Full wwPDB X-ray Structure Validation Report ⓘ

Feb 8, 2024 – 01:39 AM EST

PDB ID	:	8EYZ
Title	:	Engineered glutamine binding protein bound to GLN and a cobaloxime ligand
Authors	:	Bridwell-Rabb, J.; Boggs, D.G.; Olshansky, L.; Fatima, S.; Thompson, P.
Deposited on	:	2022-10-29
Resolution	:	2.99 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:

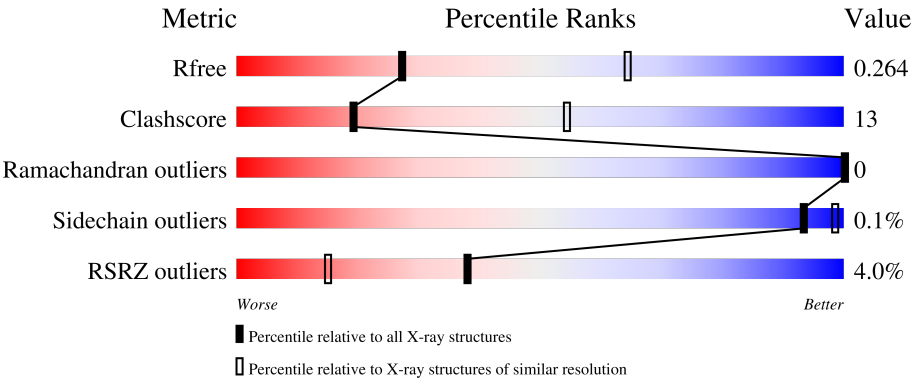
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	229	3% 71% 27% .
1	B	229	3% 69% 27% .
1	C	229	% 75% 21% .
1	D	229	% 75% 22% .
1	E	229	5% 74% 24% .

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Mol	Chain	Length	Quality of chain
1	F	229	3% 76% 21%
1	G	229	2% 74% 23%
1	H	229	% 79% 18%
1	I	229	9% 76% 22%
1	J	229	6% 76% 21%
1	K	229	9% 78% 20%
1	L	229	4% 72% 24%

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
3	SO4	A	303	-	-	-	X
4	GLN	I	302	-	-	X	-
4	GLN	K	302	-	-	X	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 21269 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 Amino acid ABC transporter substrate-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1760	1127	290	339	4			
1	B	221	Total	C	N	O	S	0	0	0
			1722	1104	284	330	4			
1	C	219	Total	C	N	O	S	0	0	0
			1706	1094	281	327	4			
1	D	221	Total	C	N	O	S	0	0	0
			1722	1104	284	330	4			
1	E	224	Total	C	N	O	S	0	0	0
			1746	1118	287	337	4			
1	F	223	Total	C	N	O	S	0	0	0
			1738	1114	286	334	4			
1	G	222	Total	C	N	O	S	0	0	0
			1731	1109	285	333	4			
1	H	221	Total	C	N	O	S	0	0	0
			1722	1103	283	332	4			
1	I	223	Total	C	N	O	S	0	0	0
			1738	1114	286	334	4			
1	J	222	Total	C	N	O	S	0	0	0
			1731	1109	285	333	4			
1	K	224	Total	C	N	O	S	0	0	0
			1747	1120	288	335	4			
1	L	220	Total	C	N	O	S	0	0	0
			1713	1098	282	329	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP C3THM2
A	-2	ASN	-	expression tag	UNP C3THM2
A	-1	ALA	-	expression tag	UNP C3THM2
A	23	ILE	LYS	engineered mutation	UNP C3THM2
A	72	CYS	THR	engineered mutation	UNP C3THM2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	SER	-	expression tag	UNP C3THM2
B	-2	ASN	-	expression tag	UNP C3THM2
B	-1	ALA	-	expression tag	UNP C3THM2
B	23	ILE	LYS	engineered mutation	UNP C3THM2
B	72	CYS	THR	engineered mutation	UNP C3THM2
C	-3	SER	-	expression tag	UNP C3THM2
C	-2	ASN	-	expression tag	UNP C3THM2
C	-1	ALA	-	expression tag	UNP C3THM2
C	23	ILE	LYS	engineered mutation	UNP C3THM2
C	72	CYS	THR	engineered mutation	UNP C3THM2
D	-3	SER	-	expression tag	UNP C3THM2
D	-2	ASN	-	expression tag	UNP C3THM2
D	-1	ALA	-	expression tag	UNP C3THM2
D	23	ILE	LYS	engineered mutation	UNP C3THM2
D	72	CYS	THR	engineered mutation	UNP C3THM2
E	-3	SER	-	expression tag	UNP C3THM2
E	-2	ASN	-	expression tag	UNP C3THM2
E	-1	ALA	-	expression tag	UNP C3THM2
E	23	ILE	LYS	engineered mutation	UNP C3THM2
E	72	CYS	THR	engineered mutation	UNP C3THM2
F	-3	SER	-	expression tag	UNP C3THM2
F	-2	ASN	-	expression tag	UNP C3THM2
F	-1	ALA	-	expression tag	UNP C3THM2
F	23	ILE	LYS	engineered mutation	UNP C3THM2
F	72	CYS	THR	engineered mutation	UNP C3THM2
G	-3	SER	-	expression tag	UNP C3THM2
G	-2	ASN	-	expression tag	UNP C3THM2
G	-1	ALA	-	expression tag	UNP C3THM2
G	23	ILE	LYS	engineered mutation	UNP C3THM2
G	72	CYS	THR	engineered mutation	UNP C3THM2
H	-3	SER	-	expression tag	UNP C3THM2
H	-2	ASN	-	expression tag	UNP C3THM2
H	-1	ALA	-	expression tag	UNP C3THM2
H	23	ILE	LYS	engineered mutation	UNP C3THM2
H	72	CYS	THR	engineered mutation	UNP C3THM2
I	-3	SER	-	expression tag	UNP C3THM2
I	-2	ASN	-	expression tag	UNP C3THM2
I	-1	ALA	-	expression tag	UNP C3THM2
I	23	ILE	LYS	engineered mutation	UNP C3THM2
I	72	CYS	THR	engineered mutation	UNP C3THM2
J	-3	SER	-	expression tag	UNP C3THM2
J	-2	ASN	-	expression tag	UNP C3THM2

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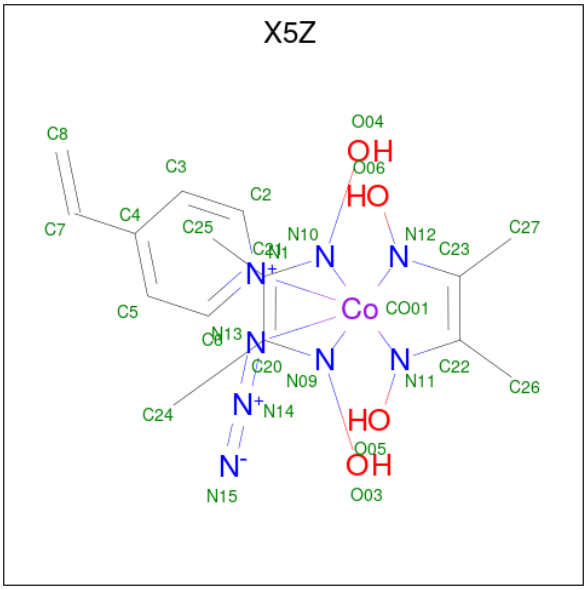
Chain	Residue	Modelled	Actual	Comment	Reference
J	-1	ALA	-	expression tag	UNP C3THM2
J	23	ILE	LYS	engineered mutation	UNP C3THM2
J	72	CYS	THR	engineered mutation	UNP C3THM2
K	-3	SER	-	expression tag	UNP C3THM2
K	-2	ASN	-	expression tag	UNP C3THM2
K	-1	ALA	-	expression tag	UNP C3THM2
K	23	ILE	LYS	engineered mutation	UNP C3THM2
K	72	CYS	THR	engineered mutation	UNP C3THM2
L	-3	SER	-	expression tag	UNP C3THM2
L	-2	ASN	-	expression tag	UNP C3THM2
L	-1	ALA	-	expression tag	UNP C3THM2
L	23	ILE	LYS	engineered mutation	UNP C3THM2
L	72	CYS	THR	engineered mutation	UNP C3THM2

- Molecule 2 is AZIDOBIS (DIMETHYLGLYOXIMATO) PYRIDINECOBALT (three-letter code: X5Z) (formula: $C_{15}H_{23}CoN_8O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		
2	B	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		
2	C	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		
2	D	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		

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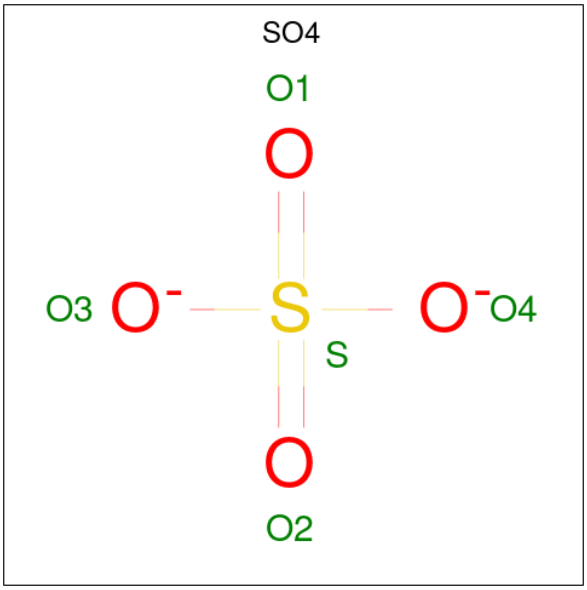
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		
2	F	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		
2	G	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		
2	H	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		
2	I	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		
2	J	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		
2	K	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		
2	L	1	Total	C	Co	N	O	0	0
			20	8	1	7	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	S		0	0
			5	4	1			
3	A	1	Total	O	S		0	0
			5	4	1			
3	B	1	Total	O	S		0	0
			5	4	1			

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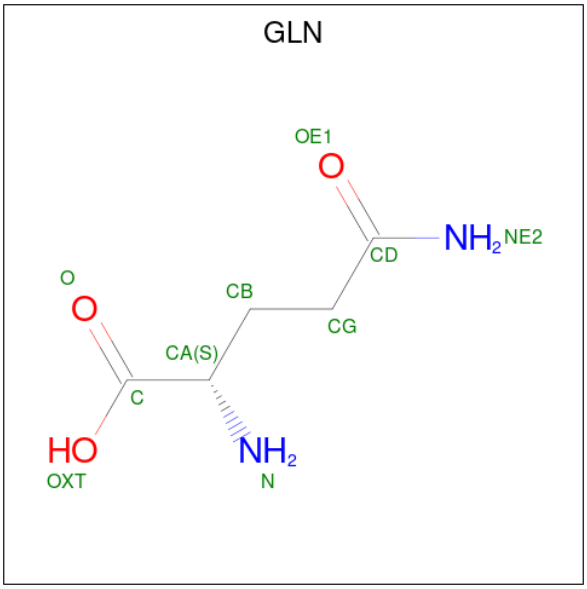
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0
3	J	1	Total O S 5 4 1	0	0

- Molecule 4 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 9 5 2 2	0	0
4	B	1	Total C N O 9 5 2 2	0	0
4	C	1	Total C N O 9 5 2 2	0	0
4	D	1	Total C N O 9 5 2 2	0	0
4	E	1	Total C N O 9 5 2 2	0	0
4	F	1	Total C N O 9 5 2 2	0	0

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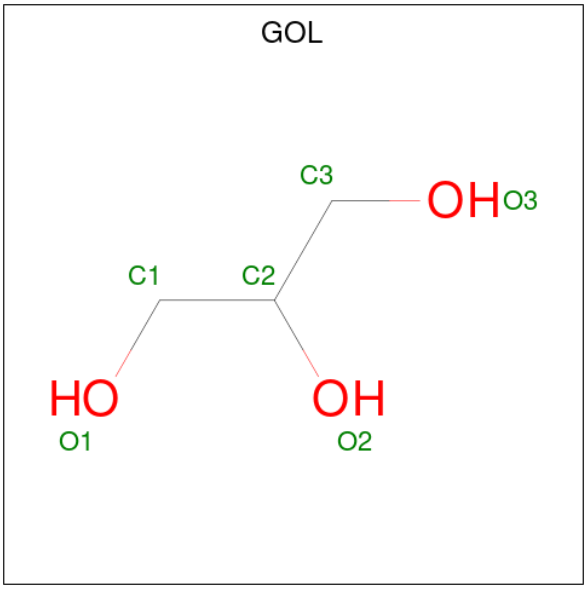
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C N O 9 5 2 2	0	0
4	H	1	Total C N O 9 5 2 2	0	0
4	I	1	Total C N O 9 5 2 2	0	0
4	J	1	Total C N O 9 5 2 2	0	0
4	K	1	Total C N O 9 5 2 2	0	0
4	L	1	Total C N O 9 5 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

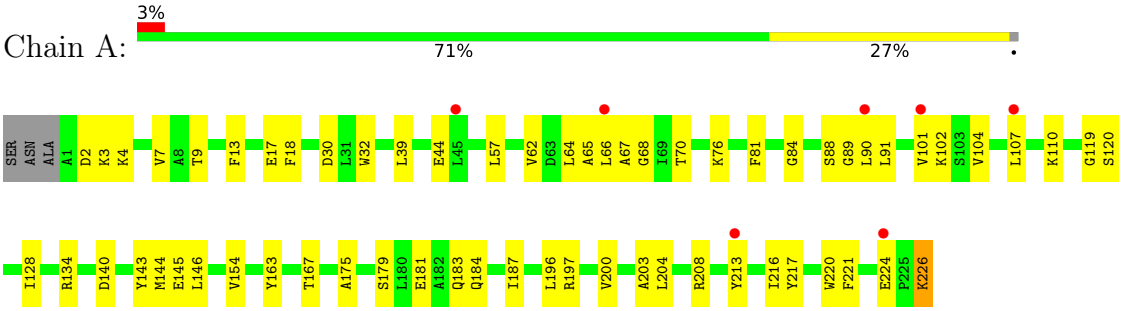
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	B	16	Total O 16 16	0	0
6	C	6	Total O 6 6	0	0
6	D	19	Total O 19 19	0	0
6	E	2	Total O 2 2	0	0
6	F	10	Total O 10 10	0	0
6	G	8	Total O 8 8	0	0
6	H	11	Total O 11 11	0	0
6	I	3	Total O 3 3	0	0
6	J	1	Total O 1 1	0	0
6	K	2	Total O 2 2	0	0
6	L	2	Total O 2 2	0	0

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.

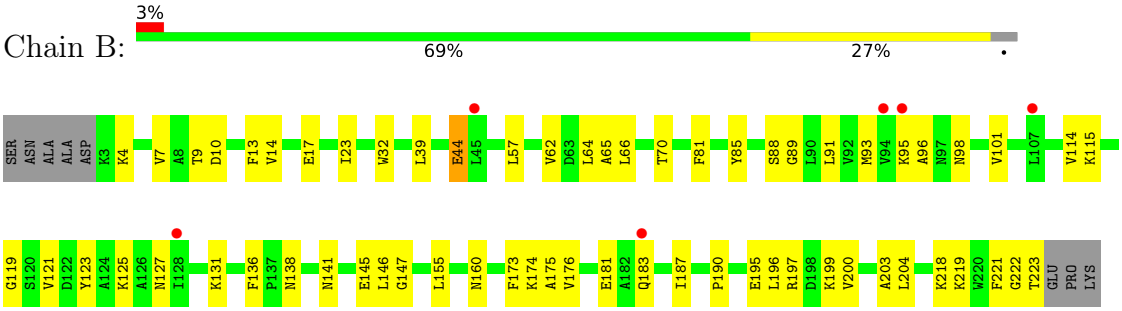
• Molecule 1: Amino acid ABC transporter substrate-binding protein

Chain A:



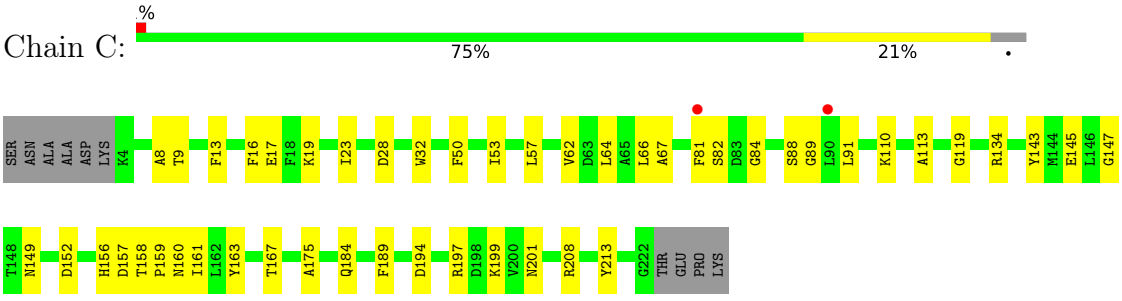
• Molecule 1: Amino acid ABC transporter substrate-binding protein

Chain B:



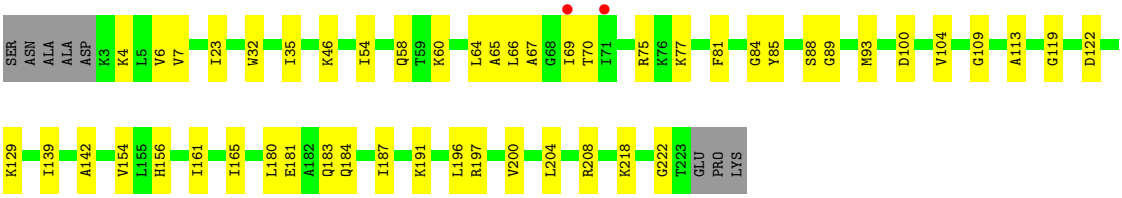
• Molecule 1: Amino acid ABC transporter substrate-binding protein

Chain C:

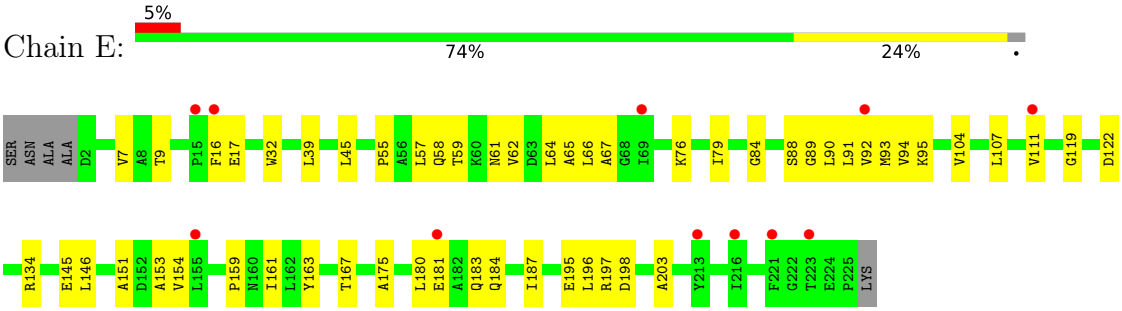


• Molecule 1: Amino acid ABC transporter substrate-binding protein

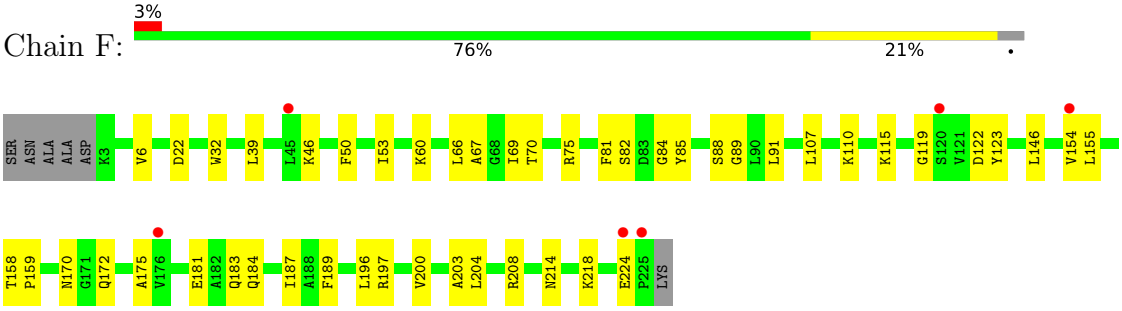
Chain D:



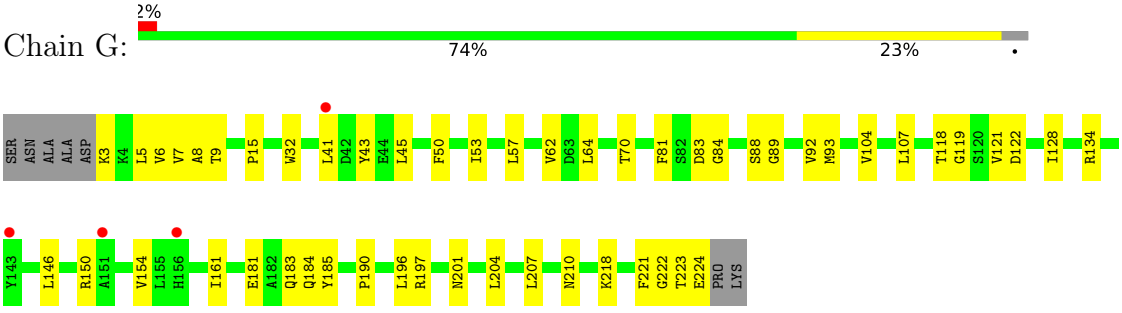
• Molecule 1: Amino acid ABC transporter substrate-binding protein



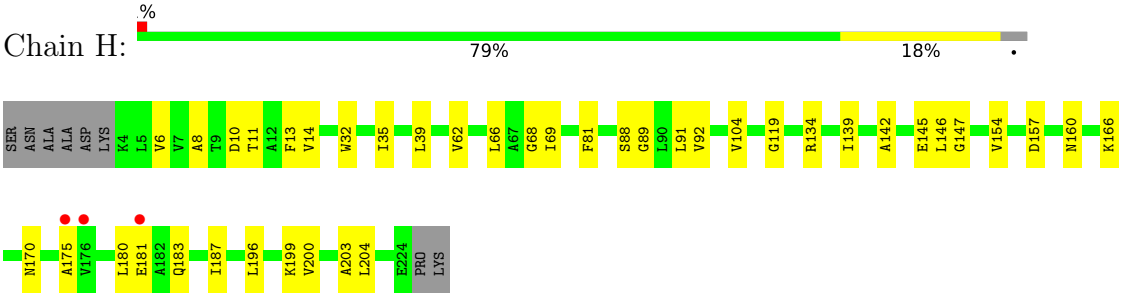
• Molecule 1: Amino acid ABC transporter substrate-binding protein



