Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 04:29 PM EST

PDB ID	:	3FBP
Title	:	STRUCTURE REFINEMENT OF FRUCTOSE-1,6-BISPHOSPHATASE AND ITS FRUCTOSE 2,6-BISPHOSPHATE COMPLEX AT 2.8 ANGSTROMS RESOLUTION
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Deposited on	:	1990-06-07
Resolution	:	2.80 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:

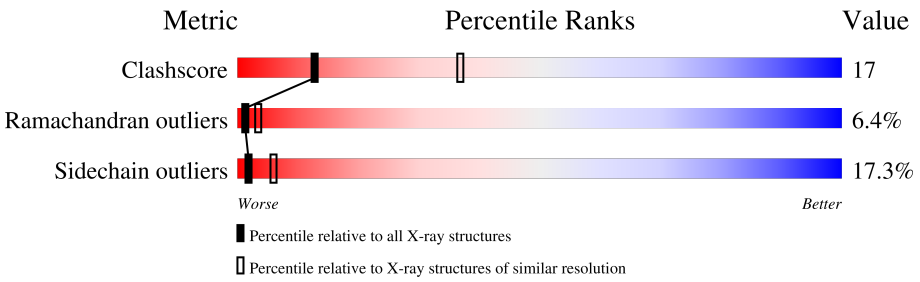
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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	335	48% 32% 11% • 6%
1	B	335	45% 35% 10% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5978 atoms, of which 1080 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.

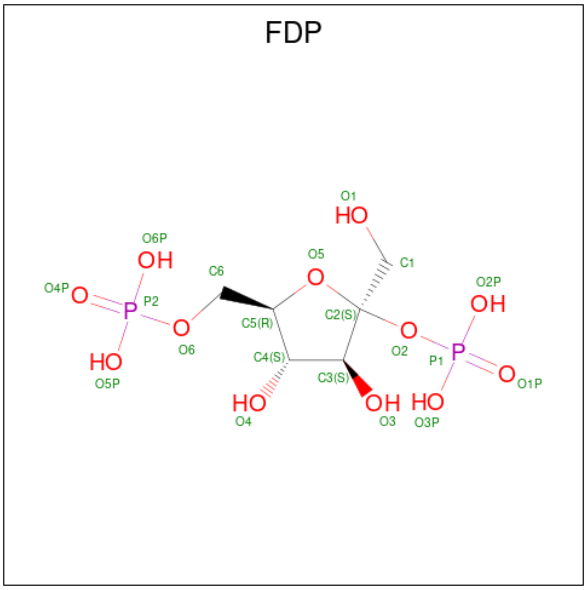
- Molecule 1 is a protein called FRUCTOSE 1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	316	2967	1546	538	408	460	15	0	0	0
1	B	316	2967	1546	538	408	460	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	conflict	UNP P00636
A	96	THR	SER	conflict	UNP P00636
A	199	ASN	ASP	conflict	UNP P00636
B	20	GLN	GLU	conflict	UNP P00636
B	96	THR	SER	conflict	UNP P00636
B	199	ASN	ASP	conflict	UNP P00636

- Molecule 2 is 2,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FDP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
2	A	1	22	6	2	12	2	0	0
			Total	C	H	O	P		
2	B	1	22	6	2	12	2	0	0

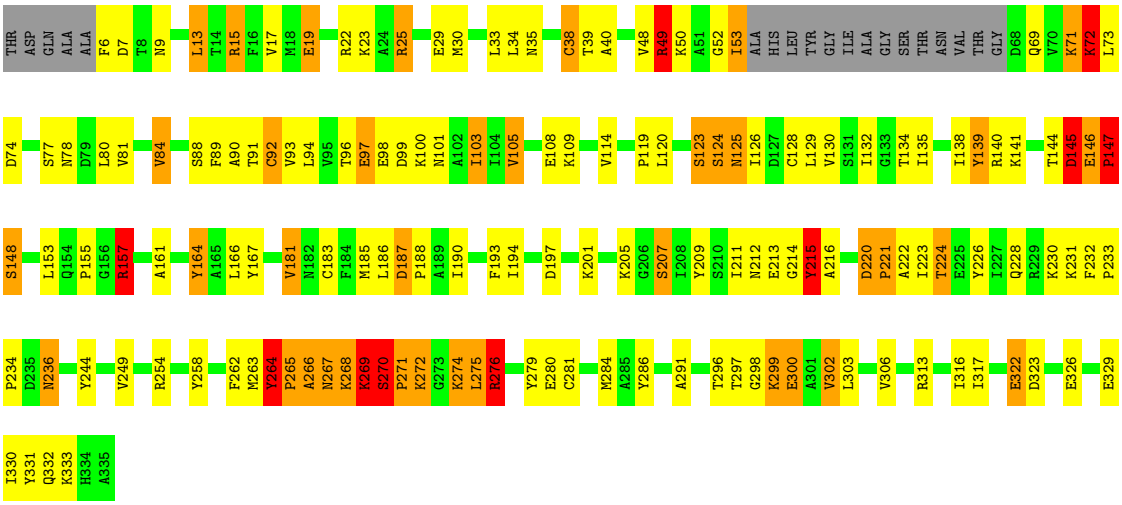
3 Residue-property plots (i)

