Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2024 – 05:03 PM EST

PDB ID	:	2FHY
Title	:	Structure of human liver FPBase complexed with a novel benzoxazole as allosteric inhibitor
Authors	:	Abad-Zapatero, C.
Deposited on	:	2005-12-27
Resolution	:	2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

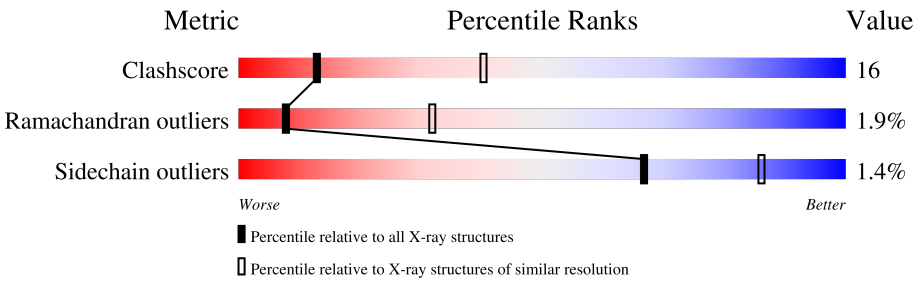
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.95 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	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	53% 30% • 15%
1	D	374	53% 30% • 15%
1	H	374	54% 30% • 15%
1	L	374	56% 28% • 15%

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	A37	A	502	-	-	X	-
3	A37	D	602	-	-	X	-
3	A37	H	702	-	-	X	-
3	A37	L	802	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9796 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 Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	318	2426	1545	407	457	17	0	0	1
1	D	318	2426	1545	407	457	17	0	0	1
1	H	318	2426	1545	407	457	17	0	0	1
1	L	318	2426	1545	407	457	17	0	0	1

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	MET	-	cloning artifact	GB 15277851
A	-35	ARG	-	cloning artifact	GB 15277851
A	-34	GLY	-	cloning artifact	GB 15277851
A	-33	SER	-	cloning artifact	GB 15277851
A	-32	HIS	-	cloning artifact	GB 15277851
A	-31	HIS	-	cloning artifact	GB 15277851
A	-30	HIS	-	cloning artifact	GB 15277851
A	-29	HIS	-	cloning artifact	GB 15277851
A	-28	HIS	-	cloning artifact	GB 15277851
A	-27	HIS	-	cloning artifact	GB 15277851
A	-26	GLY	-	cloning artifact	GB 15277851
A	-25	MET	-	cloning artifact	GB 15277851
A	-24	ALA	-	cloning artifact	GB 15277851
A	-23	SER	-	cloning artifact	GB 15277851
A	-22	MET	-	cloning artifact	GB 15277851
A	-21	THR	-	cloning artifact	GB 15277851
A	-20	GLY	-	cloning artifact	GB 15277851
A	-19	GLY	-	cloning artifact	GB 15277851
A	-18	GLN	-	cloning artifact	GB 15277851
A	-17	GLN	-	cloning artifact	GB 15277851
A	-16	MET	-	cloning artifact	GB 15277851

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	cloning artifact	GB 15277851
A	-14	ARG	-	cloning artifact	GB 15277851
A	-13	ASP	-	cloning artifact	GB 15277851
A	-12	LEU	-	cloning artifact	GB 15277851
A	-11	TYR	-	cloning artifact	GB 15277851
A	-10	ASP	-	cloning artifact	GB 15277851
A	-9	ASP	-	cloning artifact	GB 15277851
A	-8	ASP	-	cloning artifact	GB 15277851
A	-7	ASP	-	cloning artifact	GB 15277851
A	-6	LYS	-	cloning artifact	GB 15277851
A	-5	ASP	-	cloning artifact	GB 15277851
A	-4	HIS	-	cloning artifact	GB 15277851
A	-3	PRO	-	cloning artifact	GB 15277851
A	-2	PHE	-	cloning artifact	GB 15277851
A	-1	THR	-	cloning artifact	GB 15277851
A	217	LYS	ARG	variant	GB 15277851
D	-36	MET	-	cloning artifact	GB 15277851
D	-35	ARG	-	cloning artifact	GB 15277851
D	-34	GLY	-	cloning artifact	GB 15277851
D	-33	SER	-	cloning artifact	GB 15277851
D	-32	HIS	-	cloning artifact	GB 15277851
D	-31	HIS	-	cloning artifact	GB 15277851
D	-30	HIS	-	cloning artifact	GB 15277851
D	-29	HIS	-	cloning artifact	GB 15277851
D	-28	HIS	-	cloning artifact	GB 15277851
D	-27	HIS	-	cloning artifact	GB 15277851
D	-26	GLY	-	cloning artifact	GB 15277851
D	-25	MET	-	cloning artifact	GB 15277851
D	-24	ALA	-	cloning artifact	GB 15277851
D	-23	SER	-	cloning artifact	GB 15277851
D	-22	MET	-	cloning artifact	GB 15277851
D	-21	THR	-	cloning artifact	GB 15277851
D	-20	GLY	-	cloning artifact	GB 15277851
D	-19	GLY	-	cloning artifact	GB 15277851
D	-18	GLN	-	cloning artifact	GB 15277851
D	-17	GLN	-	cloning artifact	GB 15277851
D	-16	MET	-	cloning artifact	GB 15277851
D	-15	GLY	-	cloning artifact	GB 15277851
D	-14	ARG	-	cloning artifact	GB 15277851
D	-13	ASP	-	cloning artifact	GB 15277851
D	-12	LEU	-	cloning artifact	GB 15277851
D	-11	TYR	-	cloning artifact	GB 15277851

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	ASP	-	cloning artifact	GB 15277851
D	-9	ASP	-	cloning artifact	GB 15277851
D	-8	ASP	-	cloning artifact	GB 15277851
D	-7	ASP	-	cloning artifact	GB 15277851
D	-6	LYS	-	cloning artifact	GB 15277851
D	-5	ASP	-	cloning artifact	GB 15277851
D	-4	HIS	-	cloning artifact	GB 15277851
D	-3	PRO	-	cloning artifact	GB 15277851
D	-2	PHE	-	cloning artifact	GB 15277851
D	-1	THR	-	cloning artifact	GB 15277851
D	217	LYS	ARG	variant	GB 15277851
H	-36	MET	-	cloning artifact	GB 15277851
H	-35	ARG	-	cloning artifact	GB 15277851
H	-34	GLY	-	cloning artifact	GB 15277851
H	-33	SER	-	cloning artifact	GB 15277851
H	-32	HIS	-	cloning artifact	GB 15277851
H	-31	HIS	-	cloning artifact	GB 15277851
H	-30	HIS	-	cloning artifact	GB 15277851
H	-29	HIS	-	cloning artifact	GB 15277851
H	-28	HIS	-	cloning artifact	GB 15277851
H	-27	HIS	-	cloning artifact	GB 15277851
H	-26	GLY	-	cloning artifact	GB 15277851
H	-25	MET	-	cloning artifact	GB 15277851
H	-24	ALA	-	cloning artifact	GB 15277851
H	-23	SER	-	cloning artifact	GB 15277851
H	-22	MET	-	cloning artifact	GB 15277851
H	-21	THR	-	cloning artifact	GB 15277851
H	-20	GLY	-	cloning artifact	GB 15277851
H	-19	GLY	-	cloning artifact	GB 15277851
H	-18	GLN	-	cloning artifact	GB 15277851
H	-17	GLN	-	cloning artifact	GB 15277851
H	-16	MET	-	cloning artifact	GB 15277851
H	-15	GLY	-	cloning artifact	GB 15277851
H	-14	ARG	-	cloning artifact	GB 15277851
H	-13	ASP	-	cloning artifact	GB 15277851
H	-12	LEU	-	cloning artifact	GB 15277851
H	-11	TYR	-	cloning artifact	GB 15277851
H	-10	ASP	-	cloning artifact	GB 15277851
H	-9	ASP	-	cloning artifact	GB 15277851
H	-8	ASP	-	cloning artifact	GB 15277851
H	-7	ASP	-	cloning artifact	GB 15277851
H	-6	LYS	-	cloning artifact	GB 15277851

