



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 6, 2024 – 09:22 AM EDT

PDB ID : 1KEK
Title : Crystal Structure of the Free Radical Intermediate of Pyruvate:Ferredoxin Oxidoreductase
Authors : Chabriere, E.; Vernede, X.; Guigliarelli, B.; Charon, M.-H.; Hatchikian, E.C.; Fontecilla-Camps, J.C.
Deposited on : 2001-11-16
Resolution : 1.90 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

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	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

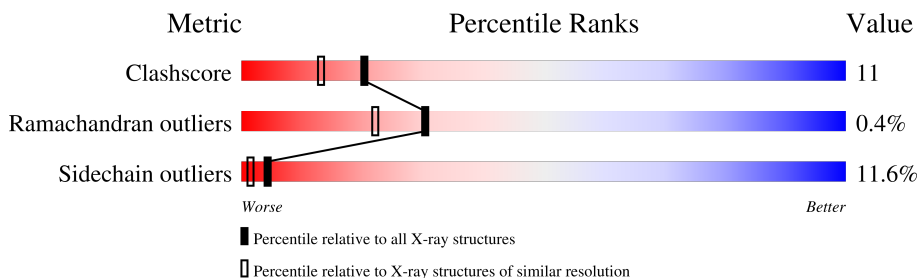
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1231	 70% 23% 5% •
1	B	1231	 73% 21% • •

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20775 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 Pyruvate-Ferredoxin Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	36	0	0
			9383	5941	1599	1784	59			
1	B	1231	Total	C	N	O	S	41	0	0
			9383	5941	1599	1784	59			

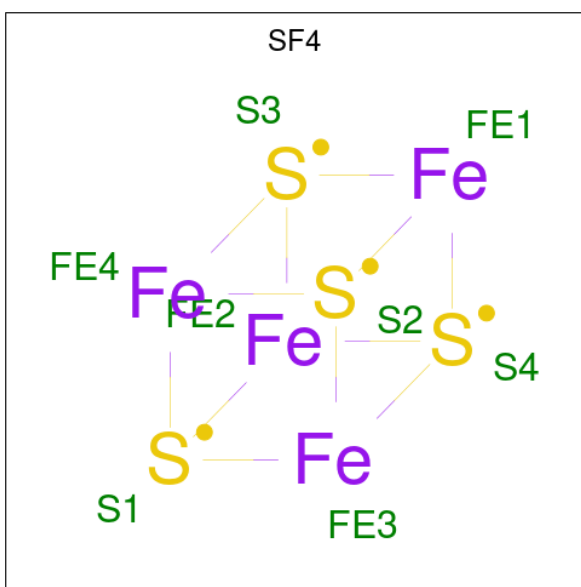
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

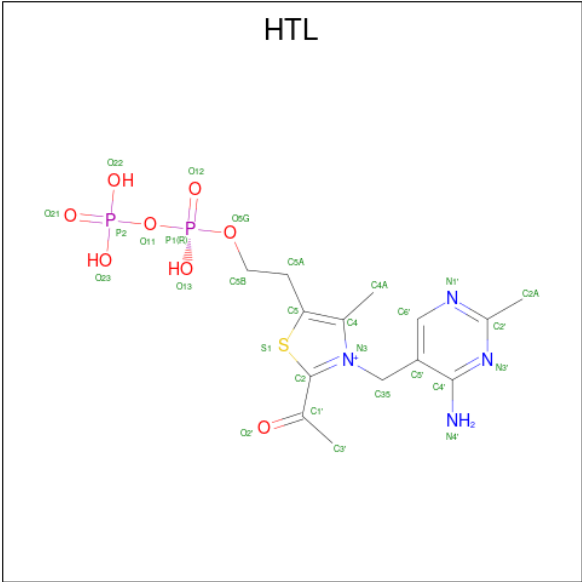
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



