



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 17, 2023 – 06:11 pm GMT

PDB ID : 4AQ6  
Title : substrate bound homogentisate 1,2-dioxygenase  
Authors : Jeoung, J.-H.; Lin, T.-Y.; Bommer, M.; Dobbek, H.  
Deposited on : 2012-04-12  
Resolution : 1.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467  
Mogul : 1.8.4, 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

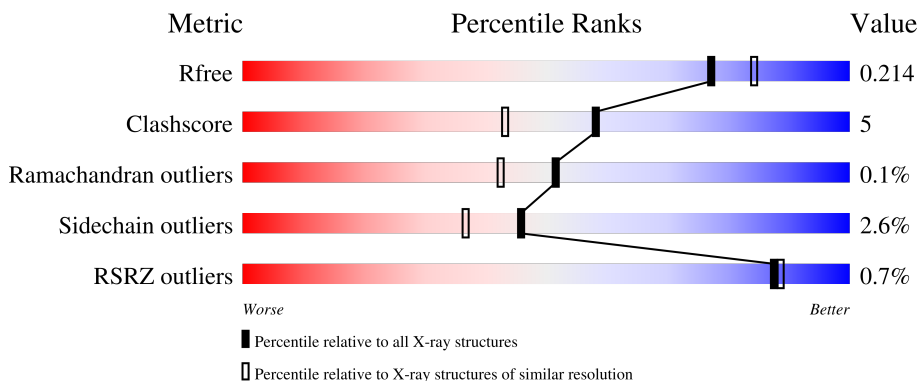
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	A	433	89% 9% .
1	B	433	88% 10% .
1	C	433	87% 10% ..
1	D	433	87% 10% ..
1	E	433	87% 11% ..

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Mol	Chain	Length	Quality of chain
1	F	433	 88% 10% .
1	G	433	 83% 14% ..
1	H	433	 86% 11% ..
1	I	433	 83% 15% .
1	J	433	 87% 11% .
1	K	433	 87% 11% .
1	L	433	 88% 9% ..

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 44389 atoms, of which 28 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 HOMOGENITISATE 1,2-DIOXYGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	425	3311	2115	2	580	597	17	0	1	0
1	B	425	3300	2110		580	593	17	0	1	0
1	C	425	3298	2109		576	596	17	0	0	0
1	D	427	3313	2117		579	600	17	0	1	0
1	E	426	3301	2111		577	596	17	0	1	0
1	F	425	3302	2112	1	578	594	17	0	1	0
1	G	425	3286	2102	2	574	591	17	0	0	0
1	H	425	3282	2101		578	586	17	0	0	0
1	I	426	3320	2121		585	597	17	0	1	0
1	J	425	3298	2111		578	592	17	0	1	0
1	K	426	3292	2106		576	593	17	0	0	0
1	L	425	3277	2098	1	575	586	17	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

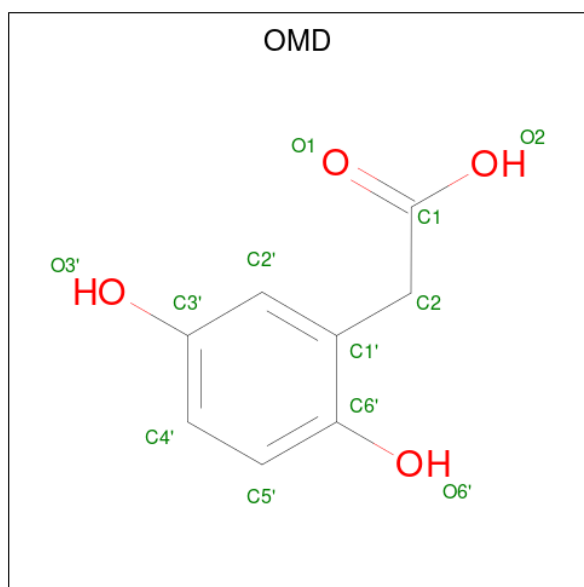
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0
2	I	1	Total Fe 1 1	0	0
2	J	1	Total Fe 1 1	0	0
2	K	1	Total Fe 1 1	0	0
2	L	1	Total Fe 1 1	0	0

- Molecule 3 is 2-(3,6-DIHYDROXYPHENYL)ACETIC ACID (three-letter code: OMD) (formula: C<sub>8</sub>H<sub>8</sub>O<sub>4</sub>).