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	ASP	-	cloning artifact	GB 15277851
H	-4	HIS	-	cloning artifact	GB 15277851
H	-3	PRO	-	cloning artifact	GB 15277851
H	-2	PHE	-	cloning artifact	GB 15277851
H	-1	THR	-	cloning artifact	GB 15277851
H	217	LYS	ARG	variant	GB 15277851
L	-36	MET	-	cloning artifact	GB 15277851
L	-35	ARG	-	cloning artifact	GB 15277851
L	-34	GLY	-	cloning artifact	GB 15277851
L	-33	SER	-	cloning artifact	GB 15277851
L	-32	HIS	-	cloning artifact	GB 15277851
L	-31	HIS	-	cloning artifact	GB 15277851
L	-30	HIS	-	cloning artifact	GB 15277851
L	-29	HIS	-	cloning artifact	GB 15277851
L	-28	HIS	-	cloning artifact	GB 15277851
L	-27	HIS	-	cloning artifact	GB 15277851
L	-26	GLY	-	cloning artifact	GB 15277851
L	-25	MET	-	cloning artifact	GB 15277851
L	-24	ALA	-	cloning artifact	GB 15277851
L	-23	SER	-	cloning artifact	GB 15277851
L	-22	MET	-	cloning artifact	GB 15277851
L	-21	THR	-	cloning artifact	GB 15277851
L	-20	GLY	-	cloning artifact	GB 15277851
L	-19	GLY	-	cloning artifact	GB 15277851
L	-18	GLN	-	cloning artifact	GB 15277851
L	-17	GLN	-	cloning artifact	GB 15277851
L	-16	MET	-	cloning artifact	GB 15277851
L	-15	GLY	-	cloning artifact	GB 15277851
L	-14	ARG	-	cloning artifact	GB 15277851
L	-13	ASP	-	cloning artifact	GB 15277851
L	-12	LEU	-	cloning artifact	GB 15277851
L	-11	TYR	-	cloning artifact	GB 15277851
L	-10	ASP	-	cloning artifact	GB 15277851
L	-9	ASP	-	cloning artifact	GB 15277851
L	-8	ASP	-	cloning artifact	GB 15277851
L	-7	ASP	-	cloning artifact	GB 15277851
L	-6	LYS	-	cloning artifact	GB 15277851
L	-5	ASP	-	cloning artifact	GB 15277851
L	-4	HIS	-	cloning artifact	GB 15277851
L	-3	PRO	-	cloning artifact	GB 15277851
L	-2	PHE	-	cloning artifact	GB 15277851
L	-1	THR	-	cloning artifact	GB 15277851

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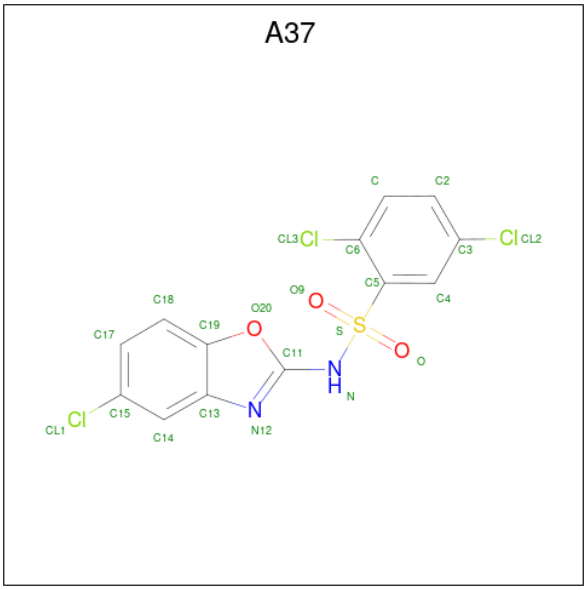
Chain	Residue	Modelled	Actual	Comment	Reference
L	217	LYS	ARG	variant	GB 15277851

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	L	1	Total Mg 1 1	0	0

- Molecule 3 is 2,5-DICHLORO-N-(5-CHLORO-1,3-BENZOXAZOL-2-YL)BENZENESULFONAMIDE (three-letter code: A37) (formula: $C_{13}H_7Cl_3N_2O_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C Cl N O S 22 13 3 2 3 1	0	0
3	D	1	Total C Cl N O S 22 13 3 2 3 1	0	0
3	H	1	Total C Cl N O S 22 13 3 2 3 1	0	0
3	L	1	Total C Cl N O S 22 13 3 2 3 1	0	0

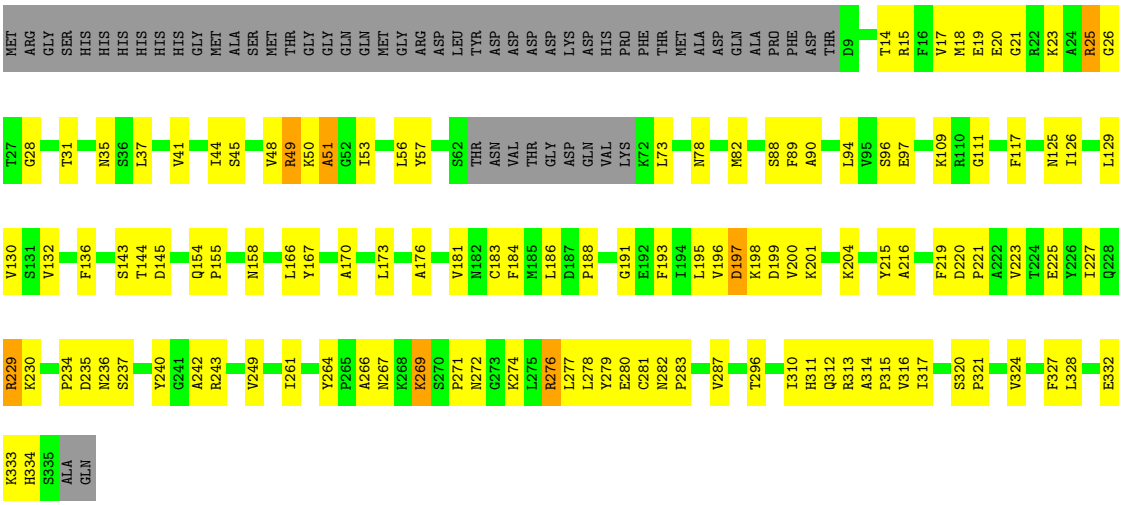
3 Residue-property plots (i)

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. 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.

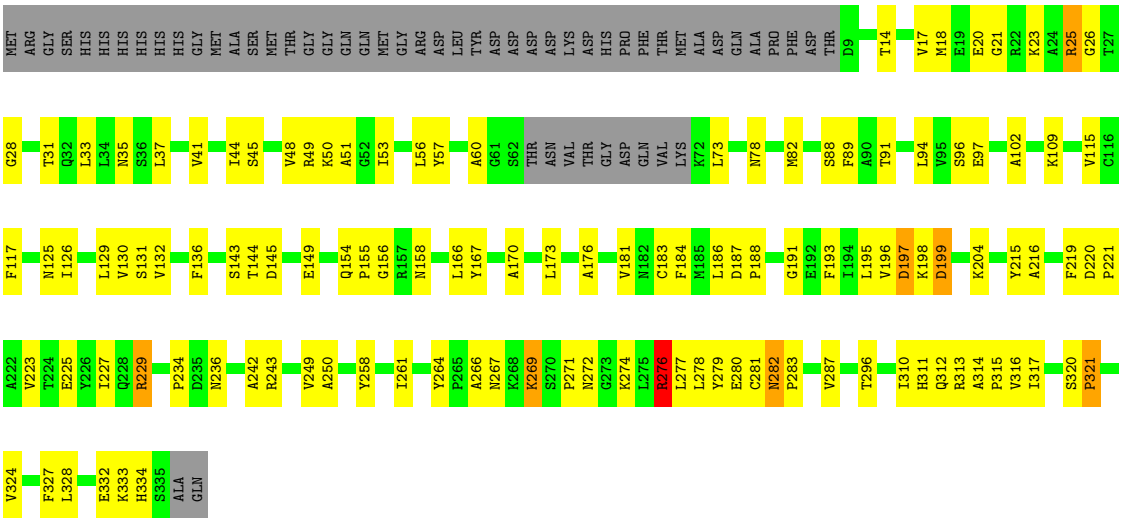
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain A: 53% 30% • 15%