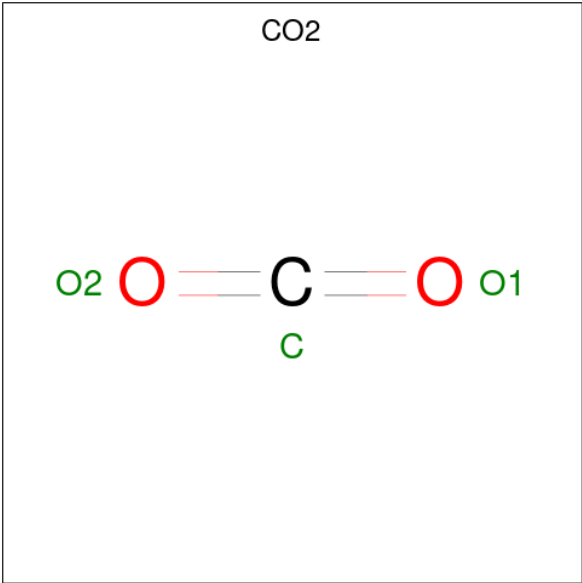
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 2-ACETYL-THIAMINE DIPHOSPHATE (three-letter code: HTL) (formula: $C_{14}H_{21}N_4O_8P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		
5	B	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		

- Molecule 6 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			3	1 2		
6	B	1	Total	C O	0	0
			3	1 2		

- Molecule 7 is water.

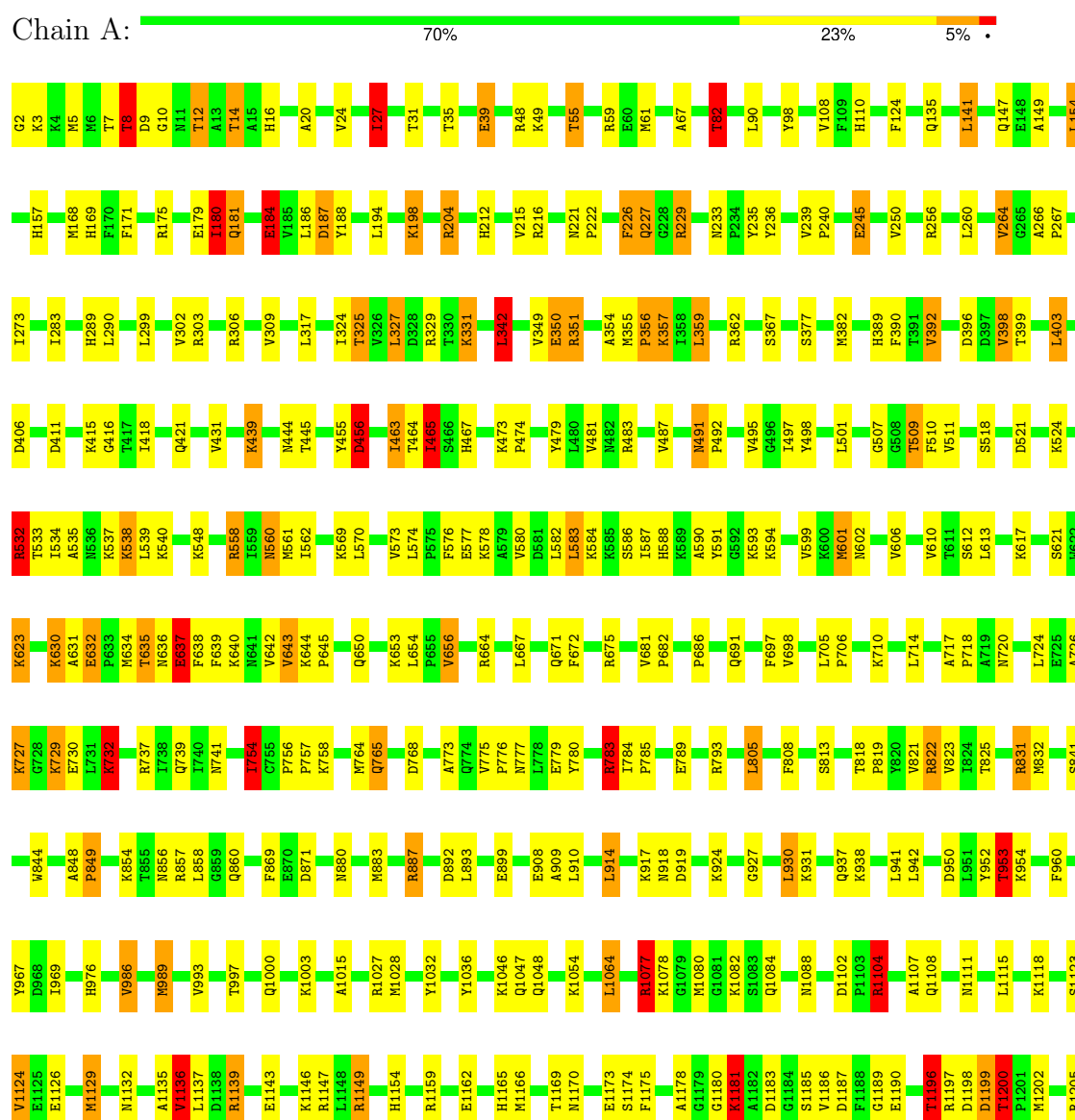
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	851	Total 851	O 851	0	0
7	B	1042	Total 1042	O 1042	0	0