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

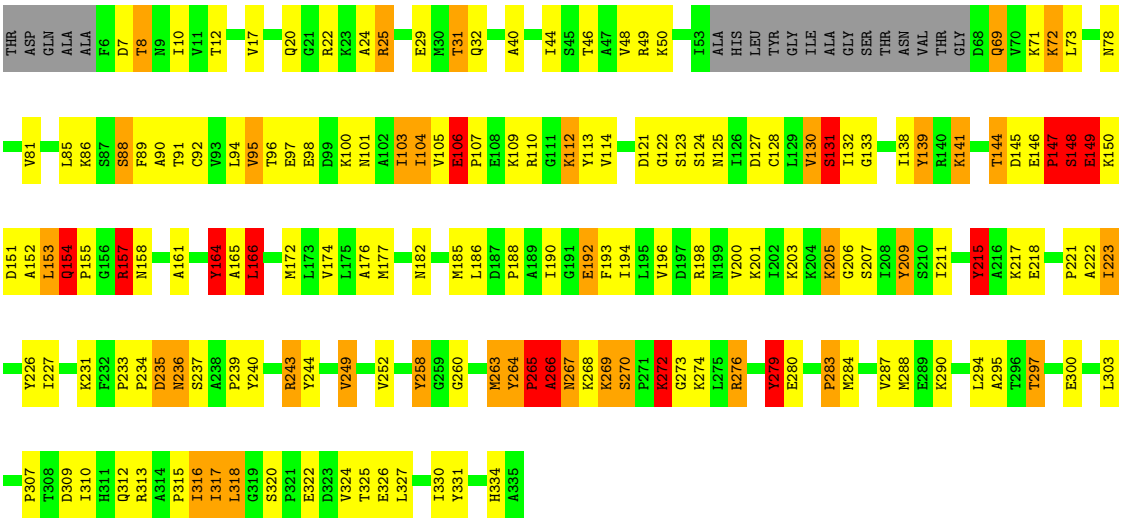
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain A: 48% 32% 11% • 6%



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain B: 45% 35% 10% • 6%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.60Å 131.60Å 68.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5978	wwPDB-VP
Average B, all atoms ($Å^2$)	24.0	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: FDP

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	0.87	0/2469	1.77	53/3337 (1.6%)
1	B	0.85	0/2469	1.77	44/3337 (1.3%)
All	All	0.86	0/4938	1.77	97/6674 (1.5%)

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	10
1	B	0	10
All	All	0	20

There are no bond length outliers.