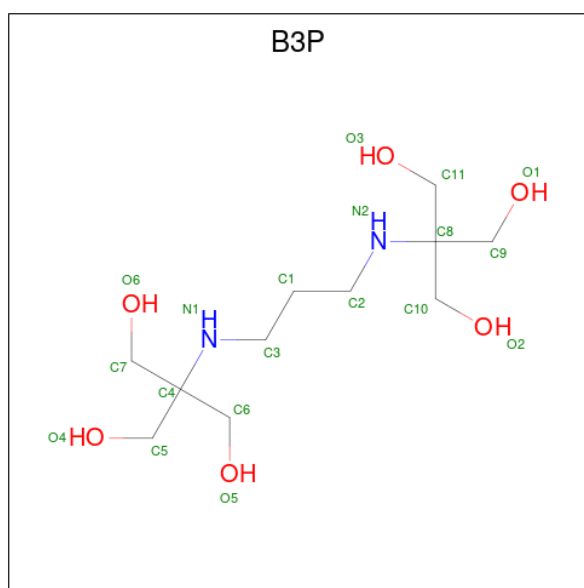
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 8 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 12 8 4	0	0
3	C	1	Total C O 12 8 4	0	0
3	D	1	Total C O 12 8 4	0	0
3	E	1	Total C O 12 8 4	0	0
3	F	1	Total C O 12 8 4	0	0
3	G	1	Total C O 12 8 4	0	0
3	H	1	Total C O 12 8 4	0	0
3	I	1	Total C O 12 8 4	0	0
3	J	1	Total C O 12 8 4	0	0
3	K	1	Total C O 12 8 4	0	0
3	L	1	Total C O 12 8 4	0	0

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:  $C_{11}H_{26}N_2O_6$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	K	1	41	11	22	2	6	0	0

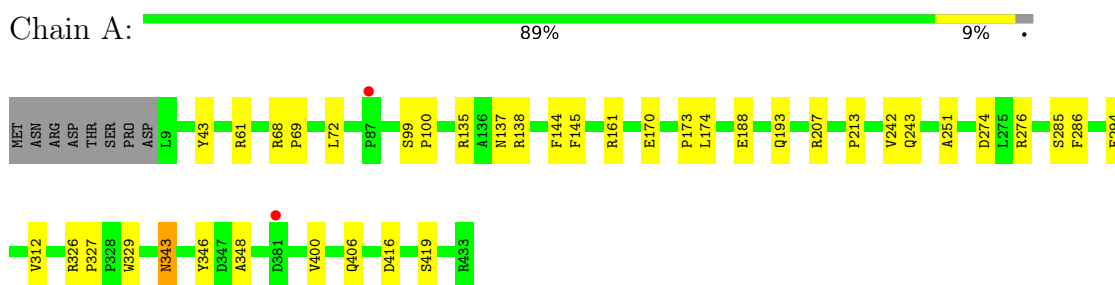
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	482	Total 488	O 488	0	6
5	B	424	Total 425	O 425	0	1
5	C	377	Total 384	O 384	0	7
5	D	439	Total 441	O 441	0	2
5	E	398	Total 401	O 401	0	3
5	F	333	Total 336	O 336	0	3
5	G	378	Total 379	O 379	0	1
5	H	365	Total 369	O 369	0	4
5	I	338	Total 340	O 340	0	2
5	J	350	Total 352	O 352	0	2
5	K	368	Total 368	O 368	0	0
5	L	328	Total 329	O 329	0	1

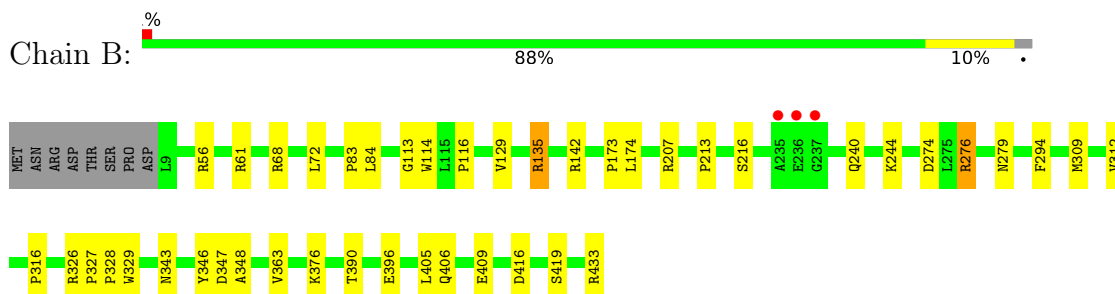
### 3 Residue-property plots [i](#)

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.

