Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 09:13 AM EDT

PDB ID	:	1LEV
Title	:	PORCINE KIDNEY FRUCTOSE-1,6-BISPHOSPHATASE COMPLEXED WITH AN AMP-SITE INHIBITOR
Authors	:	Wright, S.W.; Carlo, A.A.; Danley, D.E.; Hageman, D.L.; Karam, G.A.; Mansour, M.N.; McClure, L.D.; Pandit, J.; Schulte, G.K.; Treadway, J.L.; Wang, I.-K.; Bauer, P.H.
Deposited on	:	2002-04-10
Resolution	:	2.15 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 (i)) were used in the production of this report:

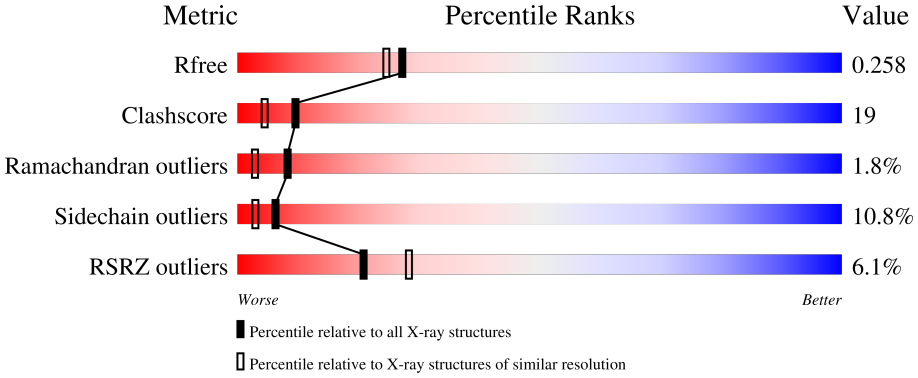
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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% 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	337	6% 58% 27% 6% • 8%
1	F	337	6% 58% 25% 8% • 8%

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
4	CLI	A	342	-	-	X	-
4	CLI	F	339	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4947 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.

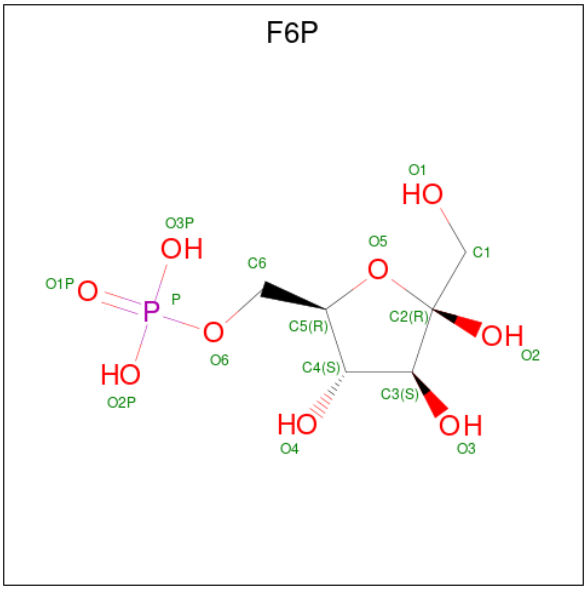
- Molecule 1 is a protein called Fructose-1,6-bisphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	311	2384	1518	401	450	15	0	0	0
1	F	311	2383	1518	400	450	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	THR	SER	conflict	UNP P00636
F	96	THR	SER	conflict	UNP P00636

- Molecule 2 is 6-O-phosphono-beta-D-fructofuranose (three-letter code: F6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	16	6	9	1	0	0

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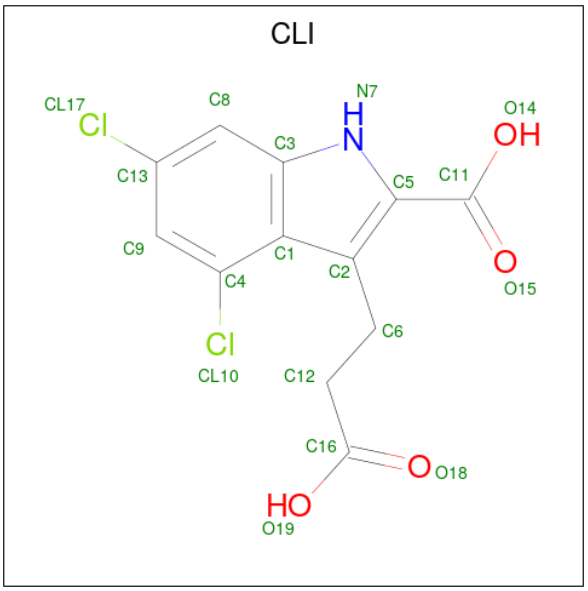
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	F	1	16	6	9	1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	2	2	2	0	0
			Total	Mn		
3	F	2	2	2	0	0

- Molecule 4 is 3-(2-CARBOXY-ETHYL)-4,6-DICHLORO-1H-INDOLE-2-CARBOXYLIC ACID (three-letter code: CLI) (formula: $C_{12}H_9Cl_2NO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
4	A	1	19	12	2	1	4	0	0
			Total	C	Cl	N	O		
4	F	1	19	12	2	1	4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	63	63	63	1	0

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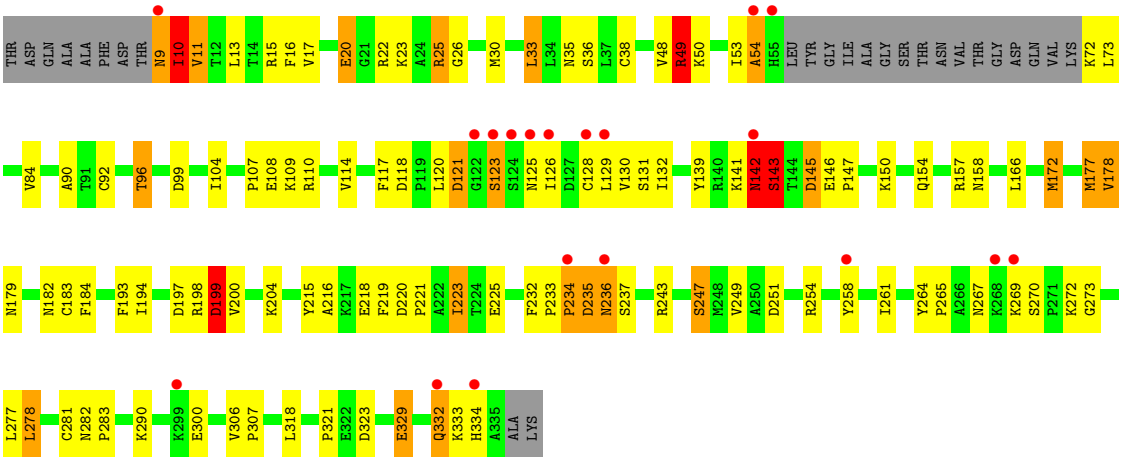
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	F	43	43	43	0	0

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 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.