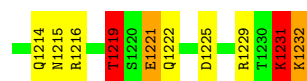
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

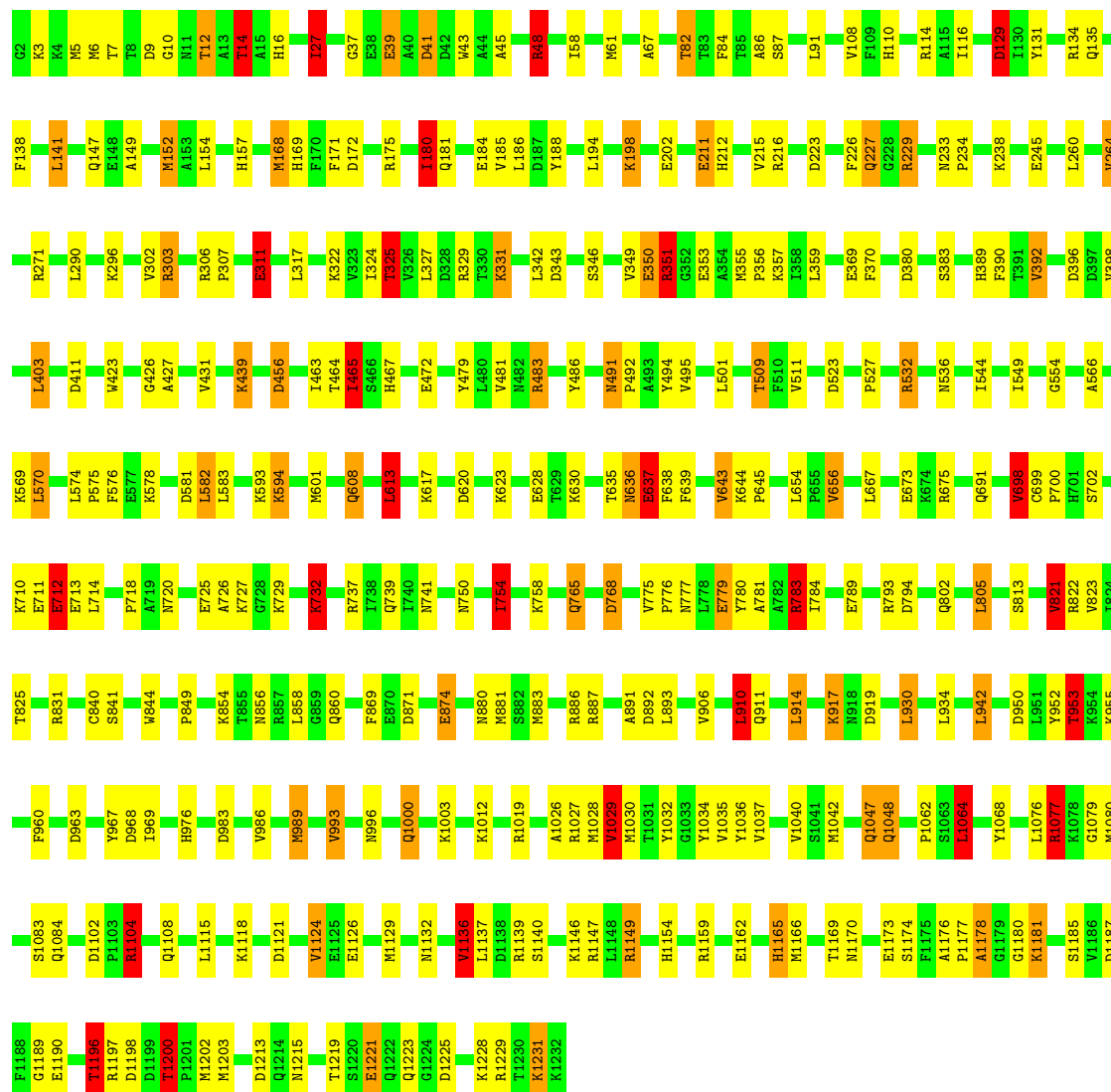
• Molecule 1: Pyruvate-Ferredoxin Oxidoreductase