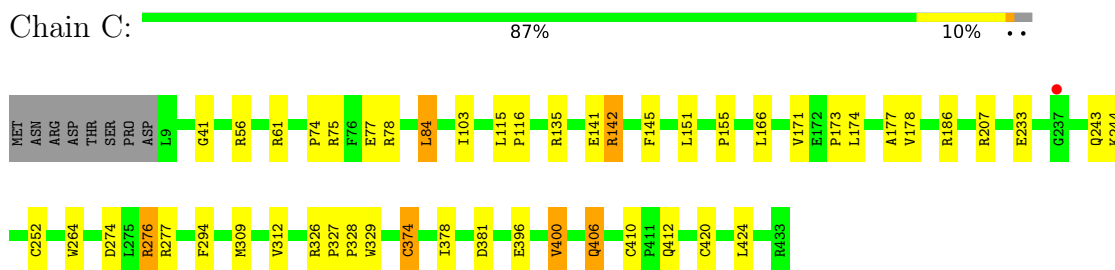
- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



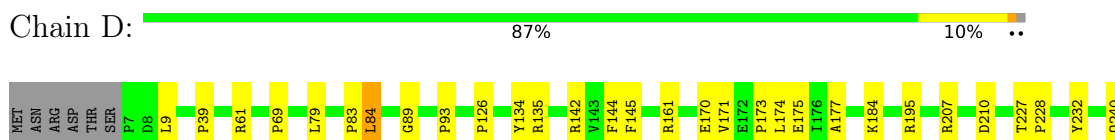
- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



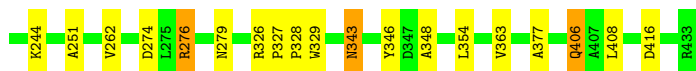
- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



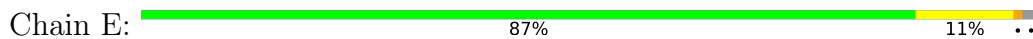
- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



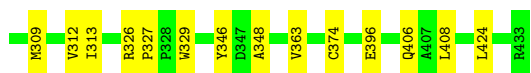
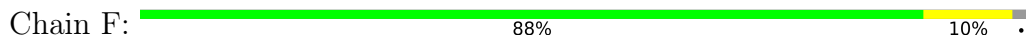




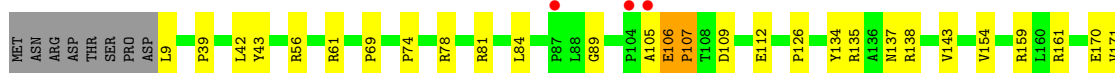
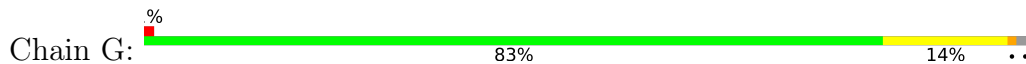
- Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



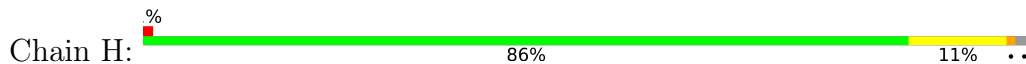
- Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



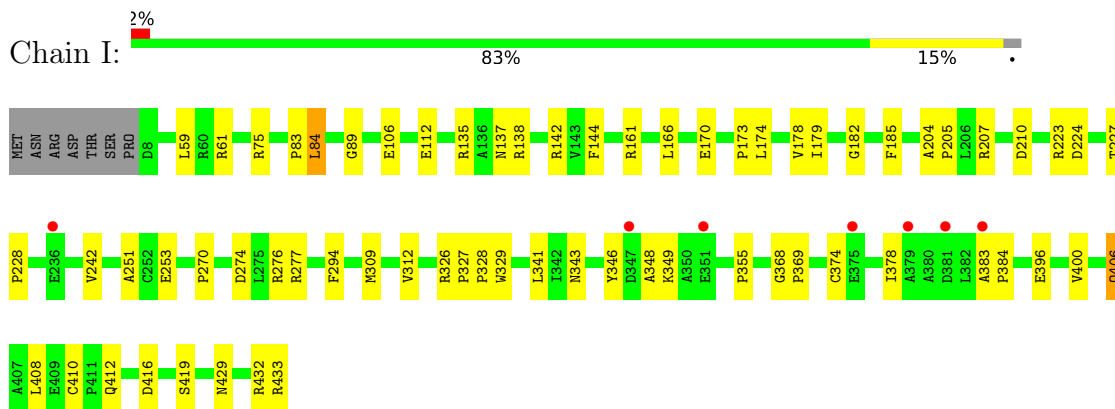
- Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