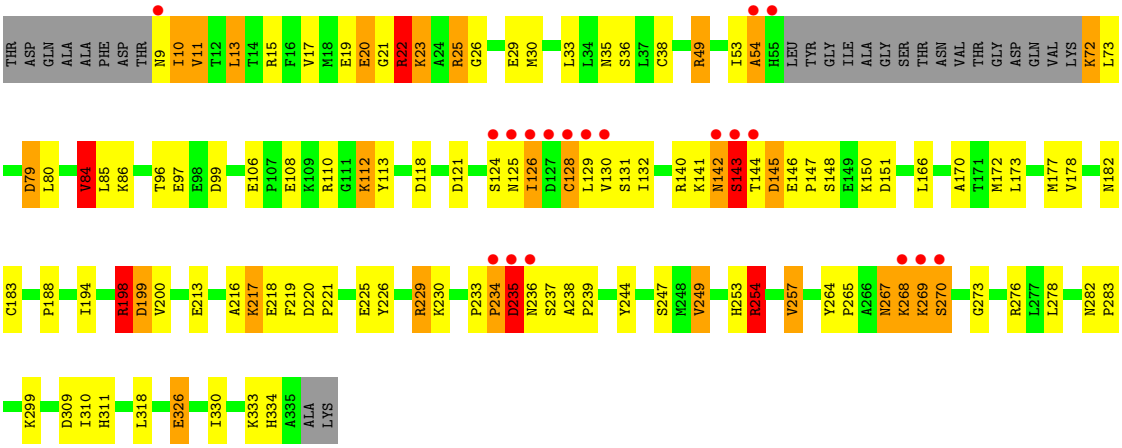
• Molecule 1: Fructose-1,6-bisphosphatase

Chain A: 6% 58% 27% 6% • 8%



• Molecule 1: Fructose-1,6-bisphosphatase

Chain F: 6% 58% 25% 8% • 8%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.87Å 73.45Å 78.03Å 90.00° 106.30° 90.00°	Depositor
Resolution (Å)	40.26 – 2.15 40.26 – 2.15	Depositor EDS
% Data completeness (in resolution range)	93.6 (40.26-2.15) 93.6 (40.26-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.193 , 0.255 0.196 , 0.258	Depositor DCC
R_{free} test set	1639 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4947	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CLI, F6P, MN

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	0.98	1/2424 (0.0%)	1.60	31/3278 (0.9%)
1	F	1.03	3/2423 (0.1%)	1.63	36/3276 (1.1%)
All	All	1.00	4/4847 (0.1%)	1.62	67/6554 (1.0%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	GLU	CD-OE2	7.13	1.33	1.25
1	F	20	GLU	CD-OE2	6.33	1.32	1.25
1	F	244	TYR	CD2-CE2	-5.95	1.30	1.39
1	F	84	VAL	CB-CG1	-5.75	1.40	1.52

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	276	ARG	NE-CZ-NH1	17.21	128.91	120.30
1	A	22	ARG	NE-CZ-NH1	13.68	127.14	120.30
1	A	49	ARG	NE-CZ-NH1	13.40	127.00	120.30
1	A	49	ARG	CD-NE-CZ	13.27	142.18	123.60
1	A	236	ASN	CB-CA-C	13.15	136.70	110.40
1	F	276	ARG	NE-CZ-NH2	-12.76	113.92	120.30
1	F	235	ASP	CA-C-N	-11.42	92.07	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	ARG	NE-CZ-NH2	-11.13	114.74	120.30
1	F	254	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	F	254	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	F	235	ASP	CB-CG-OD2	10.57	127.81	118.30
1	A	306	VAL	CG1-CB-CG2	10.41	127.56	110.90
1	F	86	LYS	CA-CB-CG	9.99	135.37	113.40
1	A	49	ARG	CA-CB-CG	9.64	134.61	113.40
1	F	79	ASP	CB-CG-OD1	9.46	126.81	118.30
1	F	235	ASP	CA-C-O	9.29	139.61	120.10
1	F	270	SER	N-CA-CB	8.99	123.99	110.50
1	A	22	ARG	CD-NE-CZ	7.93	134.70	123.60
1	F	235	ASP	N-CA-CB	7.80	124.64	110.60
1	A	157	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	F	198	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	F	199	ASP	CB-CG-OD1	7.47	125.03	118.30
1	F	22	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	A	323	ASP	CB-CG-OD2	7.31	124.88	118.30
1	A	237	SER	N-CA-CB	7.24	121.36	110.50
1	A	49	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	F	229	ARG	CA-CB-CG	7.20	129.23	113.40
1	F	86	LYS	N-CA-CB	7.04	123.27	110.60
1	A	235	ASP	CA-CB-CG	6.97	128.72	113.40
1	A	278	LEU	CA-CB-CG	6.96	131.30	115.30
1	F	22	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	143	SER	N-CA-CB	-6.67	100.49	110.50
1	A	254	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	25	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	121	ASP	CB-CG-OD1	-6.54	112.42	118.30
1	F	144	THR	N-CA-CB	6.53	122.71	110.30
1	F	276	ARG	CD-NE-CZ	6.44	132.61	123.60
1	F	244	TYR	CB-CG-CD2	-6.41	117.16	121.00
1	F	309	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	215	TYR	CB-CG-CD1	6.31	124.78	121.00
1	A	199	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	A	197	ASP	CB-CG-OD2	6.09	123.78	118.30
1	F	213	GLU	OE1-CD-OE2	-6.05	116.04	123.30
1	F	220	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	A	178	VAL	CB-CA-C	-5.97	100.06	111.40
1	A	235	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	243	ARG	CD-NE-CZ	5.78	131.70	123.60
1	F	128	CYS	CA-CB-SG	5.74	124.33	114.00
1	A	236	ASN	N-CA-CB	-5.70	100.34	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	142	ASN	N-CA-CB	-5.70	100.35	110.60
1	A	306	VAL	CB-CA-C	-5.62	100.73	111.40
1	A	329	GLU	CA-CB-CG	5.55	125.61	113.40
1	F	79	ASP	OD1-CG-OD2	-5.52	112.82	123.30
1	F	249	VAL	CG1-CB-CG2	-5.47	102.14	110.90
1	F	143	SER	N-CA-CB	-5.47	102.30	110.50
1	F	22	ARG	CG-CD-NE	5.46	123.26	111.80
1	A	92	CYS	CB-CA-C	-5.36	99.69	110.40
1	F	199	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	251	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	326	GLU	OE1-CD-OE2	5.20	129.53	123.30
1	F	49	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	F	97	GLU	CB-CG-CD	-5.15	100.28	114.20
1	F	235	ASP	C-N-CA	5.15	134.58	121.70
1	F	13	LEU	CB-CG-CD1	5.15	119.75	111.00
1	F	25	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	F	11	VAL	N-CA-C	5.04	124.62	111.00
1	A	11	VAL	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	PRO	Peptide