● Molecule 1: Pyruvate-Ferredoxin Oxidoreductase

Chain B: 73% 21%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.11Å 145.76Å 210.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.38 – 1.90	Depositor
% Data completeness (in resolution range)	97.5 (27.38-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR, REFMAC	Depositor
R, R_{free}	0.178 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20775	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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: HTL, CA, MG, SF4, CO2

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	0.78	10/9585 (0.1%)	1.56	147/12954 (1.1%)
1	B	1.07	14/9585 (0.1%)	1.63	154/12954 (1.2%)
All	All	0.94	24/19170 (0.1%)	1.60	301/25908 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	2	3
All	All	2	5

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	732	LYS	CD-CE	56.96	2.93	1.51
1	B	1231	LYS	C-N	28.83	2.00	1.34
1	B	732	LYS	CG-CD	-20.40	0.83	1.52
1	A	601	MET	C-O	-15.37	0.94	1.23
1	B	711	GLU	C-O	-15.06	0.94	1.23

The worst 5 of 301 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	532	ARG	CD-NE-CZ	35.55	173.37	123.60
1	B	48	ARG	CD-NE-CZ	30.27	165.97	123.60
1	A	204	ARG	CD-NE-CZ	29.99	165.58	123.60
1	A	48	ARG	NE-CZ-NH2	-21.39	109.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ARG	NE-CZ-NH1	21.10	130.85	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	712	GLU	CA
1	B	732	LYS	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	532	ARG	Mainchain
1	A	637	GLU	Mainchain
1	B	1029	VAL	Mainchain
1	B	129	ASP	Mainchain
1	B	712	GLU	Mainchain

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	9383	0	9263	237	0
1	B	9383	0	9261	203	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	24	0	0	0	0
4	B	24	0	0	0	0
5	A	29	0	18	3	0
5	B	29	0	18	2	0
6	A	3	0	0	1	0
6	B	3	0	0	1	0
7	A	851	0	0	37	0
7	B	1042	0	0	31	0
All	All	20775	0	18560	414	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 414 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)
5:B:3236:HTL:C2	5:B:3236:HTL:C1'	1.94	1.43
5:A:2236:HTL:C2	5:A:2236:HTL:C1'	1.97	1.39
1:A:635:THR:HG22	1:A:640:LYS:HE2	1.34	1.05
1:A:1219:THR:HG22	1:A:1222:GLN:H	1.23	0.98
1:A:892:ASP:HB3	7:A:2415:HOH:O	1.70	0.90

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	1229/1231 (100%)	1181 (96%)	42 (3%)	6 (0%)	25	17
1	B	1229/1231 (100%)	1191 (97%)	33 (3%)	5 (0%)	30	22
All	All	2458/2462 (100%)	2372 (96%)	75 (3%)	11 (0%)	30	22

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	LYS
1	B	732	LYS
1	B	1178	ALA
1	A	732	LYS
1	A	1178	ALA

5.3.2 Protein sidechains ⓘ

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	978/978 (100%)	856 (88%)	122 (12%)	3	1
1	B	978/978 (100%)	873 (89%)	105 (11%)	5	2
All	All	1956/1956 (100%)	1729 (88%)	227 (12%)	4	1

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1183	ASP
1	B	1170	ASN
1	B	311	GLU
1	B	1140	SER
1	B	880	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	212	HIS
1	B	602	ASN
1	B	221	ASN
1	B	434	ASN
1	B	720	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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$
5	HTL	A	2236	2	25,30,30	3.94	13 (52%)	32,45,45	2.15	8 (25%)
5	HTL	B	3236	2	25,30,30	4.08	10 (40%)	32,45,45	1.90	7 (21%)
6	CO2	B	3240	-	2,2,2	0.26	0	1,1,1	0.49	0
4	SF4	B	3234	1	0,12,12	-	-	-		
4	SF4	B	3235	1	0,12,12	-	-	-		
6	CO2	A	2240	-	2,2,2	0.32	0	1,1,1	0.49	0
4	SF4	A	2234	1	0,12,12	-	-	-		
4	SF4	A	2233	1	0,12,12	-	-	-		
4	SF4	B	3233	1	0,12,12	-	-	-		
4	SF4	A	2235	1	0,12,12	-	-	-		