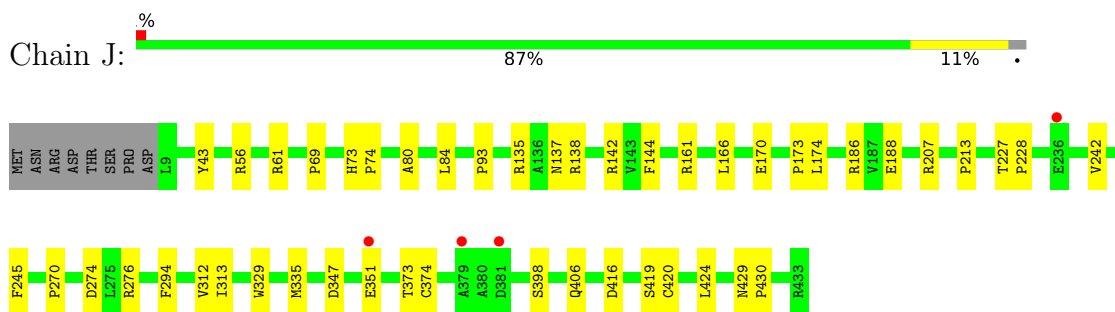
- Molecule 1: HOMOGENTISATE 1,2-DIOXYGENASE



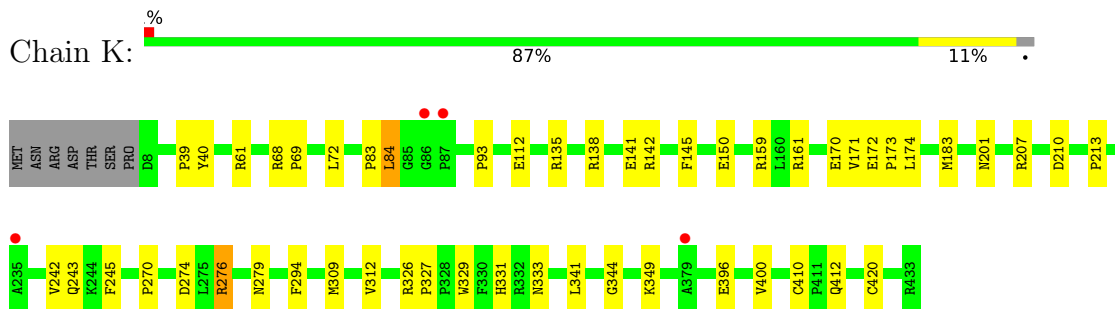
- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



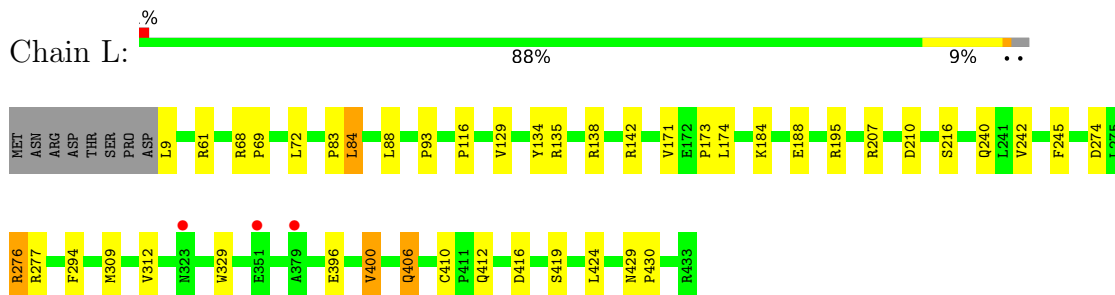
- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



- Molecule 1: HOMOGENITISATE 1,2-DIOXYGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.39Å 93.71Å 162.98Å 87.69° 80.42° 68.39°	Depositor
Resolution (Å)	34.17 – 1.98 34.17 – 1.98	Depositor EDS
% Data completeness (in resolution range)	95.6 (34.17-1.98) 95.6 (34.17-1.98)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 1.98Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.161 , 0.216 0.160 , 0.214	Depositor DCC
$R_{free}$ test set	16870 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.3	Xtrriage
Anisotropy	0.366	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	44389	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: B3P, OMD, FE