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	B	276	ARG	NE-CZ-NH2	-10.98	114.81	120.30
1	B	215	TYR	CB-CG-CD2	-10.27	114.84	121.00
1	B	276	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	215	TYR	CB-CG-CD1	8.98	126.39	121.00
1	A	268	LYS	CA-C-N	-8.85	97.73	117.20
1	B	269	LYS	N-CA-C	-8.80	87.23	111.00
1	B	196	VAL	CA-CB-CG2	-8.38	98.33	110.90
1	B	258	TYR	CB-CG-CD2	-8.33	116.00	121.00
1	B	164	TYR	CB-CG-CD2	-8.13	116.12	121.00
1	A	215	TYR	CA-CB-CG	8.04	128.67	113.40
1	B	266	ALA	N-CA-C	7.88	132.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	264	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	B	272	LYS	CA-C-N	-7.69	100.82	116.20
1	A	49	ARG	CA-CB-CG	7.68	130.29	113.40
1	A	215	TYR	CB-CG-CD2	-7.65	116.41	121.00
1	B	8	THR	N-CA-C	7.62	131.57	111.00
1	A	49	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	B	334	HIS	CA-CB-CG	-7.51	100.84	113.60
1	A	15	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	25	ARG	CA-CB-CG	7.49	129.88	113.40
1	B	334	HIS	N-CA-C	7.46	131.13	111.00
1	B	149	GLU	N-CA-C	7.44	131.10	111.00
1	A	153	LEU	CA-C-N	-7.12	101.55	117.20
1	B	270	SER	N-CA-C	7.07	130.07	111.00
1	B	166	LEU	CA-CB-CG	7.06	131.53	115.30
1	A	269	LYS	N-CA-C	-6.92	92.32	111.00
1	A	284	MET	CG-SD-CE	-6.70	89.47	100.20
1	A	13	LEU	CB-CG-CD1	-6.67	99.67	111.00
1	A	30	MET	CG-SD-CE	-6.59	89.66	100.20
1	A	9	ASN	N-CA-C	-6.56	93.29	111.00
1	B	157	ARG	CA-CB-CG	6.49	127.67	113.40
1	A	25	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	13	LEU	CB-CA-C	-6.41	98.02	110.20
1	A	145	ASP	CA-C-N	-6.41	103.10	117.20
1	B	146	GLU	CA-CB-CG	6.40	127.48	113.40
1	B	88	SER	N-CA-C	-6.38	93.78	111.00
1	A	92	CYS	CA-CB-SG	6.34	125.41	114.00
1	A	157	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	53	ILE	N-CA-C	-6.25	94.13	111.00
1	A	266	ALA	N-CA-C	6.24	127.85	111.00
1	A	187	ASP	CB-CG-OD1	6.20	123.88	118.30
1	B	106	GLU	OE1-CD-OE2	-6.08	116.00	123.30
1	A	213	GLU	CA-CB-CG	-6.02	100.15	113.40
1	B	318	LEU	CA-CB-CG	6.02	129.14	115.30
1	A	124	SER	CA-C-N	-5.99	104.02	117.20
1	A	302	VAL	CA-CB-CG2	-5.97	101.94	110.90
1	A	72	LYS	N-CA-C	5.95	127.08	111.00
1	B	196	VAL	CA-CB-CG1	5.89	119.74	110.90
1	B	215	TYR	CA-C-N	-5.82	104.40	117.20
1	A	268	LYS	O-C-N	5.82	132.01	122.70
1	A	181	VAL	CG1-CB-CG2	-5.79	101.64	110.90
1	B	249	VAL	CG1-CB-CG2	-5.75	101.69	110.90
1	B	205	LYS	CA-CB-CG	5.73	126.00	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	153	LEU	O-C-N	5.71	131.83	122.70
1	B	272	LYS	CA-CB-CG	5.68	125.89	113.40
1	A	97	GLU	CA-CB-CG	5.64	125.80	113.40
1	B	149	GLU	CA-C-N	5.61	129.54	117.20
1	B	25	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	276	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	A	274	LYS	N-CA-C	-5.54	96.04	111.00
1	A	13	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	271	PRO	CA-C-N	-5.44	105.24	117.20
1	B	209	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	A	69	GLN	N-CA-C	5.42	125.63	111.00
1	A	15	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	31	THR	CA-C-N	5.38	129.03	117.20
1	B	264	TYR	CA-CB-CG	-5.36	103.21	113.40
1	B	7	ASP	N-CA-CB	-5.35	100.96	110.60
1	B	22	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	105	VAL	CA-CB-CG2	-5.33	102.91	110.90
1	B	7	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	270	SER	N-CA-CB	-5.30	102.54	110.50
1	A	303	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	220	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	243	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	49	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	185	MET	CG-SD-CE	-5.25	91.79	100.20
1	A	302	VAL	CA-CB-CG1	5.25	118.78	110.90
1	B	112	LYS	CA-CB-CG	5.24	124.93	113.40
1	A	139	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	A	164	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	B	288	MET	CG-SD-CE	-5.23	91.83	100.20
1	A	281	CYS	CA-CB-SG	-5.22	104.61	114.00
1	A	276	ARG	CA-C-N	-5.21	105.73	117.20
1	A	39	THR	CA-CB-CG2	5.18	119.65	112.40
1	B	17	VAL	CA-CB-CG2	-5.17	103.15	110.90
1	A	38	CYS	CA-CB-SG	-5.11	104.79	114.00
1	B	263	MET	CA-C-N	-5.11	105.97	117.20
1	B	263	MET	CG-SD-CE	-5.09	92.06	100.20
1	A	207	SER	CA-C-N	5.07	128.36	117.20
1	A	88	SER	N-CA-C	-5.05	97.38	111.00
1	A	276	ARG	CG-CD-NE	5.04	122.38	111.80
1	A	272	LYS	CA-C-N	-5.04	106.13	116.20
1	A	148	SER	N-CA-CB	-5.03	102.96	110.50
1	B	300	GLU	CA-CB-CG	5.02	124.45	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	317	ILE	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	GLU	Peptide
1	A	193	PHE	Sidechain
1	A	209	TYR	Sidechain
1	A	258	TYR	Sidechain
1	A	262	PHE	Sidechain
1	A	264	TYR	Sidechain
1	A	270	SER	Peptide
1	A	279	TYR	Sidechain
1	A	286	TYR	Sidechain
1	A	6	PHE	Peptide
1	B	106	GLU	Peptide
1	B	139	TYR	Sidechain
1	B	164	TYR	Sidechain
1	B	209	TYR	Sidechain
1	B	215	TYR	Sidechain
1	B	226	TYR	Sidechain
1	B	240	TYR	Sidechain
1	B	244	TYR	Sidechain
1	B	270	SER	Peptide
1	B	279	TYR	Sidechain

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	2429	538	2486	84	0
1	B	2429	538	2486	89	0
2	A	20	2	10	2	0
2	B	20	2	10	0	0
All	All	4898	1080	4992	164	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 17.