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
5	HTL	A	2236	2	-	4/16/21/21	0/2/2/2
4	SF4	B	3234	1	-	-	0/6/5/5
4	SF4	B	3235	1	-	-	0/6/5/5
4	SF4	A	2234	1	-	-	0/6/5/5
4	SF4	B	3233	1	-	-	0/6/5/5
4	SF4	A	2233	1	-	-	0/6/5/5
5	HTL	B	3236	2	-	2/16/21/21	0/2/2/2
4	SF4	A	2235	1	-	-	0/6/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	3236	HTL	C4'-N3'	11.10	1.49	1.35
5	A	2236	HTL	C4'-N3'	9.02	1.47	1.35
5	A	2236	HTL	C2'-N1'	8.59	1.47	1.34
5	B	3236	HTL	C2'-N1'	8.46	1.47	1.34
5	A	2236	HTL	C5'-C4'	8.43	1.56	1.42

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2236	HTL	C4A-C4-N3	7.10	131.63	122.69
5	B	3236	HTL	C5A-C5-C4	-5.31	110.52	127.05
5	A	2236	HTL	C5A-C5-C4	-4.41	113.32	127.05
5	B	3236	HTL	C4-N3-C2	-4.35	106.21	108.64
5	B	3236	HTL	C2A-C2'-N1'	4.11	121.58	117.20

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2236	HTL	C4-C5-C5A-C5B
5	A	2236	HTL	C5-C5A-C5B-O5G
5	A	2236	HTL	P1-O11-P2-O23
5	B	3236	HTL	P1-O11-P2-O23
5	B	3236	HTL	P1-O11-P2-O21

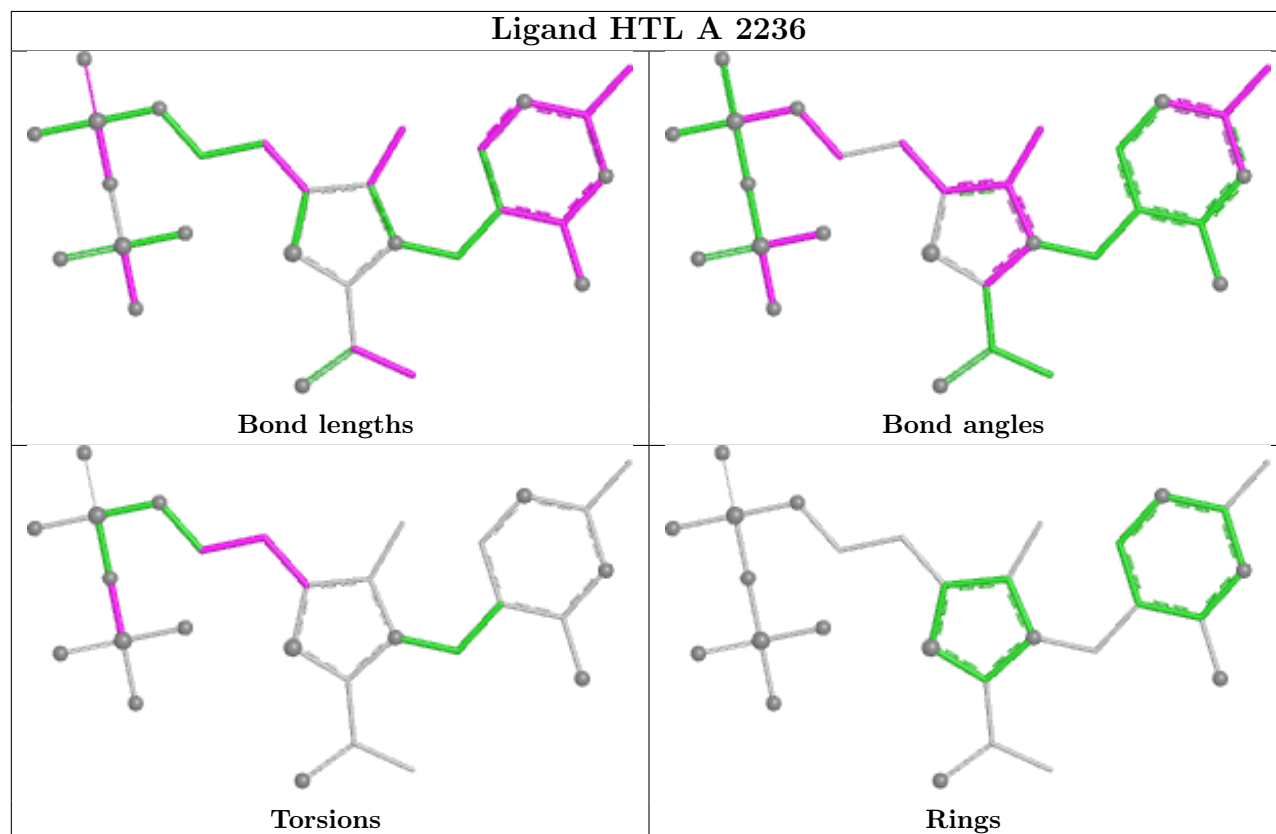
There are no ring outliers.