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	0.39	0/3411	0.55	0/4653
1	B	0.38	0/3401	0.53	0/4640
1	C	0.38	0/3399	0.54	0/4637
1	D	0.39	0/3416	0.55	0/4662
1	E	0.39	0/3403	0.55	0/4645
1	F	0.39	0/3403	0.54	0/4643
1	G	0.34	0/3385	0.51	0/4620
1	H	0.35	0/3384	0.51	0/4619
1	I	0.35	0/3422	0.51	0/4667
1	J	0.34	0/3400	0.51	0/4639
1	K	0.36	0/3394	0.53	0/4633
1	L	0.37	0/3378	0.53	0/4612
All	All	0.37	0/40796	0.53	0/55670

There are no bond length outliers.

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	A	3309	2	3196	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3300	0	3182	30	0
1	C	3298	0	3180	32	0
1	D	3313	0	3187	32	0
1	E	3301	0	3174	34	0
1	F	3301	1	3187	23	0
1	G	3284	2	3159	49	0
1	H	3282	0	3168	33	0
1	I	3320	0	3211	48	0
1	J	3298	0	3185	26	0
1	K	3292	0	3169	28	0
1	L	3276	1	3157	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	12	0	6	0	0
3	B	12	0	6	0	0
3	C	12	0	6	1	0
3	D	12	0	6	1	0
3	E	12	0	6	0	0
3	F	12	0	6	0	0
3	G	12	0	6	0	0
3	H	12	0	6	1	0
3	I	12	0	6	0	0
3	J	12	0	6	0	0
3	K	12	0	6	0	0
3	L	12	0	6	0	0
4	K	19	22	25	1	0
5	A	488	0	0	2	0
5	B	425	0	0	9	2
5	C	384	0	0	5	1
5	D	441	0	0	9	0
5	E	401	0	0	6	0
5	F	336	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	379	0	0	7	0
5	H	369	0	0	7	0
5	I	340	0	0	8	0
5	J	352	0	0	5	1
5	K	368	0	0	2	0
5	L	329	0	0	4	0
All	All	44361	28	38252	372	2

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 5.

The worst 5 of 372 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:C:56:ARG:CB	1:C:56:ARG:CD	2.48	0.91
1:B:56:ARG:CD	1:B:56:ARG:CB	2.50	0.90
1:G:56:ARG:CD	1:G:56:ARG:CB	2.51	0.88
1:G:106:GLU:HB3	1:G:107:PRO:HD3	1.55	0.87
1:G:106:GLU:CB	1:G:107:PRO:HD3	2.05	0.85

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2385:HOH:O	5:C:2379:HOH:O[1_565]	2.15	0.05
5:B:2401:HOH:O	5:J:2101:HOH:O[1_466]	2.16	0.04

## 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	424/433 (98%)	410 (97%)	14 (3%)	0	100	100
1	B	424/433 (98%)	411 (97%)	12 (3%)	1 (0%)	47	38
1	C	423/433 (98%)	408 (96%)	14 (3%)	1 (0%)	47	38
1	D	426/433 (98%)	414 (97%)	11 (3%)	1 (0%)	47	38
1	E	425/433 (98%)	414 (97%)	11 (3%)	0	100	100
1	F	424/433 (98%)	409 (96%)	14 (3%)	1 (0%)	47	38
1	G	423/433 (98%)	402 (95%)	19 (4%)	2 (0%)	29	16
1	H	423/433 (98%)	405 (96%)	18 (4%)	0	100	100
1	I	425/433 (98%)	410 (96%)	15 (4%)	0	100	100
1	J	424/433 (98%)	412 (97%)	12 (3%)	0	100	100
1	K	424/433 (98%)	412 (97%)	12 (3%)	0	100	100
1	L	423/433 (98%)	408 (96%)	15 (4%)	0	100	100
All	All	5088/5196 (98%)	4915 (97%)	167 (3%)	6 (0%)	51	42

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	106	GLU
1	C	142	ARG
1	G	107	PRO
1	B	363	VAL
1	D	363	VAL