• Molecule 1: Amino acid ABC transporter substrate-binding protein

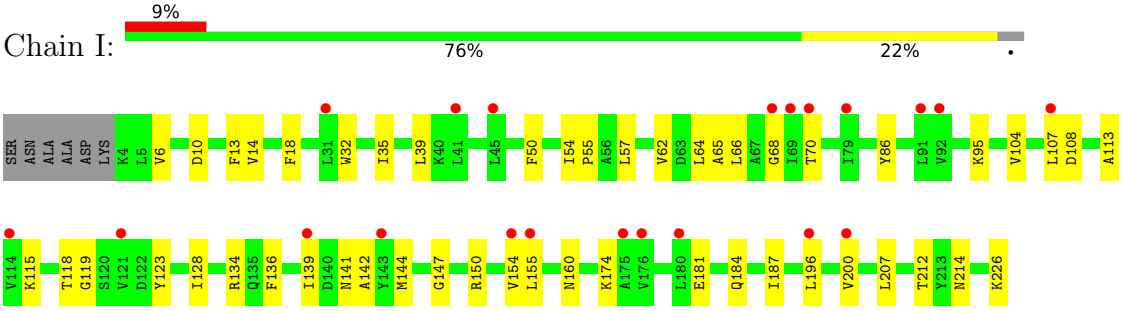


• Molecule 1: Amino acid ABC transporter substrate-binding protein



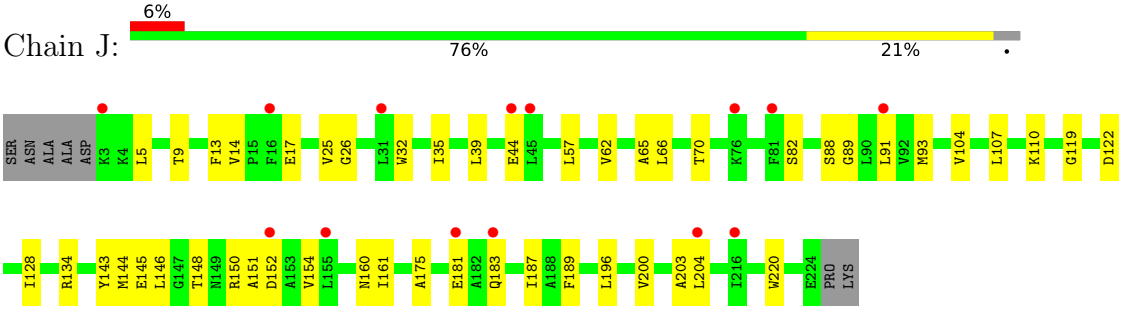
• Molecule 1: Amino acid ABC transporter substrate-binding protein

Chain I:



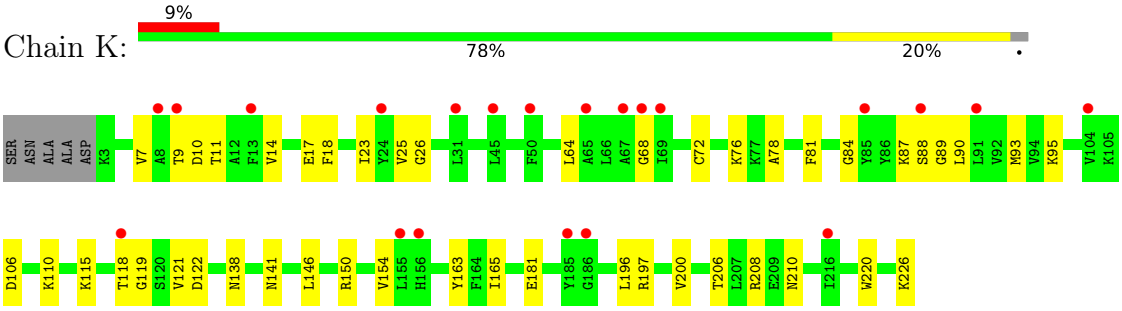
• Molecule 1: Amino acid ABC transporter substrate-binding protein

Chain J:



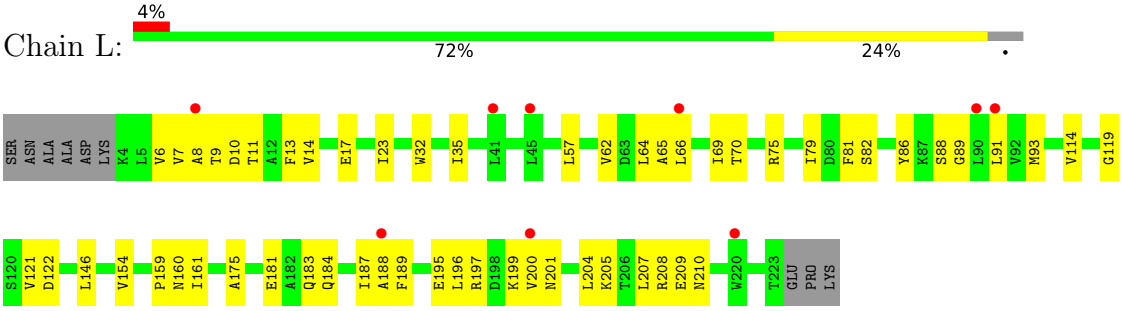
• Molecule 1: Amino acid ABC transporter substrate-binding protein

Chain K:



• Molecule 1: Amino acid ABC transporter substrate-binding protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.12Å 136.09Å 150.98Å 90.00° 90.16° 90.00°	Depositor
Resolution (Å)	41.90 – 2.99 49.65 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.90-2.99) 99.1 (49.65-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.233 , 0.266 0.233 , 0.264	Depositor DCC
R_{free} test set	6125 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å^2)	71.2	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.157 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21269	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.11% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: X5Z, SO4, GOL

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	0.38	0/1792	0.58	0/2419
1	B	0.37	0/1753	0.57	0/2366
1	C	0.31	0/1737	0.54	0/2345
1	D	0.30	0/1753	0.55	0/2366
1	E	0.32	0/1778	0.54	0/2401
1	F	0.31	0/1770	0.51	0/2390
1	G	0.33	0/1762	0.54	0/2378
1	H	0.29	0/1753	0.51	0/2367
1	I	0.33	0/1770	0.55	0/2390
1	J	0.31	0/1762	0.54	1/2378 (0.0%)
1	K	0.32	0/1779	0.54	0/2401
1	L	0.30	0/1744	0.50	0/2355
All	All	0.32	0/21153	0.54	1/28556 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	151	ALA	N-CA-CB	5.24	117.44	110.10

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	1760	0	1768	65	0
1	B	1722	0	1730	56	0
1	C	1706	0	1710	48	0
1	D	1722	0	1730	53	0
1	E	1746	0	1747	53	0
1	F	1738	0	1743	37	0
1	G	1731	0	1736	40	0
1	H	1722	0	1723	31	0
1	I	1738	0	1743	51	0
1	J	1731	0	1736	41	0
1	K	1747	0	1756	37	0
1	L	1713	0	1717	50	0
2	A	20	0	0	3	0
2	B	20	0	0	3	0
2	C	20	0	0	2	0
2	D	20	0	0	3	0
2	E	20	0	0	3	0
2	F	20	0	0	4	0
2	G	20	0	0	3	0
2	H	20	0	0	2	0
2	I	20	0	0	2	0
2	J	20	0	0	6	0
2	K	20	0	0	3	0
2	L	20	0	0	2	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	G	15	0	0	1	0
3	J	5	0	0	1	0
4	A	9	0	7	1	0
4	B	9	0	7	0	0
4	C	9	0	7	0	0
4	D	9	0	7	2	0
4	E	9	0	7	0	0
4	F	9	0	7	3	0
4	G	9	0	7	0	0
4	H	9	0	7	1	0
4	I	9	0	7	6	0
4	J	9	0	7	1	0
4	K	9	0	7	6	0
4	L	9	0	7	2	0
5	D	12	0	16	1	0
5	F	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	7	0	0	2	0
6	B	16	0	0	2	0
6	C	6	0	0	0	0
6	D	19	0	0	2	0
6	E	2	0	0	0	0
6	F	10	0	0	1	0
6	G	8	0	0	0	0
6	H	11	0	0	0	0
6	I	3	0	0	0	0
6	J	1	0	0	0	0
6	K	2	0	0	0	0
6	L	2	0	0	0	0
All	All	21269	0	20947	545	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 13.

