



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:52 AM UTC

PDB ID : 9IH9 / pdb\_00009ih9  
Title : KEAP1 complexed to linear peptide 6  
Authors : Ji, X.; Lau, K.  
Deposited on : 2025-02-20  
Resolution : 1.70 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](mailto: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>.

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

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

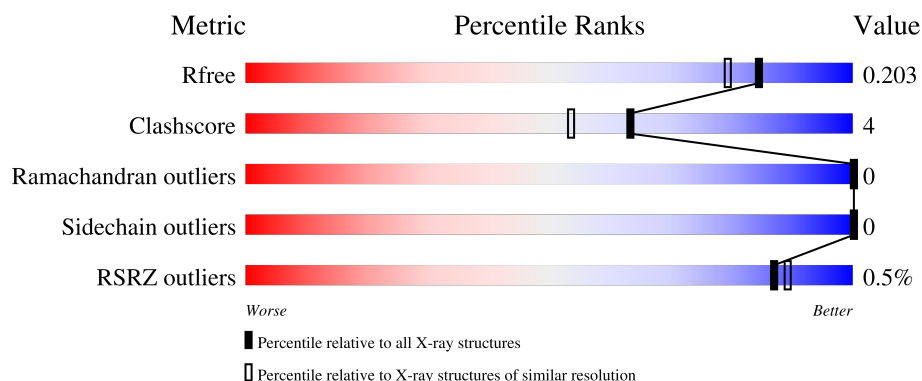
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	290	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
2	B	290	<div> <div>93%</div> <div>5%</div> <div>.</div> </div>
3	A	290	<div> <div>%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
4	X	4	<div> <div>50%</div> <div>50%</div> </div>
4	Y	4	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
4	Z	4	 75% 25%

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 13923 atoms, of which 6477 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	285	Total	C	H	N	O	S	0	1	0
			4276	1362	2083	397	419	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	320	SER	-	expression tag	UNP Q14145
C	540	ALA	GLU	engineered mutation	UNP Q14145
C	542	ALA	GLU	engineered mutation	UNP Q14145

- Molecule 2 is a protein called Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	285	Total	C	H	N	O	S	0	2	0
			4283	1363	2088	399	418	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	320	SER	-	expression tag	UNP Q14145
B	540	ALA	GLU	engineered mutation	UNP Q14145
B	542	ALA	GLU	engineered mutation	UNP Q14145

- Molecule 3 is a protein called Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	285	Total	C	H	N	O	S	0	4	0
			4304	1369	2101	399	418	17			

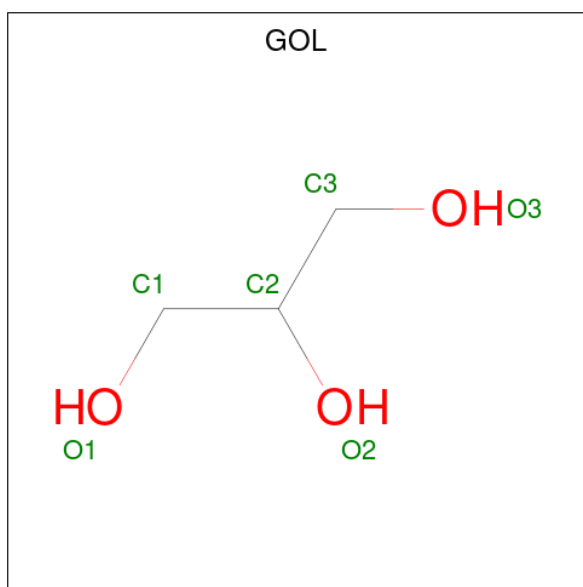
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	SER	-	expression tag	UNP Q14145
A	540	ALA	GLU	engineered mutation	UNP Q14145
A	542	ALA	GLU	engineered mutation	UNP Q14145

- Molecule 4 is a protein called Designed peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	X	4	Total	C	H	N	O	S	0	0	0
			70	23	35	5	6	1			
4	Y	4	Total	C	H	N	O	S	0	0	0
			70	23	35	5	6	1			
4	Z	4	Total	C	H	N	O	S	0	0	0
			70	23	35	5	6	1			

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			17	4	10	3		
6	B	1	Total	C	H	O	0	0
			17	4	10	3		
6	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	A	2	Total	Mg	0	0
			2	2		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).