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	2384	0	2440	95	1
1	F	2383	0	2439	100	1
2	A	16	0	10	0	0
2	F	16	0	11	0	0
3	A	2	0	0	0	0
3	F	2	0	0	0	0
4	A	19	0	7	9	0
4	F	19	0	7	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	63	0	0	7	0
5	F	43	0	0	2	0
All	All	4947	0	4914	190	1

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 19.

All (190) 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)
4:A:342:CLI:H121	4:A:342:CLI:O14	1.51	1.08
1:A:38:CYS:HB3	5:A:404:HOH:O	1.62	1.00
1:A:154:GLN:HE21	1:A:158:ASN:HD22	0.97	0.96
4:F:339:CLI:O14	4:F:339:CLI:H122	1.65	0.93
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.58	0.84
1:A:172:MET:SD	1:A:183:CYS:HB3	2.17	0.83
4:A:342:CLI:O14	4:A:342:CLI:C12	2.25	0.82
1:F:182:ASN:HD22	1:F:198:ARG:HA	1.44	0.80
1:F:267:ASN:HD22	1:F:268:LYS:H	1.28	0.79
1:A:177:MET:HE3	1:A:179:ASN:H	1.48	0.79
1:A:154:GLN:HE21	1:A:158:ASN:ND2	1.79	0.79
1:A:129:LEU:HD21	1:F:170:ALA:HB3	1.66	0.77
1:F:106:GLU:HB3	1:F:108:GLU:OE1	1.84	0.77
1:A:9:ASN:ND2	1:A:194:ILE:HG23	2.00	0.76
1:A:154:GLN:NE2	1:A:158:ASN:HD22	1.82	0.73
1:A:172:MET:CE	1:A:183:CYS:HB3	2.19	0.73
1:F:128:CYS:SG	1:F:130:VAL:CG2	2.79	0.71
1:F:172:MET:SD	1:F:183:CYS:HB3	2.32	0.70
1:F:267:ASN:ND2	1:F:269:LYS:H	1.89	0.69
1:F:9:ASN:ND2	1:F:194:ILE:HG23	2.09	0.68
4:F:339:CLI:H122	4:F:339:CLI:C11	2.24	0.67
1:A:183:CYS:SG	1:A:200:VAL:HG21	2.35	0.67
1:F:128:CYS:SG	1:F:130:VAL:HG23	2.35	0.67
1:A:177:MET:HE3	1:A:179:ASN:N	2.10	0.67
1:A:10:ILE:HD13	1:A:10:ILE:H	1.60	0.66
1:A:277:LEU:HA	1:A:281:CYS:HB2	1.75	0.66
4:A:342:CLI:H121	4:A:342:CLI:C11	2.27	0.65
1:F:96:THR:HG23	1:F:99:ASP:H	1.62	0.64
1:F:130:VAL:O	1:F:132:ILE:HG23	1.97	0.64
1:F:148:SER:OG	1:F:150:LYS:HG2	1.98	0.64
1:F:26:GLY:HA3	4:F:339:CLI:O15	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASP:O	1:A:236:ASN:HB2	1.98	0.63
1:F:131:SER:HB3	1:F:166:LEU:HD11	1.79	0.63
1:A:172:MET:HB2	1:F:129:LEU:HD11	1.80	0.62
1:A:182:ASN:HD22	1:A:198:ARG:HA	1.63	0.62
1:A:223:ILE:HD12	1:A:265:PRO:HG3	1.82	0.61
1:F:225:GLU:OE1	1:F:334:HIS:HE1	1.84	0.61
1:A:13:LEU:HD23	1:A:38:CYS:SG	2.41	0.60
1:F:13:LEU:HD23	1:F:38:CYS:SG	2.41	0.60
1:F:29:GLU:OE1	1:F:112:LYS:NZ	2.35	0.60
1:A:17:VAL:HB	4:A:342:CLI:HC8	1.84	0.59
1:F:96:THR:CG2	1:F:99:ASP:HB2	2.32	0.59
1:F:267:ASN:HD22	1:F:268:LYS:N	1.99	0.59
1:F:226:TYR:HB2	1:F:330:ILE:HD12	1.83	0.59
1:F:118:ASP:OD2	1:F:121:ASP:HB2	2.03	0.59
1:A:128:CYS:HB2	1:F:254:ARG:HA	1.85	0.59
1:A:38:CYS:CB	5:A:404:HOH:O	2.32	0.58
1:A:114:VAL:HB	1:A:139:TYR:HB2	1.84	0.58
1:A:38:CYS:SG	5:A:404:HOH:O	2.57	0.58
1:A:30:MET:HB3	4:A:342:CLI:C5	2.33	0.58
1:A:225:GLU:OE1	1:A:334:HIS:HE1	1.87	0.58
1:F:108:GLU:CD	1:F:108:GLU:H	2.06	0.58
1:F:143:SER:HB2	1:F:145:ASP:OD1	2.04	0.57
1:F:166:LEU:HD13	1:F:249:VAL:HG12	1.86	0.57
1:F:269:LYS:HG3	1:F:270:SER:N	2.18	0.57
1:F:268:LYS:HG3	1:F:269:LYS:N	2.17	0.57