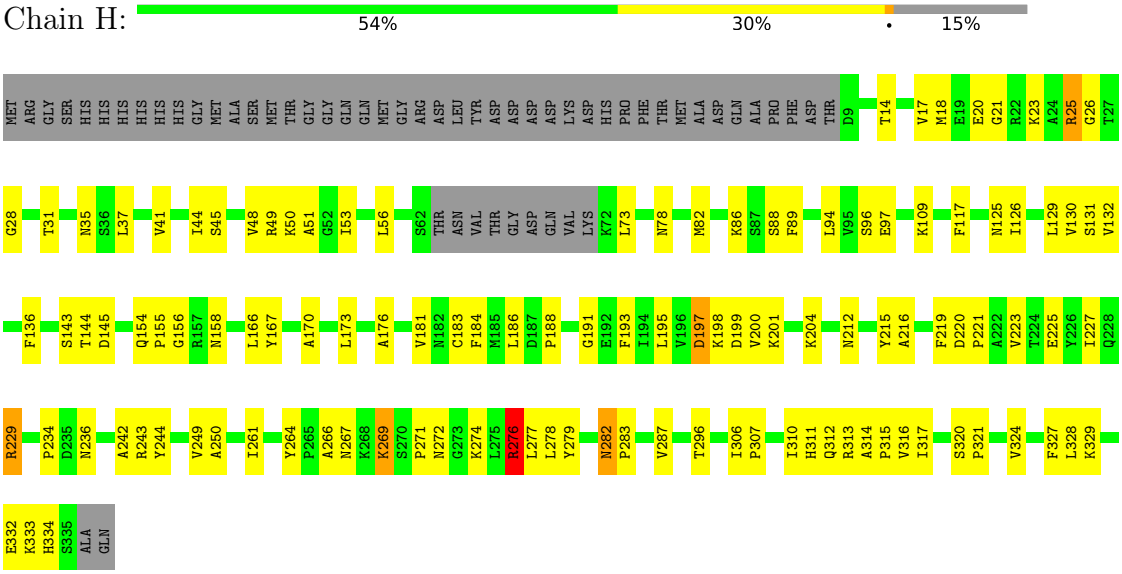
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain D: 53% 30% • 15%



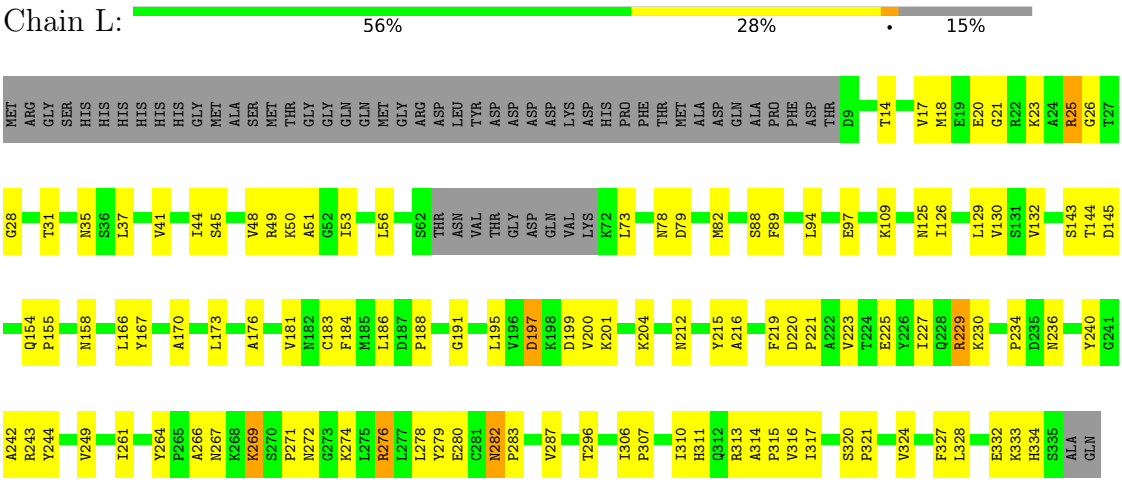
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain H:



• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain L:



4 Data and refinement statistics (i)

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	83.75Å 109.13Å 190.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.95	Depositor
% Data completeness (in resolution range)	75.1 (19.89-2.95)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.225 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9796	wwPDB-VP
Average B, all atoms (Å^2)	77.0	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: A37, MG

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	0/2469	0.93	9/3335 (0.3%)
1	D	0.38	0/2469	0.78	9/3335 (0.3%)
1	H	0.37	0/2469	0.91	10/3335 (0.3%)
1	L	0.39	0/2469	0.92	10/3335 (0.3%)
All	All	0.38	0/9876	0.89	38/13340 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	313	ARG	NE-CZ-NH1	-21.30	109.65	120.30
1	A	313	ARG	NE-CZ-NH2	19.90	130.25	120.30
1	L	229	ARG	NE-CZ-NH1	-19.86	110.37	120.30
1	H	25	ARG	NE-CZ-NH1	-19.74	110.43	120.30
1	H	25	ARG	NE-CZ-NH2	19.04	129.82	120.30
1	L	229	ARG	NE-CZ-NH2	18.95	129.78	120.30
1	A	276	ARG	NE-CZ-NH1	-13.50	113.55	120.30
1	L	276	ARG	NE-CZ-NH2	13.50	127.05	120.30
1	L	276	ARG	NE-CZ-NH1	-13.47	113.56	120.30
1	A	276	ARG	NE-CZ-NH2	13.26	126.93	120.30
1	D	276	ARG	NE-CZ-NH1	12.73	126.67	120.30
1	D	276	ARG	NE-CZ-NH2	-12.53	114.03	120.30
1	H	276	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	H	276	ARG	NE-CZ-NH1	12.33	126.47	120.30
1	A	313	ARG	CD-NE-CZ	10.47	138.25	123.60
1	L	229	ARG	CD-NE-CZ	9.57	137.00	123.60
1	H	25	ARG	CD-NE-CZ	9.41	136.78	123.60
1	D	313	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	L	313	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	D	229	ARG	NE-CZ-NH2	-7.34	116.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	313	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	25	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	D	313	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	276	ARG	CD-NE-CZ	6.85	133.19	123.60
1	H	229	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	L	25	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	L	25	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	D	276	ARG	CD-NE-CZ	6.72	133.00	123.60
1	D	25	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	L	276	ARG	CD-NE-CZ	6.70	132.99	123.60
1	H	276	ARG	CD-NE-CZ	6.67	132.94	123.60
1	L	313	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	25	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	H	313	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	D	25	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	H	229	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	D	229	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	229	ARG	NE-CZ-NH2	-5.11	117.74	120.30

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	2426	0	2469	90	0
1	D	2426	0	2469	91	0
1	H	2426	0	2469	84	0
1	L	2426	0	2469	79	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	H	1	0	0	0	0
2	L	1	0	0	0	0
3	A	22	0	7	8	0
3	D	22	0	7	8	0
3	H	22	0	7	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	22	0	7	8	0
All	All	9796	0	9904	325	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 16.