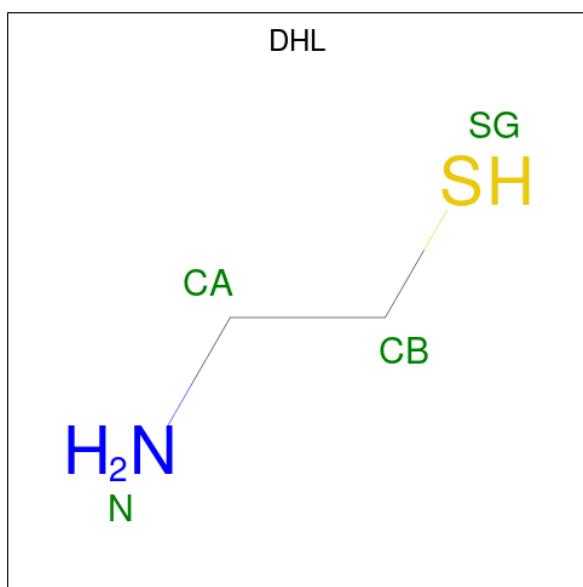


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			10	2	6	2		
8	Z	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	X	1	Total	Cl	0	0
			1	1		
9	Y	1	Total	Cl	0	0
			1	1		
9	Z	1	Total	Cl	0	0
			1	1		

- Molecule 10 is 2-AMINO-ETHANETHIOL (CCD ID: DHL) (formula: C<sub>2</sub>H<sub>7</sub>NS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	X	1	Total	C	H	N	S	0	0
			10	2	6	1	1		
10	Y	1	Total	C	H	N	S	0	0
			10	2	6	1	1		
10	Z	1	Total	C	H	N	S	0	0
			10	2	6	1	1		

- Molecule 11 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	195	Total	O	0	2
			197	197		
11	B	227	Total	O	0	0
			227	227		
11	A	238	Total	O	0	0
			238	238		
11	X	2	Total	O	0	0
			2	2		
11	Y	4	Total	O	0	0
			4	4		
11	Z	4	Total	O	0	0
			4	4		



### 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.

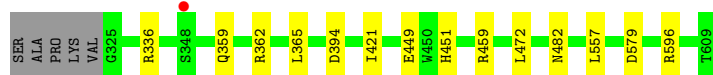
- Molecule 1: Kelch-like ECH-associated protein 1

Chain C: 



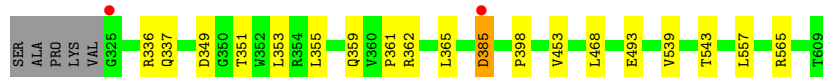
- Molecule 2: Kelch-like ECH-associated protein 1

Chain B: 



- Molecule 3: Kelch-like ECH-associated protein 1

Chain A: 



- Molecule 4: Designed peptide

Chain X: 



- Molecule 4: Designed peptide

Chain Y: 



- Molecule 4: Designed peptide

Chain Z: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.76Å 133.93Å 82.32Å 90.00° 101.36° 90.00°	Depositor
Resolution (Å)	19.74 – 1.70 19.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	76.6 (19.74-1.70) 88.4 (19.74-1.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 1.69Å)	Xtriage
Refinement program	PHENIX dev_5373	Depositor
R, $R_{free}$	0.161 , 0.203 0.160 , 0.203	Depositor DCC
$R_{free}$ test set	4247 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.3	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 53.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13923	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ABA, A1JAL, GOL, CSO, PEG, MPT, DHL, MG, CME, CL, EDO

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	C	0.41	0/2233	0.58	0/3037
2	B	0.42	0/2251	0.60	0/3062
3	A	0.52	2/2263 (0.1%)	0.62	0/3081
4	X	0.42	0/7	0.40	0/8
4	Y	0.50	0/7	0.40	0/8
4	Z	0.57	0/7	0.41	0/8
All	All	0.45	2/6768 (0.0%)	0.60	0/9204

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	385	ASP	CB-CG	-8.75	1.30	1.52
3	A	385	ASP	CG-OD2	6.88	1.38	1.25

There are no bond angle outliers.