1:A:318:LEU:C	1:A:318:LEU:HD12	2.25	0.57
1:A:220:ASP:HB2	1:A:221:PRO:CD	2.34	0.57
1:A:30:MET:HE3	1:A:33:LEU:HG	1.87	0.56
1:F:218:GLU:HB2	1:F:267:ASN:HB2	1.87	0.56
4:F:339:CLI:O14	4:F:339:CLI:C12	2.46	0.56
1:A:128:CYS:SG	1:F:254:ARG:HG3	2.45	0.56
1:F:267:ASN:ND2	1:F:268:LYS:H	1.99	0.56
1:A:218:GLU:HB2	1:A:267:ASN:HB2	1.88	0.55
1:A:235:ASP:O	1:A:236:ASN:CB	2.55	0.55
1:F:11:VAL:HG22	1:F:15:ARG:HH21	1.72	0.55
1:A:25:ARG:HH11	1:A:25:ARG:HB3	1.71	0.55
1:A:30:MET:CE	1:A:33:LEU:HG	2.37	0.54
1:F:183:CYS:SG	1:F:200:VAL:HG21	2.47	0.54
1:F:96:THR:HG23	1:F:99:ASP:N	2.22	0.54
1:A:26:GLY:HA3	4:A:342:CLI:O14	2.07	0.54
1:A:96:THR:HB	1:A:117:PHE:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:CD1	1:F:172:MET:HB2	2.37	0.54
1:A:131:SER:HB3	1:A:166:LEU:HD11	1.90	0.54
1:F:282:ASN:HB2	1:F:283:PRO:HD3	1.89	0.54
1:A:26:GLY:HA3	4:A:342:CLI:H122	1.90	0.53
1:F:30:MET:HE2	1:F:113:TYR:CZ	2.43	0.53
1:F:125:ASN:HB3	1:F:130:VAL:CG2	2.38	0.53
1:F:267:ASN:ND2	1:F:268:LYS:N	2.56	0.53
1:F:36:SER:HB3	1:F:84:VAL:HG13	1.91	0.53
4:F:339:CLI:H62	4:F:339:CLI:CL10	2.46	0.53
1:A:143:SER:HB2	1:A:145:ASP:OD1	2.08	0.53
1:F:19:GLU:O	1:F:23:LYS:HD3	2.09	0.53
1:F:229:ARG:NH1	1:F:326:GLU:OE2	2.42	0.53
1:A:13:LEU:CD2	1:A:38:CYS:SG	2.97	0.52
1:F:35:ASN:HB3	5:F:370:HOH:O	2.08	0.52
1:F:182:ASN:ND2	1:F:198:ARG:HA	2.20	0.52
1:F:216:ALA:HA	1:F:219:PHE:CD2	2.45	0.52
1:A:48:VAL:HG11	1:A:132:ILE:HD11	1.91	0.52
1:F:229:ARG:NH2	1:F:330:ILE:HG12	2.24	0.52
1:F:128:CYS:SG	1:F:130:VAL:HG21	2.49	0.52
1:F:140:ARG:HH12	4:F:339:CLI:C16	2.22	0.52
1:F:33:LEU:CD1	1:F:85:LEU:HD22	2.40	0.52
1:F:198:ARG:HG3	1:F:199:ASP:N	2.24	0.51
1:A:204:LYS:HA	1:A:321:PRO:HD2	1.93	0.51
1:F:226:TYR:CZ	1:F:230:LYS:HD3	2.46	0.51
1:F:229:ARG:HH21	1:F:330:ILE:HG12	1.74	0.51
1:F:233:PRO:C	1:F:235:ASP:H	2.14	0.51
1:A:129:LEU:CD2	1:F:170:ALA:H	2.23	0.50
1:A:50:LYS:HD2	1:F:188:PRO:HD2	1.93	0.50
1:A:125:ASN:HB3	1:A:130:VAL:CG1	2.42	0.50
1:A:130:VAL:N	5:A:355:HOH:O	2.41	0.50
1:A:13:LEU:HD23	1:A:38:CYS:HG	1.77	0.50
1:A:182:ASN:ND2	1:A:199:ASP:H	2.09	0.50
1:A:96:THR:HG23	1:A:99:ASP:HB2	1.94	0.50
1:A:118:ASP:OD2	1:A:121:ASP:HB2	2.12	0.50
1:A:270:SER:HB3	1:A:273:GLY:O	2.12	0.50
1:A:120:LEU:HD11	1:A:132:ILE:HD12	1.94	0.49
1:A:332:GLN:HA	1:A:332:GLN:OE1	2.12	0.49
1:F:17:VAL:HG12	4:F:339:CLI:CL17	2.49	0.49
1:F:17:VAL:HA	4:F:339:CLI:CL17	2.49	0.49
1:F:141:LYS:HE2	1:F:147:PRO:HB3	1.93	0.49
1:F:125:ASN:HB3	1:F:130:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:O	1:A:54:ALA:C	2.51	0.49
1:F:267:ASN:HD21	1:F:269:LYS:HB3	1.76	0.49
1:F:73:LEU:HD23	1:F:126:ILE:HD12	1.93	0.49
1:F:53:ILE:O	1:F:54:ALA:C	2.50	0.48
1:F:229:ARG:NH2	1:F:330:ILE:CG1	2.76	0.48
1:A:35:ASN:O	1:A:38:CYS:HB2	2.13	0.48
1:A:130:VAL:HG23	5:A:397:HOH:O	2.12	0.48
1:A:108:GLU:H	1:A:108:GLU:CD	2.17	0.48
1:A:172:MET:HE1	1:A:183:CYS:HB3	1.96	0.48
1:F:253:HIS:O	1:F:257:VAL:HG13	2.13	0.47