All (325) 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:296:THR:HG21	1:H:328:LEU:HD21	1.63	0.80
1:D:266:ALA:HB1	1:D:271:PRO:HA	1.68	0.76
1:L:296:THR:HG21	1:L:328:LEU:HD21	1.69	0.74
1:H:266:ALA:HB1	1:H:271:PRO:HA	1.69	0.74
1:A:296:THR:HG21	1:A:328:LEU:HD21	1.70	0.74
1:L:266:ALA:HB1	1:L:271:PRO:HA	1.70	0.74
1:D:296:THR:HG21	1:D:328:LEU:HD21	1.70	0.74
1:A:155:PRO:HD2	1:A:158:ASN:ND2	2.04	0.73
1:A:266:ALA:HB1	1:A:271:PRO:HA	1.70	0.72
1:L:26:GLY:HA3	3:L:802:A37:HN	1.54	0.72
1:L:155:PRO:HD2	1:L:158:ASN:ND2	2.04	0.72
1:H:155:PRO:HD2	1:H:158:ASN:ND2	2.03	0.72
1:D:26:GLY:HA3	3:D:602:A37:HN	1.54	0.72
1:H:26:GLY:HA3	3:H:702:A37:HN	1.53	0.71
1:L:276:ARG:HH21	1:L:311:HIS:HB3	1.54	0.71
1:A:276:ARG:HH21	1:A:311:HIS:HB3	1.54	0.71
1:D:155:PRO:HD2	1:D:158:ASN:ND2	2.04	0.70
1:H:37:LEU:O	1:H:41:VAL:HG23	1.92	0.70
1:D:276:ARG:HH21	1:D:311:HIS:HB3	1.57	0.69
1:D:37:LEU:O	1:D:41:VAL:HG23	1.92	0.69
1:A:97:GLU:HB2	1:A:279:TYR:CE1	2.28	0.69
1:L:37:LEU:O	1:L:41:VAL:HG23	1.93	0.68
1:A:26:GLY:HA3	3:A:502:A37:HN	1.58	0.67
1:H:276:ARG:HH21	1:H:311:HIS:HB3	1.59	0.67
1:H:97:GLU:HB2	1:H:279:TYR:CE1	2.30	0.67
1:D:97:GLU:HB2	1:D:279:TYR:CE1	2.30	0.66
1:L:97:GLU:HB2	1:L:279:TYR:CE1	2.30	0.66
1:D:28:GLY:HA3	3:H:702:A37:H17	1.77	0.64
1:D:183:CYS:HB2	1:D:197:ASP:HB2	1.79	0.64
1:L:225:GLU:O	1:L:229:ARG:HG3	1.97	0.64
1:A:37:LEU:O	1:A:41:VAL:HG23	1.97	0.64
1:D:89:PHE:CE2	1:D:109:LYS:HG2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:CYS:HB2	1:L:197:ASP:HB2	1.80	0.63
1:L:264:TYR:CE1	1:L:274:LYS:HB3	2.33	0.63
1:A:89:PHE:CD2	1:A:109:LYS:HA	2.34	0.62
1:A:89:PHE:CE2	1:A:109:LYS:HG2	2.33	0.62
1:D:89:PHE:CD2	1:D:109:LYS:HA	2.34	0.62
1:L:89:PHE:CD2	1:L:109:LYS:HA	2.35	0.62
1:A:45:SER:O	1:A:49:ARG:HD3	2.00	0.62
1:A:264:TYR:CE1	1:A:274:LYS:HB3	2.34	0.62
1:D:191:GLY:HA3	1:H:191:GLY:HA3	1.82	0.62
1:H:264:TYR:CE1	1:H:274:LYS:HB3	2.34	0.62
1:H:45:SER:O	1:H:49:ARG:HD3	1.99	0.62
1:H:183:CYS:HB2	1:H:197:ASP:HB2	1.80	0.62
1:L:82:MET:CE	1:L:94:LEU:HD13	2.29	0.62
1:H:89:PHE:CD2	1:H:109:LYS:HA	2.35	0.61
1:D:125:ASN:O	1:D:130:VAL:HG12	2.00	0.61
1:A:183:CYS:HB2	1:A:197:ASP:HB2	1.81	0.61
1:A:18:MET:HB2	3:A:502:A37:CL1	2.37	0.61
1:H:89:PHE:CE2	1:H:109:LYS:HG2	2.35	0.61
1:D:264:TYR:CE1	1:D:274:LYS:HB3	2.35	0.61
1:L:89:PHE:CE2	1:L:109:LYS:HG2	2.36	0.61
1:L:78:ASN:O	1:L:82:MET:HB2	2.01	0.60
1:A:89:PHE:HE2	1:A:109:LYS:HG2	1.66	0.60
1:A:89:PHE:HD2	1:A:109:LYS:HA	1.66	0.60
1:L:125:ASN:O	1:L:130:VAL:HG12	2.01	0.60
1:H:89:PHE:HE2	1:H:109:LYS:HG2	1.66	0.60
1:D:17:VAL:HG12	1:D:31:THR:HG23	1.83	0.59
1:H:26:GLY:CA	3:H:702:A37:HN	2.16	0.59
1:H:89:PHE:HD2	1:H:109:LYS:HA	1.67	0.59
1:A:14:THR:HG21	1:L:35:ASN:ND2	2.17	0.59
1:D:89:PHE:HD2	1:D:109:LYS:HA	1.65	0.59
1:A:28:GLY:HA3	3:L:802:A37:H17	1.85	0.59
1:L:89:PHE:HD2	1:L:109:LYS:HA	1.67	0.59
1:D:45:SER:O	1:D:49:ARG:HD3	2.02	0.59
1:A:125:ASN:O	1:A:130:VAL:HG12	2.04	0.58
1:D:18:MET:HB2	3:D:602:A37:CL1	2.40	0.58
1:H:82:MET:CE	1:H:94:LEU:HD13	2.33	0.58
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.38	0.58
3:A:502:A37:H17	1:L:28:GLY:HA3	1.85	0.58
1:L:216:ALA:HA	1:L:219:PHE:CD2	2.39	0.58
1:D:89:PHE:HE2	1:D:109:LYS:HG2	1.67	0.58
1:H:216:ALA:HA	1:H:219:PHE:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:MET:CE	1:A:94:LEU:HD13	2.34	0.57
1:D:35:ASN:ND2	1:H:14:THR:HG21	2.20	0.57
3:D:602:A37:H17	1:H:28:GLY:HA3	1.86	0.57
1:H:125:ASN:O	1:H:130:VAL:HG12	2.04	0.57
1:D:14:THR:HG21	1:H:35:ASN:ND2	2.18	0.57
1:D:26:GLY:CA	3:D:602:A37:HN	2.17	0.57
1:L:26:GLY:CA	3:L:802:A37:HN	2.16	0.57
1:A:170:ALA:HB3	1:D:129:LEU:HD22	1.87	0.57
1:L:82:MET:HE2	1:L:94:LEU:HD13	1.86	0.57
1:D:316:VAL:C	1:D:317:ILE:HD12	2.24	0.57
1:H:316:VAL:C	1:H:317:ILE:HD12	2.25	0.57
1:D:78:ASN:O	1:D:82:MET:HB2	2.05	0.56
1:D:82:MET:HE2	1:D:94:LEU:HD13	1.87	0.56
1:L:316:VAL:C	1:L:317:ILE:HD12	2.25	0.56
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.86	0.56
1:L:89:PHE:HE2	1:L:109:LYS:HG2	1.68	0.56
1:D:82:MET:CE	1:D:94:LEU:HD13	2.35	0.56
1:A:17:VAL:HG12	1:A:31:THR:HG23	1.88	0.56
1:H:28:GLY:HA2	3:H:702:A37:N12	2.20	0.56
1:H:78:ASN:O	1:H:82:MET:HB2	2.06	0.56
1:A:129:LEU:HD22	1:D:170:ALA:HB3	1.86	0.56
1:A:316:VAL:C	1:A:317:ILE:HD12	2.26	0.55
1:D:216:ALA:HA	1:D:219:PHE:CD2	2.41	0.55
1:A:78:ASN:O	1:A:82:MET:HB2	2.06	0.55
1:D:17:VAL:HG13	3:D:602:A37:CL2	2.43	0.55
1:L:166:LEU:HD13	1:L:249:VAL:HG12	1.88	0.55
1:H:17:VAL:HG12	1:H:31:THR:HG23	1.88	0.55
1:A:82:MET:HE2	1:A:94:LEU:HD13	1.88	0.55
1:L:17:VAL:HG12	1:L:31:THR:HG23	1.89	0.55
1:L:45:SER:O	1:L:49:ARG:HD3	2.07	0.54
1:D:154:GLN:HB3	1:D:158:ASN:HD22	1.72	0.54
1:L:18:MET:HB2	3:L:802:A37:CL1	2.45	0.54
1:H:166:LEU:HD13	1:H:249:VAL:HG12	1.88	0.54
1:A:234:PRO:C	1:A:236:ASN:H	2.11	0.54
1:A:191:GLY:HA3	1:L:191:GLY:HA3	1.89	0.54
1:D:269:LYS:O	1:D:271:PRO:HD3	2.08	0.53
1:L:17:VAL:HG13	3:L:802:A37:CL2	2.45	0.53