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	C	2193	2083	2083	19	0
2	B	2195	2088	2073	13	0
3	A	2203	2101	2084	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	X	35	35	16	1	0
4	Y	35	35	16	1	0
4	Z	35	35	16	0	0
5	A	18	24	24	1	0
5	B	6	8	8	0	0
5	C	6	8	8	1	0
6	A	7	10	10	1	0
6	B	7	10	10	3	0
6	C	7	10	10	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	4	6	6	2	0
8	Z	4	6	6	0	0
9	X	1	0	0	0	0
9	Y	1	0	0	0	0
9	Z	1	0	0	0	0
10	X	4	6	5	0	0
10	Y	4	6	5	0	0
10	Z	4	6	5	0	0
11	A	238	0	0	10	0
11	B	227	0	0	6	0
11	C	197	0	0	4	0
11	X	2	0	0	0	0
11	Y	4	0	0	0	0
11	Z	4	0	0	0	0
All	All	7446	6477	6385	53	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 4.

All (53) 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)
3:A:385:ASP:OD2	11:A:801:HOH:O	1.78	1.02
1:C:385:ASP:HB2	11:A:801:HOH:O	1.63	0.96
3:A:385:ASP:OD2	11:A:802:HOH:O	2.03	0.74
2:B:459:ARG:HE	6:B:703:PEG:H21	1.58	0.69
6:B:703:PEG:H42	11:B:830:HOH:O	2.01	0.61
2:B:362:ARG:NH2	2:B:394:ASP:OD2	2.35	0.60
1:C:362:ARG:NH2	1:C:394:ASP:OD2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:557:LEU:HD23	3:A:557:LEU:H	1.68	0.58
3:A:543:THR:HG21	11:A:1008:HOH:O	2.04	0.58
3:A:385:ASP:CG	11:A:801:HOH:O	2.40	0.56
2:B:421:ILE:HD11	2:B:472:LEU:HB2	1.90	0.54
3:A:365:LEU:HD23	3:A:365:LEU:H	1.73	0.53
11:C:974:HOH:O	4:X:1:MPT:HB1	2.08	0.53
2:B:482:ASN:ND2	11:B:802:HOH:O	2.22	0.53
2:B:557:LEU:H	2:B:557:LEU:HD23	1.73	0.53
1:C:557:LEU:H	1:C:557:LEU:HD23	1.74	0.53
1:C:606:VAL:O	5:C:701:GOL:H2	2.09	0.53
2:B:365:LEU:H	2:B:365:LEU:HD23	1.74	0.52
3:A:349:ASP:OD1	3:A:351:THR:HG22	2.10	0.52
3:A:337:GLN:HB3	11:A:994:HOH:O	2.10	0.49
11:A:912:HOH:O	4:Y:1:MPT:HB1	2.13	0.49
3:A:353:LEU:HG	3:A:355:LEU:HD21	1.94	0.48
2:B:359:GLN:OE1	11:B:801:HOH:O	2.20	0.48
1:C:365:LEU:H	1:C:365:LEU:HD23	1.77	0.48
1:C:515:LEU:HD22	1:C:566:ILE:HG13	1.97	0.46
1:C:362:ARG:HD2	1:C:378:GLY:O	2.17	0.45
3:A:565:ARG:HD2	11:A:982:HOH:O	2.17	0.45
2:B:459:ARG:CG	6:B:703:PEG:H41	2.47	0.45
2:B:362:ARG:HG2	11:B:903:HOH:O	2.16	0.45
1:C:424:HIS:CD2	1:C:444:GLU:HG2	2.52	0.44
1:C:493:GLU:HG2	11:C:961:HOH:O	2.17	0.44
2:B:336:ARG:NE	11:B:811:HOH:O	2.50	0.44
3:A:353:LEU:CD1	11:A:1004:HOH:O	2.65	0.44
1:C:468:LEU:HD23	1:C:539:VAL:HG21	1.99	0.44
1:C:505:THR:HG22	1:C:506:ILE:O	2.17	0.44
2:B:459:ARG:HH12	8:B:701:EDO:H12	1.83	0.44
1:C:380:ARG:NH2	3:A:336:ARG:NH2	2.66	0.43
1:C:421:ILE:HD11	1:C:472:LEU:HB2	1.99	0.43
1:C:359:GLN:H	1:C:359:GLN:CD	2.26	0.43
3:A:468:LEU:HD23	3:A:539:VAL:HG21	2.00	0.43
1:C:442:ARG:NH1	11:C:806:HOH:O	2.45	0.42
3:A:361:PRO:O	3:A:362:ARG:HG3	2.20	0.42
3:A:493:GLU:O	6:A:704:PEG:H22	2.20	0.42
1:C:380:ARG:HD3	1:C:382:ASN:OD1	2.20	0.42
8:B:701:EDO:H11	11:B:814:HOH:O	2.19	0.42
1:C:452:LEU:HD23	11:C:959:HOH:O	2.20	0.41
3:A:359:GLN:HG3	11:A:960:HOH:O	2.20	0.41
3:A:398:PRO:O	5:A:701:GOL:H12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:MET:HE3	1:C:550:MET:HB2	1.93	0.41
2:B:579:ASP:OD2	2:B:596:ARG:NH2	2.54	0.41
1:C:432:HIS:NE2	3:A:336:ARG:HG2	2.37	0.40
2:B:449:GLU:HG2	2:B:451:HIS:CE1	2.57	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	C	282/290 (97%)	277 (98%)	5 (2%)	0	100	100
2	B	284/290 (98%)	278 (98%)	6 (2%)	0	100	100
3	A	286/290 (99%)	282 (99%)	4 (1%)	0	100	100
4	X	1/4 (25%)	1 (100%)	0	0	100	100
4	Y	1/4 (25%)	1 (100%)	0	0	100	100
4	Z	1/4 (25%)	1 (100%)	0	0	100	100
All	All	855/882 (97%)	840 (98%)	15 (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	C	228/231 (99%)	228 (100%)	0	100	100
2	B	230/232 (99%)	230 (100%)	0	100	100
3	A	231/232 (100%)	231 (100%)	0	100	100
4	X	1/1 (100%)	1 (100%)	0	100	100
4	Y	1/1 (100%)	1 (100%)	0	100	100
4	Z	1/1 (100%)	1 (100%)	0	100	100
All	All	692/698 (99%)	692 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	414	ASN
1	C	469	ASN
1	C	517	ASN
2	B	337	GLN
2	B	359	GLN
2	B	424	HIS
2	B	552	HIS
3	A	359	GLN
3	A	414	ASN
3	A	451	HIS
3	A	482	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues 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
1	CSO	C	583	1	3,6,7	0.67	0	1,6,8	0.03	0
4	ABA	Z	4	10,4	4,5,6	0.72	0	1,5,7	0.28	0
3	CME	A	583	3	8,9,10	0.47	0	6,9,11	0.61	0
4	A1JAL	X	2	4	14,17,18	0.54	0	18,22,24	0.87	1 (5%)
4	A1JAL	Y	2	4	14,17,18	0.42	0	18,22,24	0.90	1 (5%)
2	CSO	B	518	2	3,6,7	0.50	0	1,6,8	0.06	0
4	ABA	X	4	10,4	4,5,6	0.70	0	1,5,7	0.13	0
1	CSO	C	518	1	3,6,7	0.61	0	1,6,8	0.68	0
4	ABA	Y	4	10,4	4,5,6	0.58	0	1,5,7	0.02	0
4	A1JAL	Z	2	4	14,17,18	0.64	0	18,22,24	0.87	1 (5%)