### 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	342/355 (96%)	336 (98%)	6 (2%)	59	51
1	B	339/355 (96%)	333 (98%)	6 (2%)	59	51
1	C	340/355 (96%)	329 (97%)	11 (3%)	39	28
1	D	342/355 (96%)	331 (97%)	11 (3%)	39	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	339/355 (96%)	330 (97%)	9 (3%)	44	35
1	F	340/355 (96%)	333 (98%)	7 (2%)	53	47
1	G	336/355 (95%)	323 (96%)	13 (4%)	32	19
1	H	336/355 (95%)	326 (97%)	10 (3%)	41	29
1	I	343/355 (97%)	334 (97%)	9 (3%)	46	37
1	J	339/355 (96%)	330 (97%)	9 (3%)	44	35
1	K	338/355 (95%)	328 (97%)	10 (3%)	41	29
1	L	335/355 (94%)	326 (97%)	9 (3%)	44	35
All	All	4069/4260 (96%)	3959 (97%)	110 (3%)	46	35

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	329	TRP
1	H	406	GLN
1	L	406	GLN
1	K	400	VAL
1	G	374	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	101	GLN
1	H	304	HIS
1	L	343	ASN
1	J	101	GLN
1	K	304	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 12 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
3	OMD	J	838	2	12,12,12	0.76	0	16,16,16	0.84	0
3	OMD	F	838	2	12,12,12	0.83	0	16,16,16	0.83	0
3	OMD	B	838	2	12,12,12	0.63	0	16,16,16	0.84	0
3	OMD	E	838	2	12,12,12	0.79	0	16,16,16	1.02	1 (6%)
3	OMD	G	838	2	12,12,12	0.67	0	16,16,16	0.80	0
4	B3P	K	1436	-	18,18,18	1.28	3 (16%)	21,23,23	0.87	0
3	OMD	I	838	2	12,12,12	0.67	0	16,16,16	0.69	0
3	OMD	K	838	2	12,12,12	0.65	0	16,16,16	0.87	0
3	OMD	H	838	2	12,12,12	0.77	0	16,16,16	0.87	0
3	OMD	D	838	2	12,12,12	0.81	0	16,16,16	0.83	0
3	OMD	L	838	2	12,12,12	0.78	0	16,16,16	1.05	1 (6%)
3	OMD	C	838	2	12,12,12	0.83	0	16,16,16	1.00	1 (6%)
3	OMD	A	838	2	12,12,12	0.86	0	16,16,16	1.12	2 (12%)

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
3	OMD	J	838	2	-	0/4/4/4	0/1/1/1
3	OMD	F	838	2	-	0/4/4/4	0/1/1/1
3	OMD	B	838	2	-	0/4/4/4	0/1/1/1
3	OMD	E	838	2	-	0/4/4/4	0/1/1/1
3	OMD	G	838	2	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	B3P	K	1436	-	-	4/28/28/28	-
3	OMD	I	838	2	-	0/4/4/4	0/1/1/1
3	OMD	K	838	2	-	0/4/4/4	0/1/1/1
3	OMD	H	838	2	-	0/4/4/4	0/1/1/1
3	OMD	D	838	2	-	0/4/4/4	0/1/1/1
3	OMD	L	838	2	-	0/4/4/4	0/1/1/1
3	OMD	C	838	2	-	0/4/4/4	0/1/1/1
3	OMD	A	838	2	-	0/4/4/4	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1436	B3P	C2-N2	3.23	1.50	1.46
4	K	1436	B3P	C7-C4	2.50	1.56	1.53
4	K	1436	B3P	O3-C11	-2.02	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	838	OMD	C2-C1'-C6'	-2.35	118.28	120.88
3	C	838	OMD	C2-C1'-C6'	-2.23	118.41	120.88
3	A	838	OMD	C2-C1'-C6'	-2.08	118.58	120.88
3	A	838	OMD	C2'-C1'-C6'	2.02	120.59	118.17
3	L	838	OMD	O2-C1-C2	2.01	121.64	114.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	1436	B3P	C3-C1-C2-N2
4	K	1436	B3P	N2-C8-C9-O1
4	K	1436	B3P	C11-C8-C9-O1
4	K	1436	B3P	C10-C8-C9-O1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