1:D:234:PRO:C	1:D:236:ASN:H	2.12	0.53
1:H:221:PRO:HB2	1:H:334:HIS:ND1	2.23	0.53
1:H:269:LYS:O	1:H:271:PRO:HD3	2.08	0.53
1:A:35:ASN:ND2	1:L:14:THR:HG21	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:132:VAL:HG23	1:L:167:TYR:HD2	1.74	0.53
1:L:269:LYS:O	1:L:271:PRO:HD3	2.08	0.53
1:A:283:PRO:O	1:A:287:VAL:HG23	2.09	0.53
1:L:243:ARG:HG2	1:L:243:ARG:HH11	1.73	0.53
1:A:269:LYS:O	1:A:271:PRO:HD3	2.09	0.53
1:D:225:GLU:O	1:D:229:ARG:HG3	2.09	0.53
1:D:242:ALA:O	1:D:243:ARG:HG2	2.07	0.53
1:D:173:LEU:HD23	1:D:173:LEU:C	2.28	0.53
1:L:234:PRO:C	1:L:236:ASN:H	2.12	0.52
1:D:243:ARG:HG2	1:D:243:ARG:HH11	1.74	0.52
1:H:170:ALA:HB3	1:L:129:LEU:HD22	1.92	0.52
1:A:176:ALA:HB2	1:A:181:VAL:HG22	1.91	0.52
1:H:18:MET:HB2	3:H:702:A37:CL1	2.46	0.52
1:H:234:PRO:C	1:H:236:ASN:H	2.12	0.52
1:A:173:LEU:C	1:A:173:LEU:HD23	2.30	0.52
1:L:154:GLN:HB3	1:L:158:ASN:HD22	1.75	0.52
1:A:17:VAL:HG13	3:A:502:A37:CL2	2.46	0.52
1:D:132:VAL:HG23	1:D:167:TYR:HD2	1.75	0.52
1:A:132:VAL:HG23	1:A:167:TYR:HD2	1.75	0.52
1:D:166:LEU:HD13	1:D:249:VAL:HG12	1.91	0.51
1:H:132:VAL:HG23	1:H:167:TYR:HD2	1.74	0.51
1:L:324:VAL:O	1:L:327:PHE:HB3	2.11	0.51
1:A:26:GLY:CA	3:A:502:A37:HN	2.22	0.51
1:D:176:ALA:CB	1:D:181:VAL:HG22	2.41	0.51
1:H:17:VAL:HG13	3:H:702:A37:CL2	2.47	0.51
1:L:173:LEU:C	1:L:173:LEU:HD23	2.31	0.51
1:H:173:LEU:C	1:H:173:LEU:HD23	2.30	0.51
1:A:176:ALA:CB	1:A:181:VAL:HG22	2.41	0.51
1:A:243:ARG:HG2	1:A:243:ARG:HH11	1.74	0.51
1:H:154:GLN:HB3	1:H:158:ASN:HD22	1.75	0.51
1:D:223:VAL:O	1:D:227:ILE:HG12	2.11	0.50
1:L:88:SER:O	1:L:89:PHE:HB2	2.12	0.50
1:H:176:ALA:CB	1:H:181:VAL:HG22	2.40	0.50
1:D:53:ILE:HA	1:D:56:LEU:HD13	1.94	0.50
1:D:272:ASN:O	1:D:314:ALA:CA	2.60	0.50
1:D:176:ALA:HB2	1:D:181:VAL:HG22	1.93	0.50
1:H:82:MET:HE2	1:H:94:LEU:HD13	1.94	0.50
1:L:221:PRO:HB2	1:L:334:HIS:ND1	2.26	0.50
1:H:283:PRO:O	1:H:287:VAL:HG23	2.12	0.50
1:L:220:ASP:HB2	1:L:221:PRO:HD2	1.93	0.50
1:D:221:PRO:HB2	1:D:334:HIS:ND1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:ALA:HB2	1:H:181:VAL:HG22	1.93	0.49
1:H:28:GLY:HA2	3:H:702:A37:C11	2.43	0.49
1:H:44:ILE:O	1:H:48:VAL:HG23	2.12	0.49
1:A:225:GLU:O	1:A:229:ARG:HG3	2.12	0.49
1:A:272:ASN:O	1:A:314:ALA:CA	2.60	0.49
1:A:324:VAL:O	1:A:327:PHE:HB3	2.12	0.49
1:H:49:ARG:O	1:H:50:LYS:HB2	2.13	0.49
1:H:129:LEU:HD22	1:L:170:ALA:HB3	1.94	0.48
1:H:243:ARG:HG2	1:H:243:ARG:HH11	1.78	0.48
1:A:50:LYS:O	1:D:188:PRO:HD2	2.12	0.48
1:D:220:ASP:HB2	1:D:221:PRO:HD2	1.96	0.48
1:D:324:VAL:O	1:D:327:PHE:HB3	2.14	0.48
1:H:88:SER:O	1:H:89:PHE:HB2	2.14	0.48
1:L:272:ASN:O	1:L:314:ALA:CA	2.61	0.48
1:A:154:GLN:HB3	1:A:158:ASN:HD22	1.78	0.48
1:H:220:ASP:HB2	1:H:221:PRO:HD2	1.95	0.48
1:A:53:ILE:HA	1:A:56:LEU:HD13	1.95	0.48
1:A:221:PRO:HB2	1:A:334:HIS:ND1	2.29	0.48
1:A:186:LEU:O	1:A:188:PRO:HD3	2.14	0.48
1:A:220:ASP:HB2	1:A:221:PRO:HD2	1.96	0.48
1:D:49:ARG:O	1:D:50:LYS:HB2	2.14	0.48
1:H:223:VAL:O	1:H:227:ILE:HG12	2.13	0.48
1:D:183:CYS:O	1:D:195:LEU:HD12	2.14	0.47
1:H:306:ILE:HA	1:H:307:PRO:HD3	1.74	0.47
1:L:28:GLY:HA2	3:L:802:A37:N12	2.28	0.47
1:D:20:GLU:OE1	1:D:20:GLU:HA	2.14	0.47
1:L:204:LYS:O	1:L:320:SER:HB3	2.13	0.47
1:D:44:ILE:O	1:D:48:VAL:HG23	2.14	0.47
1:H:21:GLY:HA2	3:H:702:A37:C6	2.45	0.47
1:H:272:ASN:O	1:H:314:ALA:CA	2.63	0.47
1:L:223:VAL:O	1:L:227:ILE:HG12	2.15	0.47
1:H:225:GLU:O	1:H:229:ARG:HG3	2.14	0.47
1:L:216:ALA:HA	1:L:219:PHE:CE2	2.50	0.47
1:L:242:ALA:O	1:L:243:ARG:HG2	2.15	0.47
1:L:283:PRO:O	1:L:287:VAL:HG23	2.14	0.47
1:H:53:ILE:HA	1:H:56:LEU:HD13	1.97	0.47
1:A:215:TYR:N	1:A:215:TYR:CD2	2.83	0.46
1:A:216:ALA:HA	1:A:219:PHE:CE2	2.50	0.46
1:A:44:ILE:O	1:A:48:VAL:HG23	2.15	0.46
1:D:276:ARG:O	1:D:280:GLU:HB2	2.16	0.46
1:A:88:SER:O	1:A:89:PHE:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ALA:O	1:A:243:ARG:HG2	2.15	0.46
1:D:186:LEU:HB2	1:D:193:PHE:CE1	2.50	0.46
1:D:283:PRO:O	1:D:287:VAL:HG23	2.14	0.46
1:H:20:GLU:OE1	1:H:20:GLU:HA	2.15	0.46
1:D:332:GLU:O	1:D:334:HIS:N	2.49	0.46
1:L:53:ILE:HA	1:L:56:LEU:HD13	1.96	0.46
1:H:324:VAL:O	1:H:327:PHE:HB3	2.16	0.46
1:L:186:LEU:O	1:L:188:PRO:HD3	2.16	0.46
1:A:276:ARG:NH2	1:A:311:HIS:HB3	2.28	0.46
1:L:184:PHE:CE2	1:L:195:LEU:HD13	2.51	0.46
1:H:278:LEU:HD12	1:H:310:ILE:HA	1.98	0.45
1:A:332:GLU:O	1:A:334:HIS:N	2.50	0.45
1:D:96:SER:HB2	1:D:117:PHE:CZ	2.51	0.45
1:L:21:GLY:HA2	3:L:802:A37:C6	2.46	0.45
1:H:242:ALA:O	1:H:243:ARG:HG2	2.17	0.45
1:A:223:VAL:O	1:A:227:ILE:HG12	2.16	0.45
1:A:21:GLY:HA2	3:A:502:A37:C6	2.47	0.45
1:H:73:LEU:HD23	1:H:126:ILE:HD13	1.98	0.45
1:D:88:SER:O	1:D:89:PHE:HB2	2.16	0.45
1:H:184:PHE:CE2	1:H:195:LEU:HD13	2.52	0.45
1:H:186:LEU:O	1:H:188:PRO:HD3	2.16	0.45
1:L:176:ALA:HB2	1:L:181:VAL:HG22	1.98	0.45
1:A:183:CYS:O	1:A:195:LEU:HD12	2.17	0.45
1:D:28:GLY:HA2	3:D:602:A37:C11	2.47	0.45
1:H:96:SER:HB2	1:H:117:PHE:CZ	2.52	0.45