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
1	CSO	C	583	1	-	0/1/5/7	-
4	ABA	Z	4	10,4	-	0/3/4/6	-
3	CME	A	583	3	-	0/5/8/10	-
4	A1JAL	X	2	4	-	0/9/28/30	0/2/2/2
4	A1JAL	Y	2	4	-	0/9/28/30	0/2/2/2
2	CSO	B	518	2	-	0/1/5/7	-
4	ABA	X	4	10,4	-	0/3/4/6	-
1	CSO	C	518	1	-	0/1/5/7	-
4	ABA	Y	4	10,4	-	0/3/4/6	-
4	A1JAL	Z	2	4	-	0/9/28/30	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	2	A1JAL	O-C-CA	-2.59	118.11	124.77
4	Z	2	A1JAL	O-C-CA	-2.43	118.52	124.77
4	X	2	A1JAL	O-C-CA	-2.16	119.22	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	EDO	B	701	-	3,3,3	0.26	0	2,2,2	0.43	0
5	GOL	A	703	-	5,5,5	0.37	0	5,5,5	0.29	0
5	GOL	B	702	-	5,5,5	0.54	0	5,5,5	1.01	0
6	PEG	B	703	-	6,6,6	0.29	0	5,5,5	0.85	0
8	EDO	Z	701	-	3,3,3	0.27	0	2,2,2	0.35	0
10	DHL	Z	703	4	2,3,3	0.27	0	1,2,2	0.52	0
5	GOL	C	701	-	5,5,5	0.42	0	5,5,5	0.94	0
10	DHL	X	702	4	2,3,3	0.14	0	1,2,2	1.46	0
5	GOL	A	702	-	5,5,5	0.39	0	5,5,5	0.68	0
6	PEG	C	702	-	6,6,6	0.28	0	5,5,5	0.27	0
10	DHL	Y	702	4	2,3,3	0.16	0	1,2,2	1.17	0
6	PEG	A	704	-	6,6,6	0.29	0	5,5,5	0.35	0
5	GOL	A	701	-	5,5,5	0.40	0	5,5,5	0.38	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
8	EDO	B	701	-	-	1/1/1/1	-
5	GOL	A	703	-	-	4/4/4/4	-
5	GOL	B	702	-	-	2/4/4/4	-
6	PEG	B	703	-	-	4/4/4/4	-
8	EDO	Z	701	-	-	0/1/1/1	-
10	DHL	Z	703	4	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	701	-	-	2/4/4/4	-
10	DHL	X	702	4	-	0/1/1/1	-
5	GOL	A	702	-	-	0/4/4/4	-
6	PEG	C	702	-	-	4/4/4/4	-
10	DHL	Y	702	4	-	0/1/1/1	-
6	PEG	A	704	-	-	1/4/4/4	-
5	GOL	A	701	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	701	GOL	O1-C1-C2-C3
5	B	702	GOL	O1-C1-C2-O2
5	B	702	GOL	O1-C1-C2-C3
5	C	701	GOL	O1-C1-C2-O2
6	B	703	PEG	C1-C2-O2-C3
6	C	702	PEG	O2-C3-C4-O4
5	A	703	GOL	O1-C1-C2-C3
5	A	703	GOL	C1-C2-C3-O3
6	B	703	PEG	O2-C3-C4-O4
6	B	703	PEG	O1-C1-C2-O2
6	C	702	PEG	O1-C1-C2-O2
5	A	703	GOL	O2-C2-C3-O3
6	C	702	PEG	C1-C2-O2-C3
5	A	703	GOL	O1-C1-C2-O2
6	C	702	PEG	C4-C3-O2-C2
6	B	703	PEG	C4-C3-O2-C2
8	B	701	EDO	O1-C1-C2-O2
6	A	704	PEG	C1-C2-O2-C3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