All (164) 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:A:141:LYS:HE3	1:A:148:SER:HA	1.45	0.96
1:A:270:SER:HA	1:A:272:LYS:HG3	1.55	0.88
1:A:188:PRO:HD2	1:B:50:LYS:HD3	1.65	0.78
1:B:223:ILE:HD13	1:B:265:PRO:HG3	1.65	0.76
1:B:94:LEU:HB2	1:B:103:ILE:HG23	1.69	0.74
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.71	0.72
1:B:176:ALA:HB2	1:B:287:VAL:HG22	1.69	0.72
1:B:96:THR:HG22	1:B:98:GLU:N	2.04	0.71
1:B:190:ILE:HD11	1:B:194:ILE:HD11	1.72	0.70
1:A:96:THR:HG23	1:A:119:PRO:HD3	1.73	0.70
1:A:329:GLU:O	1:A:332:GLN:HG2	1.92	0.70
1:B:104:ILE:HG13	1:B:149:GLU:HG3	1.73	0.70
1:A:183:CYS:HB2	1:A:197:ASP:HB3	1.75	0.68
1:A:80:LEU:O	1:A:84:VAL:HB	1.94	0.68
1:B:130:VAL:HG13	1:B:131:SER:H	1.58	0.67
1:A:91:THR:HG23	1:A:105:VAL:HG21	1.77	0.65
1:A:221:PRO:HD2	1:A:223:ILE:HD12	1.79	0.65
1:B:269:LYS:O	1:B:272:LYS:HA	1.96	0.65
1:B:107:PRO:HA	1:B:110:ARG:HD2	1.79	0.65
1:B:166:LEU:HD23	1:B:249:VAL:HG12	1.80	0.63
1:A:187:ASP:HB2	1:A:194:ILE:HD12	1.79	0.63
1:B:29:GLU:HB2	1:B:113:TYR:HE1	1.63	0.63
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.80	0.62
1:A:223:ILE:HD11	1:A:265:PRO:HG2	1.82	0.62
1:A:215:TYR:HD1	1:A:216:ALA:H	1.48	0.62
1:B:40:ALA:O	1:B:44:ILE:HG13	2.00	0.61
1:B:69:GLN:HG2	1:B:72:LYS:HB2	1.83	0.61
1:A:215:TYR:HD1	1:A:216:ALA:N	1.99	0.61
1:B:81:VAL:O	1:B:85:LEU:HG	2.01	0.61
1:A:96:THR:HG22	1:A:98:GLU:H	1.65	0.60
1:A:129:LEU:HD11	1:B:172:MET:HB2	1.84	0.60
1:A:190:ILE:HD11	1:A:194:ILE:HD11	1.84	0.60
1:A:52:GLY:O	1:A:53:ILE:HG13	2.01	0.60
1:A:267:ASN:HA	1:A:272:LYS:HG2	1.82	0.60
1:A:329:GLU:HA	1:A:332:GLN:NE2	2.18	0.59
1:B:316:ILE:HD12	1:B:318:LEU:HD23	1.84	0.58
1:B:264:TYR:HD2	1:B:273:GLY:HA2	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:HD3	1:A:306:VAL:HG22	1.84	0.58
1:B:252:VAL:HG11	1:B:284:MET:SD	2.43	0.58
1:B:91:THR:HG23	1:B:105:VAL:HG21	1.87	0.57
1:A:94:LEU:HD12	1:A:103:ILE:HD11	1.88	0.56
1:A:276:ARG:NH2	2:A:336:FDP:H11	2.21	0.56
1:B:264:TYR:CD2	1:B:273:GLY:HA2	2.40	0.56
1:B:205:LYS:NZ	1:B:322:GLU:HB3	2.20	0.56
1:B:153:LEU:HD21	1:B:310:ILE:HG22	1.88	0.56
1:A:329:GLU:HA	1:A:332:GLN:HE21	1.70	0.55
1:A:13:LEU:CD1	1:A:38:CYS:SG	2.95	0.55
1:B:252:VAL:HG22	1:B:318:LEU:HD11	1.89	0.55
1:A:269:LYS:O	1:A:272:LYS:HA	2.07	0.55
1:B:231:LYS:O	1:B:239:PRO:HB3	2.07	0.55
1:B:233:PRO:HG3	1:B:239:PRO:HD3	1.88	0.55
1:A:40:ALA:HA	1:A:80:LEU:HD22	1.89	0.54
1:A:92:CYS:HA	1:A:105:VAL:HB	1.88	0.54
1:B:92:CYS:HA	1:B:105:VAL:HB	1.90	0.54
1:B:309:ASP:O	1:B:312:GLN:HB2	2.08	0.54
1:A:223:ILE:CD1	1:A:265:PRO:HG2	2.38	0.54
1:B:12:THR:HG22	1:B:192:GLU:HG2	1.90	0.53
1:A:181:VAL:HG21	1:A:291:ALA:HB2	1.91	0.53
1:A:71:LYS:H	1:A:71:LYS:HD2	1.73	0.53
1:A:267:ASN:OD1	1:A:268:LYS:NZ	2.39	0.52
1:A:78:ASN:OD1	1:A:96:THR:HG21	2.08	0.52
1:B:89:PHE:HD2	1:B:109:LYS:HA	1.75	0.52
1:A:132:ILE:HG13	1:A:167:TYR:HB2	1.91	0.52
1:B:205:LYS:HZ1	1:B:322:GLU:HB3	1.75	0.52
1:B:186:LEU:O	1:B:188:PRO:HD3	2.10	0.52
1:B:91:THR:O	1:B:110:ARG:HA	2.11	0.51
1:A:145:ASP:CG	1:A:147:PRO:HA	2.32	0.50
1:B:235:ASP:CG	1:B:236:ASN:H	2.15	0.50
1:A:96:THR:HG22	1:A:98:GLU:N	2.27	0.50
1:A:129:LEU:HD12	1:B:166:LEU:HD12	1.94	0.49
1:A:215:TYR:CD1	1:A:216:ALA:N	2.80	0.49
1:B:211:ILE:HD13	1:B:227:ILE:HD11	1.93	0.49
1:B:157:ARG:O	1:B:157:ARG:HG3	2.12	0.49
1:A:254:ARG:HA	1:B:128:CYS:HB2	1.95	0.49
1:B:104:ILE:HG21	1:B:149:GLU:OE2	2.11	0.49
1:A:244:TYR:HE2	1:B:243:ARG:NH1	2.11	0.48
1:A:94:LEU:HB2	1:A:103:ILE:HG13	1.95	0.48
1:A:96:THR:HG22	1:A:97:GLU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ALA:HB2	1:A:84:VAL:HG11	1.95	0.48
1:B:206:GLY:HA3	1:B:260:GLY:N	2.28	0.48
1:B:269:LYS:HD3	1:B:274:LYS:HB2	1.95	0.48
1:A:231:LYS:O	1:A:233:PRO:HD3	2.14	0.48
1:B:86:LYS:HA	1:B:91:THR:CG2	2.43	0.48