1:H:216:ALA:HA	1:H:219:PHE:CE2	2.51	0.45
1:A:188:PRO:HD2	1:D:50:LYS:O	2.16	0.45
1:A:200:VAL:CG1	1:A:201:LYS:N	2.80	0.44
1:D:216:ALA:HA	1:D:219:PHE:CE2	2.52	0.44
1:D:215:TYR:N	1:D:215:TYR:CD2	2.83	0.44
1:D:261:ILE:HD11	1:D:317:ILE:HG23	2.00	0.44
1:L:176:ALA:CB	1:L:181:VAL:HG22	2.47	0.44
1:A:15:ARG:O	1:A:19:GLU:HG3	2.17	0.44
1:H:215:TYR:N	1:H:215:TYR:CD2	2.83	0.44
1:L:314:ALA:HA	1:L:315:PRO:HD3	1.80	0.44
1:A:184:PHE:CE2	1:A:195:LEU:HD13	2.51	0.44
1:A:204:LYS:O	1:A:320:SER:HB3	2.17	0.44
1:H:332:GLU:O	1:H:334:HIS:N	2.50	0.44
1:L:73:LEU:HD23	1:L:126:ILE:HD13	1.99	0.44
1:L:28:GLY:HA2	3:L:802:A37:C11	2.48	0.44
1:A:314:ALA:HA	1:A:315:PRO:HD3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:GLY:HA2	3:D:602:A37:N12	2.32	0.44
1:H:183:CYS:O	1:H:195:LEU:HD12	2.18	0.44
1:L:20:GLU:HA	1:L:20:GLU:OE1	2.16	0.44
1:D:21:GLY:HA2	3:D:602:A37:C6	2.47	0.44
1:L:215:TYR:N	1:L:215:TYR:CD2	2.83	0.44
1:L:278:LEU:HD12	1:L:310:ILE:HA	2.00	0.44
1:D:277:LEU:HD22	1:D:312:GLN:NE2	2.33	0.44
1:H:143:SER:HB2	1:H:145:ASP:OD2	2.18	0.44
1:L:183:CYS:O	1:L:195:LEU:HD12	2.18	0.44
1:A:51:ALA:O	1:D:187:ASP:OD1	2.36	0.43
1:A:28:GLY:HA2	3:A:502:A37:N12	2.33	0.43
1:D:60:ALA:O	1:L:79:ASP:HB3	2.18	0.43
1:H:282:ASN:HD22	1:H:282:ASN:HA	1.69	0.43
1:D:143:SER:HB2	1:D:145:ASP:OD2	2.18	0.43
1:D:314:ALA:HA	1:D:315:PRO:HD3	1.81	0.43
1:H:204:LYS:O	1:H:320:SER:HB3	2.19	0.43
1:L:49:ARG:O	1:L:50:LYS:HB2	2.17	0.43
1:A:20:GLU:OE1	1:A:20:GLU:HA	2.18	0.43
1:D:102:ALA:HB2	1:D:149:GLU:HG3	2.01	0.43
1:L:276:ARG:NH2	1:L:311:HIS:HB3	2.28	0.43
1:A:23:LYS:C	1:A:25:ARG:H	2.22	0.43
1:D:41:VAL:HG13	1:D:167:TYR:OH	2.18	0.43
1:A:73:LEU:HD23	1:A:126:ILE:HD13	2.00	0.43
1:D:23:LYS:C	1:D:25:ARG:H	2.21	0.43
1:A:278:LEU:HD12	1:A:310:ILE:HA	2.01	0.43
1:H:82:MET:HG3	1:H:86:LYS:HE3	2.01	0.43
1:A:276:ARG:O	1:A:280:GLU:HB2	2.19	0.42
1:H:37:LEU:HD21	1:H:136:PHE:CG	2.54	0.42
1:D:14:THR:HG21	1:H:35:ASN:HD21	1.83	0.42
1:D:186:LEU:O	1:D:188:PRO:HD3	2.19	0.42
1:D:204:LYS:O	1:D:320:SER:HB3	2.19	0.42
1:L:41:VAL:HG13	1:L:167:TYR:OH	2.19	0.42
1:L:332:GLU:O	1:L:334:HIS:N	2.52	0.42
1:A:125:ASN:HA	1:D:258:TYR:OH	2.18	0.42
1:D:73:LEU:HD23	1:D:126:ILE:HD13	2.00	0.42
1:A:96:SER:HB2	1:A:117:PHE:CZ	2.55	0.42
1:A:143:SER:HB2	1:A:145:ASP:OD2	2.20	0.42
1:A:198:LYS:HE3	1:A:198:LYS:HB2	1.75	0.42
1:L:143:SER:HB2	1:L:145:ASP:OD2	2.20	0.42
1:A:90:ALA:C	1:A:111:GLY:HA3	2.40	0.42
1:D:184:PHE:CE2	1:D:195:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:306:ILE:HA	1:L:307:PRO:HD3	1.74	0.42
1:A:281:CYS:SG	1:A:316:VAL:HG21	2.60	0.42
1:D:131:SER:HB2	1:D:250:ALA:HB2	2.01	0.42
1:A:14:THR:HG21	1:L:35:ASN:HD21	1.83	0.42
1:D:281:CYS:SG	1:D:316:VAL:HG21	2.60	0.42
1:H:14:THR:O	1:H:18:MET:HG2	2.19	0.42
1:L:23:LYS:C	1:L:25:ARG:H	2.23	0.42
1:L:44:ILE:O	1:L:48:VAL:HG23	2.20	0.42
1:L:261:ILE:HD11	1:L:317:ILE:HG23	2.00	0.42
1:H:212:ASN:HB2	1:H:244:TYR:CE2	2.55	0.42
1:L:276:ARG:HA	1:L:276:ARG:HD3	1.93	0.42
1:L:282:ASN:HD22	1:L:282:ASN:HA	1.70	0.42
1:A:277:LEU:HD22	1:A:312:GLN:NE2	2.35	0.41
1:H:200:VAL:CG1	1:H:201:LYS:N	2.82	0.41
1:D:278:LEU:HD12	1:D:310:ILE:HA	2.01	0.41
1:H:186:LEU:HB2	1:H:193:PHE:CE1	2.55	0.41
1:D:332:GLU:C	1:D:334:HIS:N	2.72	0.41
1:H:156:GLY:HA3	1:H:282:ASN:ND2	2.34	0.41
1:L:212:ASN:HB2	1:L:244:TYR:CE2	2.55	0.41
1:A:28:GLY:HA2	3:A:502:A37:C11	2.50	0.41
1:H:198:LYS:HE3	1:H:198:LYS:HB2	1.76	0.41
1:H:261:ILE:HD11	1:H:317:ILE:HG23	2.01	0.41
1:A:332:GLU:C	1:A:334:HIS:N	2.74	0.41
1:A:49:ARG:O	1:A:50:LYS:HB2	2.20	0.41
1:L:200:VAL:CG1	1:L:201:LYS:N	2.83	0.41
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.90	0.41
1:D:37:LEU:HD21	1:D:136:PHE:CG	2.56	0.41
1:H:131:SER:HB2	1:H:250:ALA:HB2	2.02	0.41
1:D:33:LEU:CD2	1:D:91:THR:HG23	2.51	0.41
1:D:320:SER:HA	1:D:321:PRO:HD3	1.91	0.41
1:H:23:LYS:C	1:H:25:ARG:H	2.22	0.41
1:H:277:LEU:HD22	1:H:312:GLN:NE2	2.36	0.41
1:H:314:ALA:HA	1:H:315:PRO:HD3	1.84	0.41
1:A:235:ASP:OD2	1:A:237:SER:HB3	2.22	0.41
1:L:276:ARG:O	1:L:280:GLU:HB2	2.21	0.41
1:D:94:LEU:HD23	1:D:115:VAL:HB	2.03	0.40
1:D:198:LYS:O	1:D:199:ASP:C	2.59	0.40
1:H:332:GLU:C	1:H:334:HIS:N	2.74	0.40
1:A:196:VAL:HG12	1:D:57:TYR:CE2	2.56	0.40
1:A:230:LYS:HE2	1:A:240:TYR:CE2	2.57	0.40
1:A:261:ILE:HD11	1:A:317:ILE:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:329:LYS:HB2	1:H:329:LYS:HE2	1.85	0.40
1:L:230:LYS:HE2	1:L:240:TYR:CE2	2.57	0.40
1:A:37:LEU:HD21	1:A:136:PHE:CG	2.56	0.40
1:A:57:TYR:CE2	1:D:196:VAL:HG12	2.56	0.40
1:D:156:GLY:HA3	1:D:282:ASN:ND2	2.36	0.40
1:A:186:LEU:HB2	1:A:193:PHE:CE1	2.56	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	314/374 (84%)	286 (91%)	22 (7%)	6 (2%)	8 32
1	D	314/374 (84%)	287 (91%)	21 (7%)	6 (2%)	8 32
1	H	314/374 (84%)	289 (92%)	19 (6%)	6 (2%)	8 32
1	L	314/374 (84%)	286 (91%)	22 (7%)	6 (2%)	8 32
All	All	1256/1496 (84%)	1148 (91%)	84 (7%)	24 (2%)	8 32