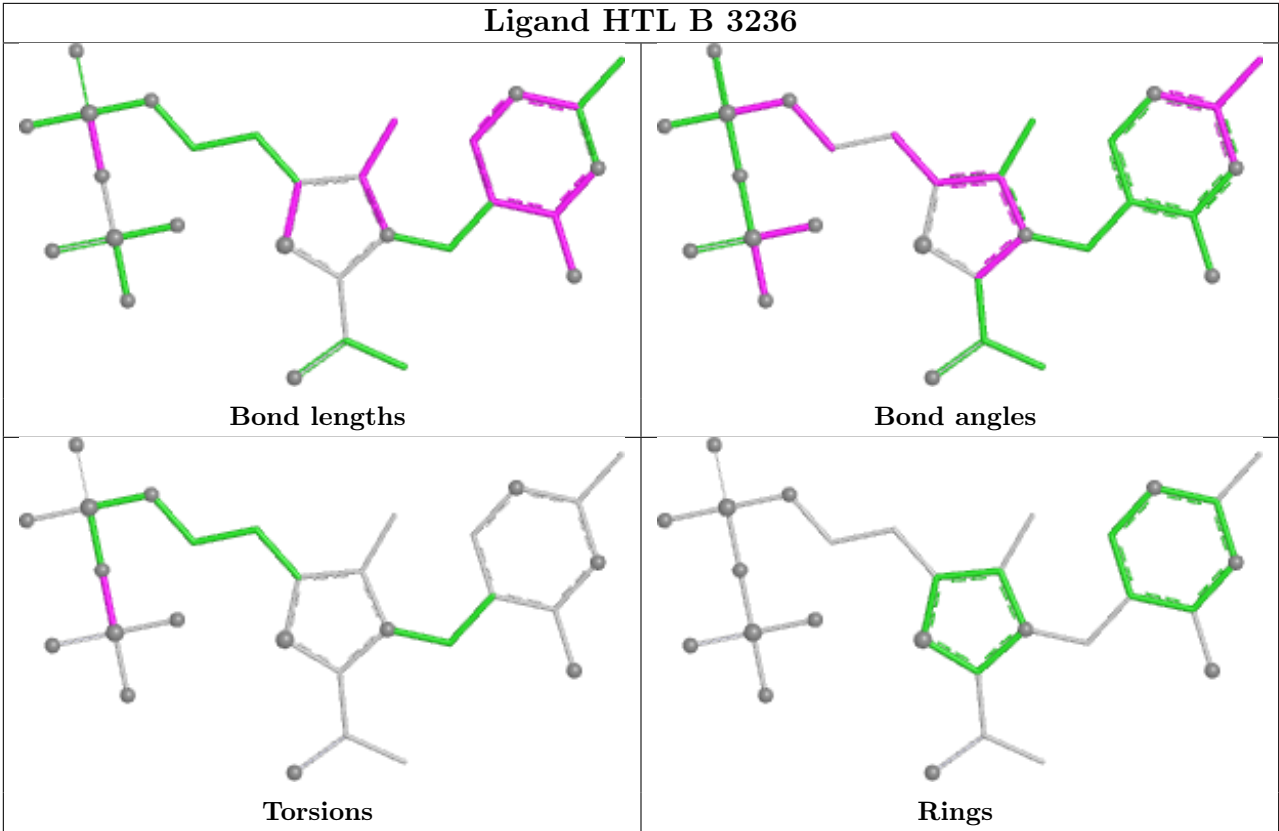
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2236	HTL	3	0
5	B	3236	HTL	2	0
6	B	3240	CO2	1	0
6	A	2240	CO2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1231:LYS	C	1232:LYS	N	2.00

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.