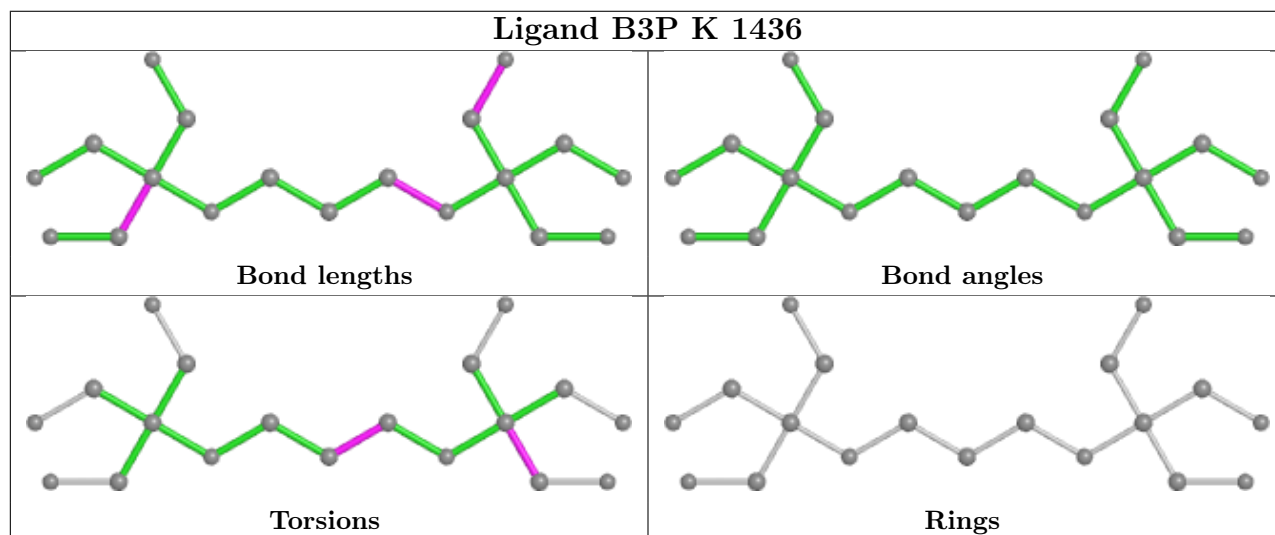
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1436	B3P	1	0
3	H	838	OMD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	838	OMD	1	0
3	C	838	OMD	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	A	425/433 (98%)	-0.47	2 (0%) 91 91	9, 16, 30, 41	0
1	B	425/433 (98%)	-0.44	3 (0%) 87 88	11, 18, 31, 52	0
1	C	425/433 (98%)	-0.44	1 (0%) 95 95	10, 17, 30, 52	5 (1%)
1	D	427/433 (98%)	-0.45	0 100 100	10, 17, 29, 48	0
1	E	426/433 (98%)	-0.43	2 (0%) 91 91	11, 17, 31, 51	1 (0%)
1	F	425/433 (98%)	-0.41	0 100 100	10, 18, 30, 57	0
1	G	425/433 (98%)	-0.16	5 (1%) 79 80	15, 24, 38, 63	2 (0%)
1	H	425/433 (98%)	-0.24	3 (0%) 87 88	14, 22, 37, 53	0
1	I	426/433 (98%)	-0.22	7 (1%) 72 73	14, 23, 37, 56	0
1	J	425/433 (98%)	-0.30	4 (0%) 84 85	14, 23, 38, 60	0
1	K	426/433 (98%)	-0.35	4 (0%) 84 85	11, 19, 33, 55	0
1	L	425/433 (98%)	-0.34	3 (0%) 87 88	13, 20, 35, 53	0
All	All	5105/5196 (98%)	-0.35	34 (0%) 87 88	9, 19, 35, 63	8 (0%)

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	105	ALA	5.0
1	K	86	GLY	4.2
1	H	379	ALA	4.0
1	G	235	ALA	4.0
1	K	235	ALA	3.8