All (545) 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:H:104:VAL:HG21	1:H:180:LEU:CD1	1.76	1.17
1:A:2:ASP:O	1:A:3:LYS:HG3	1.46	1.16
2:J:301:X5Z:N15	1:L:209:GLU:HA	1.60	1.15
1:C:66:LEU:HD12	1:C:66:LEU:O	1.49	1.13
1:A:221:PHE:O	1:A:224:GLU:HG2	1.48	1.13
1:A:217:TYR:OH	1:A:224:GLU:HB3	1.51	1.10
1:C:28:ASP:HB3	1:C:66:LEU:CD1	1.85	1.06
1:A:221:PHE:HB3	1:A:224:GLU:CG	1.90	1.01
1:K:118:THR:OG1	4:K:302:GLN:HB2	1.61	0.99
1:A:217:TYR:CE1	1:A:224:GLU:HB2	1.99	0.97
1:D:104:VAL:HG21	1:D:180:LEU:HD11	1.49	0.94
1:E:84:GLY:HA3	1:E:184:GLN:NE2	1.82	0.94
1:H:104:VAL:HG21	1:H:180:LEU:HD12	1.50	0.93
1:D:181:GLU:O	1:D:183:GLN:HG3	1.68	0.93
1:I:13:PHE:CE1	1:I:160:ASN:ND2	2.36	0.93
1:C:32:TRP:HB2	1:C:66:LEU:HD21	1.50	0.92
1:H:119:GLY:HA2	2:H:301:X5Z:C25	2.00	0.92
1:D:32:TRP:HB2	1:D:66:LEU:HD22	1.52	0.91
1:E:104:VAL:HG21	1:E:180:LEU:CD1	2.01	0.91
1:I:32:TRP:HB2	1:I:66:LEU:HD22	1.53	0.91
1:B:96:ALA:HA	1:B:174:LYS:HZ2	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:65:ALA:O	1:L:66:LEU:HD12	1.71	0.90
1:B:32:TRP:HB2	1:B:66:LEU:HD22	1.54	0.89
1:B:9:THR:OG1	1:B:17:GLU:HG2	1.72	0.88
1:I:65:ALA:O	1:I:66:LEU:HD12	1.73	0.88
1:A:221:PHE:HB3	1:A:224:GLU:HG3	1.56	0.87
1:H:104:VAL:HG21	1:H:180:LEU:HD11	1.56	0.87
1:J:32:TRP:HB2	1:J:66:LEU:CD2	2.05	0.86
1:I:119:GLY:HA2	2:I:301:X5Z:C25	2.06	0.85
1:G:6:VAL:HG12	1:G:62:VAL:HG23	1.59	0.84
1:B:32:TRP:HB2	1:B:66:LEU:CD2	2.08	0.83
1:A:2:ASP:O	1:A:3:LYS:CG	2.25	0.83
1:A:221:PHE:HB3	1:A:224:GLU:HG2	1.60	0.83
1:A:226:LYS:H	1:A:226:LYS:HD3	1.44	0.83
1:J:32:TRP:HB2	1:J:66:LEU:HD22	1.59	0.83
1:A:119:GLY:HA2	2:A:301:X5Z:C25	2.09	0.83
1:L:6:VAL:HG12	1:L:62:VAL:HG23	1.60	0.82
1:E:122:ASP:OD2	2:E:301:X5Z:C24	2.28	0.82
1:G:84:GLY:HA3	1:G:184:GLN:HG2	1.61	0.81
1:J:91:LEU:HD21	1:J:175:ALA:HB1	1.61	0.81
1:E:104:VAL:HG21	1:E:180:LEU:HD12	1.62	0.81
1:K:115:LYS:NZ	4:K:302:GLN:HE22	1.77	0.81
1:D:32:TRP:HB2	1:D:66:LEU:CD2	2.11	0.80
1:I:32:TRP:HB2	1:I:66:LEU:CD2	2.11	0.80
1:E:104:VAL:CG2	1:E:180:LEU:CD1	2.60	0.79
1:A:217:TYR:OH	1:A:224:GLU:CB	2.29	0.79
1:F:66:LEU:HD21	1:F:187:ILE:HG12	1.63	0.79
1:G:134:ARG:HH12	1:G:150:ARG:HB3	1.49	0.78
1:A:226:LYS:H	1:A:226:LYS:CD	1.95	0.78
1:E:84:GLY:HA3	1:E:184:GLN:HE21	1.45	0.77
1:F:196:LEU:O	1:F:200:VAL:HG23	1.85	0.77
1:L:65:ALA:C	1:L:66:LEU:HD12	2.06	0.77
1:I:134:ARG:HH12	1:I:150:ARG:HB3	1.49	0.76
1:H:6:VAL:HG12	1:H:62:VAL:HG13	1.68	0.75
1:G:84:GLY:HA3	1:G:184:GLN:CG	2.17	0.74
1:J:146:LEU:HD22	1:J:154:VAL:HG23	1.68	0.74
1:A:4:LYS:HD2	1:A:44:GLU:HB3	1.69	0.74
1:I:214:ASN:OD1	1:I:226:LYS:NZ	2.21	0.74
1:C:28:ASP:HB3	1:C:66:LEU:HD13	1.70	0.73
1:E:119:GLY:HA2	2:E:301:X5Z:C25	2.18	0.73
1:B:114:VAL:HG12	1:B:115:LYS:N	2.02	0.73
1:B:218:LYS:HA	1:B:222:GLY:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TYR:HE1	1:A:224:GLU:HB2	1.53	0.72
1:K:115:LYS:O	1:K:118:THR:HG22	1.88	0.72
1:B:96:ALA:HA	1:B:174:LYS:NZ	2.04	0.71
1:C:119:GLY:HA2	2:C:301:X5Z:C25	2.19	0.71
1:G:104:VAL:HA	1:G:107:LEU:HD13	1.72	0.71
1:B:181:GLU:O	1:B:183:GLN:HG3	1.91	0.71
1:I:65:ALA:C	1:I:66:LEU:HD12	2.10	0.71
1:G:181:GLU:O	1:G:183:GLN:HG3	1.91	0.71
1:H:104:VAL:CG2	1:H:180:LEU:HD11	2.19	0.71
1:B:65:ALA:O	1:B:66:LEU:HD12	1.91	0.70
1:A:32:TRP:HB2	1:A:66:LEU:HD22	1.73	0.70
1:A:119:GLY:CA	2:A:301:X5Z:C25	2.69	0.70
1:D:119:GLY:HA2	2:D:301:X5Z:C25	2.21	0.70
1:F:181:GLU:O	1:F:183:GLN:HG3	1.92	0.70
1:J:25:VAL:HG12	1:J:220:TRP:CZ2	2.27	0.70
1:B:222:GLY:O	1:B:223:THR:C	2.31	0.69
1:C:147:GLY:HA3	1:D:23:ILE:HG22	1.73	0.69
1:K:146:LEU:HD22	1:K:154:VAL:HG23	1.74	0.69
1:E:65:ALA:O	1:E:66:LEU:HD12	1.92	0.69
1:I:66:LEU:HD11	1:I:187:ILE:HG23	1.74	0.69
1:I:66:LEU:CD1	1:I:187:ILE:HG23	2.23	0.69
1:L:14:VAL:O	1:L:160:ASN:ND2	2.24	0.69
1:L:146:LEU:HD22	1:L:154:VAL:HG23	1.75	0.69
1:A:104:VAL:HG22	1:A:128:ILE:HD11	1.74	0.69
1:C:66:LEU:O	1:C:66:LEU:CD1	2.36	0.69
1:A:32:TRP:HB2	1:A:66:LEU:CD2	2.22	0.68
1:B:65:ALA:C	1:B:66:LEU:HD12	2.14	0.68
1:F:67:ALA:O	4:F:303:GLN:NE2	2.26	0.68
1:L:7:VAL:HG22	1:L:64:LEU:HD11	1.76	0.68
1:G:119:GLY:HA2	2:G:301:X5Z:C25	2.24	0.68
1:J:119:GLY:HA2	2:J:301:X5Z:C25	2.24	0.68
1:E:65:ALA:C	1:E:66:LEU:HD12	2.13	0.68
1:C:19:LYS:HD2	1:I:144:MET:HE1	1.75	0.68
1:B:219:LYS:NZ	6:B:401:HOH:O	2.27	0.67
1:D:93:MET:CE	1:D:161:ILE:HG23	2.25	0.67
1:F:146:LEU:HD22	1:F:154:VAL:HG23	1.77	0.67
1:D:93:MET:HE1	1:D:165:ILE:HG13	1.77	0.67
1:G:223:THR:O	1:G:224:GLU:C	2.32	0.67
1:A:224:GLU:HA	1:A:224:GLU:OE1	1.94	0.67
1:E:32:TRP:HB2	1:E:66:LEU:CD2	2.25	0.67
1:H:146:LEU:HD22	1:H:154:VAL:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:32:TRP:HB2	1:L:66:LEU:HD22	1.76	0.66
1:B:57:LEU:HD23	1:B:62:VAL:HG23	1.77	0.66
1:C:19:LYS:HD2	1:I:144:MET:CE	2.25	0.66
1:G:5:LEU:CD1	1:G:41:LEU:HD13	2.26	0.66
1:C:28:ASP:HB3	1:C:66:LEU:HD11	1.76	0.66
1:K:196:LEU:O	1:K:200:VAL:HG23	1.95	0.66
1:J:181:GLU:O	1:J:183:GLN:HG3	1.95	0.66
1:G:104:VAL:HG12	1:G:128:ILE:HD11	1.77	0.65
1:D:67:ALA:H	1:D:69:ILE:HD12	1.61	0.65
1:I:70:THR:HG1	4:I:302:GLN:N	1.95	0.65
1:E:32:TRP:HB2	1:E:66:LEU:HD22	1.79	0.65
1:F:115:LYS:NZ	4:F:303:GLN:OE1	2.28	0.65
1:L:93:MET:HE2	1:L:161:ILE:HD12	1.78	0.65
1:E:104:VAL:CG2	1:E:180:LEU:HD12	2.27	0.64
1:I:13:PHE:HE1	1:I:160:ASN:HD21	1.35	0.64
1:K:68:GLY:O	4:K:302:GLN:N	2.30	0.64
1:C:156:HIS:HB3	1:C:161:ILE:HD11	1.80	0.64
1:D:109:GLY:N	1:D:129:LYS:O	2.23	0.64
1:D:66:LEU:CD1	1:D:187:ILE:HG23	2.27	0.64
1:D:69:ILE:HG22	1:D:81:PHE:HE1	1.62	0.64
1:F:119:GLY:HA2	2:F:301:X5Z:C25	2.28	0.63
1:L:66:LEU:HD11	1:L:187:ILE:HG23	1.81	0.63
1:L:82:SER:HB3	1:L:189:PHE:HE1	1.63	0.63
1:A:144:MET:HE2	1:F:22:ASP:HA	1.79	0.63
1:D:93:MET:HE3	1:D:161:ILE:HG23	1.79	0.63
1:H:181:GLU:O	1:H:183:GLN:HG3	1.99	0.63
1:E:84:GLY:CA	1:E:184:GLN:HE21	2.12	0.63
1:F:119:GLY:CA	2:F:301:X5Z:C25	2.77	0.63
1:G:8:ALA:HB2	1:G:62:VAL:HG21	1.81	0.62
1:L:7:VAL:HG13	1:L:64:LEU:HD12	1.81	0.62
1:A:217:TYR:CE1	1:A:224:GLU:CB	2.79	0.62
1:J:91:LEU:HD21	1:J:175:ALA:CB	2.28	0.62
1:B:123:TYR:HD2	1:B:155:LEU:HD21	1.64	0.61
1:E:39:LEU:HD21	1:E:203:ALA:HB2	1.82	0.61
1:L:32:TRP:HB2	1:L:66:LEU:CD2	2.30	0.61
1:C:119:GLY:CA	2:C:301:X5Z:C25	2.77	0.61
1:K:90:LEU:HD13	1:K:181:GLU:HB3	1.82	0.61
1:L:183:GLN:HG3	1:L:184:GLN:H	1.65	0.61
1:E:59:THR:CG2	1:E:61:ASN:OD1	2.48	0.61
1:H:119:GLY:CA	2:H:301:X5Z:C25	2.76	0.61
1:L:183:GLN:HG3	1:L:184:GLN:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:TYR:CZ	1:A:224:GLU:HB2	2.36	0.61
1:L:66:LEU:CD1	1:L:187:ILE:HG23	2.31	0.61
1:I:35:ILE:HG21	1:I:200:VAL:HG13	1.83	0.60
1:B:114:VAL:CG1	1:B:115:LYS:N	2.64	0.60
1:L:207:LEU:HD23	1:L:210:ASN:HD21	1.66	0.60
1:K:115:LYS:CE	4:K:302:GLN:HE22	2.14	0.60
1:D:100:ASP:OD1	1:D:100:ASP:O	2.20	0.60
1:A:217:TYR:CZ	1:A:224:GLU:CB	2.85	0.60
1:E:146:LEU:HD22	1:E:154:VAL:HG23	1.82	0.60
1:K:93:MET:HG3	1:K:165:ILE:HD11	1.82	0.60
1:A:221:PHE:O	1:A:224:GLU:CG	2.36	0.60
1:D:54:ILE:O	1:D:58:GLN:HG3	2.02	0.59
1:H:39:LEU:HD13	1:H:199:LYS:HG2	1.82	0.59
1:C:19:LYS:CD	1:I:144:MET:CE	2.79	0.59
1:L:91:LEU:HD21	1:L:175:ALA:HB1	1.84	0.59
1:I:119:GLY:CA	2:I:301:X5Z:C25	2.78	0.59
1:A:221:PHE:CB	1:A:224:GLU:HG2	2.31	0.59
1:G:146:LEU:HD22	1:G:154:VAL:HG23	1.82	0.59
1:F:214:ASN:ND2	1:H:166:LYS:O	2.34	0.58
1:H:134:ARG:NH1	1:H:145:GLU:OE1	2.36	0.58
1:H:66:LEU:HG	1:H:187:ILE:HG12	1.86	0.58
1:E:119:GLY:CA	2:E:301:X5Z:C25	2.81	0.58
1:F:218:LYS:HD2	1:H:170:ASN:OD1	2.03	0.58
1:K:119:GLY:HA2	2:K:301:X5Z:C25	2.32	0.58
1:A:216:ILE:HD13	6:A:406:HOH:O	2.04	0.58
1:E:104:VAL:HG23	1:E:180:LEU:HD11	1.84	0.58
1:B:119:GLY:CA	2:B:301:X5Z:C25	2.81	0.58
1:G:70:THR:HG23	1:G:183:GLN:HB3	1.86	0.58
1:I:104:VAL:HG13	1:I:128:ILE:HD11	1.85	0.57
1:F:70:THR:HG23	1:F:183:GLN:HB3	1.85	0.57
1:D:122:ASP:OD2	2:D:301:X5Z:C24	2.52	0.57
1:I:70:THR:H	4:I:302:GLN:N	2.02	0.57
1:J:82:SER:HB3	1:J:189:PHE:HE1	1.70	0.57
1:J:93:MET:HE2	1:J:161:ILE:HD12	1.85	0.57
1:B:119:GLY:HA2	2:B:301:X5Z:C25	2.35	0.57
1:I:10:ASP:OD2	1:I:115:LYS:NZ	2.36	0.57
1:J:145:GLU:HG2	1:J:150:ARG:HH21	1.69	0.57
1:B:7:VAL:HG13	1:B:64:LEU:HD12	1.85	0.57
1:E:59:THR:HG21	1:E:61:ASN:OD1	2.04	0.57
1:F:158:THR:HB	1:F:159:PRO:HD3	1.86	0.57
1:G:218:LYS:HA	1:G:222:GLY:CA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ALA:HB3	1:D:154:VAL:HG12	1.84	0.57
1:B:81:PHE:O	1:B:197:ARG:HD2	2.05	0.57
1:A:13:PHE:HB3	1:A:17:GLU:OE1	2.05	0.56
1:B:101:VAL:HG12	1:B:176:VAL:HG21	1.86	0.56
1:B:114:VAL:HG12	1:B:115:LYS:H	1.70	0.56
1:B:114:VAL:CG1	1:B:115:LYS:H	2.19	0.56
1:E:55:PRO:HA	1:E:58:GLN:HE21	1.68	0.56
1:L:86:TYR:HE2	1:L:159:PRO:CG	2.18	0.56
1:A:179:SER:HB3	3:A:303:SO4:O3	2.05	0.56
1:H:14:VAL:O	1:H:160:ASN:ND2	2.38	0.56
1:E:104:VAL:CG2	1:E:180:LEU:HD11	2.35	0.56
1:L:8:ALA:HB2	1:L:62:VAL:HG21	1.87	0.56
1:D:84:GLY:HA3	1:D:184:GLN:HG2	1.87	0.56
1:D:66:LEU:HD11	1:D:187:ILE:HG23	1.87	0.56
1:I:108:ASP:OD1	1:I:128:ILE:HG23	2.06	0.56
1:C:82:SER:HB3	1:C:189:PHE:HE1	1.70	0.56
1:A:66:LEU:HG	1:A:187:ILE:HG12	1.88	0.56
1:K:10:ASP:OD1	1:K:11:THR:N	2.39	0.56
1:K:106:ASP:O	1:K:110:LYS:NZ	2.22	0.56
1:K:122:ASP:OD2	2:K:301:X5Z:C24	2.54	0.56
1:G:218:LYS:HA	1:G:222:GLY:HA2	1.87	0.55
1:D:65:ALA:C	1:D:66:LEU:HD12	2.27	0.55
1:F:67:ALA:H	1:F:69:ILE:HD12	1.70	0.55
1:I:196:LEU:O	1:I:200:VAL:HG23	2.05	0.55
1:J:39:LEU:HD21	1:J:203:ALA:HB2	1.87	0.55
1:G:83:ASP:HB2	1:G:201:ASN:OD1	2.06	0.55
1:D:119:GLY:CA	2:D:301:X5Z:C25	2.84	0.55
1:I:50:PHE:CZ	4:I:302:GLN:HG2	2.42	0.55
1:G:7:VAL:HG23	1:G:45:LEU:HD23	1.88	0.55
1:H:91:LEU:HD21	1:H:175:ALA:HB1	1.88	0.55
1:J:25:VAL:HG12	1:J:26:GLY:N	2.22	0.55
1:C:9:THR:OG1	1:C:17:GLU:HG2	2.07	0.55
1:J:66:LEU:CD1	1:J:187:ILE:HG23	2.36	0.55
1:C:8:ALA:HB2	1:C:62:VAL:HG21	1.89	0.54
1:L:114:VAL:HG21	1:L:121:VAL:HG22	1.89	0.54
1:B:7:VAL:HG13	1:B:64:LEU:CD1	2.38	0.54
1:J:5:LEU:O	1:J:44:GLU:HG2	2.07	0.54
1:E:7:VAL:HG13	1:E:64:LEU:HD12	1.88	0.54
1:I:68:GLY:O	4:I:302:GLN:N	2.41	0.54
1:C:19:LYS:CD	1:I:144:MET:HE1	2.37	0.54
1:D:85:TYR:HB3	1:D:204:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:196:LEU:O	1:J:200:VAL:HG23	2.08	0.54
1:G:134:ARG:HH12	1:G:150:ARG:CB	2.19	0.54
1:B:85:TYR:HB3	1:B:204:LEU:HD21	1.89	0.54
1:C:28:ASP:CB	1:C:66:LEU:HD13	2.37	0.54
1:C:113:ALA:HA	1:C:134:ARG:HB2	1.89	0.54
1:H:32:TRP:HB2	1:H:66:LEU:HD22	1.90	0.54
1:G:50:PHE:HD1	1:G:53:ILE:HD12	1.73	0.53
1:C:19:LYS:HD3	1:I:144:MET:HE3	1.89	0.53
1:H:157:ASP:OD2	4:H:302:GLN:N	2.41	0.53
1:L:205:LYS:O	1:L:209:GLU:HG2	2.07	0.53
1:F:91:LEU:HD21	1:F:175:ALA:HB1	1.91	0.53
1:G:122:ASP:OD2	2:G:301:X5Z:C24	2.57	0.53
1:I:50:PHE:CE1	4:I:302:GLN:HG2	2.43	0.53
1:B:95:LYS:O	1:B:174:LYS:NZ	2.42	0.53
1:E:17:GLU:OE2	1:E:67:ALA:HA	2.09	0.53
1:A:196:LEU:O	1:A:200:VAL:HG23	2.09	0.53
1:J:14:VAL:O	1:J:160:ASN:ND2	2.42	0.53
1:I:86:TYR:O	1:I:184:GLN:HA	2.08	0.53
1:G:207:LEU:HD23	1:G:210:ASN:HD21	1.74	0.53
1:I:181:GLU:O	1:I:181:GLU:HG3	2.09	0.53
1:D:93:MET:HB3	1:D:154:VAL:CG2	2.39	0.52
1:E:91:LEU:HD21	1:E:175:ALA:HB1	1.90	0.52
1:I:95:LYS:O	1:I:174:LYS:HE2	2.09	0.52
1:J:65:ALA:C	1:J:66:LEU:HD12	2.29	0.52
1:G:118:THR:O	1:G:121:VAL:HG12	2.09	0.52
1:L:196:LEU:O	1:L:200:VAL:HG23	2.09	0.52
1:I:13:PHE:HE1	1:I:160:ASN:ND2	2.00	0.52
1:H:104:VAL:CG2	1:H:180:LEU:CD1	2.65	0.52
1:A:30:ASP:HB3	1:A:216:ILE:HD12	1.92	0.51
1:I:134:ARG:NH1	1:I:150:ARG:HB3	2.20	0.51
1:F:119:GLY:HA3	2:F:301:X5Z:C25	2.41	0.51
1:K:7:VAL:HG22	1:K:64:LEU:HD11	1.92	0.51
1:A:70:THR:HG23	1:A:183:GLN:HB2	1.93	0.51
1:B:13:PHE:CZ	1:B:160:ASN:OD1	2.64	0.51
1:C:149:ASN:O	1:D:4:LYS:NZ	2.27	0.51
1:E:92:VAL:HG21	1:E:104:VAL:HG22	1.92	0.51
1:E:93:MET:HE2	1:E:161:ILE:HD12	1.93	0.51
1:F:32:TRP:HB2	1:F:66:LEU:CD1	2.40	0.51
1:I:118:THR:HG22	4:I:302:GLN:HG3	1.93	0.51
1:C:84:GLY:HA3	1:C:184:GLN:HG2	1.91	0.51
1:C:208:ARG:HD2	1:C:213:TYR:CG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:LEU:O	1:H:200:VAL:HG23	2.10	0.51
1:A:9:THR:HG23	1:A:17:GLU:HG2	1.93	0.51
1:J:25:VAL:HG12	1:J:220:TRP:HZ2	1.75	0.51
1:B:95:LYS:HD2	1:B:146:LEU:O	2.11	0.51
1:B:138:ASN:HB3	1:B:141:ASN:OD1	2.10	0.51
1:D:6:VAL:CG1	1:D:46:LYS:HD3	2.41	0.51
1:D:69:ILE:HG22	1:D:81:PHE:CE1	2.44	0.51
1:D:93:MET:HB3	1:D:154:VAL:HG23	1.93	0.51
1:F:170:ASN:ND2	6:F:404:HOH:O	2.44	0.50
1:L:122:ASP:OD2	2:L:301:X5Z:C24	2.59	0.50
1:B:119:GLY:HA3	2:B:301:X5Z:C25	2.41	0.50
1:L:195:GLU:O	1:L:199:LYS:HG3	2.10	0.50
1:F:6:VAL:HG11	1:F:46:LYS:HE3	1.92	0.50
1:F:50:PHE:HD1	1:F:53:ILE:HD12	1.76	0.50
1:L:75:ARG:NH2	4:L:302:GLN:O	2.37	0.50
1:L:86:TYR:HE2	1:L:159:PRO:HG2	1.75	0.50
1:I:113:ALA:HB3	1:I:154:VAL:HG22	1.93	0.50
1:C:19:LYS:CD	1:I:144:MET:HE3	2.41	0.50
1:C:32:TRP:HB2	1:C:66:LEU:CD2	2.31	0.50
1:D:64:LEU:HD13	1:D:66:LEU:CD1	2.41	0.50
1:E:7:VAL:HB	1:E:45:LEU:HD23	1.92	0.50
1:G:119:GLY:CA	2:G:301:X5Z:C25	2.90	0.50
1:I:39:LEU:HD11	1:I:200:VAL:HA	1.94	0.50
1:K:150:ARG:HG2	1:K:150:ARG:HH11	1.76	0.50
1:I:66:LEU:HD11	1:I:187:ILE:CG2	2.42	0.50
1:J:35:ILE:HD11	1:J:204:LEU:HD13	1.94	0.50
1:F:75:ARG:NH2	4:F:303:GLN:O	2.38	0.50
1:G:5:LEU:HD11	1:G:41:LEU:HD13	1.93	0.49
1:K:118:THR:O	1:K:121:VAL:HG12	2.12	0.49
1:E:104:VAL:HG23	1:E:180:LEU:CD1	2.38	0.49
1:L:70:THR:HG1	4:L:302:GLN:N	2.09	0.49
1:A:146:LEU:HD22	1:A:154:VAL:HG23	1.93	0.49
1:E:111:VAL:HG11	1:E:151:ALA:HA	1.95	0.49
1:H:92:VAL:CG2	1:H:104:VAL:HG22	2.43	0.49
1:G:15:PRO:HG2	1:G:221:PHE:CZ	2.48	0.49
1:C:64:LEU:C	1:C:64:LEU:HD12	2.33	0.49
1:E:84:GLY:CA	1:E:184:GLN:NE2	2.64	0.49
1:H:139:ILE:HD12	1:H:142:ALA:HB3	1.94	0.49
1:H:8:ALA:HB2	1:H:62:VAL:HG11	1.95	0.49
1:D:75:ARG:HH22	4:D:304:GLN:C	2.16	0.48
1:E:181:GLU:O	1:E:183:GLN:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:SER:OG	1:C:89:GLY:N	2.46	0.48
1:A:65:ALA:C	1:A:66:LEU:HD12	2.33	0.48
1:J:25:VAL:CG1	1:J:220:TRP:HZ2	2.26	0.48
1:K:9:THR:CG2	1:K:17:GLU:HG3	2.43	0.48
1:A:39:LEU:HD21	1:A:203:ALA:HB2	1.95	0.48
1:B:7:VAL:HG22	1:B:64:LEU:HD11	1.95	0.48
1:B:13:PHE:CE1	1:B:160:ASN:OD1	2.67	0.48
1:J:25:VAL:CG1	1:J:220:TRP:CZ2	2.96	0.48
1:L:7:VAL:HG22	1:L:64:LEU:CD1	2.40	0.48
1:K:81:PHE:O	1:K:197:ARG:HD2	2.14	0.48
1:B:195:GLU:O	1:B:199:LYS:HG3	2.14	0.48
1:D:93:MET:HE2	1:D:161:ILE:HG23	1.94	0.48
1:E:88:SER:OG	1:E:89:GLY:N	2.47	0.48
1:L:9:THR:HG22	1:L:10:ASP:N	2.29	0.48
1:G:81:PHE:O	1:G:197:ARG:HD2	2.14	0.48
1:A:91:LEU:HD21	1:A:175:ALA:HB1	1.96	0.47
1:A:204:LEU:O	1:A:208:ARG:HG2	2.13	0.47
1:C:82:SER:HB2	1:C:201:ASN:OD1	2.14	0.47
1:I:14:VAL:HG12	1:I:18:PHE:CG	2.49	0.47
1:A:221:PHE:C	1:A:224:GLU:HG2	2.29	0.47
1:K:88:SER:OG	1:K:89:GLY:N	2.47	0.47
1:F:39:LEU:HD21	1:F:203:ALA:HB2	1.96	0.47
1:G:218:LYS:HA	1:G:222:GLY:N	2.29	0.47
1:I:207:LEU:HD22	1:I:212:THR:HB	1.97	0.47
1:J:122:ASP:OD2	2:J:301:X5Z:C24	2.62	0.47
1:A:17:GLU:OE2	1:A:67:ALA:HA	2.15	0.47
1:B:91:LEU:HD21	1:B:175:ALA:HB1	1.96	0.47
1:D:64:LEU:HD12	1:D:64:LEU:C	2.35	0.47
1:F:123:TYR:HD2	1:F:155:LEU:HD21	1.80	0.47
1:E:9:THR:OG1	1:E:17:GLU:HG2	2.14	0.47
1:J:25:VAL:HG12	1:J:220:TRP:CH2	2.48	0.47
1:L:79:ILE:HD12	1:L:188:ALA:HB1	1.97	0.47
1:B:32:TRP:CH2	1:B:64:LEU:HD21	2.50	0.47
1:A:119:GLY:HA3	2:A:301:X5Z:C25	2.43	0.47
1:C:163:TYR:CZ	1:C:167:THR:HG21	2.50	0.47
1:G:9:THR:HG21	1:G:45:LEU:HD22	1.97	0.47
1:D:67:ALA:H	1:D:69:ILE:CD1	2.26	0.47
1:F:172:GLN:HG3	1:L:23:ILE:HD13	1.96	0.47
1:D:70:THR:HG1	4:D:304:GLN:N	2.13	0.47
1:D:77:LYS:NZ	6:D:406:HOH:O	2.47	0.47
1:G:88:SER:OG	1:G:89:GLY:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:VAL:HG21	1:H:104:VAL:HG22	1.96	0.47
1:J:13:PHE:CZ	4:J:303:GLN:HG3	2.50	0.47
1:F:218:LYS:HE2	1:F:224:GLU:HB3	1.97	0.46
1:K:87:LYS:HE2	1:K:226:LYS:HG3	1.97	0.46
1:D:32:TRP:CH2	1:D:64:LEU:HD21	2.50	0.46
1:D:218:LYS:HG2	1:D:222:GLY:O	2.15	0.46
1:L:69:ILE:HG22	1:L:81:PHE:HE1	1.80	0.46
1:D:156:HIS:HB3	1:D:161:ILE:HD11	1.97	0.46
1:K:7:VAL:HG13	1:K:64:LEU:HD12	1.98	0.46
1:B:136:PHE:CZ	1:B:145:GLU:HG3	2.51	0.46
1:A:2:ASP:C	1:A:3:LYS:HG3	2.27	0.46
1:J:110:LYS:HD2	1:J:152:ASP:OD2	2.15	0.46
1:B:10:ASP:OD2	1:B:115:LYS:NZ	2.48	0.46
1:K:25:VAL:HG12	1:K:26:GLY:N	2.30	0.46
1:K:119:GLY:CA	2:K:301:X5Z:C25	2.93	0.46
1:E:134:ARG:NH1	1:E:145:GLU:OE2	2.42	0.46
1:K:25:VAL:HG12	1:K:220:TRP:CZ2	2.50	0.46
1:B:131:LYS:NZ	6:B:404:HOH:O	2.49	0.46
1:B:88:SER:OG	1:B:89:GLY:N	2.48	0.46
1:C:143:TYR:OH	1:C:160:ASN:OD1	2.33	0.46
1:E:59:THR:HG23	1:E:61:ASN:OD1	2.15	0.46
1:K:14:VAL:HG23	1:K:18:PHE:CD1	2.50	0.46
1:L:35:ILE:HG21	1:L:200:VAL:HG13	1.98	0.46
1:B:195:GLU:HG2	1:B:199:LYS:HE3	1.98	0.46
1:C:23:ILE:HG22	1:I:147:GLY:HA3	1.98	0.46
1:E:76:LYS:HA	1:E:79:ILE:O	2.16	0.46
1:C:16:PHE:O	1:C:17:GLU:HG3	2.15	0.45
1:C:91:LEU:HD21	1:C:175:ALA:HB1	1.98	0.45
1:C:194:ASP:HA	1:C:197:ARG:HB3	1.98	0.45
1:D:88:SER:OG	1:D:89:GLY:N	2.49	0.45
1:J:134:ARG:NH1	3:J:302:SO4:O1	2.47	0.45
1:I:139:ILE:HD12	1:I:142:ALA:HB3	1.98	0.45
1:J:88:SER:OG	1:J:89:GLY:N	2.48	0.45
1:E:111:VAL:CG1	1:E:151:ALA:HA	2.46	0.45
1:I:57:LEU:HD23	1:I:62:VAL:HG23	1.99	0.45
1:J:25:VAL:CG1	1:J:26:GLY:N	2.79	0.45
1:A:7:VAL:HG22	1:A:64:LEU:HD11	1.97	0.45
1:A:81:PHE:O	1:A:197:ARG:HD2	2.17	0.45
1:D:35:ILE:HD11	1:D:204:LEU:HD13	1.98	0.45
1:F:88:SER:OG	1:F:89:GLY:N	2.49	0.45
1:J:104:VAL:CG1	1:J:128:ILE:HG12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:TRP:CZ2	1:B:64:LEU:HD21	2.52	0.45
1:K:138:ASN:HB3	1:K:141:ASN:OD1	2.16	0.45
1:L:86:TYR:CE2	1:L:159:PRO:CG	2.98	0.45
1:F:107:LEU:HA	1:F:110:LYS:HD2	1.98	0.45
1:H:39:LEU:HD21	1:H:203:ALA:HB2	1.99	0.45
1:K:115:LYS:HZ1	4:K:302:GLN:HE22	1.61	0.45
1:B:121:VAL:HG12	1:B:125:LYS:HE2	1.99	0.45
1:C:19:LYS:HD3	1:I:144:MET:CE	2.45	0.45
1:B:96:ALA:CA	1:B:174:LYS:HZ2	2.19	0.45
1:C:110:LYS:HD2	1:C:152:ASP:OD2	2.15	0.45
1:E:181:GLU:HG3	1:E:183:GLN:HE21	1.81	0.45
1:G:5:LEU:O	1:G:43:TYR:HA	2.17	0.45
1:I:64:LEU:HD23	1:I:196:LEU:HD21	1.98	0.45
1:B:196:LEU:O	1:B:200:VAL:HG23	2.17	0.45
1:B:221:PHE:O	1:B:222:GLY:C	2.55	0.45
1:D:93:MET:HE2	1:D:165:ILE:HD11	1.97	0.45
1:F:84:GLY:HA3	1:F:184:GLN:CG	2.47	0.45
1:A:90:LEU:HD21	1:A:120:SER:HA	1.99	0.44
1:B:57:LEU:HD22	1:B:190:PRO:HD3	1.99	0.44
1:E:16:PHE:HE2	1:E:159:PRO:HB2	1.81	0.44
1:E:196:LEU:O	1:E:197:ARG:C	2.56	0.44
1:F:82:SER:HB3	1:F:189:PHE:HE1	1.82	0.44
1:K:7:VAL:HG22	1:K:64:LEU:CD1	2.47	0.44
1:A:226:LYS:NZ	1:A:226:LYS:N	2.66	0.44
1:D:7:VAL:HG13	1:D:64:LEU:CD1	2.48	0.44
1:E:88:SER:O	1:E:183:GLN:N	2.39	0.44
1:J:66:LEU:HD12	1:J:187:ILE:HG23	1.98	0.44
1:L:181:GLU:O	1:L:181:GLU:HG2	2.17	0.44
1:C:57:LEU:HD23	1:C:62:VAL:HG13	2.00	0.44
1:G:57:LEU:HD22	1:G:190:PRO:HD3	1.98	0.44
2:J:301:X5Z:N15	1:L:209:GLU:OE1	2.51	0.44
1:K:72:CYS:O	1:K:76:LYS:HG3	2.17	0.44
1:A:84:GLY:HA3	1:A:184:GLN:OE1	2.18	0.44
1:C:147:GLY:CA	1:D:23:ILE:HG22	2.43	0.44
1:B:23:ILE:HG22	1:H:147:GLY:HA3	2.00	0.44
1:C:81:PHE:O	1:C:197:ARG:NE	2.51	0.44
1:D:66:LEU:HD12	1:D:187:ILE:HG23	1.98	0.44
1:H:88:SER:OG	1:H:89:GLY:N	2.51	0.44
1:A:18:PHE:HZ	1:A:220:TRP:CZ3	2.35	0.44
1:A:88:SER:OG	1:A:89:GLY:N	2.50	0.44
1:B:66:LEU:HG	1:B:187:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:THR:HG23	1:B:183:GLN:HB3	2.00	0.44
1:B:95:LYS:O	1:B:98:ASN:HB3	2.18	0.44
1:I:123:TYR:HD2	1:I:155:LEU:HD21	1.83	0.44
1:C:17:GLU:OE2	1:C:67:ALA:HA	2.18	0.44
1:F:81:PHE:O	1:F:197:ARG:HD2	2.17	0.44
1:G:92:VAL:HG21	1:G:104:VAL:HG22	1.99	0.44
1:J:144:MET:O	1:J:148:THR:HG22	2.18	0.44
1:E:95:LYS:HD2	1:E:146:LEU:O	2.17	0.44
1:F:85:TYR:HA	1:F:208:ARG:HH12	1.83	0.44
1:K:115:LYS:HZ3	4:K:302:GLN:HE22	1.63	0.44
1:J:9:THR:HG22	1:J:17:GLU:HG3	2.00	0.43
1:A:76:LYS:HG2	1:A:81:PHE:HD2	1.83	0.43
1:D:85:TYR:HA	1:D:208:ARG:HH21	1.83	0.43
1:I:66:LEU:HD12	1:I:187:ILE:HG23	2.00	0.43
1:K:84:GLY:O	1:K:208:ARG:NH2	2.51	0.43
1:C:50:PHE:HD1	1:C:53:ILE:HD12	1.83	0.43
1:J:119:GLY:CA	2:J:301:X5Z:C25	2.95	0.43
1:C:28:ASP:CB	1:C:66:LEU:CD1	2.75	0.43
1:K:95:LYS:HD2	1:K:146:LEU:O	2.17	0.43
1:D:69:ILE:CG2	1:D:81:PHE:HE1	2.30	0.43
1:E:163:TYR:CZ	1:E:167:THR:HG21	2.54	0.43
1:H:13:PHE:CE2	1:H:68:GLY:HA3	2.54	0.43
1:I:136:PHE:HB3	1:I:141:ASN:HB2	1.99	0.43
1:L:88:SER:OG	1:L:89:GLY:N	2.50	0.43
1:A:102:LYS:NZ	6:A:401:HOH:O	2.52	0.43
1:A:163:TYR:CZ	1:A:167:THR:HG21	2.54	0.43
1:E:94:VAL:HG12	1:E:153:ALA:HB2	2.01	0.43
1:K:206:THR:HG22	1:K:210:ASN:ND2	2.34	0.43
1:L:7:VAL:HG13	1:L:64:LEU:CD1	2.49	0.43
1:L:7:VAL:CG2	1:L:64:LEU:HD11	2.48	0.43
1:F:69:ILE:HG22	1:F:81:PHE:HE1	1.83	0.43
1:I:54:ILE:HB	1:I:55:PRO:HD3	2.01	0.43
1:A:208:ARG:HD2	1:A:213:TYR:CG	2.53	0.42
1:A:217:TYR:HH	1:A:224:GLU:HB3	1.74	0.42
1:C:13:PHE:HZ	1:C:157:ASP:OD2	2.02	0.42
1:E:16:PHE:O	1:E:17:GLU:HG3	2.19	0.42
1:F:69:ILE:HG22	1:F:81:PHE:CE1	2.54	0.42
1:G:7:VAL:HG11	1:G:32:TRP:NE1	2.34	0.42
1:G:64:LEU:HD23	1:G:196:LEU:HD21	2.01	0.42
1:L:10:ASP:OD1	1:L:11:THR:N	2.52	0.42
1:A:68:GLY:O	4:A:304:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:ARG:HD2	3:G:304:SO4:O1	2.19	0.42
1:B:39:LEU:HD21	1:B:203:ALA:HB2	2.01	0.42
1:C:158:THR:N	1:C:159:PRO:HD2	2.34	0.42
1:I:107:LEU:HD12	1:I:128:ILE:HD13	2.02	0.42
1:L:197:ARG:HD2	1:L:201:ASN:ND2	2.34	0.42
1:A:134:ARG:NH1	1:A:145:GLU:OE2	2.48	0.42
1:A:226:LYS:H	1:A:226:LYS:NZ	2.18	0.42
1:H:10:ASP:OD1	1:H:11:THR:N	2.52	0.42
1:B:127:ASN:OD1	1:C:199:LYS:HD2	2.20	0.42
1:D:7:VAL:HG13	1:D:64:LEU:HD12	2.02	0.42
1:D:196:LEU:O	1:D:200:VAL:HG23	2.19	0.42
1:E:16:PHE:CE2	1:E:159:PRO:HB2	2.55	0.42
1:F:122:ASP:OD2	2:F:301:X5Z:C24	2.68	0.42
1:B:136:PHE:CE2	1:B:145:GLU:HG3	2.55	0.42
1:H:69:ILE:HG22	1:H:81:PHE:HE1	1.84	0.42
1:J:65:ALA:O	1:J:66:LEU:HD12	2.19	0.42
1:J:104:VAL:HA	1:J:107:LEU:HD12	2.02	0.42
1:D:66:LEU:HD11	1:D:187:ILE:CG2	2.50	0.42
1:J:66:LEU:HD11	1:J:187:ILE:HG23	2.01	0.42
1:I:6:VAL:CG1	1:I:62:VAL:HG12	2.50	0.42
1:K:76:LYS:C	1:K:78:ALA:N	2.73	0.42
1:E:195:GLU:O	1:E:198:ASP:N	2.53	0.41
1:A:140:ASP:HA	1:A:143:TYR:CD2	2.56	0.41
1:E:66:LEU:CD1	1:E:187:ILE:HG23	2.50	0.41
1:J:57:LEU:HD23	1:J:62:VAL:HG23	2.02	0.41
1:L:86:TYR:HE2	1:L:159:PRO:HG3	1.84	0.41
1:A:181:GLU:O	1:A:181:GLU:HG3	2.20	0.41
1:B:93:MET:SD	1:B:173:PHE:HB3	2.60	0.41
1:E:90:LEU:HG	1:E:183:GLN:HE22	1.85	0.41
1:J:70:THR:HG23	1:J:183:GLN:HB3	2.01	0.41
1:L:13:PHE:HB3	1:L:17:GLU:OE2	2.20	0.41
1:F:204:LEU:O	1:F:208:ARG:HG3	2.20	0.41
1:J:93:MET:HE1	1:J:143:TYR:CE1	2.56	0.41
1:L:57:LEU:HD23	1:L:62:VAL:HG13	2.03	0.41
1:A:101:VAL:HG22	1:A:110:LYS:NZ	2.35	0.41
2:J:301:X5Z:N15	1:L:209:GLU:CD	2.74	0.41
1:L:66:LEU:HD11	1:L:187:ILE:CG2	2.50	0.41
1:A:57:LEU:HD23	1:A:62:VAL:HG23	2.03	0.41
1:C:134:ARG:NH1	1:C:145:GLU:OE2	2.53	0.41
1:D:81:PHE:O	1:D:197:ARG:HD2	2.21	0.41
1:K:9:THR:HG22	1:K:17:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:HG22	1:A:110:LYS:HZ2	1.85	0.41
1:C:28:ASP:HB3	1:C:66:LEU:HD12	1.89	0.41
1:E:57:LEU:HD23	1:E:62:VAL:HG23	2.02	0.41
1:E:104:VAL:O	1:E:107:LEU:HB2	2.21	0.41
1:G:93:MET:HB2	1:G:161:ILE:HG21	2.02	0.41
1:H:35:ILE:HD11	1:H:204:LEU:HD13	2.03	0.41
1:B:4:LYS:HD3	1:B:44:GLU:HB3	2.03	0.41
5:D:303:GOL:O3	6:D:401:HOH:O	2.20	0.41
1:E:196:LEU:HD12	1:E:196:LEU:HA	1.89	0.41
1:F:60:LYS:O	1:F:60:LYS:HG2	2.20	0.41
1:F:84:GLY:HA3	1:F:184:GLN:HG2	2.03	0.41
1:A:107:LEU:HA	1:A:110:LYS:HD2	2.03	0.41
1:G:3:LYS:HE2	1:G:3:LYS:HB3	1.85	0.41
1:G:204:LEU:HD12	1:G:204:LEU:HA	1.91	0.41
1:C:84:GLY:HA3	1:C:184:GLN:CG	2.51	0.41
1:D:66:LEU:HG	1:D:187:ILE:HG12	2.02	0.40
1:G:84:GLY:HA2	1:G:185:TYR:O	2.21	0.40
1:G:128:ILE:HD13	1:G:128:ILE:HA	1.83	0.40
1:L:119:GLY:HA2	2:L:301:X5Z:C25	2.51	0.40
1:B:14:VAL:O	1:B:160:ASN:ND2	2.54	0.40
1:B:147:GLY:HA3	1:K:23:ILE:HG22	2.02	0.40
1:D:6:VAL:HG11	1:D:46:LYS:HD3	2.03	0.40
1:A:226:LYS:CD	1:A:226:LYS:N	2.73	0.40
1:A:226:LYS:HB2	1:A:226:LYS:HE2	1.71	0.40
1:I:66:LEU:HG	1:I:187:ILE:HG12	2.02	0.40
1:L:183:GLN:CG	1:L:184:GLN:N	2.84	0.40
1:D:60:LYS:NZ	1:D:191:LYS:O	2.53	0.40
1:E:84:GLY:HA3	1:E:184:GLN:CD	2.40	0.40
1:J:148:THR:HG21	1:J:150:ARG:NH1	2.36	0.40
1:K:14:VAL:HG22	1:K:163:TYR:CE1	2.56	0.40
1:L:204:LEU:O	1:L:208:ARG:HG2	2.21	0.40
1:D:139:ILE:HD12	1:D:142:ALA:HB3	2.03	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	224/229 (98%)	212 (95%)	12 (5%)	0	100	100
1	B	219/229 (96%)	211 (96%)	8 (4%)	0	100	100
1	C	217/229 (95%)	210 (97%)	7 (3%)	0	100	100
1	D	219/229 (96%)	213 (97%)	6 (3%)	0	100	100
1	E	222/229 (97%)	212 (96%)	10 (4%)	0	100	100
1	F	221/229 (96%)	216 (98%)	5 (2%)	0	100	100
1	G	220/229 (96%)	214 (97%)	6 (3%)	0	100	100
1	H	219/229 (96%)	214 (98%)	5 (2%)	0	100	100
1	I	221/229 (96%)	213 (96%)	8 (4%)	0	100	100
1	J	220/229 (96%)	212 (96%)	8 (4%)	0	100	100
1	K	222/229 (97%)	213 (96%)	9 (4%)	0	100	100
1	L	218/229 (95%)	212 (97%)	6 (3%)	0	100	100
All	All	2642/2748 (96%)	2552 (97%)	90 (3%)	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	186/188 (99%)	185 (100%)	1 (0%)	88	96
1	B	182/188 (97%)	181 (100%)	1 (0%)	88	96
1	C	180/188 (96%)	180 (100%)	0	100	100
1	D	182/188 (97%)	182 (100%)	0	100	100
1	E	185/188 (98%)	185 (100%)	0	100	100
1	F	184/188 (98%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	183/188 (97%)	183 (100%)	0	100 100
1	H	182/188 (97%)	182 (100%)	0	100 100
1	I	184/188 (98%)	184 (100%)	0	100 100
1	J	183/188 (97%)	183 (100%)	0	100 100
1	K	185/188 (98%)	185 (100%)	0	100 100
1	L	181/188 (96%)	181 (100%)	0	100 100
All	All	2197/2256 (97%)	2195 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	LYS
1	B	44	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	B	184	GLN
1	E	183	GLN
1	E	184	GLN
1	G	183	GLN
1	I	184	GLN