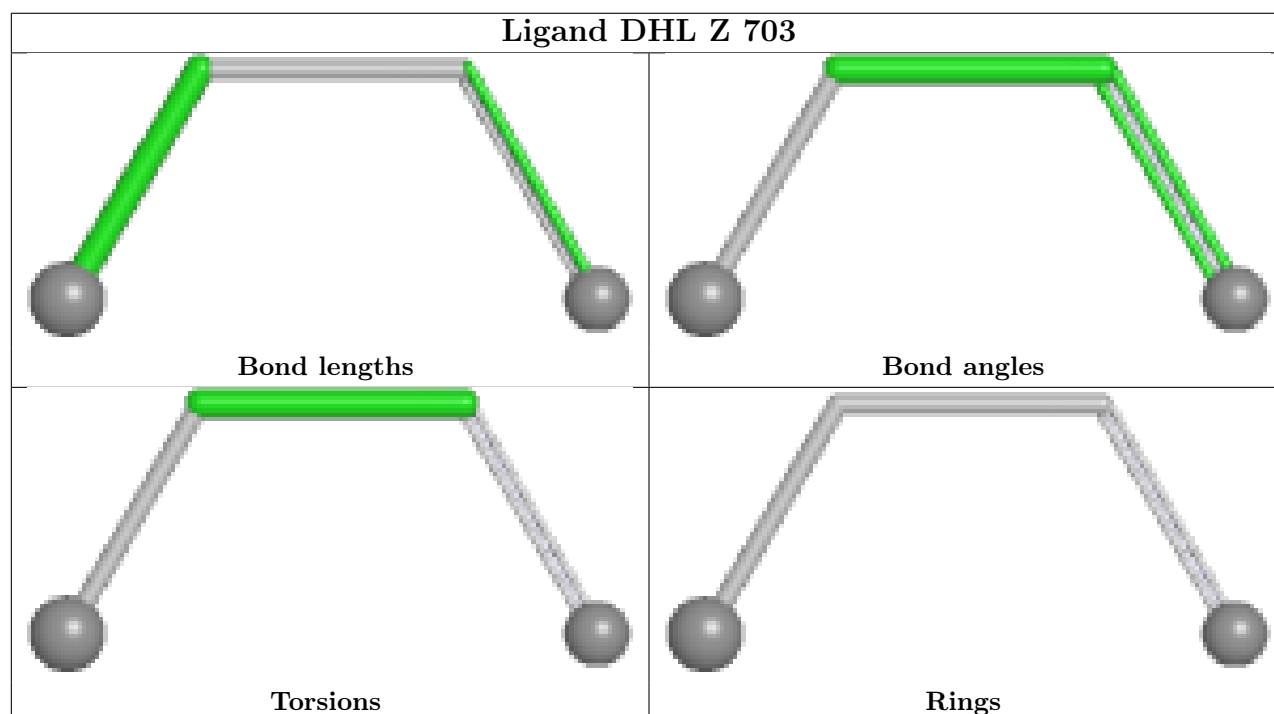
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	701	EDO	2	0
6	B	703	PEG	3	0
5	C	701	GOL	1	0