1:A:96:THR:HB	1:A:117:PHE:CZ	2.49	0.47
1:A:96:THR:HG21	1:A:99:ASP:OD2	2.14	0.47
1:A:258:TYR:OH	1:F:125:ASN:HA	2.14	0.47
1:A:130:VAL:O	1:A:132:ILE:HG23	2.15	0.46
4:A:342:CLI:C12	4:A:342:CLI:C11	2.90	0.46
1:A:129:LEU:HD21	1:F:170:ALA:CB	2.39	0.46
1:A:269:LYS:HD3	5:A:401:HOH:O	2.15	0.46
1:F:13:LEU:CD2	1:F:38:CYS:SG	3.03	0.46
1:A:73:LEU:HD23	1:A:126:ILE:HD13	1.98	0.46
1:F:13:LEU:HD12	1:F:17:VAL:HG13	1.97	0.46
1:A:184:PHE:HB3	1:A:193:PHE:HB3	1.97	0.46
1:F:10:ILE:HG22	1:F:15:ARG:NH2	2.30	0.46
1:A:166:LEU:HD23	1:F:129:LEU:HD12	1.98	0.46
1:F:233:PRO:O	1:F:235:ASP:N	2.49	0.46
1:F:9:ASN:ND2	1:F:11:VAL:N	2.64	0.45
1:F:145:ASP:OD1	1:F:145:ASP:N	2.46	0.45
1:F:9:ASN:ND2	1:F:194:ILE:CG2	2.79	0.45
1:A:10:ILE:H	1:A:10:ILE:CD1	2.12	0.45
1:A:107:PRO:HA	1:A:110:ARG:HG3	1.98	0.45
1:F:25:ARG:HH11	1:F:25:ARG:HD2	1.56	0.45
1:A:49:ARG:NH1	5:A:357:HOH:O	2.50	0.44
1:A:16:PHE:O	1:A:20:GLU:HG2	2.16	0.44
1:F:96:THR:HG22	1:F:99:ASP:HB2	1.99	0.44
1:F:282:ASN:N	1:F:283:PRO:CD	2.80	0.44
1:A:130:VAL:O	1:A:131:SER:C	2.55	0.44
1:F:22:ARG:HH11	1:F:22:ARG:CB	2.30	0.44
1:F:33:LEU:HD11	1:F:85:LEU:HD22	2.00	0.44
1:F:282:ASN:CB	1:F:283:PRO:HD3	2.48	0.44
1:A:109:LYS:HB2	1:A:109:LYS:HE3	1.77	0.43
1:A:290:LYS:HA	1:A:290:LYS:HD3	1.84	0.43
1:A:232:PHE:CE2	1:F:217:LYS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:ARG:HH11	1:F:22:ARG:CG	2.32	0.43
1:A:10:ILE:HB	1:A:11:VAL:HG23	2.00	0.43
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.53	0.42
1:F:21:GLY:HA2	4:F:339:CLI:N7	2.34	0.42
1:F:150:LYS:HG3	1:F:151:ASP:N	2.33	0.42
1:A:25:ARG:HB3	1:A:25:ARG:NH1	2.34	0.42
1:F:221:PRO:HB2	1:F:334:HIS:CD2	2.55	0.42
1:A:49:ARG:HD2	1:F:49:ARG:NH2	2.34	0.42
1:F:125:ASN:HB3	1:F:130:VAL:HB	2.02	0.42
1:F:172:MET:HG3	1:F:173:LEU:N	2.34	0.42
1:A:33:LEU:HB2	1:A:90:ALA:HB3	2.01	0.42
1:A:30:MET:HE2	1:A:30:MET:O	2.20	0.42
1:A:282:ASN:HD22	1:A:282:ASN:HA	1.63	0.41
1:F:318:LEU:C	1:F:318:LEU:HD12	2.40	0.41
1:A:125:ASN:ND2	1:A:247:SER:HB2	2.35	0.41
1:A:141:LYS:CE	1:A:147:PRO:HA	2.51	0.41
1:A:30:MET:HG2	4:A:342:CLI:C1	2.50	0.41
1:A:36:SER:HB3	1:A:84:VAL:HB	2.02	0.41
1:F:20:GLU:OE1	1:F:23:LYS:HE3	2.20	0.41
1:F:310:ILE:HG13	1:F:311:HIS:CD2	2.55	0.41
1:A:261:ILE:HD13	1:A:261:ILE:HG21	1.79	0.41
1:F:238:ALA:HA	1:F:239:PRO:HD3	1.92	0.41
1:F:270:SER:HB3	1:F:273:GLY:O	2.21	0.41
1:A:282:ASN:N	1:A:283:PRO:CD	2.84	0.41
1:F:10:ILE:HB	1:F:11:VAL:HG23	2.02	0.41
1:A:96:THR:CG2	1:A:99:ASP:OD2	2.69	0.41
1:F:72:LYS:HD3	1:F:72:LYS:HA	1.62	0.41
1:F:178:VAL:HG13	5:F:349:HOH:O	2.21	0.41
1:F:229:ARG:HH12	1:F:326:GLU:HG3	1.85	0.41
1:A:220:ASP:HB2	1:A:221:PRO:HD3	2.03	0.41
1:A:141:LYS:HE3	1:A:147:PRO:HB3	2.03	0.40
1:A:233:PRO:HA	1:A:234:PRO:HD3	1.67	0.40
1:F:80:LEU:HD23	1:F:80:LEU:HA	1.97	0.40
1:A:129:LEU:HD21	1:F:170:ALA:H	1.87	0.40
1:F:225:GLU:OE1	1:F:334:HIS:CE1	2.70	0.40
1:A:9:ASN:ND2	1:A:11:VAL:N	2.70	0.40