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)

35 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	$\#\|Z\| > 2$
2	X5Z	K	301	-	8,21,30	3.63	6 (75%)	1,36,52	1.92	0
3	SO4	G	304	-	4,4,4	0.53	0	6,6,6	0.11	0
2	X5Z	G	301	-	8,21,30	3.63	6 (75%)	1,36,52	1.95	0
3	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	302	-	4,4,4	0.81	0	6,6,6	1.38	1 (16%)
2	X5Z	I	301	-	8,21,30	3.63	6 (75%)	1,36,52	1.98	0
4	GLN	L	302	-	7,8,9	0.45	0	4,9,11	0.07	0
3	SO4	A	303	-	4,4,4	0.49	0	6,6,6	0.09	0
4	GLN	G	305	-	7,8,9	0.44	0	4,9,11	0.06	0
2	X5Z	H	301	-	8,21,30	3.63	6 (75%)	1,36,52	1.90	0
3	SO4	G	303	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	G	302	-	4,4,4	0.14	0	6,6,6	0.05	0
2	X5Z	B	301	-	8,21,30	3.62	6 (75%)	1,36,52	1.94	0
4	GLN	J	303	-	7,8,9	0.44	0	4,9,11	0.05	0
4	GLN	H	302	-	7,8,9	0.43	0	4,9,11	0.03	0
4	GLN	D	304	-	7,8,9	0.37	0	4,9,11	0.21	0
2	X5Z	D	301	-	8,21,30	3.63	6 (75%)	1,36,52	1.91	0
5	GOL	F	302	-	5,5,5	0.89	0	5,5,5	1.00	0
4	GLN	K	302	-	7,8,9	0.48	0	4,9,11	0.07	0
4	GLN	C	303	-	7,8,9	0.45	0	4,9,11	0.06	0
2	X5Z	F	301	-	8,21,30	3.63	6 (75%)	1,36,52	1.93	0
4	GLN	E	302	-	7,8,9	0.44	0	4,9,11	0.05	0
5	GOL	D	302	-	5,5,5	0.89	0	5,5,5	1.01	0
4	GLN	A	304	-	7,8,9	0.42	0	4,9,11	0.29	0
2	X5Z	A	301	-	8,21,30	3.63	6 (75%)	1,36,52	1.95	0
3	SO4	J	302	-	4,4,4	0.14	0	6,6,6	0.07	0
4	GLN	B	303	-	7,8,9	0.44	0	4,9,11	0.05	0
2	X5Z	L	301	-	8,21,30	3.63	6 (75%)	1,36,52	1.94	0
4	GLN	F	303	-	7,8,9	0.44	0	4,9,11	0.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	D	303	-	5,5,5	0.91	0	5,5,5	0.99	0
2	X5Z	C	301	-	8,21,30	3.62	6 (75%)	1,36,52	1.90	0
4	GLN	I	302	-	7,8,9	0.43	0	4,9,11	0.12	0
2	X5Z	E	301	-	8,21,30	3.64	6 (75%)	1,36,52	1.96	0
2	X5Z	J	301	-	8,21,30	3.62	6 (75%)	1,36,52	1.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	X5Z	K	301	-	-	-	0/2/2/3
2	X5Z	G	301	-	-	-	0/2/2/3
4	GLN	L	302	-	-	0/6/7/9	-
2	X5Z	I	301	-	-	-	0/2/2/3
4	GLN	G	305	-	-	0/6/7/9	-
2	X5Z	H	301	-	-	-	0/2/2/3
2	X5Z	B	301	-	-	-	0/2/2/3
4	GLN	J	303	-	-	0/6/7/9	-
4	GLN	H	302	-	-	0/6/7/9	-
4	GLN	D	304	-	-	3/6/7/9	-
5	GOL	F	302	-	-	0/4/4/4	-
2	X5Z	D	301	-	-	-	0/2/2/3
4	GLN	K	302	-	-	0/6/7/9	-
4	GLN	C	303	-	-	0/6/7/9	-
2	X5Z	F	301	-	-	-	0/2/2/3
4	GLN	E	302	-	-	0/6/7/9	-
5	GOL	D	302	-	-	0/4/4/4	-
4	GLN	A	304	-	-	1/6/7/9	-
4	GLN	F	303	-	-	1/6/7/9	-
4	GLN	B	303	-	-	1/6/7/9	-
2	X5Z	A	301	-	-	-	0/2/2/3
2	X5Z	L	301	-	-	-	0/2/2/3
5	GOL	D	303	-	-	0/4/4/4	-
2	X5Z	C	301	-	-	-	0/2/2/3
4	GLN	I	302	-	-	1/6/7/9	-
2	X5Z	E	301	-	-	-	0/2/2/3
2	X5Z	J	301	-	-	-	0/2/2/3

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	X5Z	CO01-N10	-4.67	1.88	2.10
2	C	301	X5Z	CO01-N10	-4.66	1.88	2.10
2	J	301	X5Z	CO01-N10	-4.66	1.88	2.10
2	H	301	X5Z	CO01-N10	-4.66	1.88	2.10
2	I	301	X5Z	CO01-N10	-4.65	1.88	2.10
2	D	301	X5Z	CO01-N10	-4.64	1.88	2.10
2	L	301	X5Z	CO01-N10	-4.64	1.88	2.10
2	E	301	X5Z	CO01-N10	-4.64	1.88	2.10
2	G	301	X5Z	CO01-N10	-4.64	1.88	2.10
2	F	301	X5Z	CO01-N10	-4.63	1.88	2.10
2	K	301	X5Z	CO01-N10	-4.63	1.88	2.10
2	B	301	X5Z	CO01-N10	-4.63	1.88	2.10
2	K	301	X5Z	CO01-N12	-4.39	1.89	2.10
2	I	301	X5Z	CO01-N12	-4.38	1.89	2.10
2	G	301	X5Z	CO01-N12	-4.38	1.89	2.10
2	L	301	X5Z	CO01-N12	-4.37	1.89	2.10
2	B	301	X5Z	CO01-N12	-4.37	1.90	2.10
2	D	301	X5Z	CO01-N12	-4.37	1.90	2.10
2	E	301	X5Z	CO01-N12	-4.36	1.90	2.10
2	A	301	X5Z	CO01-N12	-4.36	1.90	2.10
2	F	301	X5Z	CO01-N12	-4.35	1.90	2.10
2	C	301	X5Z	CO01-N12	-4.35	1.90	2.10
2	A	301	X5Z	CO01-N09	-4.35	1.90	2.10
2	H	301	X5Z	CO01-N12	-4.34	1.90	2.10
2	I	301	X5Z	CO01-N09	-4.34	1.90	2.10
2	J	301	X5Z	CO01-N12	-4.33	1.90	2.10
2	G	301	X5Z	CO01-N09	-4.33	1.90	2.10
2	B	301	X5Z	CO01-N09	-4.33	1.90	2.10
2	F	301	X5Z	CO01-N09	-4.32	1.90	2.10
2	K	301	X5Z	CO01-N09	-4.32	1.90	2.10
2	E	301	X5Z	CO01-N09	-4.32	1.90	2.10
2	L	301	X5Z	CO01-N09	-4.32	1.90	2.10
2	J	301	X5Z	CO01-N09	-4.32	1.90	2.10
2	H	301	X5Z	CO01-N09	-4.31	1.90	2.10
2	C	301	X5Z	CO01-N09	-4.31	1.90	2.10
2	D	301	X5Z	CO01-N09	-4.31	1.90	2.10
2	L	301	X5Z	CO01-N11	-4.27	1.90	2.10
2	E	301	X5Z	CO01-N11	-4.26	1.90	2.10
2	K	301	X5Z	CO01-N11	-4.26	1.90	2.10
2	H	301	X5Z	CO01-N11	-4.26	1.90	2.10
2	J	301	X5Z	CO01-N11	-4.26	1.90	2.10
2	F	301	X5Z	CO01-N11	-4.26	1.90	2.10
2	C	301	X5Z	CO01-N11	-4.25	1.90	2.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	X5Z	CO01-N11	-4.25	1.90	2.10
2	D	301	X5Z	CO01-N11	-4.25	1.90	2.10
2	B	301	X5Z	CO01-N11	-4.24	1.90	2.10
2	I	301	X5Z	CO01-N11	-4.24	1.90	2.10
2	A	301	X5Z	CO01-N11	-4.23	1.90	2.10
2	E	301	X5Z	C20-C21	3.73	1.47	1.36
2	K	301	X5Z	C20-C21	3.72	1.47	1.36
2	G	301	X5Z	C20-C21	3.72	1.47	1.36
2	F	301	X5Z	C20-C21	3.72	1.47	1.36
2	D	301	X5Z	C20-C21	3.70	1.47	1.36
2	I	301	X5Z	C20-C21	3.70	1.47	1.36
2	B	301	X5Z	C20-C21	3.70	1.47	1.36
2	H	301	X5Z	C20-C21	3.70	1.47	1.36
2	C	301	X5Z	C20-C21	3.69	1.47	1.36
2	A	301	X5Z	C20-C21	3.69	1.47	1.36
2	L	301	X5Z	C20-C21	3.67	1.46	1.36
2	J	301	X5Z	C20-C21	3.67	1.46	1.36
2	E	301	X5Z	C22-C23	3.60	1.46	1.36
2	F	301	X5Z	C22-C23	3.59	1.46	1.36
2	L	301	X5Z	C22-C23	3.58	1.46	1.36
2	J	301	X5Z	C22-C23	3.58	1.46	1.36
2	H	301	X5Z	C22-C23	3.57	1.46	1.36
2	D	301	X5Z	C22-C23	3.56	1.46	1.36
2	K	301	X5Z	C22-C23	3.56	1.46	1.36
2	I	301	X5Z	C22-C23	3.56	1.46	1.36
2	C	301	X5Z	C22-C23	3.55	1.46	1.36
2	B	301	X5Z	C22-C23	3.55	1.46	1.36
2	A	301	X5Z	C22-C23	3.55	1.46	1.36
2	G	301	X5Z	C22-C23	3.54	1.46	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	302	SO4	O4-S-O1	3.08	125.40	109.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	304	GLN	O-C-CA-CB
4	B	303	GLN	O-C-CA-CB
4	F	303	GLN	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	I	302	GLN	C-CA-CB-CG
4	D	304	GLN	OE1-CD-CG-CB
4	D	304	GLN	NE2-CD-CG-CB
4	D	304	GLN	N-CA-CB-CG

There are no ring outliers.