1:B:185:MET:O	1:B:193:PHE:HA	2.13	0.48
1:B:125:ASN:HB3	1:B:130:VAL:HG11	1.95	0.47
1:B:266:ALA:HB1	1:B:269:LYS:HB2	1.96	0.47
1:A:48:VAL:HG11	1:A:132:ILE:HD11	1.97	0.47
1:B:48:VAL:HG22	1:B:73:LEU:HD21	1.95	0.47
1:B:141:LYS:HE2	1:B:148:SER:HB3	1.97	0.47
1:A:268:LYS:HD3	1:A:268:LYS:HA	1.60	0.47
1:B:157:ARG:HD3	1:B:303:LEU:HD13	1.97	0.47
1:B:294:LEU:O	1:B:318:LEU:HA	2.15	0.47
1:B:233:PRO:HA	1:B:234:PRO:HD3	1.82	0.47
1:A:93:VAL:HB	1:A:114:VAL:HG22	1.96	0.47
1:B:133:GLY:HA3	1:B:249:VAL:HG21	1.97	0.47
1:B:154:GLN:HB2	1:B:307:PRO:HB2	1.97	0.47
1:B:203:LYS:HG2	1:B:205:LYS:O	2.15	0.47
1:A:296:THR:HG22	1:A:298:GLY:H	1.80	0.46
1:B:267:ASN:HA	1:B:272:LYS:NZ	2.30	0.46
1:B:100:LYS:O	1:B:310:ILE:HD11	2.15	0.46
1:B:133:GLY:HA3	1:B:165:ALA:O	2.16	0.46
1:A:128:CYS:HG	1:B:258:TYR:HE2	1.63	0.46
1:B:122:GLY:HA3	1:B:132:ILE:HG22	1.97	0.46
1:B:268:LYS:HA	1:B:268:LYS:HD2	1.67	0.46
1:A:29:GLU:HG2	1:A:90:ALA:HA	1.97	0.46
1:A:297:THR:HB	1:A:300:GLU:O	2.16	0.46
1:B:88:SER:O	1:B:90:ALA:N	2.49	0.46
1:B:297:THR:HG22	1:B:315:PRO:HG2	1.97	0.46
1:A:120:LEU:HD23	1:A:123:SER:HB3	1.98	0.45
1:A:214:GLY:O	1:A:216:ALA:N	2.49	0.45
1:A:77:SER:O	1:A:81:VAL:HG23	2.17	0.45
1:B:110:ARG:HH12	1:B:147:PRO:HB3	1.82	0.45
1:B:95:VAL:HG22	1:B:153:LEU:HD12	1.99	0.45
1:B:279:TYR:O	1:B:283:PRO:HD2	2.17	0.45
1:A:124:SER:O	1:A:125:ASN:HB2	2.16	0.44
1:B:166:LEU:CD2	1:B:249:VAL:HG12	2.46	0.44
1:A:212:ASN:HB2	1:A:244:TYR:CZ	2.51	0.44
1:A:114:VAL:HB	1:A:139:TYR:HB2	1.98	0.44
1:A:157:ARG:NH1	1:A:157:ARG:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:TYR:HB2	1:A:330:ILE:HD12	1.99	0.44
1:A:49:ARG:HD2	1:B:49:ARG:NH1	2.32	0.44
1:B:157:ARG:HB2	1:B:303:LEU:HB3	2.00	0.44
1:B:29:GLU:OE1	1:B:112:LYS:NZ	2.51	0.44
1:A:108:GLU:HG2	1:A:109:LYS:HG3	1.99	0.44
1:A:17:VAL:HG11	1:A:34:LEU:HD12	2.00	0.44
1:A:222:ALA:HB1	1:A:330:ILE:HG22	2.00	0.43
1:A:119:PRO:HA	1:A:134:THR:HG23	1.99	0.43
1:A:275:LEU:HD13	1:A:316:ILE:HG22	2.00	0.43
1:B:264:TYR:CE2	1:B:266:ALA:HB2	2.53	0.43
1:A:80:LEU:O	1:A:80:LEU:HD23	2.18	0.43
1:A:332:GLN:HG3	1:A:333:LYS:HG3	2.00	0.43
1:B:200:VAL:O	1:B:201:LYS:NZ	2.52	0.43
1:B:96:THR:HG22	1:B:98:GLU:H	1.79	0.43
1:B:290:LYS:HD3	1:B:290:LYS:HA	1.74	0.43
1:A:19:GLU:OE1	1:A:23:LYS:NZ	2.50	0.43
1:A:128:CYS:SG	1:B:258:TYR:HE2	2.42	0.43
1:B:164:TYR:OH	1:B:174:VAL:HG21	2.19	0.43
1:A:138:ILE:HB	1:A:161:ALA:HB3	2.01	0.43
1:A:164:TYR:CD1	1:A:249:VAL:HG13	2.54	0.43
1:B:12:THR:CG2	1:B:192:GLU:HG2	2.48	0.43
1:A:126:ILE:HG21	1:A:132:ILE:HD13	2.01	0.43
1:B:327:LEU:O	1:B:330:ILE:HB	2.19	0.43
1:B:222:ALA:HB3	1:B:331:TYR:CE1	2.54	0.42
1:B:272:LYS:HB3	1:B:272:LYS:HZ3	1.84	0.42
1:B:266:ALA:CB	1:B:269:LYS:HB2	2.50	0.42
1:A:71:LYS:HG2	1:A:72:LYS:H	1.85	0.41
1:B:203:LYS:HE2	1:B:205:LYS:O	2.20	0.41
1:A:216:ALA:O	1:A:220:ASP:N	2.53	0.41
1:B:294:LEU:HB3	1:B:324:VAL:HG11	2.02	0.41
1:A:89:PHE:HD1	1:A:109:LYS:HA	1.85	0.41
1:A:264:TYR:HB3	1:A:275:LEU:HD11	2.03	0.41
1:A:323:ASP:O	1:A:326:GLU:HB3	2.21	0.41
1:A:276:ARG:HH22	2:A:336:FDP:H11	1.85	0.41
1:A:29:GLU:O	1:A:33:LEU:HB2	2.21	0.41
1:B:78:ASN:OD1	1:B:96:THR:HG21	2.21	0.41
1:A:135:ILE:HG23	1:A:164:TYR:HB3	2.04	0.41
1:B:138:ILE:HD12	1:B:161:ALA:O	2.21	0.41
1:A:205:LYS:HG3	1:A:322:GLU:HB3	2.03	0.40
1:B:89:PHE:CD2	1:B:109:LYS:HA	2.54	0.40
1:B:141:LYS:HG2	1:B:152:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASP:OD2	1:B:50:LYS:NZ	2.53	0.40
1:A:299:LYS:HE3	1:A:299:LYS:HA	2.02	0.40
1:A:263:MET:HB2	1:A:317:ILE:HG12	2.04	0.40
1:B:295:ALA:HA	1:B:317:ILE:O	2.22	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	312/335 (93%)	260 (83%)	33 (11%)	19 (6%)	1 4
1	B	312/335 (93%)	253 (81%)	38 (12%)	21 (7%)	1 3
All	All	624/670 (93%)	513 (82%)	71 (11%)	40 (6%)	1 3