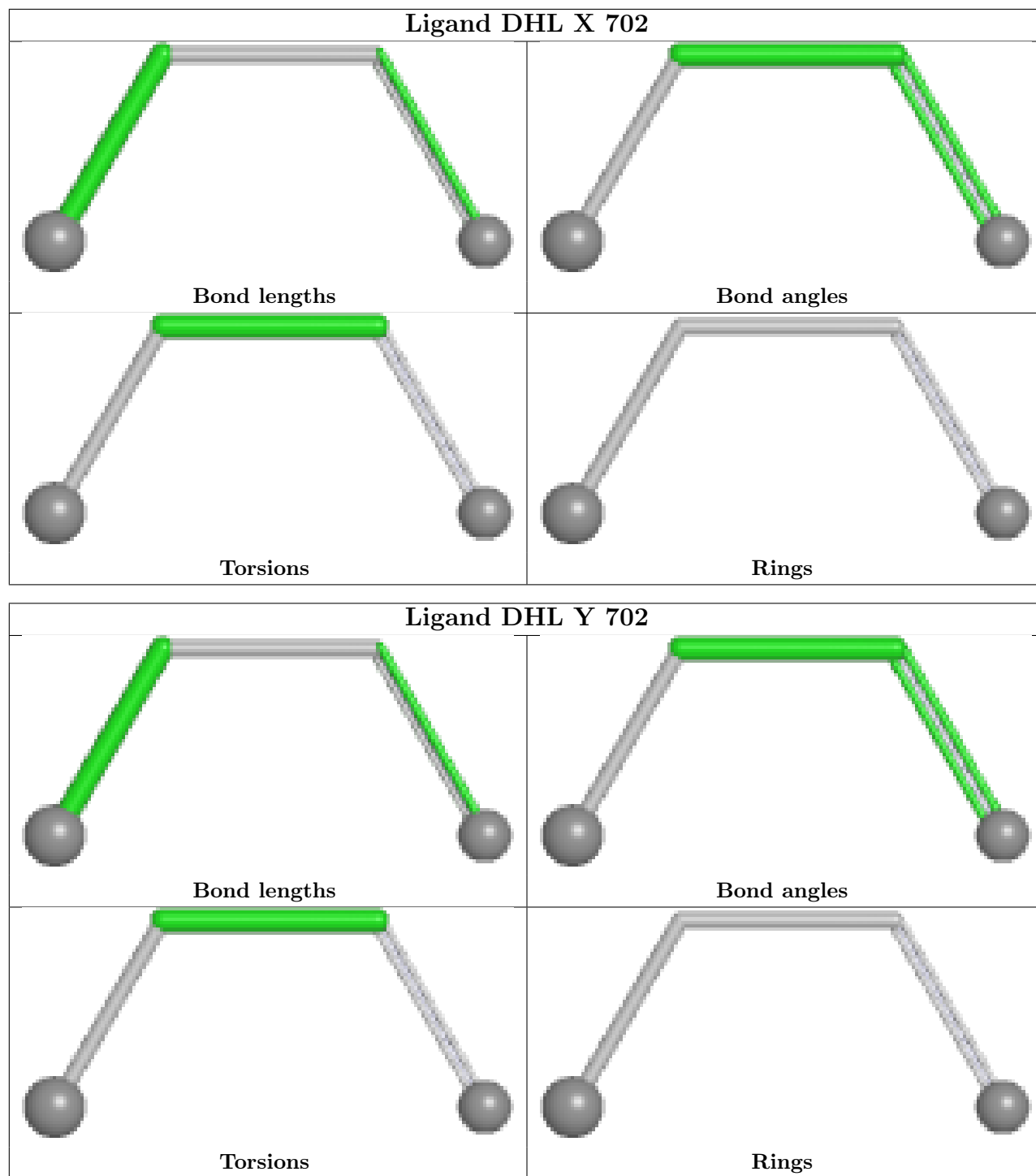
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	704	PEG	1	0
5	A	701	GOL	1	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	283/290 (97%)	-0.27	1 (0%) 88 90	8, 17, 41, 61	1 (0%)
2	B	284/290 (97%)	-0.31	1 (0%) 88 90	8, 17, 38, 55	1 (0%)
3	A	284/290 (97%)	-0.44	2 (0%) 84 86	5, 15, 34, 48	2 (0%)
4	X	1/4 (25%)	-0.95	0 100 100	12, 12, 12, 12	0
4	Y	1/4 (25%)	-0.95	0 100 100	12, 12, 12, 12	0
4	Z	1/4 (25%)	-0.84	0 100 100	13, 13, 13, 13	0
All	All	854/882 (96%)	-0.34	4 (0%) 87 89	5, 16, 38, 61	4 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	385	ASP	3.6
3	A	325	GLY	2.4
1	C	386	GLY	2.3
2	B	348	SER	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CSO	B	518	7/8	0.93	0.07	14,24,30,43	0
1	CSO	C	583	7/8	0.94	0.08	17,23,30,37	0
1	CSO	C	518	7/8	0.96	0.06	11,21,28,32	0
4	ABA	Z	4	6/7	0.96	0.06	10,14,15,17	0
4	A1JAL	X	2	16/17	0.97	0.04	5,10,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	A1JAL	Z	2	16/17	0.97	0.05	8,12,16,16	0
4	ABA	Y	4	6/7	0.97	0.04	14,18,22,22	0
3	CME	A	583	10/11	0.97	0.07	13,21,62,74	0
4	A1JAL	Y	2	16/17	0.98	0.04	7,10,13,13	0
4	ABA	X	4	6/7	0.98	0.04	9,13,16,17	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