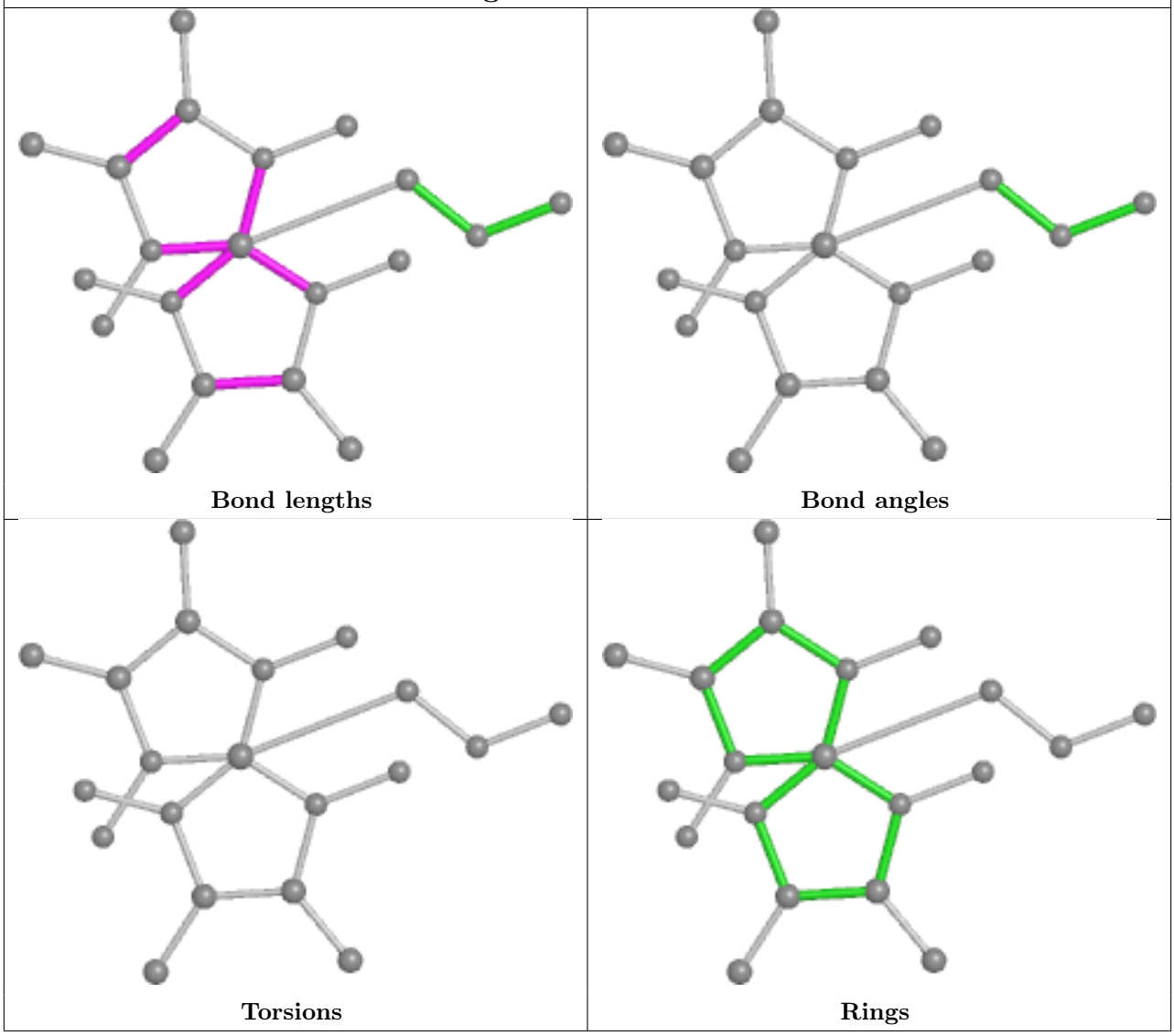
24 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	301	X5Z	3	0
3	G	304	SO4	1	0
2	G	301	X5Z	3	0
2	I	301	X5Z	2	0
4	L	302	GLN	2	0
3	A	303	SO4	1	0
2	H	301	X5Z	2	0
2	B	301	X5Z	3	0
4	J	303	GLN	1	0
4	H	302	GLN	1	0
4	D	304	GLN	2	0
2	D	301	X5Z	3	0
4	K	302	GLN	6	0
2	F	301	X5Z	4	0
4	A	304	GLN	1	0
2	A	301	X5Z	3	0
3	J	302	SO4	1	0
2	L	301	X5Z	2	0
4	F	303	GLN	3	0
5	D	303	GOL	1	0
2	C	301	X5Z	2	0
4	I	302	GLN	6	0
2	E	301	X5Z	3	0
2	J	301	X5Z	6	0

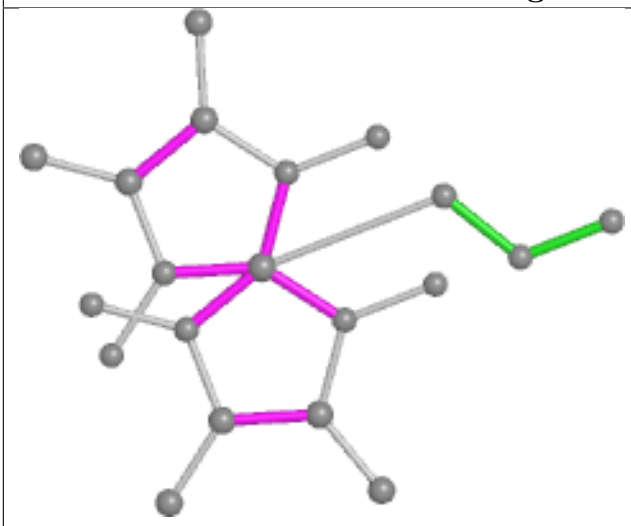
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

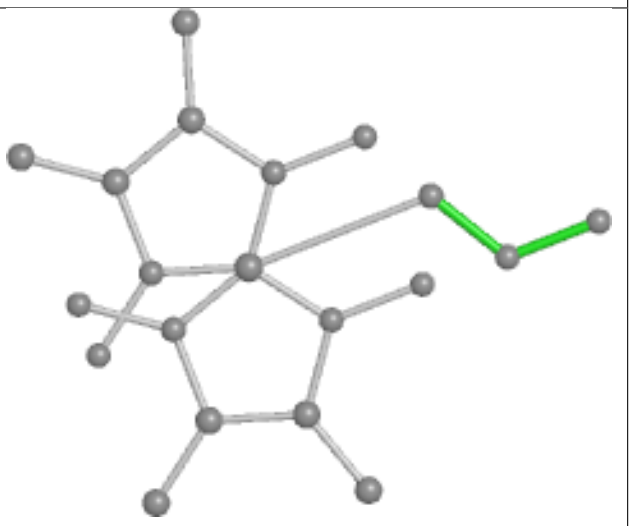
Ligand X5Z K 301



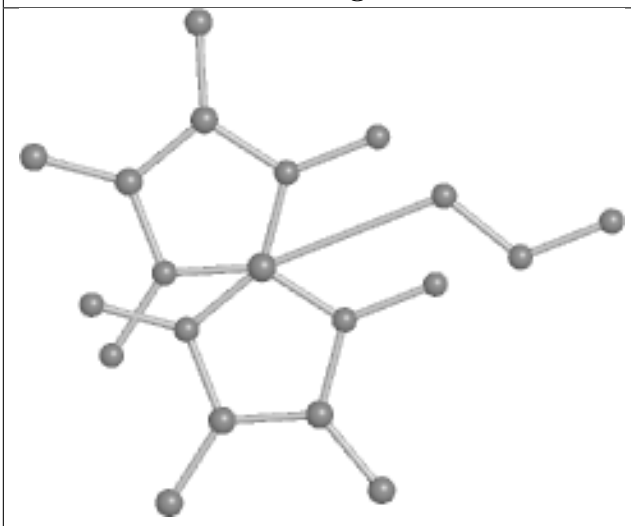
Ligand X5Z G 301



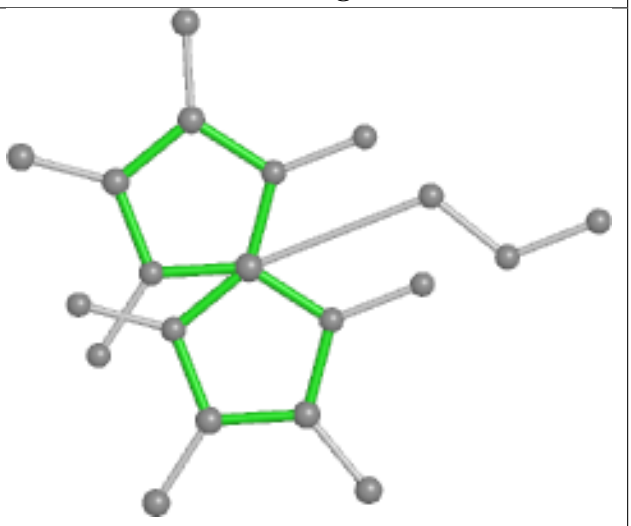
Bond lengths



Bond angles

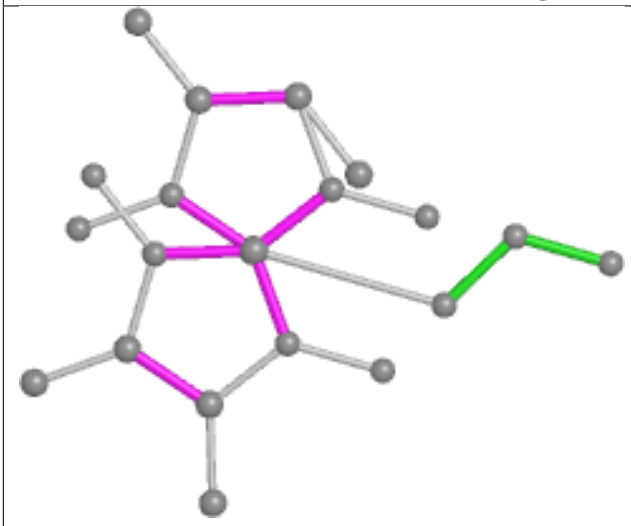


Torsions

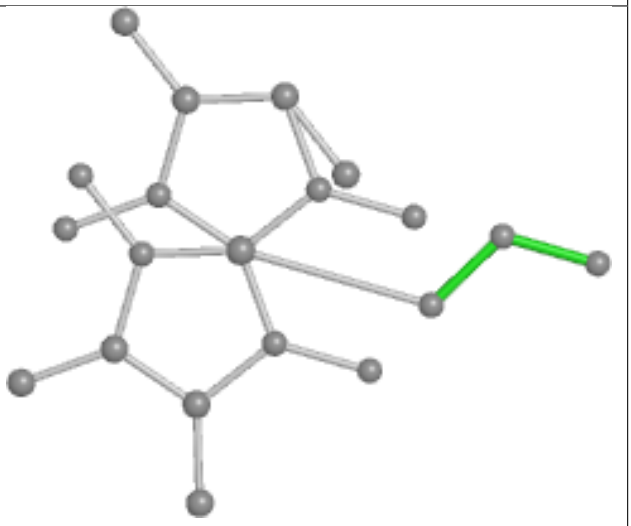


Rings

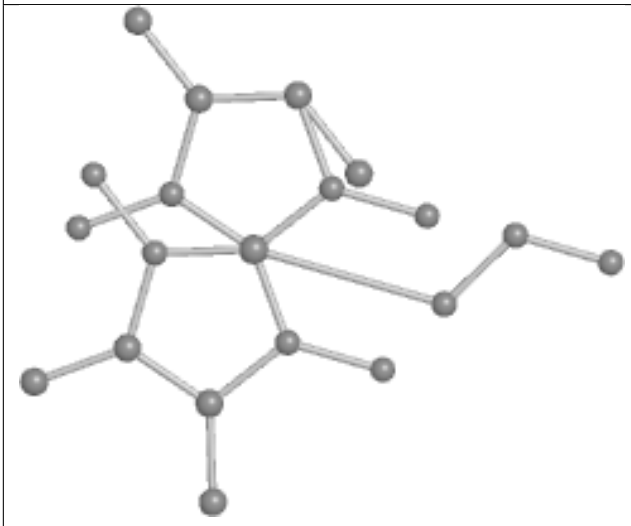
Ligand X5Z I 301



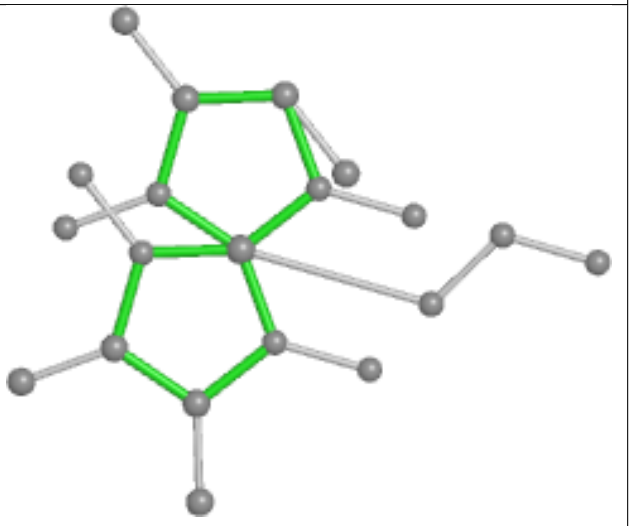
Bond lengths



Bond angles

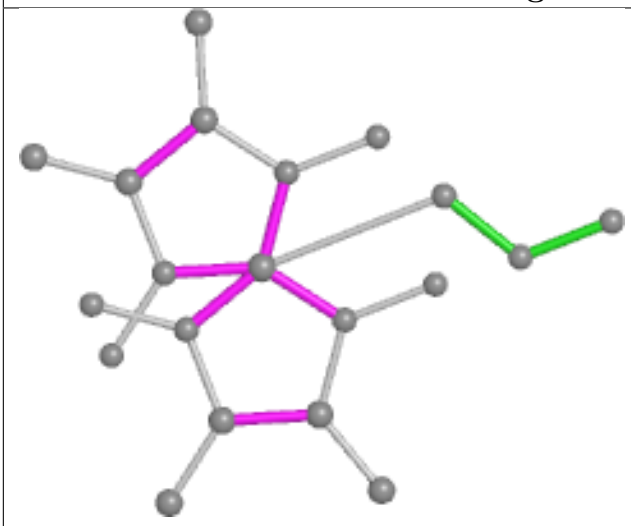


Torsions

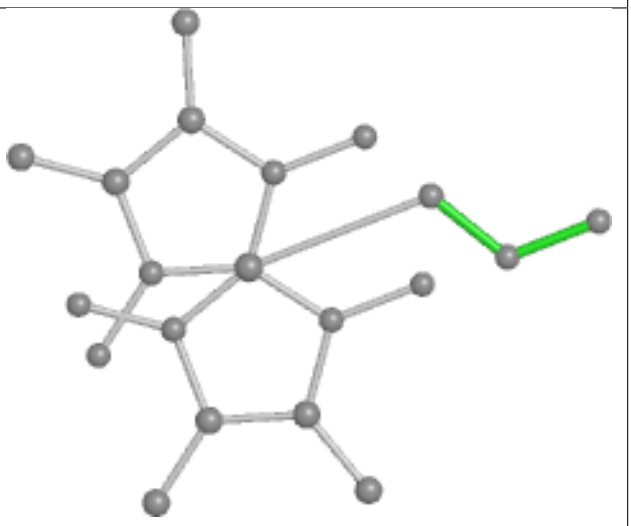


Rings

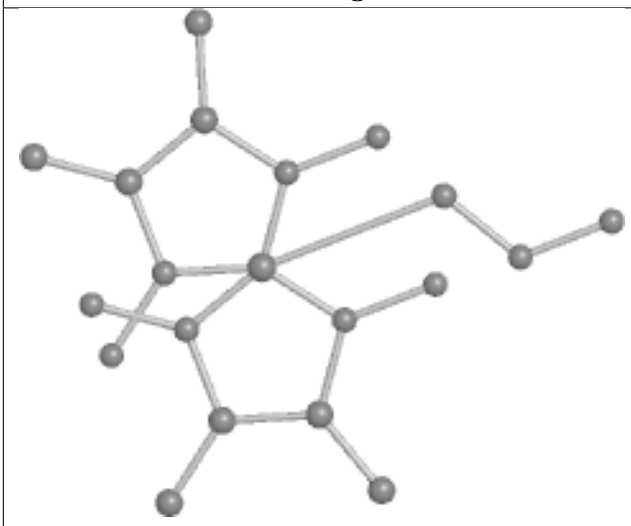
Ligand X5Z H 301



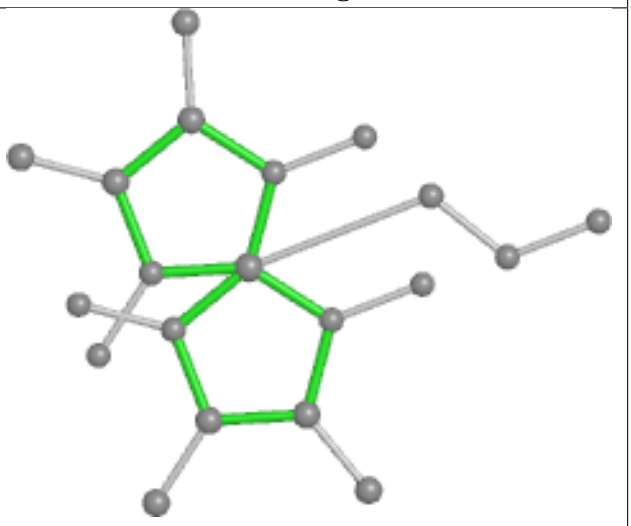
Bond lengths



Bond angles

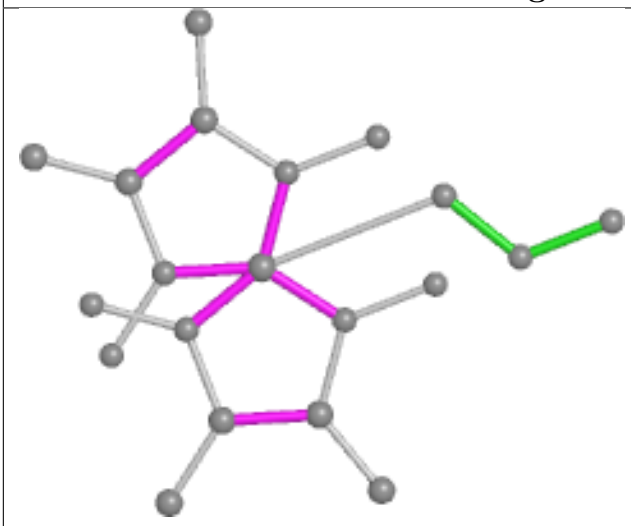


Torsions



Rings

Ligand X5Z B 301



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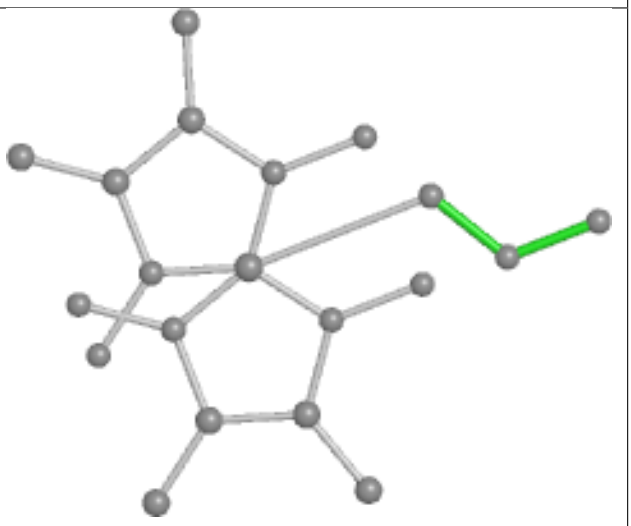
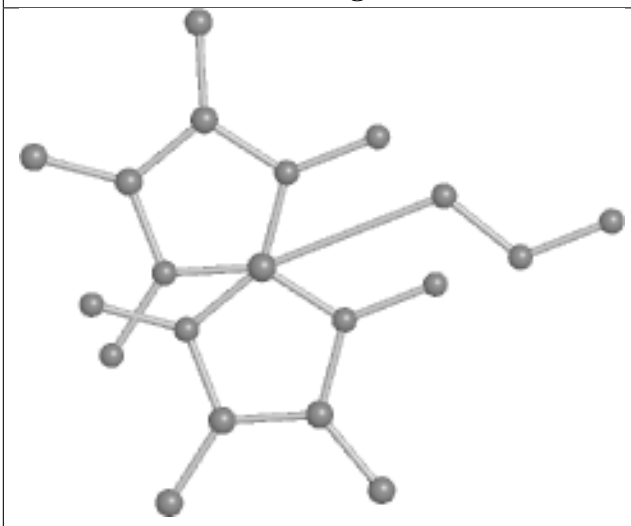


Bond angles



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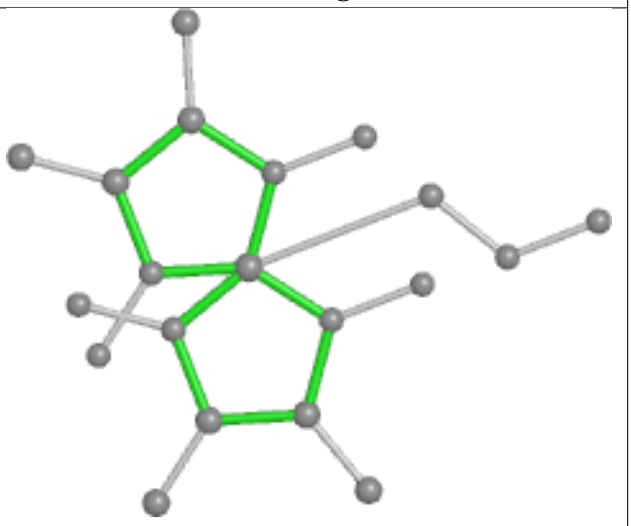
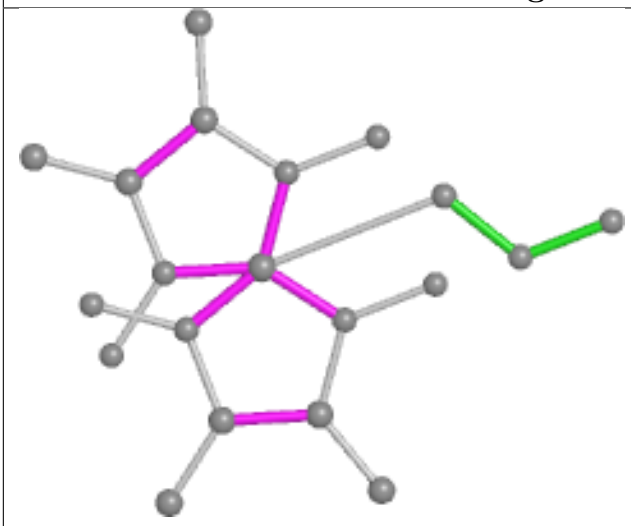