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ALA
1	A	269	LYS
1	D	51	ALA
1	D	269	LYS
1	H	51	ALA
1	H	269	LYS
1	L	51	ALA
1	L	269	LYS
1	A	333	LYS

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Mol	Chain	Res	Type
1	D	333	LYS
1	H	333	LYS
1	L	333	LYS
1	D	199	ASP
1	D	267	ASN
1	L	199	ASP
1	A	199	ASP
1	A	267	ASN
1	H	199	ASP
1	H	267	ASN
1	L	267	ASN
1	A	321	PRO
1	D	321	PRO
1	H	321	PRO
1	L	321	PRO

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	264/311 (85%)	260 (98%)	4 (2%)	65	85
1	D	264/311 (85%)	260 (98%)	4 (2%)	65	85
1	H	264/311 (85%)	260 (98%)	4 (2%)	65	85
1	L	264/311 (85%)	261 (99%)	3 (1%)	73	89
All	All	1056/1244 (85%)	1041 (99%)	15 (1%)	67	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	144	THR
1	A	197	ASP
1	A	282	ASN
1	D	144	THR
1	D	197	ASP

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Mol	Chain	Res	Type
1	D	276	ARG
1	D	282	ASN
1	H	144	THR
1	H	197	ASP
1	H	276	ARG
1	H	282	ASN
1	L	144	THR
1	L	197	ASP
1	L	282	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	158	ASN
1	A	228	GLN
1	A	282	ASN
1	D	35	ASN
1	D	158	ASN
1	D	228	GLN
1	D	282	ASN
1	H	35	ASN
1	H	158	ASN
1	H	228	GLN
1	H	282	ASN
1	L	35	ASN
1	L	158	ASN
1	L	228	GLN
1	L	282	ASN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	A37	D	602	-	21,24,24	3.71	14 (66%)	28,36,36	0.98	0
3	A37	A	502	-	21,24,24	3.77	12 (57%)	28,36,36	0.91	1 (3%)
3	A37	H	702	-	21,24,24	3.97	14 (66%)	28,36,36	0.86	0
3	A37	L	802	-	21,24,24	4.07	14 (66%)	28,36,36	0.99	1 (3%)

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	A37	D	602	-	-	1/9/11/11	0/3/3/3
3	A37	A	502	-	-	2/9/11/11	0/3/3/3
3	A37	H	702	-	-	1/9/11/11	0/3/3/3
3	A37	L	802	-	-	0/9/11/11	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	802	A37	O9-S	10.11	1.55	1.43
3	A	502	A37	O9-S	9.09	1.53	1.43
3	L	802	A37	O-S	8.82	1.53	1.43
3	H	702	A37	O-S	8.31	1.53	1.43
3	D	602	A37	O9-S	7.54	1.52	1.43
3	H	702	A37	O9-S	6.94	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	A37	O-S	6.35	1.50	1.43
3	H	702	A37	C11-N	6.27	1.53	1.39
3	A	502	A37	C11-N	5.65	1.51	1.39
3	D	602	A37	C11-N	5.59	1.51	1.39
3	L	802	A37	C14-C15	5.45	1.47	1.36
3	D	602	A37	O-S	5.30	1.49	1.43
3	D	602	A37	C4-C5	5.20	1.47	1.39
3	H	702	A37	C4-C5	5.13	1.47	1.39
3	H	702	A37	C14-C15	5.12	1.46	1.36
3	H	702	A37	C5-S	5.07	1.84	1.77
3	L	802	A37	C11-N	4.96	1.50	1.39
3	D	602	A37	C14-C15	4.93	1.46	1.36
3	A	502	A37	S-N	4.88	1.71	1.63
3	A	502	A37	C4-C3	4.70	1.46	1.38
3	D	602	A37	C5-S	4.49	1.84	1.77
3	H	702	A37	C18-C17	4.33	1.45	1.36
3	L	802	A37	C18-C17	4.28	1.45	1.36
3	A	502	A37	C14-C15	4.16	1.44	1.36
3	L	802	A37	C4-C5	4.08	1.45	1.39
3	L	802	A37	C4-C3	4.00	1.44	1.38
3	H	702	A37	C11-N12	3.95	1.40	1.35
3	D	602	A37	C18-C17	3.90	1.44	1.36
3	A	502	A37	C18-C17	3.89	1.44	1.36
3	A	502	A37	C4-C5	3.79	1.45	1.39
3	D	602	A37	C2-C	3.77	1.45	1.38
3	H	702	A37	S-N	3.73	1.69	1.63
3	A	502	A37	C2-C	3.57	1.45	1.38
3	L	802	A37	C2-C	3.53	1.45	1.38
3	D	602	A37	C4-C3	3.50	1.44	1.38
3	D	602	A37	C11-N12	3.38	1.39	1.35
3	D	602	A37	C6-C5	3.35	1.44	1.40
3	H	702	A37	C4-C3	3.35	1.43	1.38
3	H	702	A37	C2-C	3.29	1.44	1.38
3	L	802	A37	C11-N12	3.27	1.39	1.35
3	D	602	A37	S-N	3.23	1.69	1.63
3	A	502	A37	C17-C15	3.16	1.44	1.38
3	L	802	A37	S-N	3.09	1.68	1.63
3	A	502	A37	C-C6	3.04	1.45	1.38
3	L	802	A37	C17-C15	2.80	1.43	1.38
3	A	502	A37	C11-N12	2.79	1.38	1.35
3	D	602	A37	C2-C3	2.77	1.43	1.38
3	D	602	A37	C17-C15	2.74	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	702	A37	C6-C5	2.62	1.43	1.40
3	H	702	A37	C17-C15	2.39	1.42	1.38
3	L	802	A37	C-C6	2.18	1.43	1.38
3	L	802	A37	C5-S	2.18	1.80	1.77
3	H	702	A37	C2-C3	2.13	1.42	1.38
3	L	802	A37	C13-C19	2.03	1.49	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	802	A37	C5-S-N	2.64	110.36	107.27
3	A	502	A37	O9-S-O	-2.48	116.50	119.55

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	602	A37	C11-N-S-O
3	H	702	A37	C11-N-S-O
3	A	502	A37	C11-N-S-O9
3	A	502	A37	C11-N-S-O

There are no ring outliers.

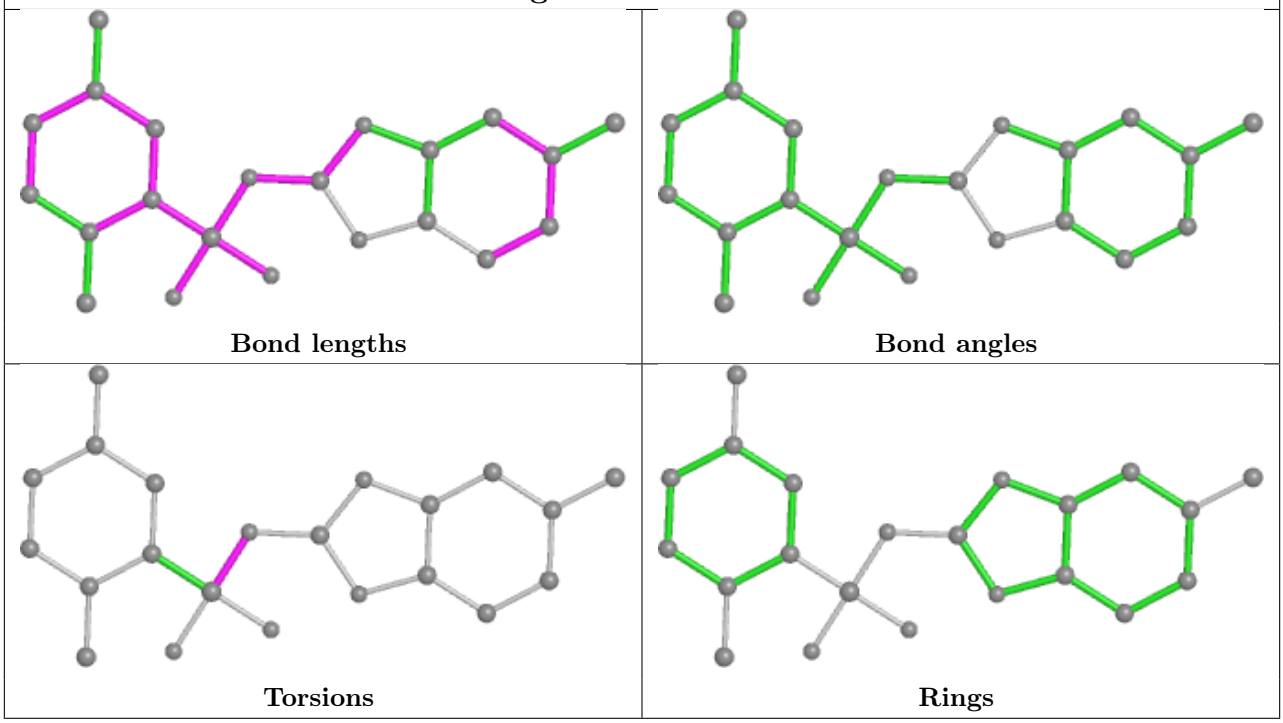
4 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	A37	8	0
3	A	502	A37	8	0
3	H	702	A37	8	0
3	L	802	A37	8	0

