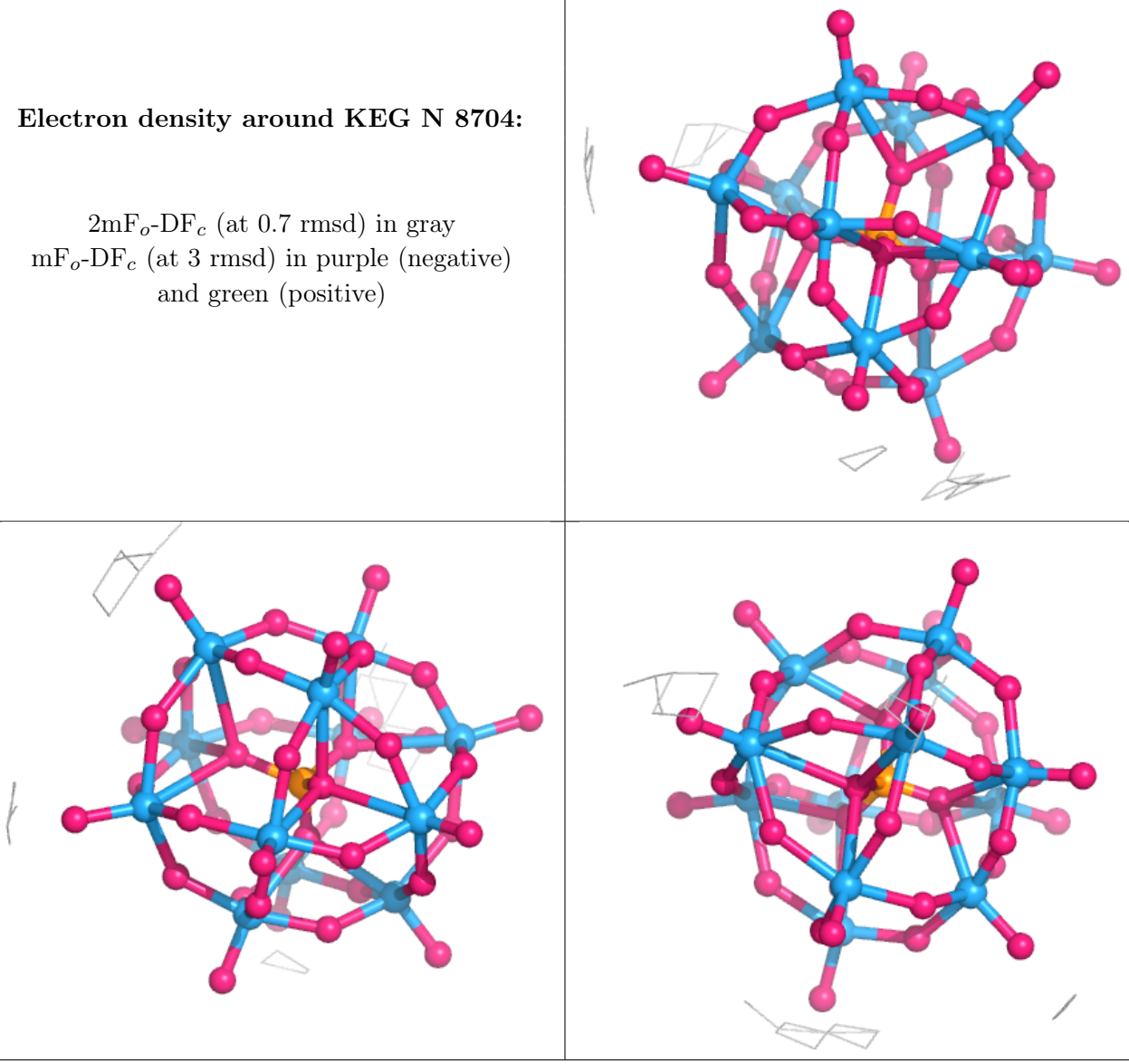
Electron density around KEG M 8703:

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



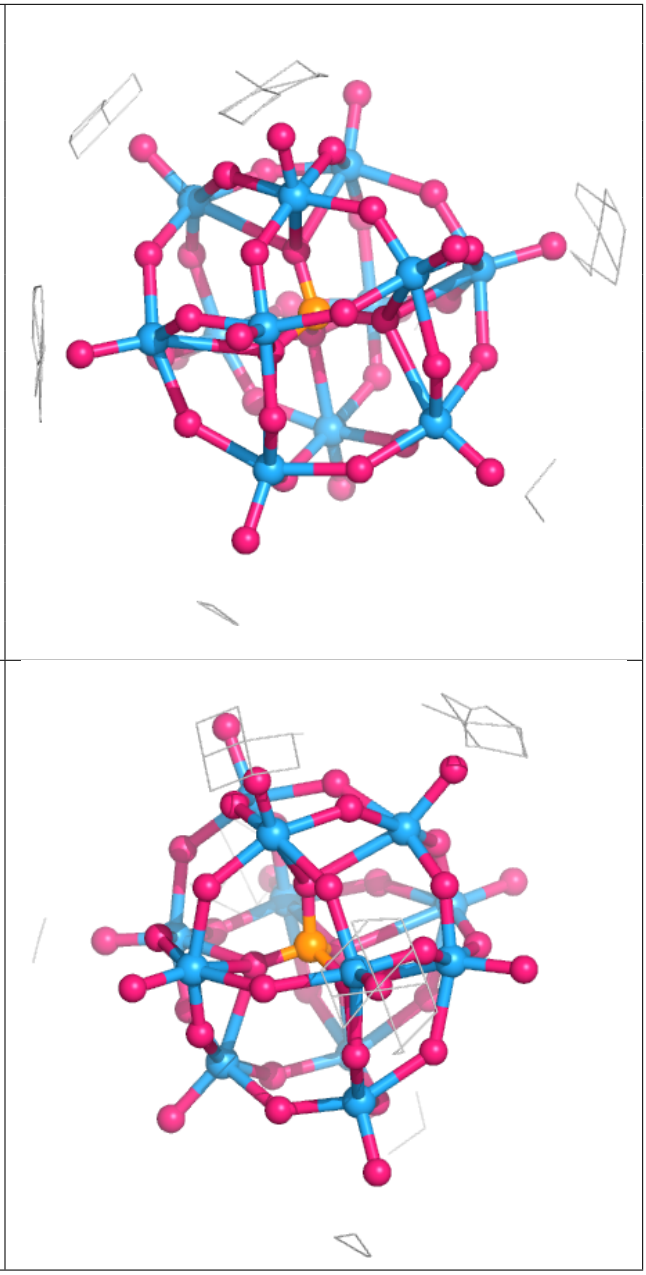
Electron density around KEG N 8704:

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



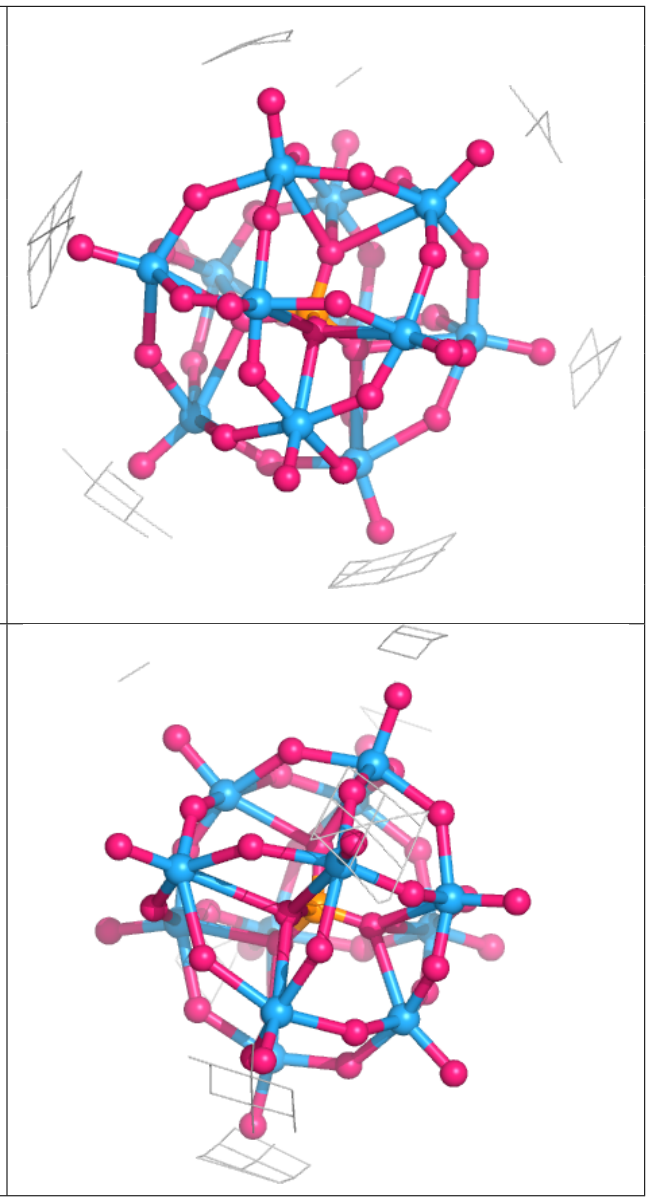
Electron density around KEG N 8705:

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 8702:

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.