Rings

Ligand X5Z D 301



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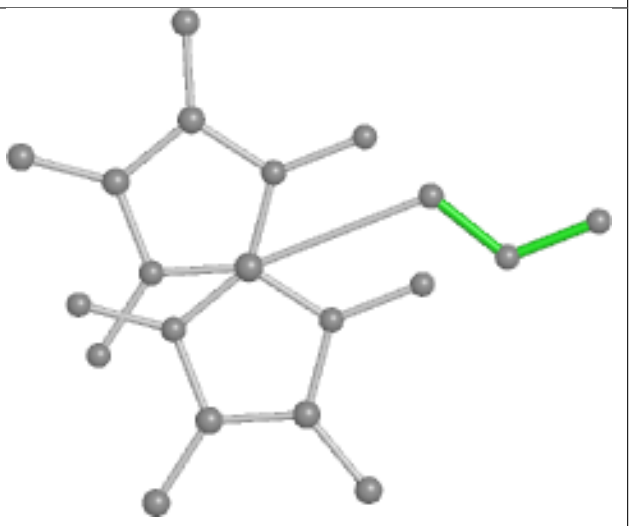
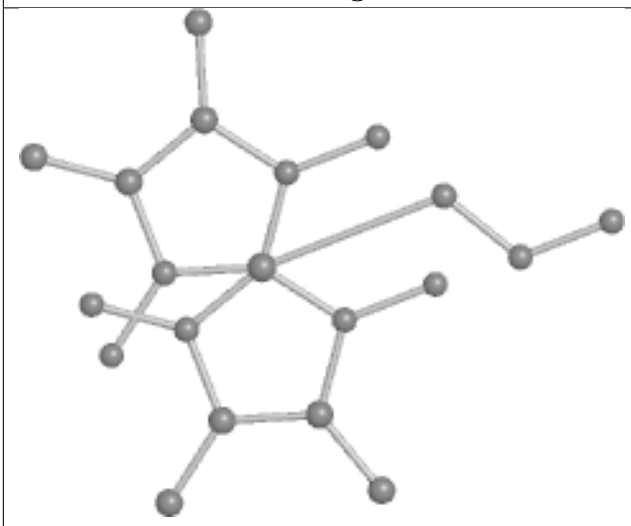


Bond angles



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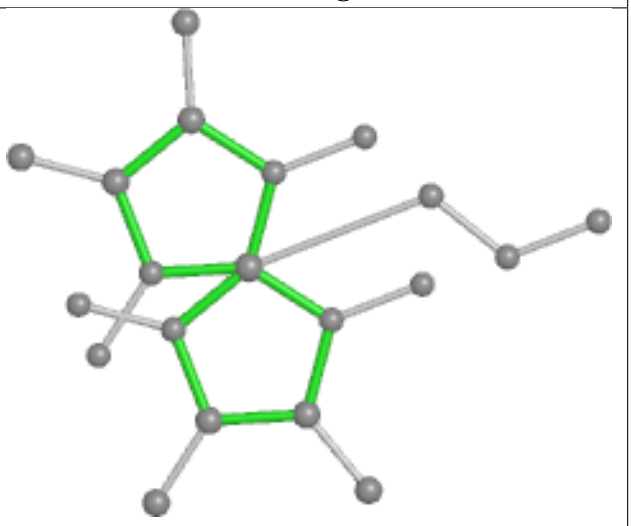
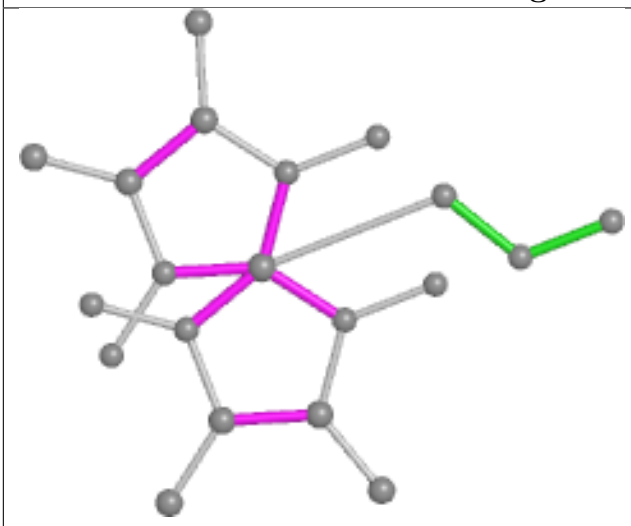
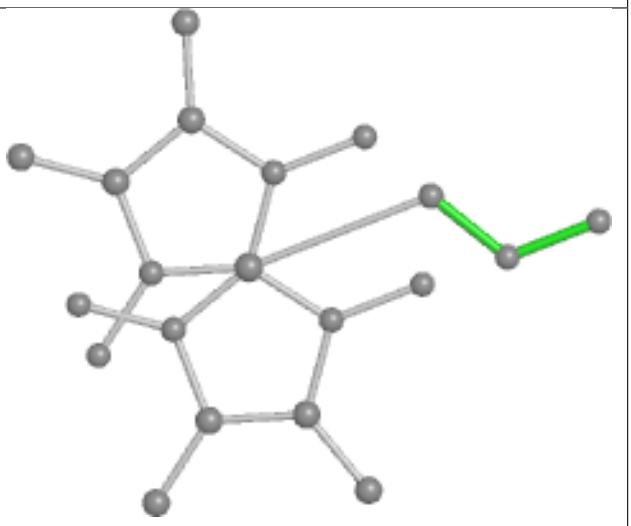


Rings

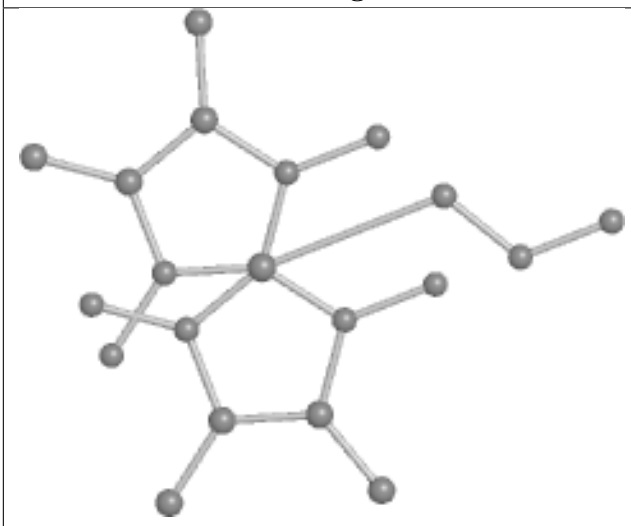
Ligand X5Z F 301



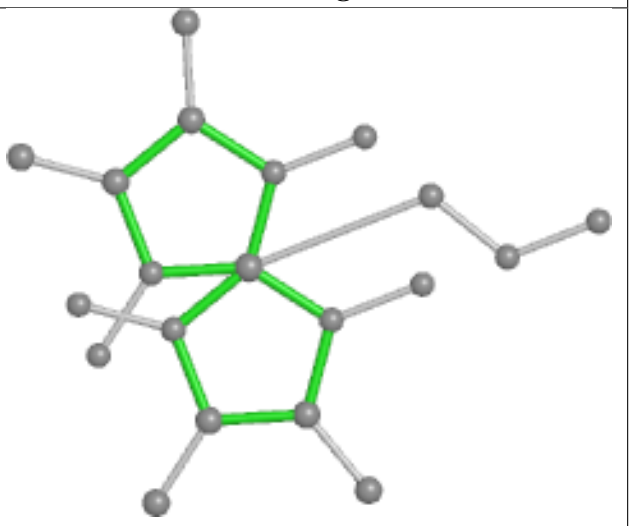
Bond lengths



Bond angles

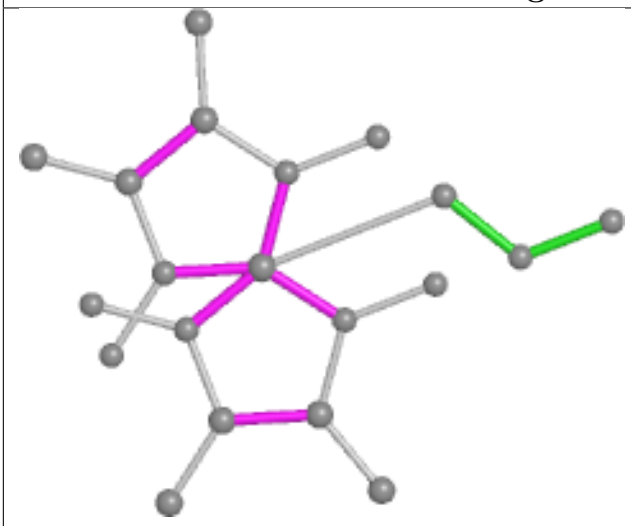


Torsions



Rings

Ligand X5Z A 301



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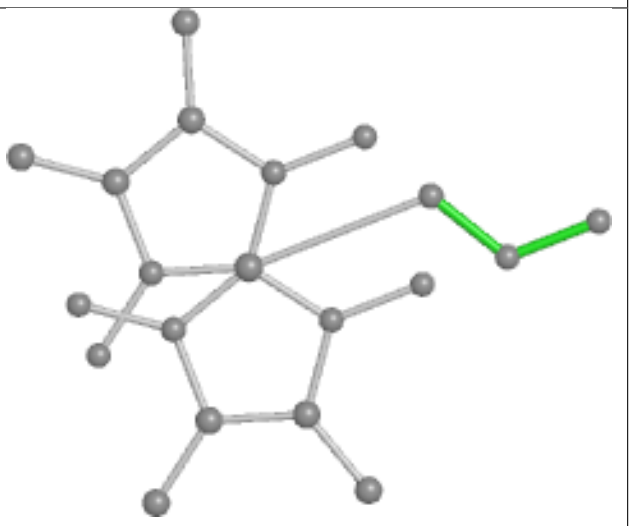
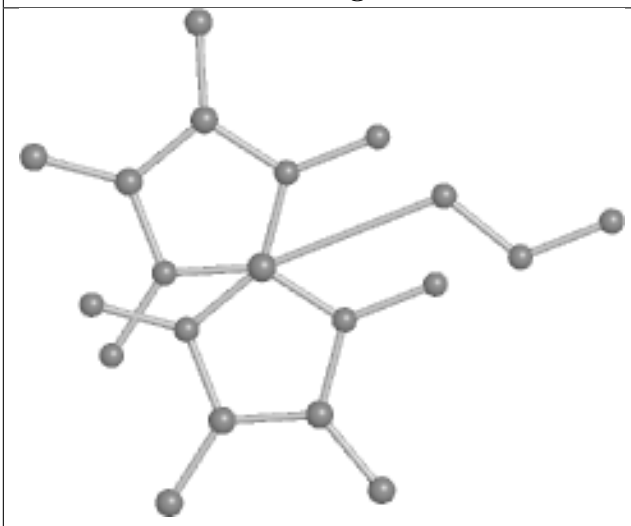


Bond angles



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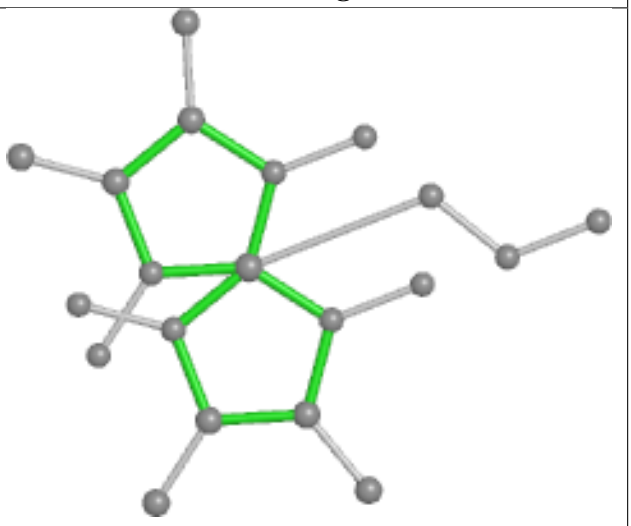
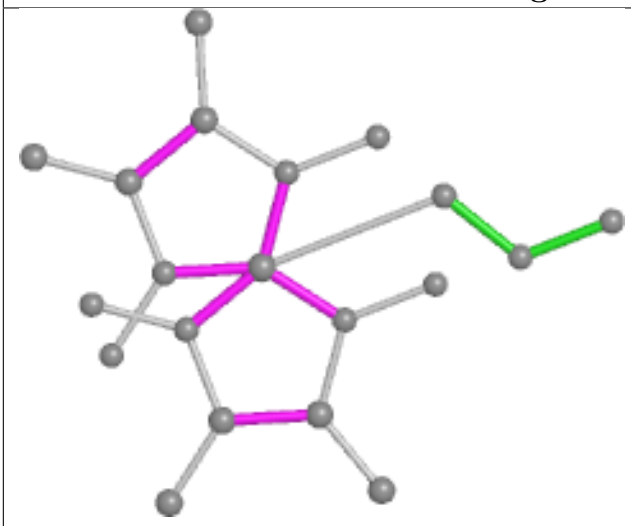
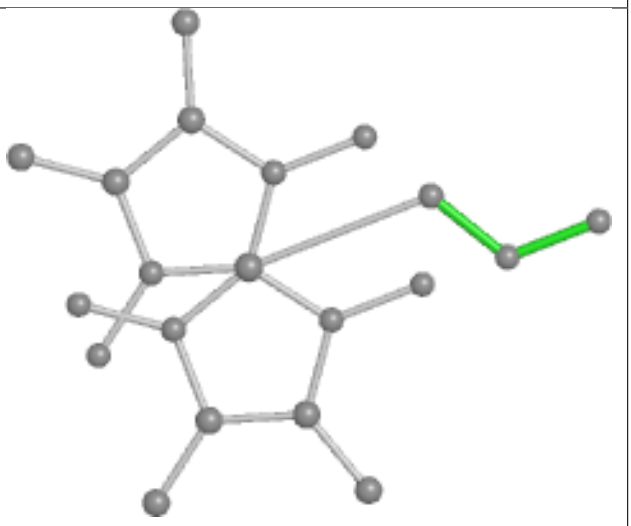


Rings

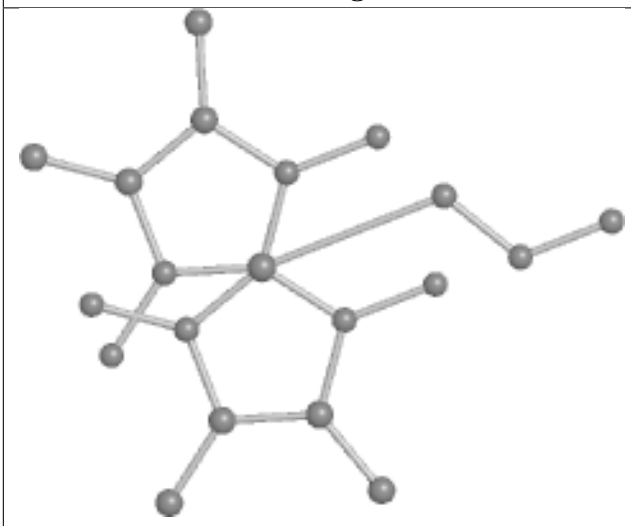
Ligand X5Z L 301



Bond lengths



Bond angles



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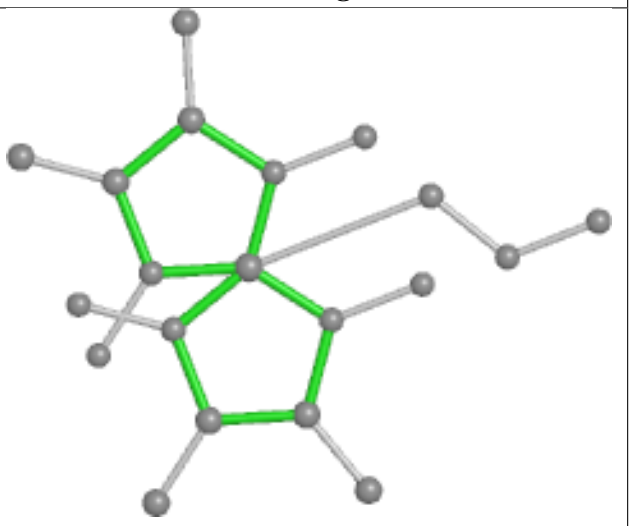
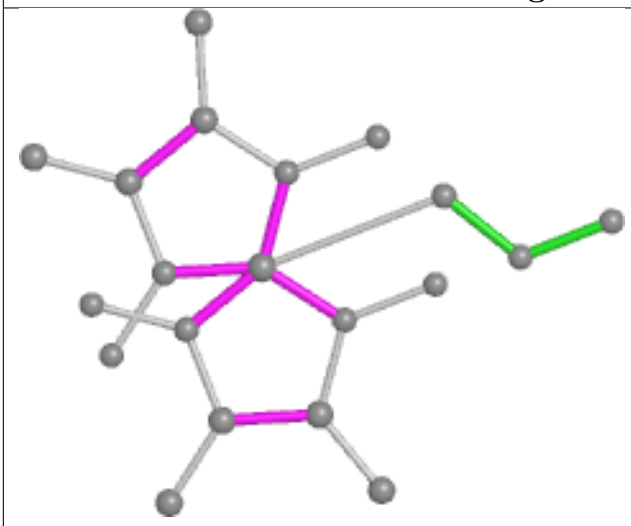
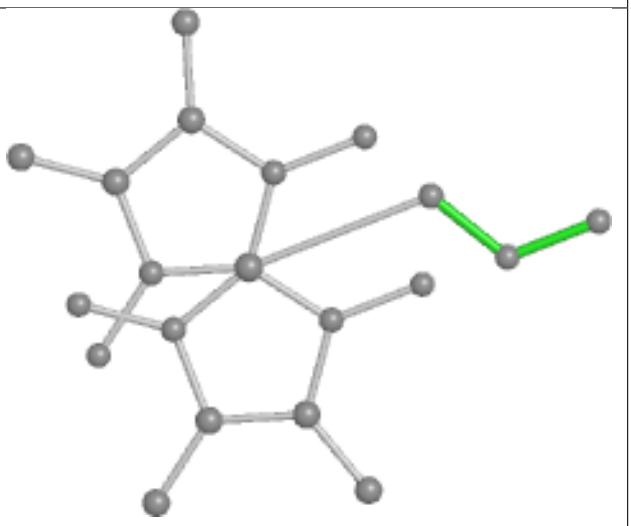