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	LYS
1	A	123	SER
1	A	125	ASN
1	A	147	PRO
1	A	207	SER
1	A	215	TYR
1	A	221	PRO
1	A	224	THR
1	A	266	ALA
1	A	267	ASN
1	A	269	LYS
1	B	8	THR
1	B	131	SER
1	B	144	THR

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Mol	Chain	Res	Type
1	B	150	LYS
1	B	221	PRO
1	B	266	ALA
1	B	267	ASN
1	B	272	LYS
1	A	265	PRO
1	A	274	LYS
1	B	24	ALA
1	B	157	ARG
1	B	223	ILE
1	B	235	ASP
1	A	49	ARG
1	A	234	PRO
1	A	236	ASN
1	A	271	PRO
1	B	130	VAL
1	B	147	PRO
1	B	148	SER
1	B	149	GLU
1	B	72	LYS
1	B	154	GLN
1	A	146	GLU
1	B	280	GLU
1	B	265	PRO
1	A	270	SER
1	B	155	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	266/278 (96%)	226 (85%)	40 (15%)	3 9
1	B	266/278 (96%)	214 (80%)	52 (20%)	1 4
All	All	532/556 (96%)	440 (83%)	92 (17%)	2 6

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	15	ARG
1	A	19	GLU
1	A	25	ARG
1	A	35	ASN
1	A	50	LYS
1	A	71	LYS
1	A	73	LEU
1	A	74	ASP
1	A	84	VAL
1	A	99	ASP
1	A	100	LYS
1	A	101	ASN
1	A	103	ILE
1	A	130	VAL
1	A	140	ARG
1	A	144	THR
1	A	145	ASP
1	A	147	PRO
1	A	157	ARG
1	A	186	LEU
1	A	201	LYS
1	A	211	ILE
1	A	215	TYR
1	A	224	THR
1	A	228	GLN
1	A	230	LYS
1	A	232	PHE
1	A	236	ASN
1	A	264	TYR
1	A	270	SER
1	A	275	LEU
1	A	276	ARG
1	A	280	GLU
1	A	299	LYS
1	A	300	GLU
1	A	302	VAL
1	A	313	ARG
1	A	322	GLU
1	A	331	TYR
1	B	10	ILE
1	B	20	GLN
1	B	25	ARG