All (1) 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)
1:A:307:PRO:O	1:F:234:PRO:CG[4_546]	2.18	0.02

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	307/337 (91%)	292 (95%)	10 (3%)	5 (2%)	9 4
1	F	307/337 (91%)	288 (94%)	13 (4%)	6 (2%)	7 2
All	All	614/674 (91%)	580 (94%)	23 (4%)	11 (2%)	8 3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ALA
1	F	54	ALA
1	A	123	SER
1	A	143	SER
1	F	143	SER
1	F	236	ASN
1	A	142	ASN
1	F	142	ASN
1	A	10	ILE
1	F	235	ASP
1	F	234	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	260/279 (93%)	232 (89%)	28 (11%)	6 3
1	F	259/279 (93%)	231 (89%)	28 (11%)	6 3
All	All	519/558 (93%)	463 (89%)	56 (11%)	6 3

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	10	ILE
1	A	15	ARG
1	A	23	LYS
1	A	33	LEU
1	A	49	ARG
1	A	72	LYS
1	A	96	THR
1	A	104	ILE
1	A	123	SER
1	A	142	ASN
1	A	143	SER
1	A	145	ASP
1	A	146	GLU
1	A	150	LYS
1	A	172	MET
1	A	177	MET
1	A	178	VAL
1	A	199	ASP
1	A	223	ILE
1	A	247	SER
1	A	264	TYR
1	A	272	LYS
1	A	278	LEU
1	A	300	GLU
1	A	329	GLU
1	A	332	GLN
1	A	333	LYS
1	F	10	ILE
1	F	22	ARG
1	F	23	LYS
1	F	72	LYS
1	F	79	ASP
1	F	84	VAL
1	F	110	ARG

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Mol	Chain	Res	Type
1	F	112	LYS
1	F	124	SER
1	F	126	ILE
1	F	142	ASN
1	F	145	ASP
1	F	146	GLU
1	F	177	MET
1	F	198	ARG
1	F	217	LYS
1	F	237	SER
1	F	247	SER
1	F	254	ARG
1	F	257	VAL
1	F	264	TYR
1	F	265	PRO
1	F	267	ASN
1	F	268	LYS
1	F	269	LYS
1	F	278	LEU
1	F	299	LYS
1	F	333	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	35	ASN
1	A	125	ASN
1	A	154	GLN
1	A	182	ASN
1	A	282	ASN
1	A	334	HIS
1	F	35	ASN
1	F	142	ASN
1	F	182	ASN
1	F	267	ASN
1	F	282	ASN
1	F	334	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 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	$\#\|Z\| > 2$
4	CLI	A	342	-	18,20,20	1.86	5 (27%)	22,29,29	1.85	8 (36%)
4	CLI	F	339	-	18,20,20	2.00	5 (27%)	22,29,29	1.71	7 (31%)
2	F6P	A	338	-	15,16,16	1.34	2 (13%)	17,25,25	1.76	2 (11%)
2	F6P	F	338	-	15,16,16	0.70	0	17,25,25	1.03	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLI	A	342	-	-	4/9/9/9	0/2/2/2
4	CLI	F	339	-	-	5/9/9/9	0/2/2/2
2	F6P	A	338	-	-	1/9/28/28	0/1/1/1
2	F6P	F	338	-	-	3/9/28/28	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	339	CLI	C5-C2	-4.76	1.33	1.41
4	A	342	CLI	C5-C2	-4.14	1.34	1.41
4	A	342	CLI	O18-C16	3.95	1.35	1.22
4	F	339	CLI	C5-C11	-3.04	1.46	1.51
4	F	339	CLI	C2-C1	2.97	1.48	1.40
4	F	339	CLI	O18-C16	2.97	1.32	1.22
2	A	338	F6P	P-O3P	-2.96	1.43	1.54
4	A	342	CLI	C2-C1	2.62	1.47	1.40
4	F	339	CLI	O19-C16	-2.57	1.22	1.30
4	A	342	CLI	C9-C13	2.28	1.42	1.38
2	A	338	F6P	O2-C2	2.21	1.44	1.40
4	A	342	CLI	C12-C16	2.01	1.55	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	338	F6P	O2-C2-O5	5.29	119.71	109.50
4	A	342	CLI	O19-C16-C12	3.63	125.68	114.03
4	F	339	CLI	C6-C12-C16	-3.21	104.75	113.76
4	A	342	CLI	O14-C11-C5	3.06	124.39	114.46
4	A	342	CLI	C13-C8-C3	-3.03	116.94	119.50
4	A	342	CLI	C5-N7-C3	2.79	109.63	103.90
4	A	342	CLI	O19-C16-O18	-2.76	116.42	123.30
2	A	338	F6P	O1-C1-C2	-2.69	106.15	111.86
4	F	339	CLI	C5-N7-C3	2.57	109.18	103.90
4	F	339	CLI	O14-C11-C5	2.41	122.27	114.46
4	F	339	CLI	C4-C9-C13	-2.36	116.04	118.72
4	F	339	CLI	C9-C13-CL17	-2.26	116.33	119.15
2	F	338	F6P	O1-C1-C2	-2.26	107.06	111.86
4	F	339	CLI	O19-C16-C12	2.23	121.20	114.03
4	A	342	CLI	C6-C12-C16	2.17	119.84	113.76
4	F	339	CLI	C8-C3-C1	-2.17	118.37	121.16
4	A	342	CLI	O14-C11-O15	-2.12	118.65	123.35
4	A	342	CLI	C1-C4-CL10	-2.02	117.98	122.81

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	338	F6P	O1-C1-C2-O2
2	F	338	F6P	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	342	CLI	C1-C2-C6-C12
4	A	342	CLI	C5-C2-C6-C12
4	F	339	CLI	C1-C2-C6-C12
4	F	339	CLI	C5-C2-C6-C12
2	F	338	F6P	O1-C1-C2-O5
4	F	339	CLI	C16-C12-C6-C2
2	A	338	F6P	C6-O6-P-O1P
4	F	339	CLI	C6-C12-C16-O19
4	F	339	CLI	C6-C12-C16-O18
4	A	342	CLI	C6-C12-C16-O18
4	A	342	CLI	C6-C12-C16-O19

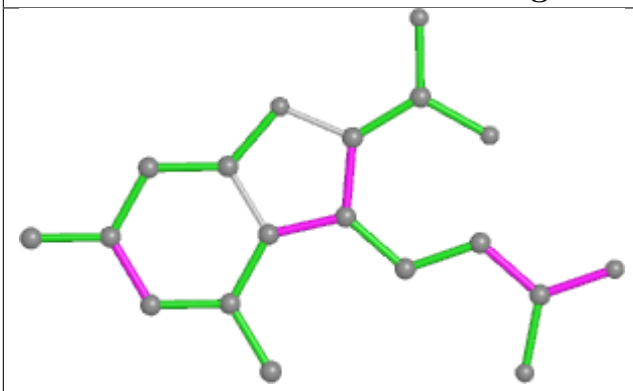
There are no ring outliers.