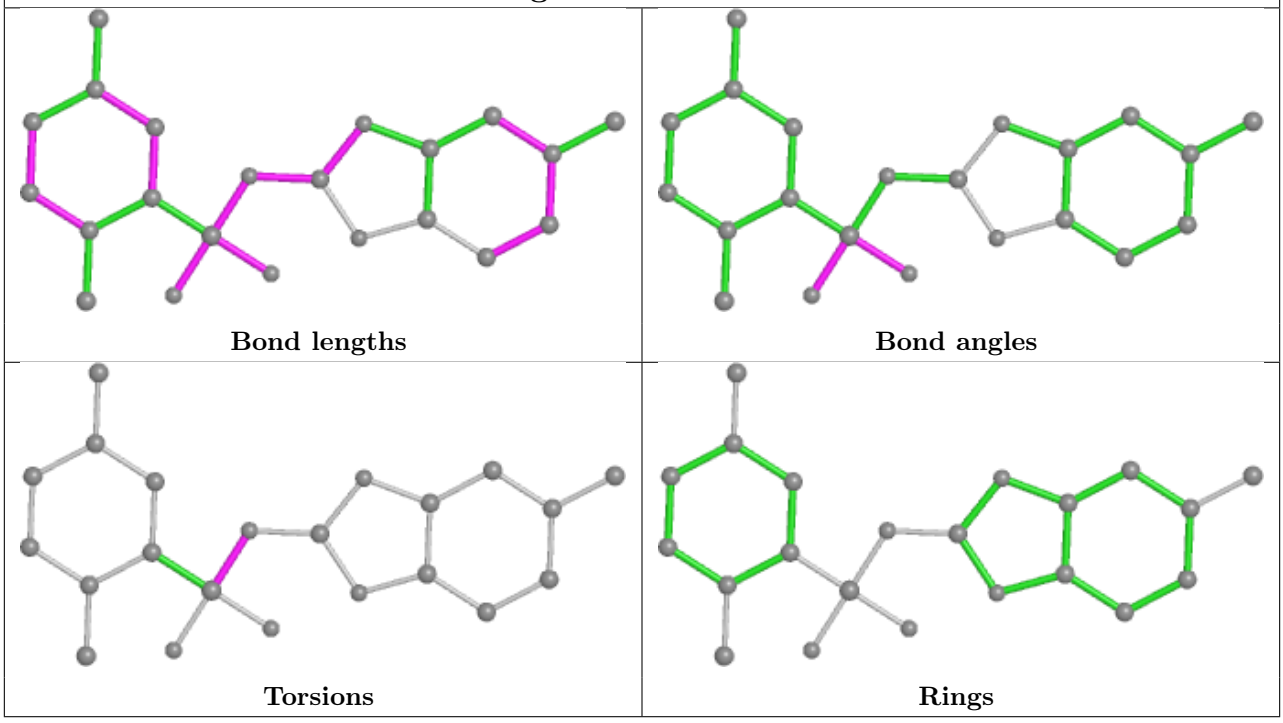
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

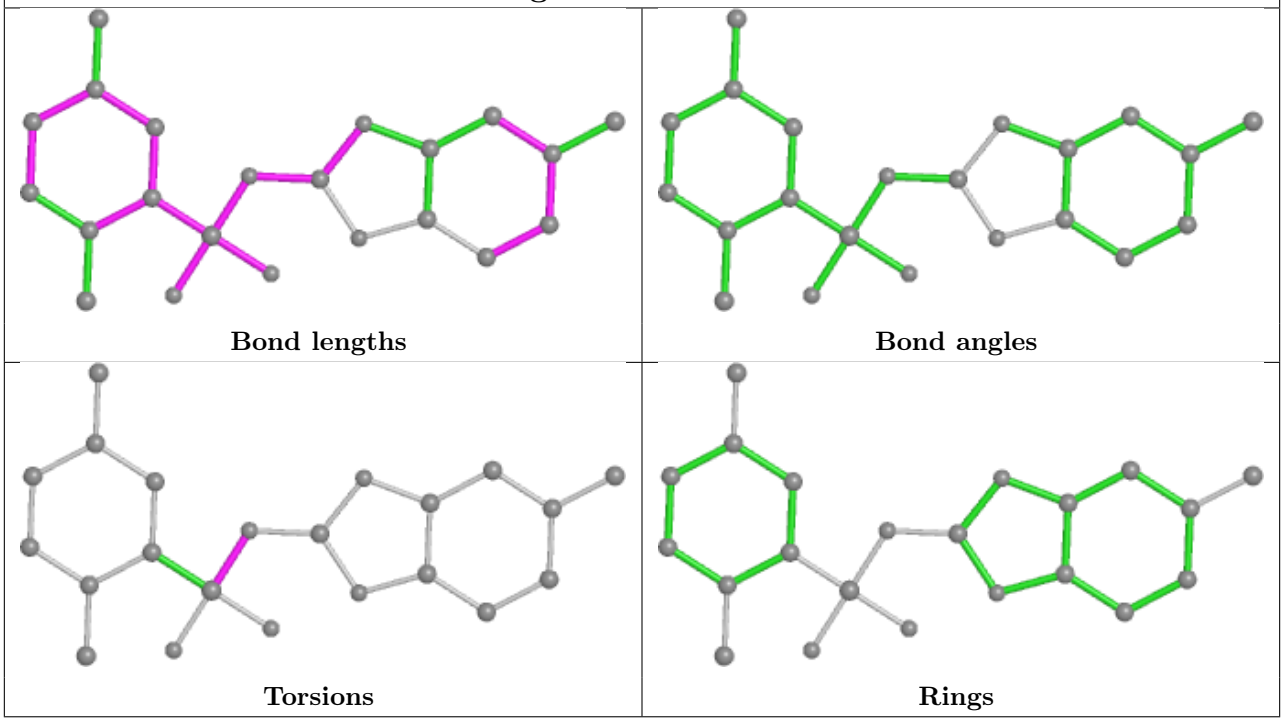
Ligand A37 D 602



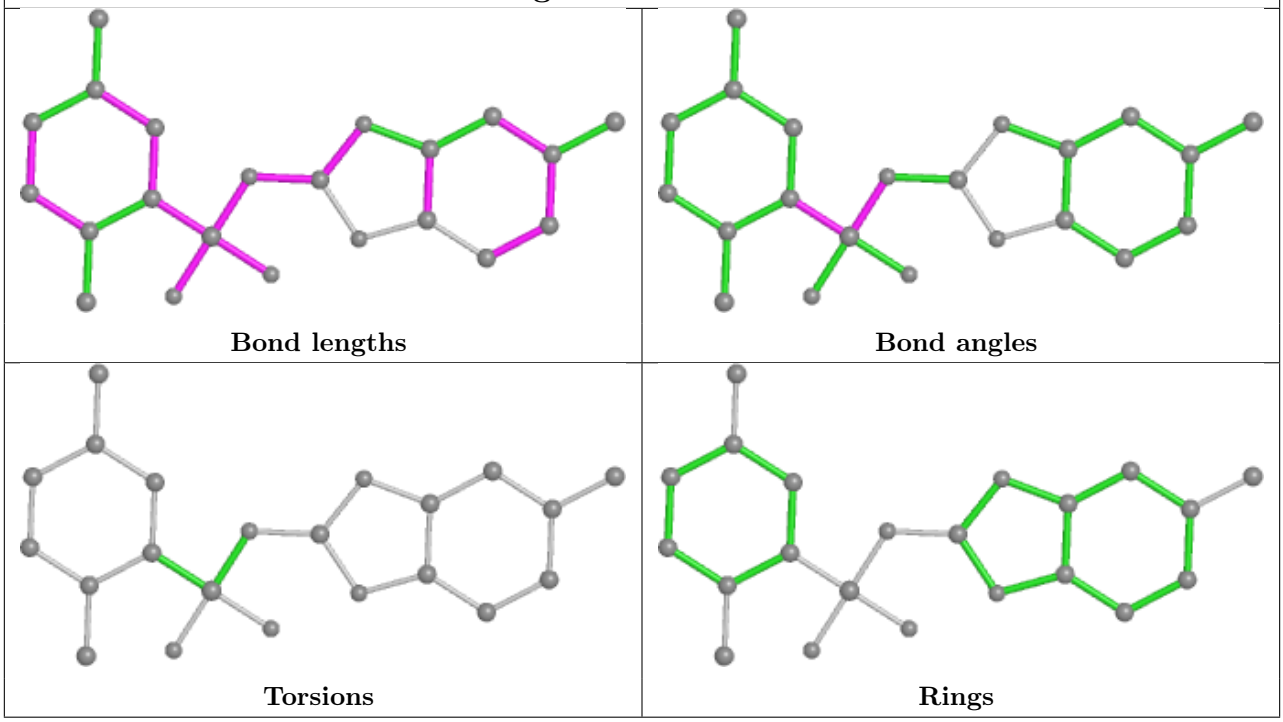
Ligand A37 A 502



Ligand A37 H 702



Ligand A37 L 802



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.