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Mol	Chain	Res	Type
1	B	31	THR
1	B	32	GLN
1	B	46	THR
1	B	69	GLN
1	B	71	LYS
1	B	95	VAL
1	B	97	GLU
1	B	101	ASN
1	B	103	ILE
1	B	104	ILE
1	B	106	GLU
1	B	121	ASP
1	B	123	SER
1	B	124	SER
1	B	127	ASP
1	B	131	SER
1	B	141	LYS
1	B	144	THR
1	B	145	ASP
1	B	147	PRO
1	B	148	SER
1	B	151	ASP
1	B	153	LEU
1	B	154	GLN
1	B	157	ARG
1	B	158	ASN
1	B	166	LEU
1	B	177	MET
1	B	182	ASN
1	B	192	GLU
1	B	198	ARG
1	B	207	SER
1	B	215	TYR
1	B	217	LYS
1	B	218	GLU
1	B	236	ASN
1	B	237	SER
1	B	263	MET
1	B	265	PRO
1	B	272	LYS
1	B	276	ARG
1	B	279	TYR

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Mol	Chain	Res	Type
1	B	283	PRO
1	B	297	THR
1	B	313	ARG
1	B	316	ILE
1	B	320	SER
1	B	325	THR
1	B	326	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	B	142	ASN
1	B	154	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FDP	A	336	-	19,20,20	0.65	0	30,32,32	1.14	3 (10%)
2	FDP	B	336	-	19,20,20	0.71	0	30,32,32	1.07	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
2	FDP	A	336	-	-	6/12/34/34	0/1/1/1
2	FDP	B	336	-	-	3/12/34/34	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	336	FDP	P2-O6-C6	2.63	125.55	118.30
2	B	336	FDP	C1-C2-C3	-2.47	107.27	114.56
2	A	336	FDP	C1-C2-C3	-2.31	107.73	114.56
2	A	336	FDP	O5P-P2-O6	2.06	112.22	106.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	336	FDP	O1-C1-C2-O5
2	A	336	FDP	C6-O6-P2-O5P
2	A	336	FDP	C6-O6-P2-O6P
2	B	336	FDP	C6-O6-P2-O4P
2	B	336	FDP	C6-O6-P2-O5P
2	B	336	FDP	C6-O6-P2-O6P
2	A	336	FDP	O1-C1-C2-O2
2	A	336	FDP	O1-C1-C2-C3
2	A	336	FDP	C6-O6-P2-O4P

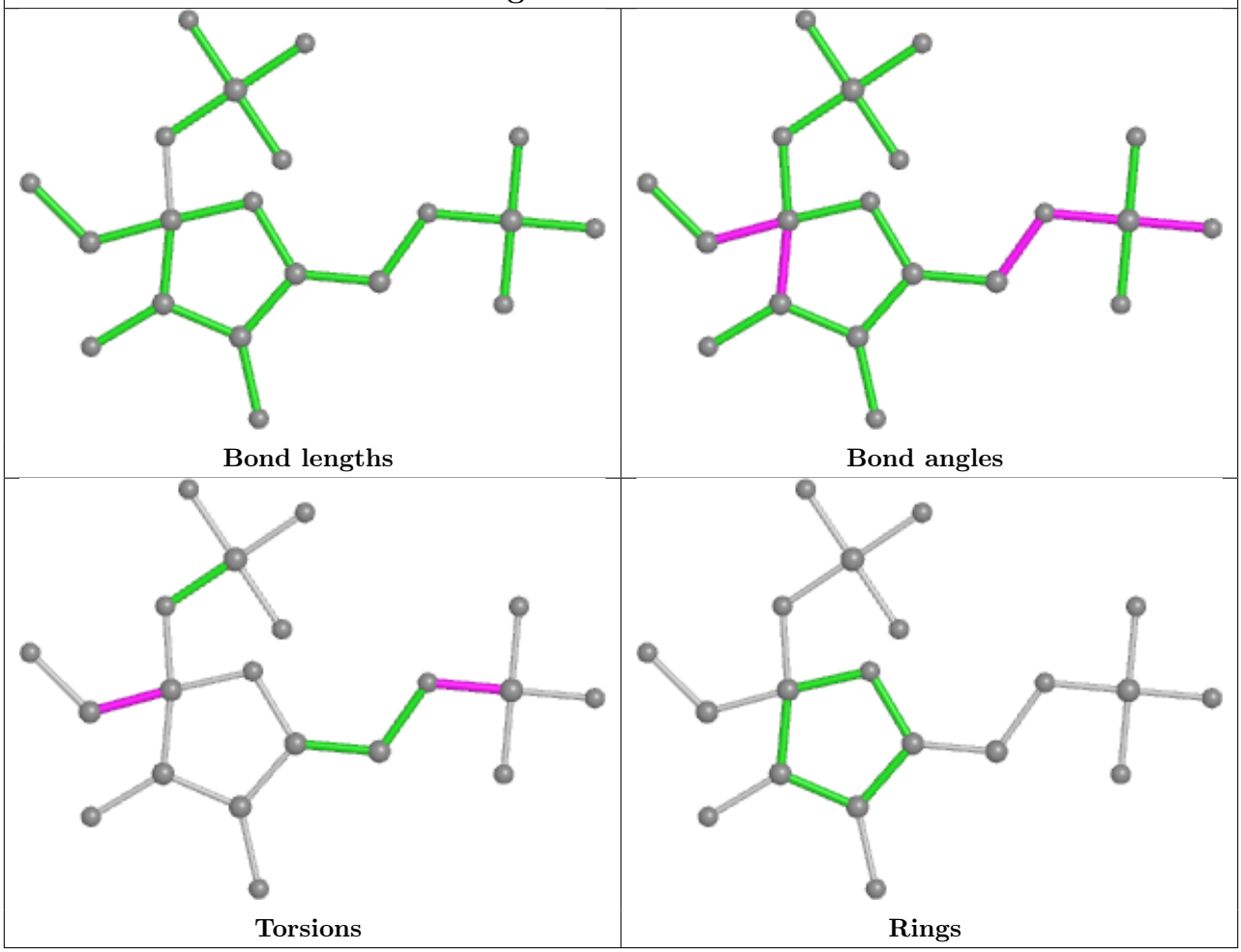
There are no ring outliers.