2 monomers are involved in 18 short contacts:

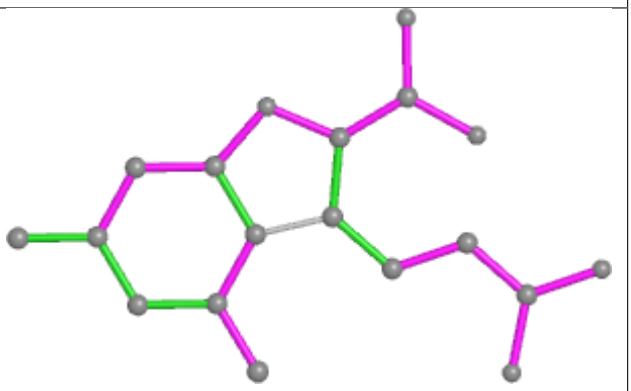
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	342	CLI	9	0
4	F	339	CLI	9	0

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.

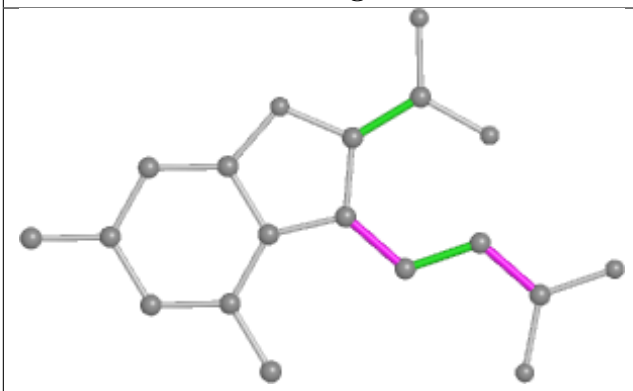
Ligand CLI A 342



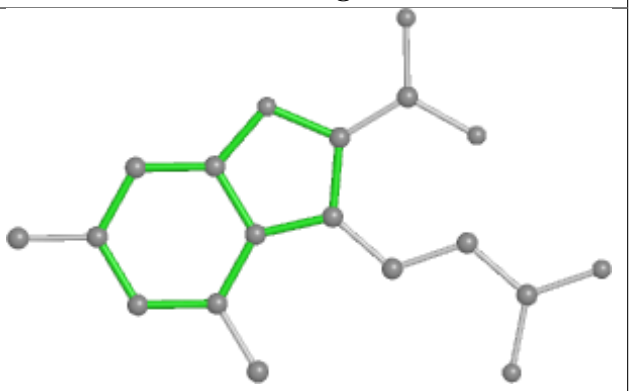
Bond lengths



Bond angles

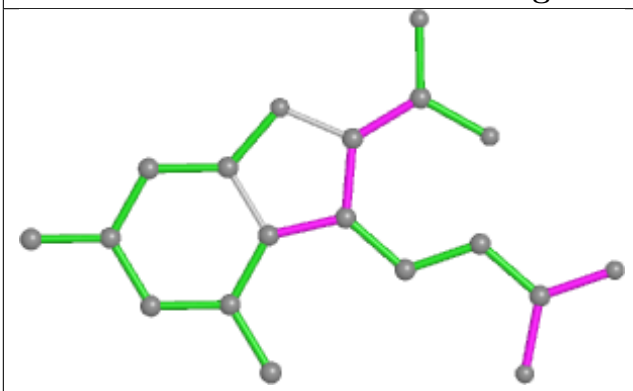


Torsions

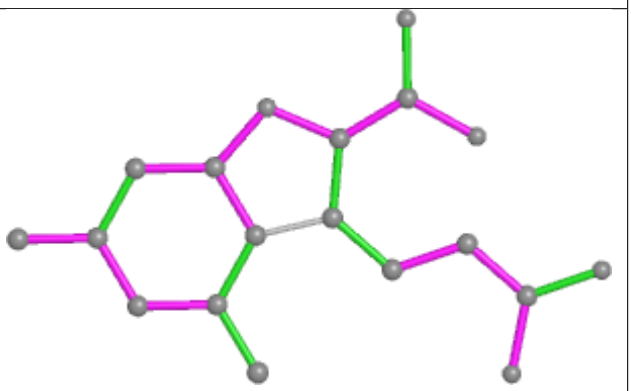


Rings

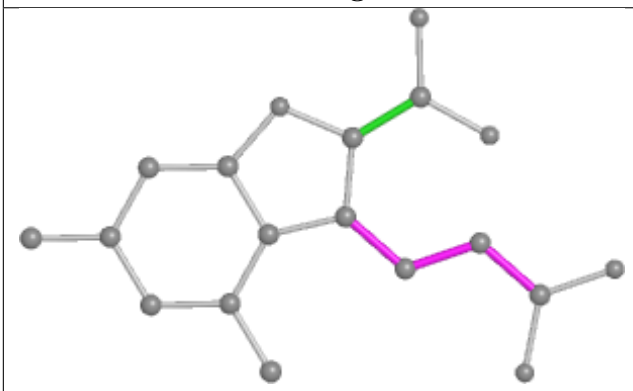
Ligand CLI F 339



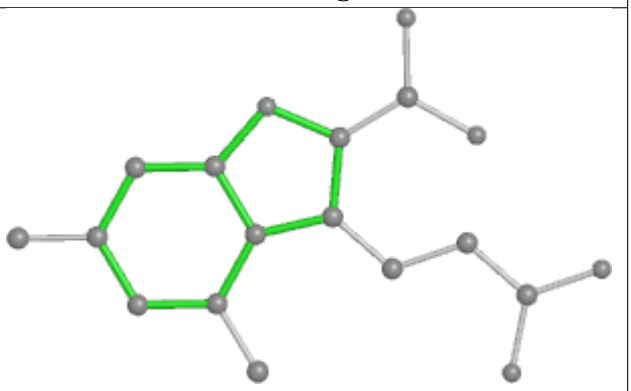