### 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](#)

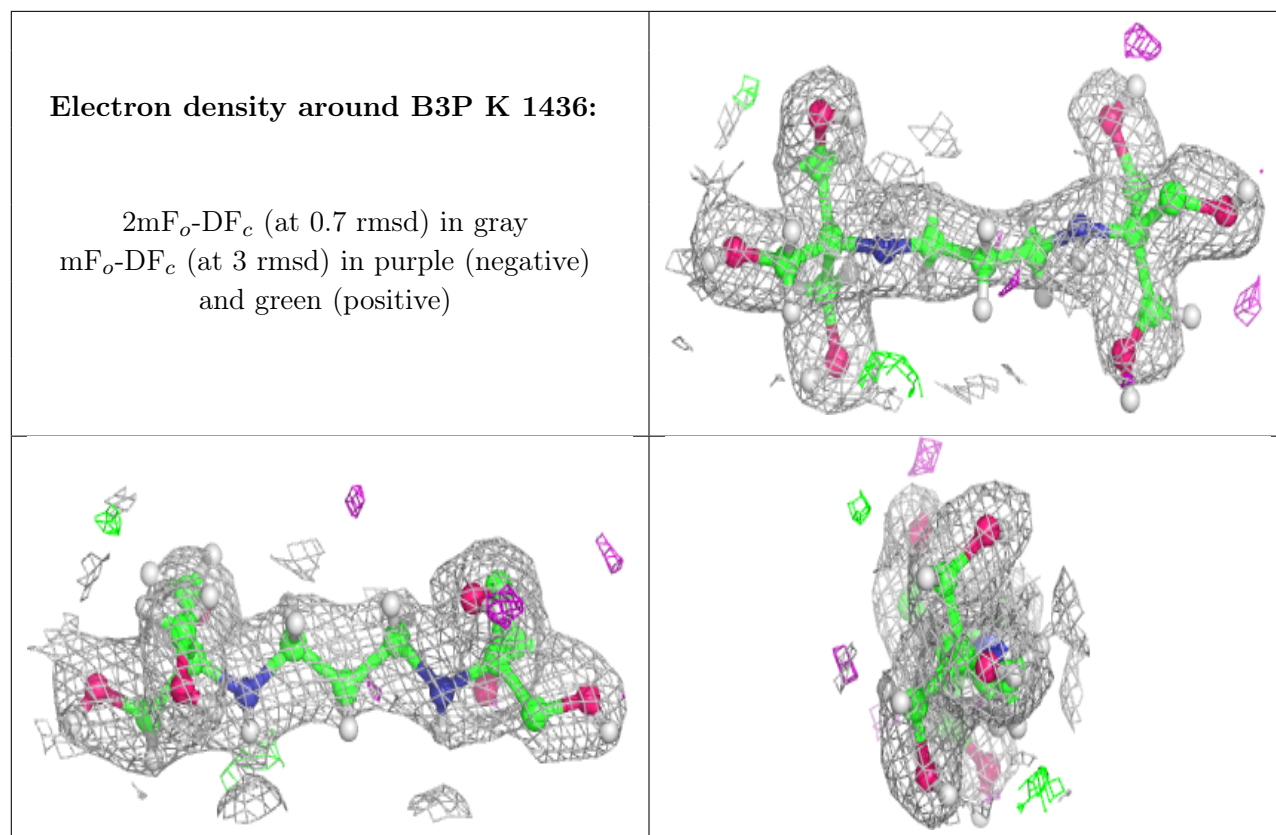
There are no monosaccharides in this entry.

### 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<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
4	B3P	K	1436	19/19	0.94	0.14	18,26,33,39	0
3	OMD	L	838	12/12	0.95	0.13	18,23,24,30	0
3	OMD	D	838	12/12	0.96	0.14	12,17,19,22	0
3	OMD	F	838	12/12	0.96	0.12	13,17,18,20	0
3	OMD	G	838	12/12	0.96	0.13	17,19,23,24	0
3	OMD	J	838	12/12	0.96	0.15	18,23,25,26	12
3	OMD	A	838	12/12	0.96	0.12	8,12,15,16	0
3	OMD	C	838	12/12	0.96	0.12	9,14,16,17	12
3	OMD	H	838	12/12	0.97	0.12	18,21,24,26	0
3	OMD	E	838	12/12	0.97	0.09	11,13,15,18	0
3	OMD	K	838	12/12	0.98	0.12	15,17,20,20	0
3	OMD	I	838	12/12	0.98	0.11	20,24,26,28	0
3	OMD	B	838	12/12	0.98	0.10	13,16,18,18	0
2	FE	F	837	1/1	0.99	0.09	13,13,13,13	0
2	FE	D	837	1/1	1.00	0.07	11,11,11,11	0
2	FE	E	837	1/1	1.00	0.06	13,13,13,13	0
2	FE	A	837	1/1	1.00	0.08	11,11,11,11	0
2	FE	G	837	1/1	1.00	0.07	16,16,16,16	0
2	FE	H	837	1/1	1.00	0.07	17,17,17,17	0
2	FE	I	837	1/1	1.00	0.07	18,18,18,18	0
2	FE	J	837	1/1	1.00	0.06	16,16,16,16	0
2	FE	K	837	1/1	1.00	0.08	15,15,15,15	0
2	FE	L	837	1/1	1.00	0.07	14,14,14,14	0
2	FE	B	837	1/1	1.00	0.07	12,12,12,12	0
2	FE	C	837	1/1	1.00	0.08	11,11,11,11	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.