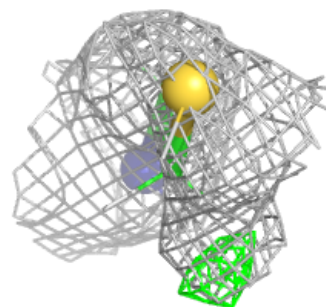
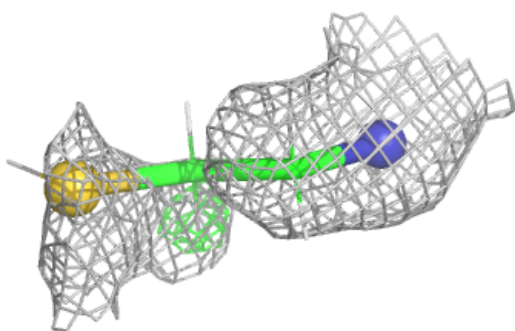
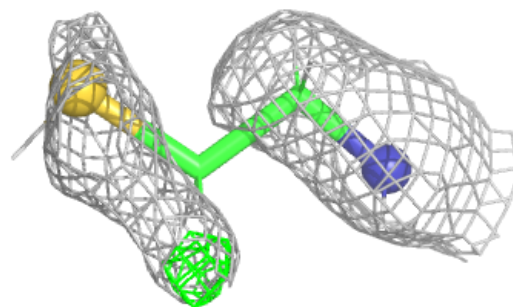
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PEG	A	704	7/7	0.74	0.17	36,50,60,67	0
6	PEG	C	702	7/7	0.76	0.15	36,49,65,65	0
8	EDO	Z	701	4/4	0.83	0.14	31,39,45,50	0
5	GOL	A	701	6/6	0.86	0.11	25,35,43,51	0
6	PEG	B	703	7/7	0.86	0.13	24,37,48,54	0
10	DHL	X	702	4/4	0.86	0.14	19,29,65,78	0
8	EDO	B	701	4/4	0.88	0.16	30,37,44,51	0
10	DHL	Y	702	4/4	0.88	0.12	16,25,77,92	0
10	DHL	Z	703	4/4	0.90	0.13	13,25,72,87	0
5	GOL	A	703	6/6	0.91	0.11	16,31,49,56	0
5	GOL	C	701	6/6	0.93	0.10	16,23,30,35	0
5	GOL	B	702	6/6	0.95	0.11	16,25,39,39	0
7	MG	B	704	1/1	0.96	0.05	15,15,15,15	0
7	MG	A	706	1/1	0.97	0.06	35,35,35,35	0
5	GOL	A	702	6/6	0.97	0.06	12,16,21,21	0
7	MG	C	703	1/1	0.98	0.03	14,14,14,14	0
7	MG	A	705	1/1	0.98	0.03	12,12,12,12	0
9	CL	Y	701	1/1	0.99	0.03	12,12,12,12	0
9	CL	Z	702	1/1	1.00	0.02	11,11,11,11	0
9	CL	X	701	1/1	1.00	0.01	10,10,10,10	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 DHL X 702:**