Rings

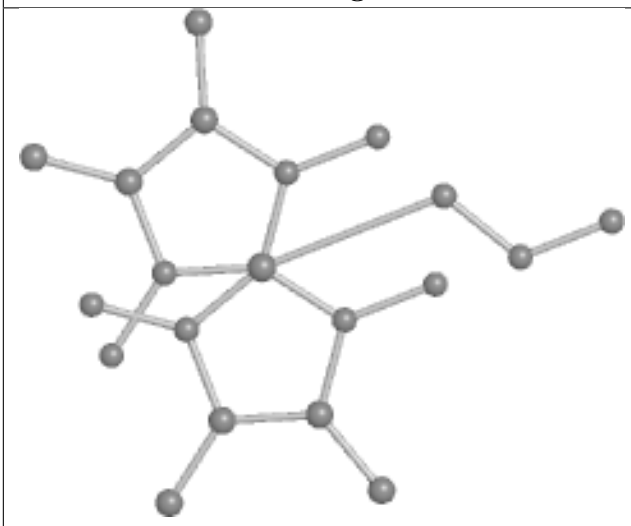
Ligand X5Z C 301



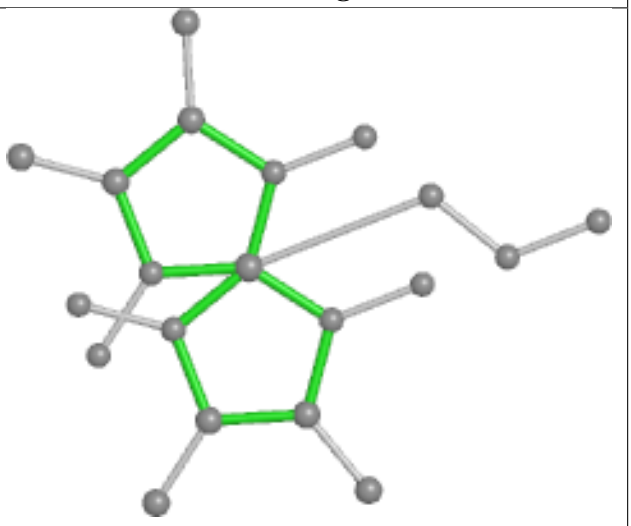
Bond lengths



Bond angles

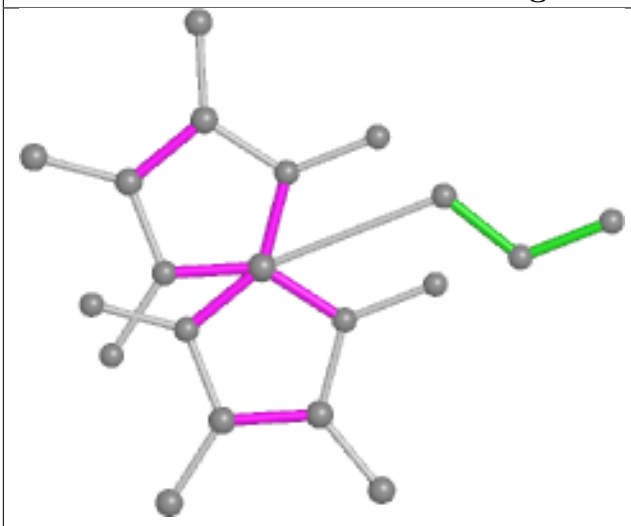


Torsions

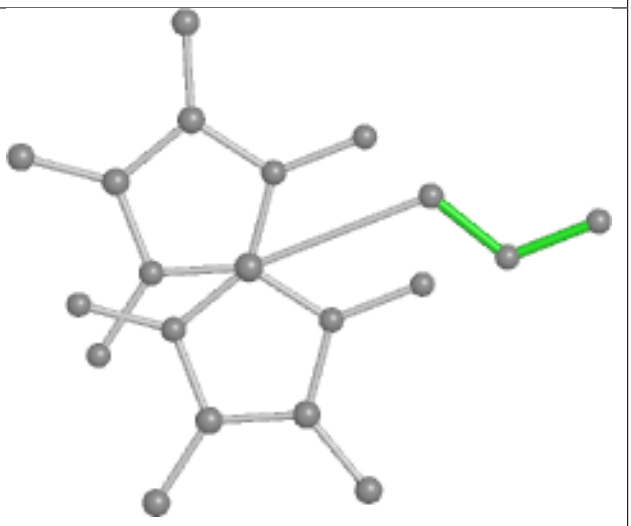


Rings

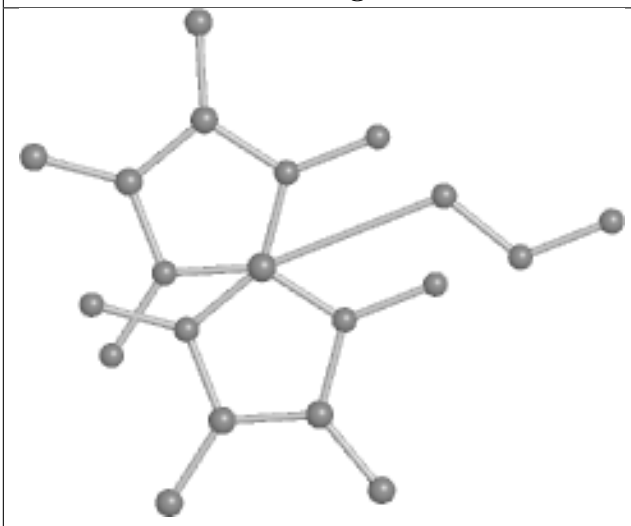
Ligand X5Z E 301



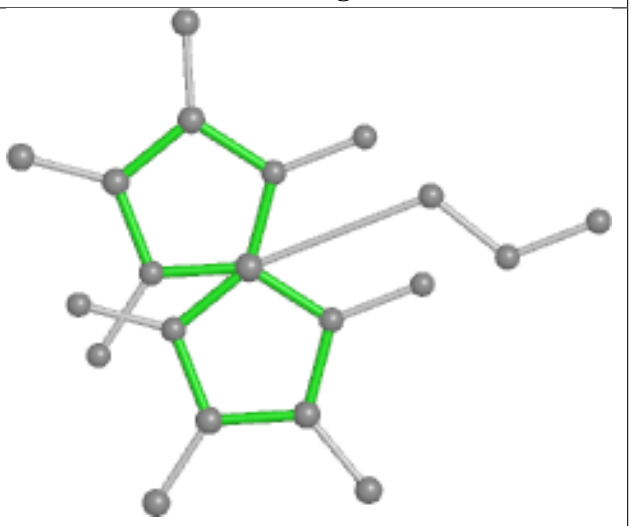
Bond lengths



Bond angles

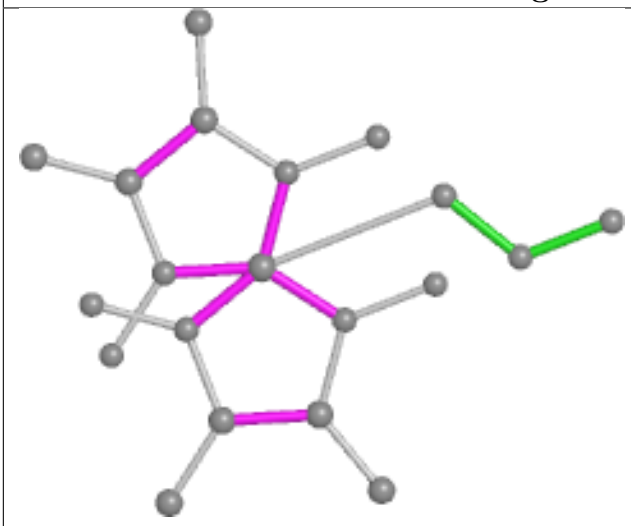


Torsions

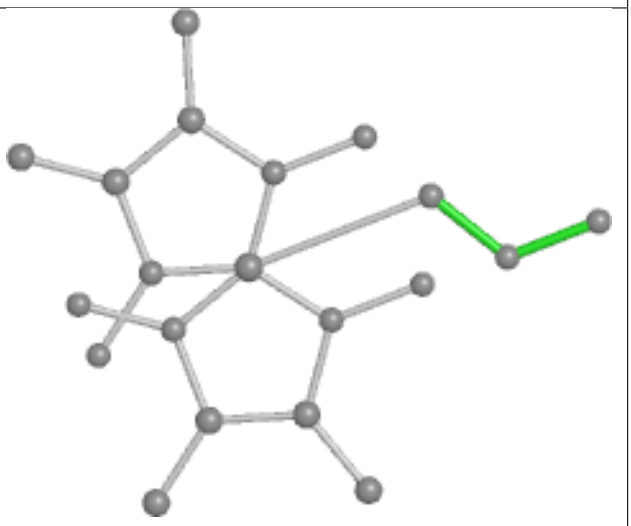


Rings

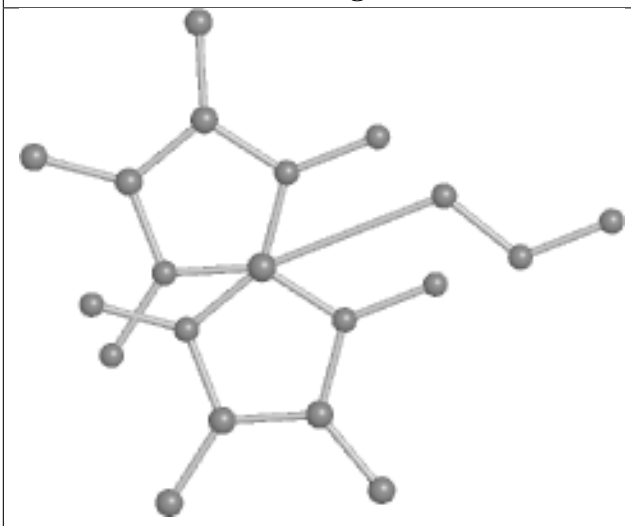
Ligand X5Z J 301



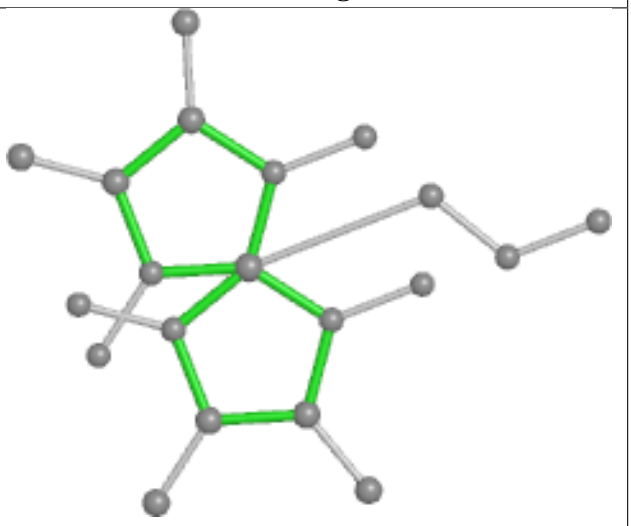
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

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, 95^{th} 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	226/229 (98%)	0.37	7 (3%) 49 21	38, 56, 90, 117	0
1	B	221/229 (96%)	0.29	6 (2%) 54 26	32, 53, 78, 97	0
1	C	219/229 (95%)	0.29	2 (0%) 84 63	44, 57, 80, 99	0
1	D	221/229 (96%)	0.19	2 (0%) 84 63	34, 55, 80, 94	0
1	E	224/229 (97%)	0.52	11 (4%) 29 11	52, 70, 97, 124	0
1	F	223/229 (97%)	0.37	6 (2%) 54 26	42, 59, 88, 111	0
1	G	222/229 (96%)	0.30	4 (1%) 68 40	43, 61, 85, 98	0
1	H	221/229 (96%)	0.30	3 (1%) 75 49	39, 57, 83, 96	0
1	I	223/229 (97%)	0.65	21 (9%) 8 3	56, 77, 102, 113	0
1	J	222/229 (96%)	0.47	14 (6%) 20 6	50, 71, 100, 117	0
1	K	224/229 (97%)	0.56	21 (9%) 8 3	55, 74, 92, 107	0
1	L	220/229 (96%)	0.44	9 (4%) 37 14	45, 69, 93, 107	0
All	All	2666/2748 (97%)	0.39	106 (3%) 38 15	32, 64, 93, 124	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	GLU	5.6
1	I	91	LEU	5.4
1	I	155	LEU	5.3
1	E	181	GLU	4.9
1	A	107	LEU	4.5
1	F	154	VAL	4.4
1	L	45	LEU	4.3
1	K	67	ALA	4.3
1	L	66	LEU	4.2
1	L	41	LEU	4.1
1	I	154	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	I	41	LEU	4.1
1	F	224	GLU	3.9
1	J	91	LEU	3.7
1	H	181	GLU	3.7
1	I	200	VAL	3.5
1	I	92	VAL	3.4
1	E	223	THR	3.3
1	I	69	ILE	3.2
1	K	24	TYR	3.2
1	J	45	LEU	3.2
1	K	31	LEU	3.1
1	I	45	LEU	3.1
1	D	71	ILE	3.1
1	K	104	VAL	3.0
1	B	45	LEU	3.0
1	G	143	TYR	3.0
1	E	213	TYR	2.9
1	J	183	GLN	2.9
1	J	155	LEU	2.9
1	G	41	LEU	2.9
1	I	176	VAL	2.8
1	J	181	GLU	2.8
1	K	50	PHE	2.8
1	I	175	ALA	2.8
1	E	16	PHE	2.8
1	I	143	TYR	2.8
1	J	204	LEU	2.7
1	E	221	PHE	2.7
1	L	8	ALA	2.7
1	K	156	HIS	2.6
1	L	200	VAL	2.6
1	J	44	GLU	2.6
1	A	66	LEU	2.5
1	J	81	PHE	2.5
1	L	188	ALA	2.5
1	A	90	LEU	2.5
1	J	76	LYS	2.5
1	I	107	LEU	2.5
1	I	79	ILE	2.5
1	E	155	LEU	2.5
1	D	69	ILE	2.5
1	K	155	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	101	VAL	2.4
1	K	91	LEU	2.4
1	I	180	LEU	2.4
1	K	13	PHE	2.4
1	K	186	GLY	2.4
1	F	45	LEU	2.4
1	K	118	THR	2.3
1	A	213	TYR	2.3
1	G	151	ALA	2.3
1	K	65	ALA	2.3
1	L	91	LEU	2.3
1	J	152	ASP	2.3
1	E	216	ILE	2.3
1	L	90	LEU	2.3
1	C	81	PHE	2.3
1	F	176	VAL	2.3
1	A	45	LEU	2.3
1	H	175	ALA	2.3
1	K	216	ILE	2.3
1	E	92	VAL	2.2
1	K	9	THR	2.2
1	B	107	LEU	2.2
1	K	8	ALA	2.2
1	K	68	GLY	2.2
1	I	139	ILE	2.2
1	J	3	LYS	2.2
1	K	88	SER	2.2
1	F	225	PRO	2.2
1	L	220	TRP	2.1
1	G	156	HIS	2.1
1	I	121	VAL	2.1
1	C	90	LEU	2.1
1	K	45	LEU	2.1
1	E	69	ILE	2.1
1	I	31	LEU	2.1
1	K	185	TYR	2.1
1	B	95	LYS	2.1
1	E	15	PRO	2.1
1	F	120	SER	2.1
1	J	31	LEU	2.1
1	I	70	THR	2.1
1	K	69	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	68	GLY	2.1
1	E	111	VAL	2.1
1	B	94	VAL	2.0
1	J	16	PHE	2.0
1	B	183	GLN	2.0
1	K	85	TYR	2.0
1	I	196	LEU	2.0
1	B	128	ILE	2.0
1	J	216	ILE	2.0
1	H	176	VAL	2.0
1	I	114	VAL	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, 95^{th} 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	GLN	K	302	9/10	0.57	0.81	62,74,87,90	0
3	SO4	A	303	5/5	0.71	0.42	111,120,131,132	0
3	SO4	G	303	5/5	0.78	0.29	77,86,98,105	0
5	GOL	D	302	6/6	0.82	0.22	46,56,56,64	0
5	GOL	F	302	6/6	0.82	0.20	39,49,52,53	0
4	GLN	I	302	9/10	0.85	0.41	63,67,74,75	0
4	GLN	J	303	9/10	0.88	0.35	62,67,74,79	0
5	GOL	D	303	6/6	0.88	0.23	39,46,59,64	0
3	SO4	A	302	5/5	0.88	0.15	81,91,106,110	0
3	SO4	C	302	5/5	0.89	0.25	92,106,114,125	0
2	X5Z	A	301	20/28	0.89	0.32	85,99,106,117	0
4	GLN	D	304	9/10	0.90	0.30	39,45,52,59	0

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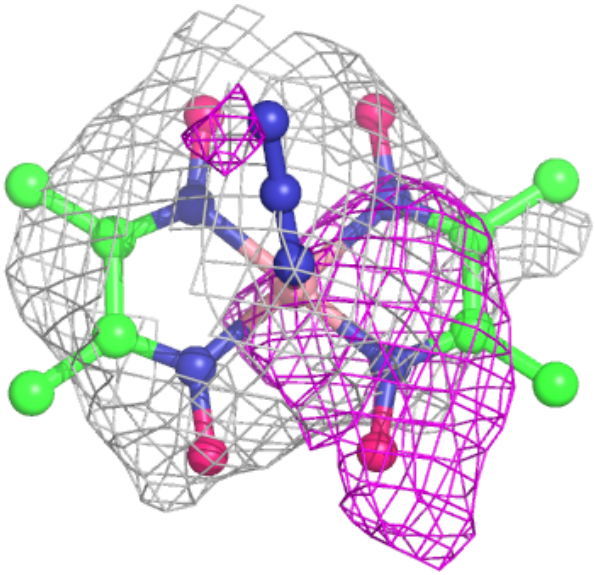
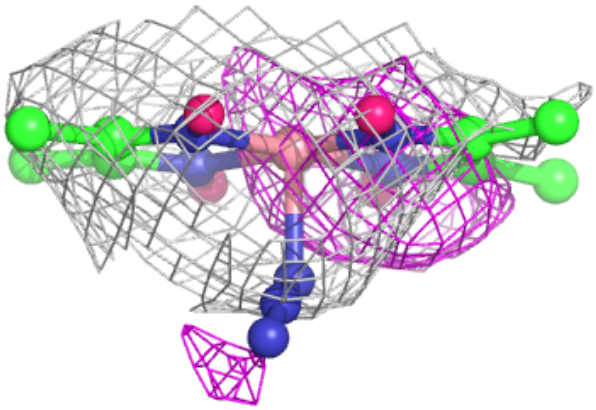
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GLN	L	302	9/10	0.90	0.29	53,60,66,66	0
4	GLN	F	303	9/10	0.90	0.34	51,53,56,57	0
3	SO4	G	302	5/5	0.90	0.22	73,77,103,111	0
2	X5Z	I	301	20/28	0.90	0.35	102,118,134,153	0
3	SO4	G	304	5/5	0.91	0.14	92,95,111,111	0
3	SO4	B	302	5/5	0.91	0.18	81,84,98,103	0
2	X5Z	J	301	20/28	0.91	0.28	99,107,117,131	0
2	X5Z	F	301	20/28	0.91	0.28	87,113,120,139	0
2	X5Z	D	301	20/28	0.91	0.28	84,103,119,130	0
2	X5Z	K	301	20/28	0.92	0.24	99,116,132,143	0
4	GLN	E	302	9/10	0.92	0.24	54,57,61,64	0
2	X5Z	E	301	20/28	0.92	0.27	98,126,137,155	0
4	GLN	A	304	9/10	0.92	0.30	36,38,43,48	0
4	GLN	C	303	9/10	0.92	0.28	43,50,55,60	0
2	X5Z	B	301	20/28	0.93	0.23	68,86,103,116	0
2	X5Z	G	301	20/28	0.93	0.32	89,113,131,149	0
3	SO4	J	302	5/5	0.93	0.14	69,70,79,89	0
2	X5Z	L	301	20/28	0.93	0.20	95,116,123,146	0
2	X5Z	C	301	20/28	0.93	0.26	85,115,125,145	0
4	GLN	G	305	9/10	0.94	0.36	44,51,63,63	0
4	GLN	H	302	9/10	0.94	0.29	41,43,49,53	0
2	X5Z	H	301	20/28	0.94	0.20	91,106,120,129	0
4	GLN	B	303	9/10	0.96	0.25	38,45,53,53	0

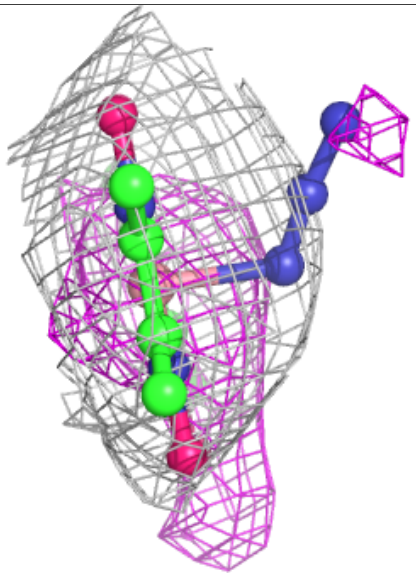
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around X5Z A 301:

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

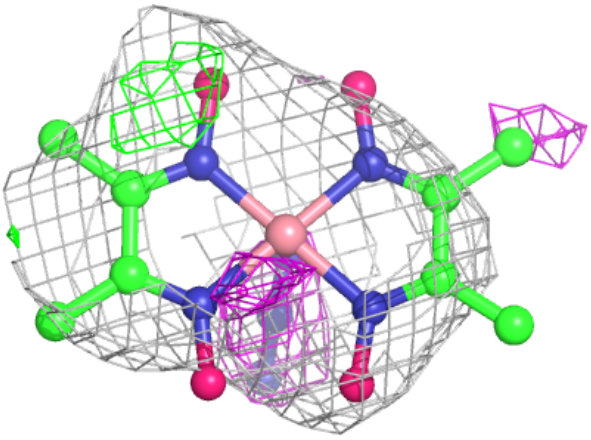


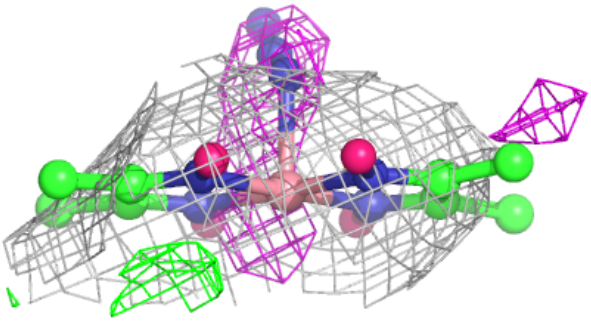


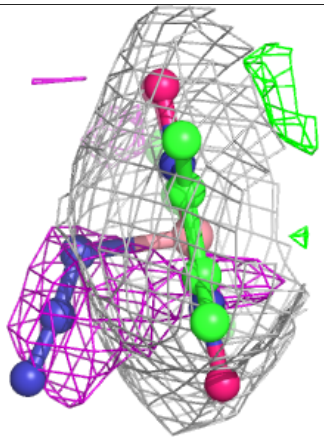


Electron density around X5Z I 301:

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

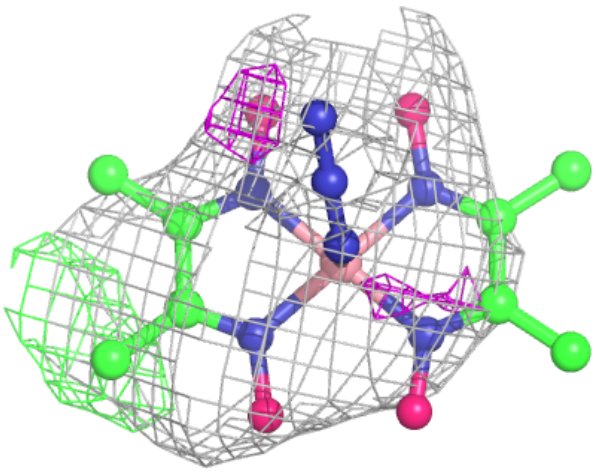


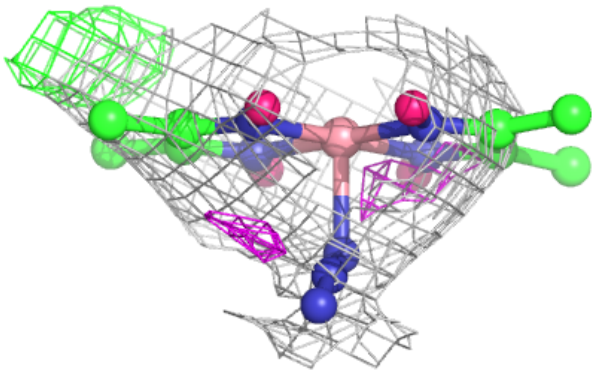


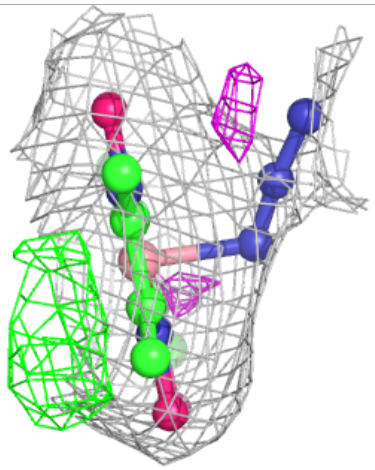


Electron density around X5Z J 301:

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

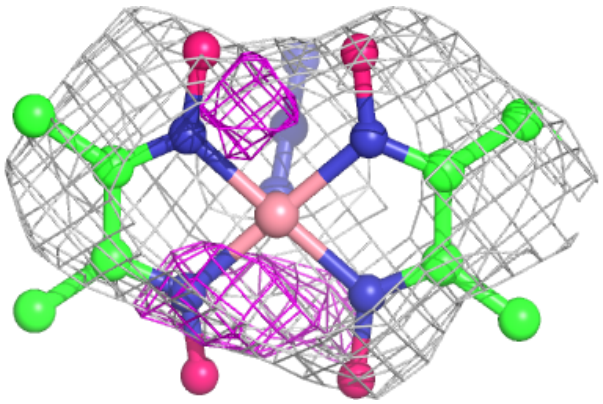


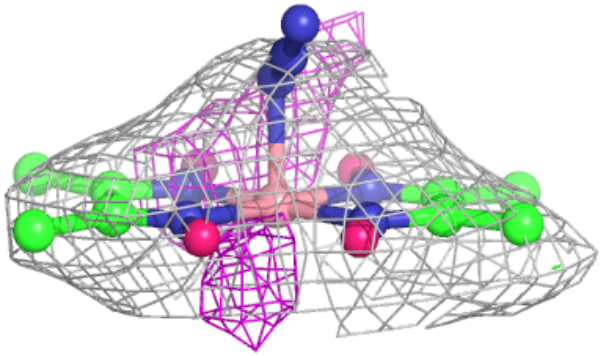


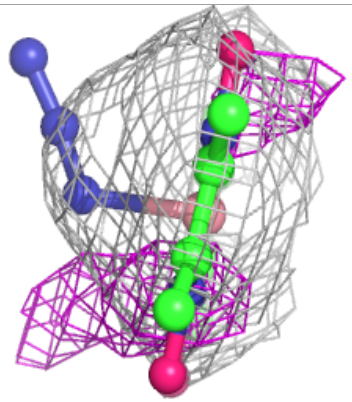


Electron density around X5Z F 301:

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

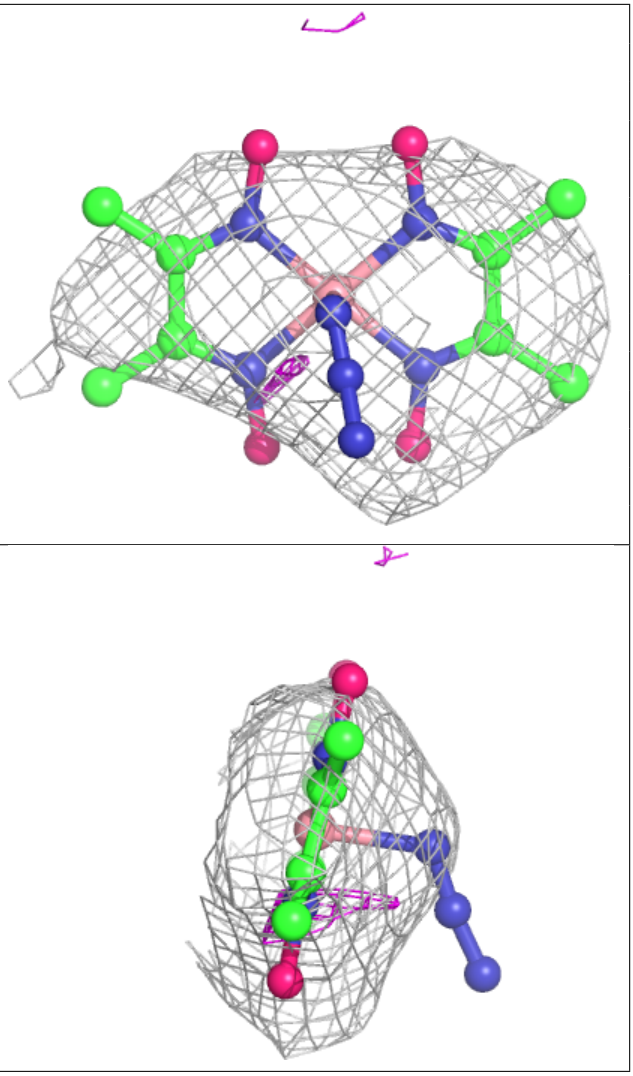






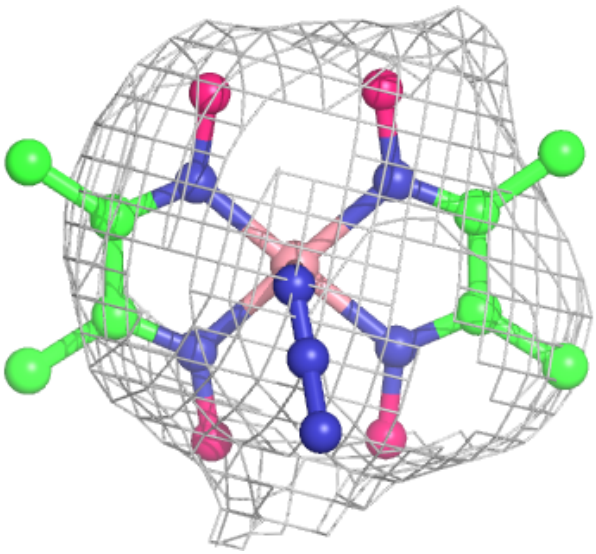
Electron density around X5Z D 301:

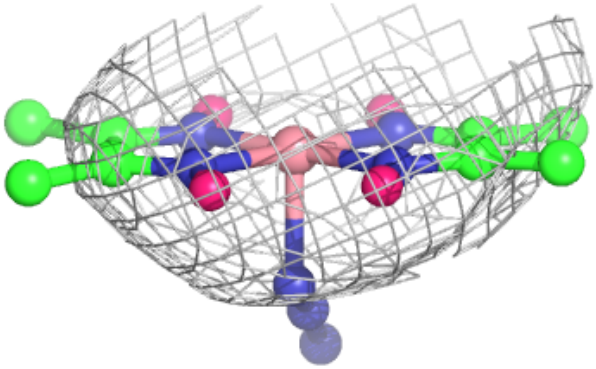
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

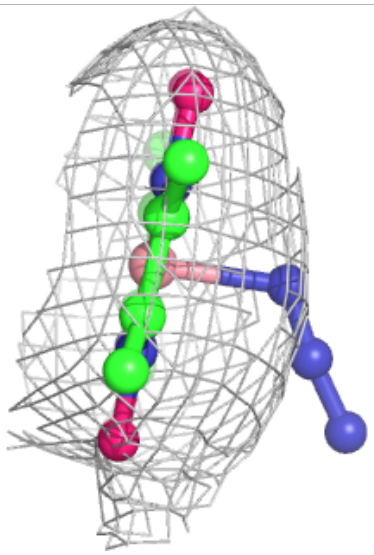


Electron density around X5Z K 301:

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

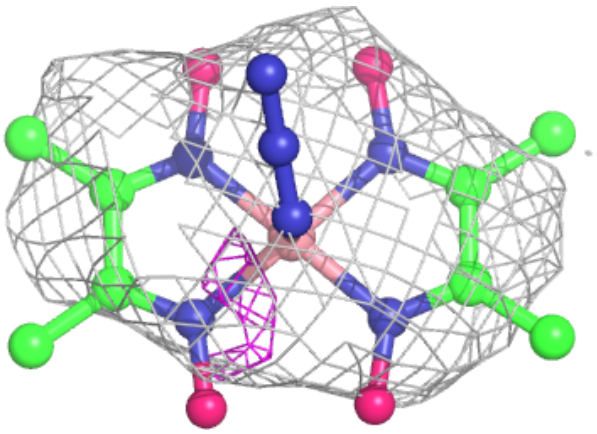


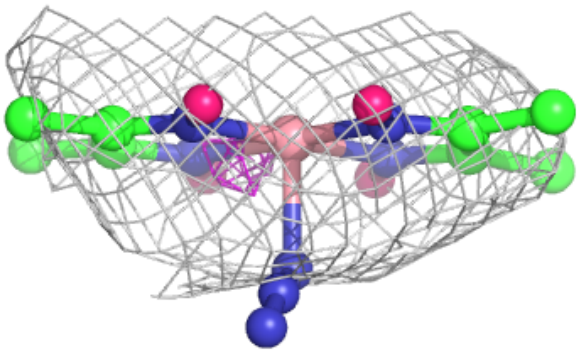


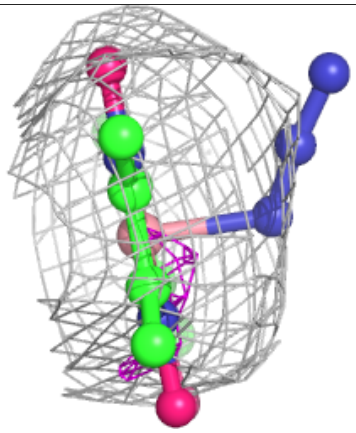


Electron density around X5Z E 301:

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

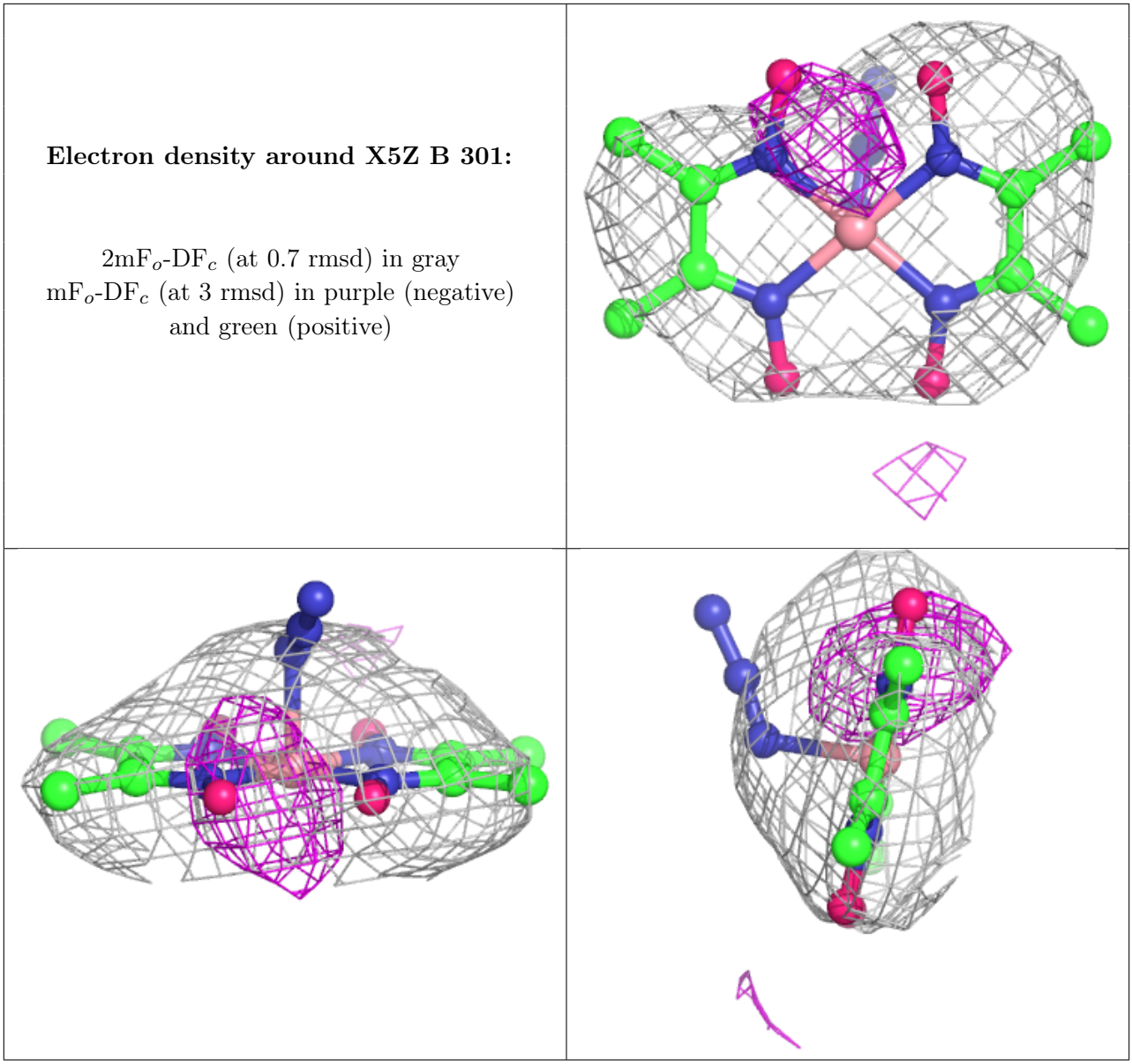






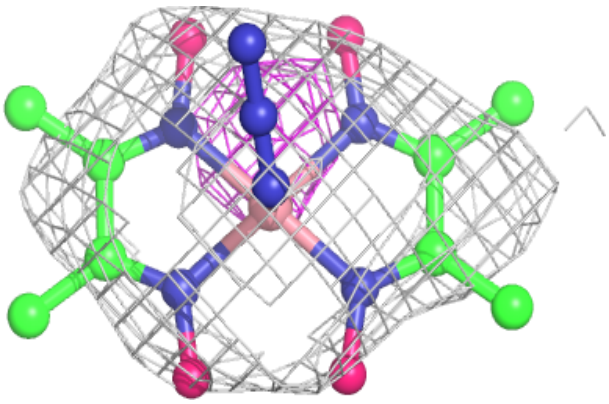
Electron density around X5Z B 301:

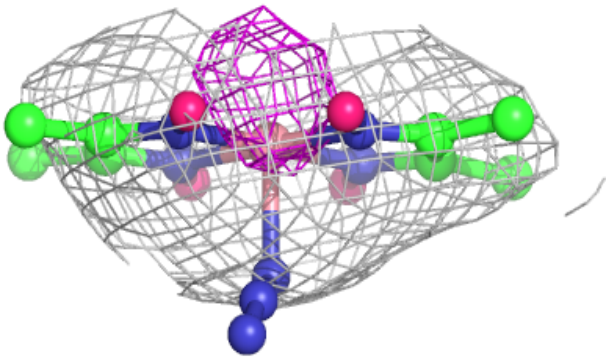
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

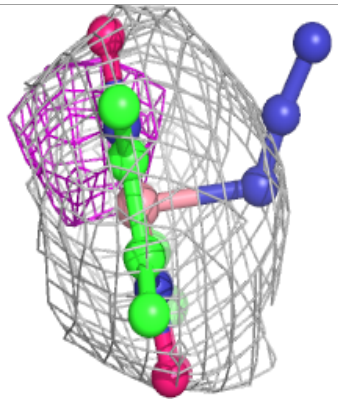


Electron density around X5Z G 301:

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

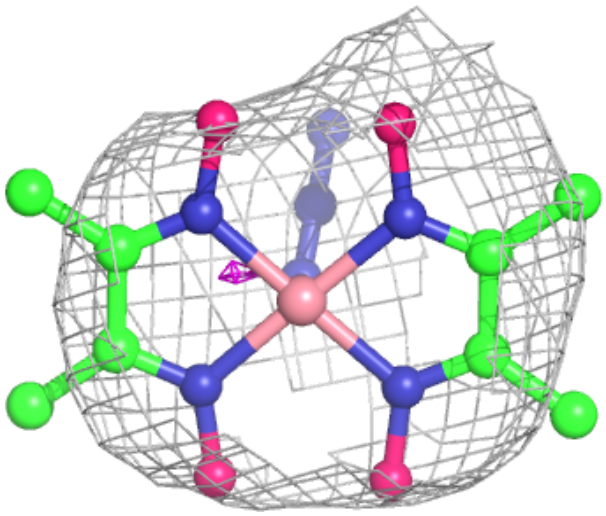


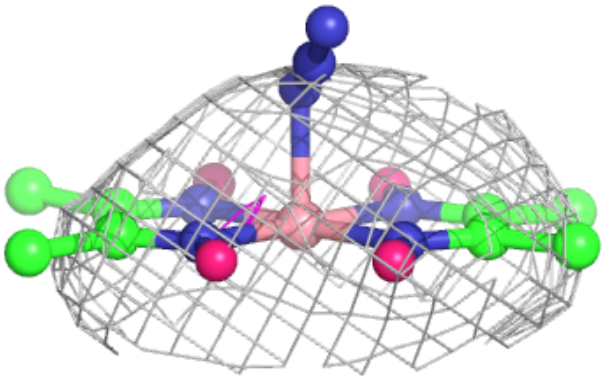


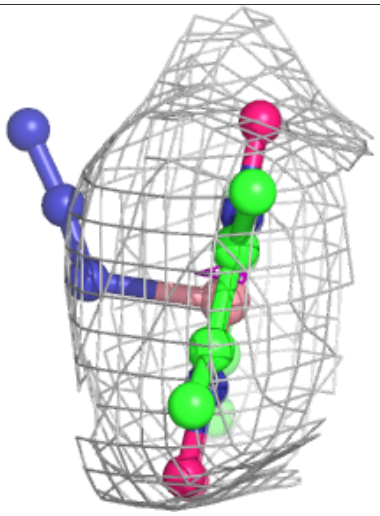


Electron density around X5Z L 301:

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

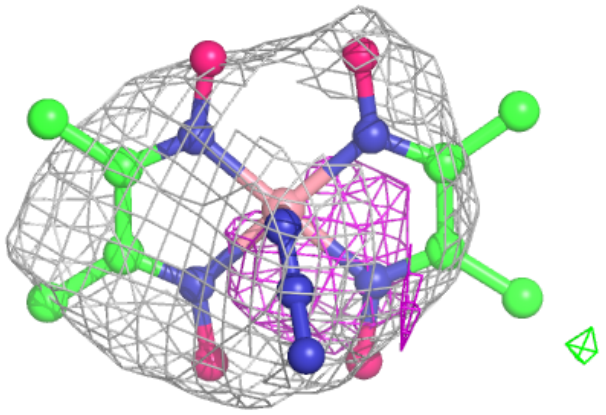


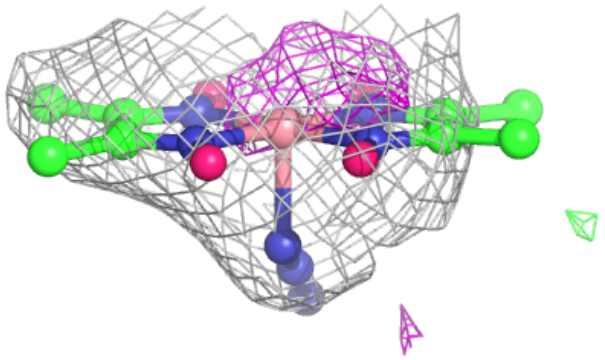


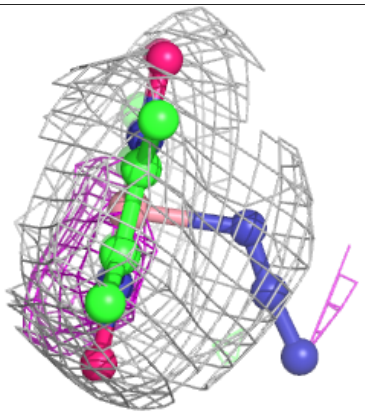


Electron density around X5Z C 301:

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

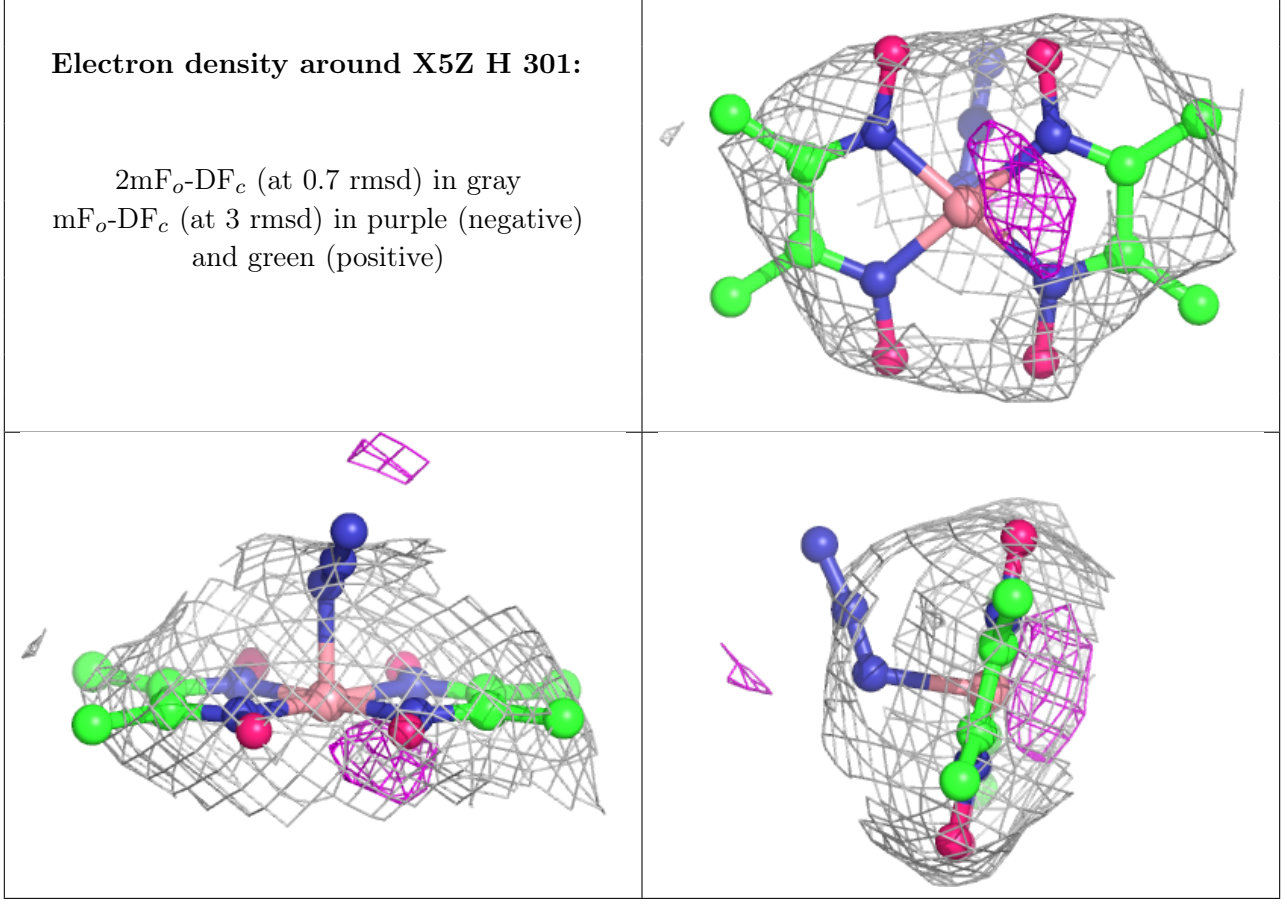






Electron density around X5Z H 301:

$2mF_o$-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

There are no such residues in this entry.