1 monomer is involved in 2 short contacts:

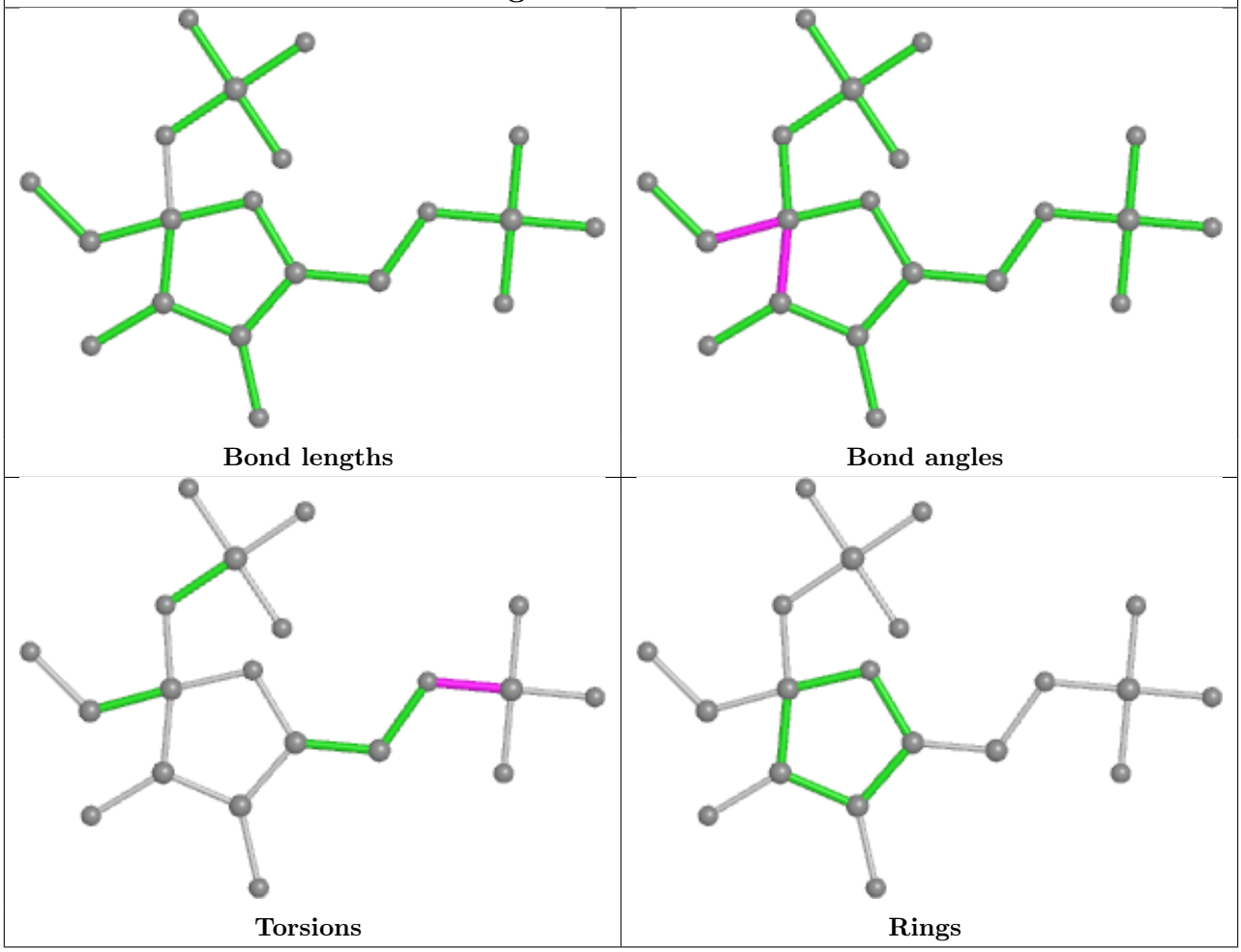
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	336	FDP	2	0

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 FDP A 336



Ligand FDP B 336



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.