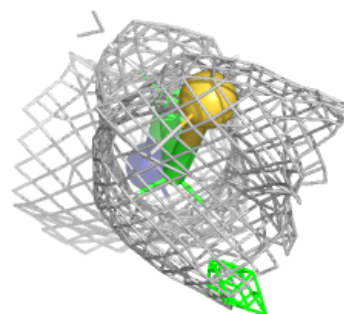
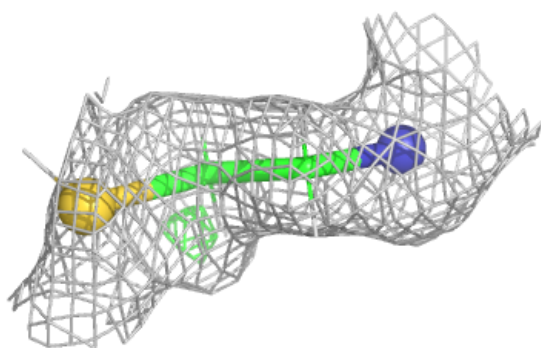
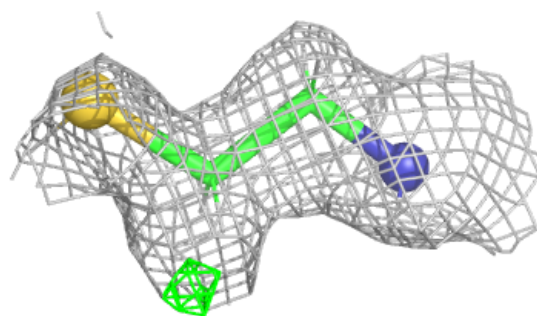
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



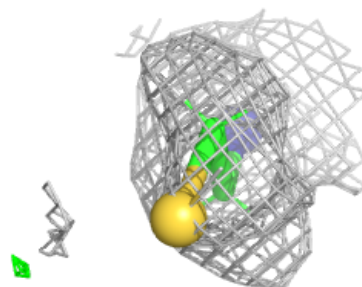
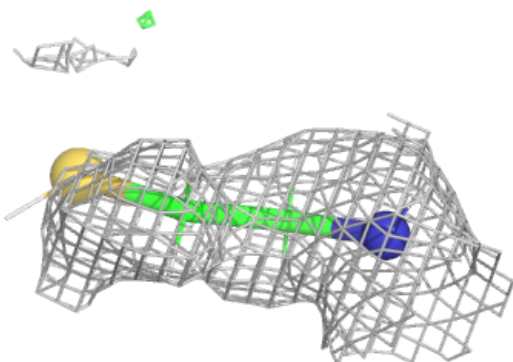
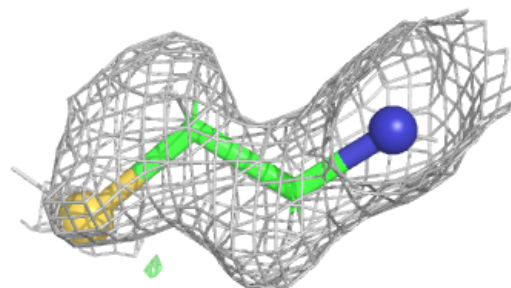


**Electron density around DHL Y 702:**

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

**Electron density around DHL Z 703:**

$2mF_o-DF_c$  (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.