Bond lengths



Bond angles

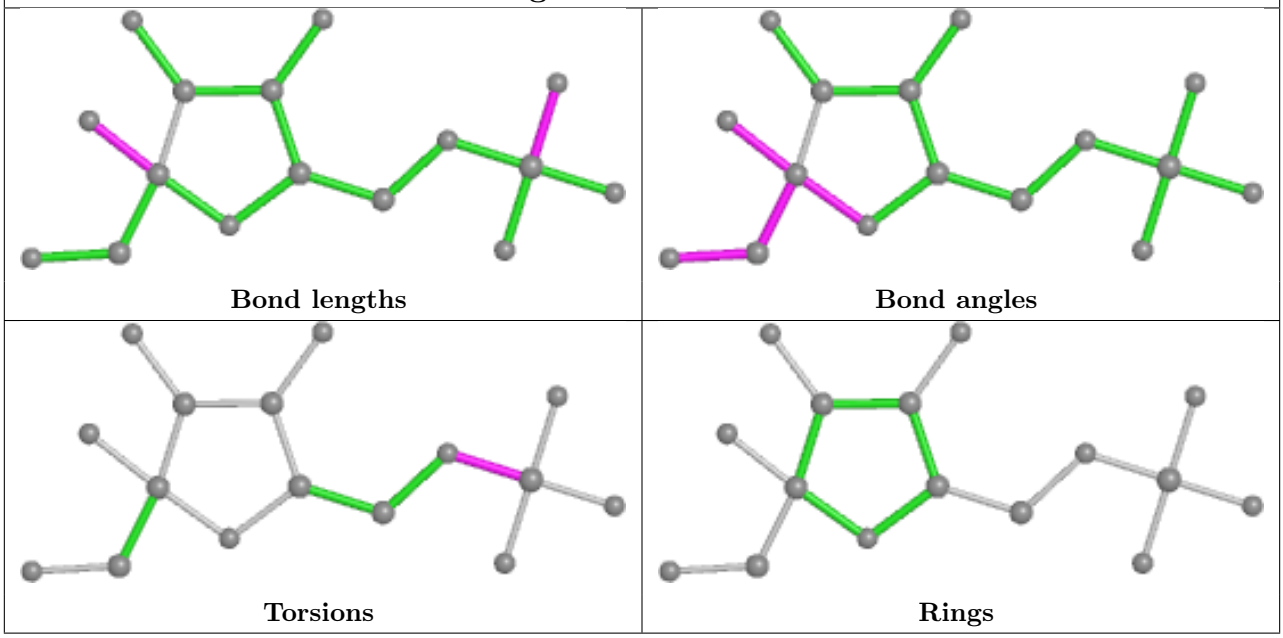


Torsions

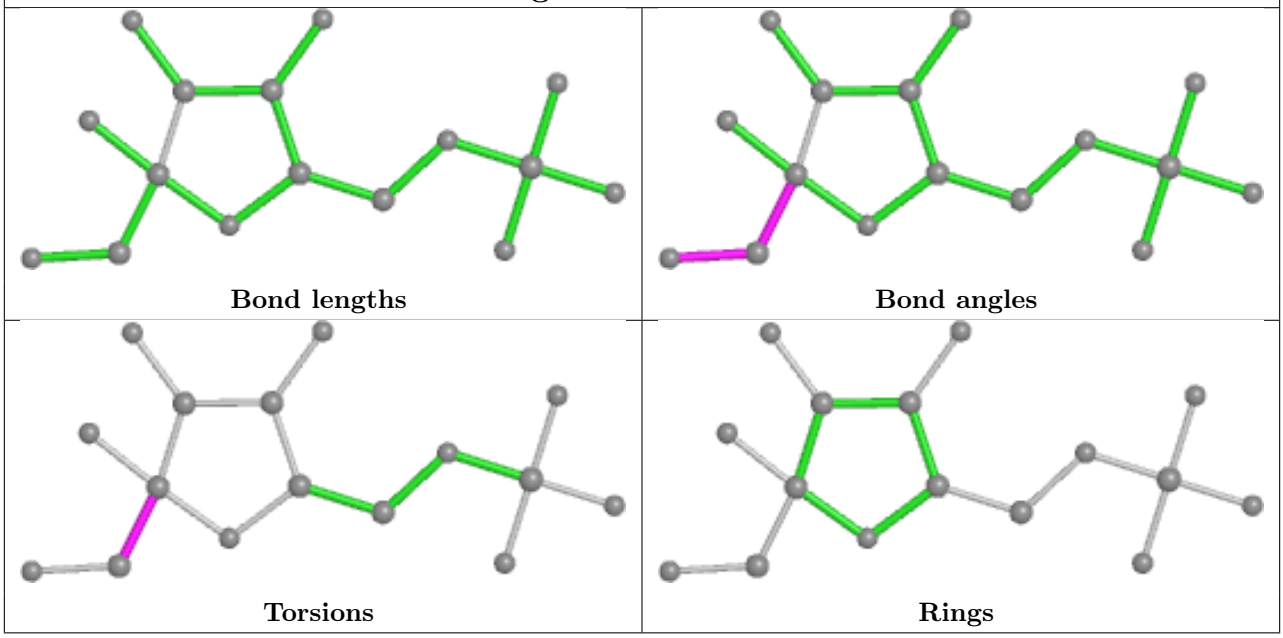


Rings

Ligand F6P A 338



Ligand F6P F 338



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, 95th 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^2)	Q<0.9
1	A	311/337 (92%)	-0.01	19 (6%)	21	28	16, 27, 74, 101	0
1	F	311/337 (92%)	0.06	19 (6%)	21	28	15, 27, 76, 102	0
All	All	622/674 (92%)	0.02	38 (6%)	21	28	15, 27, 75, 102	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	ASN	10.9
1	F	9	ASN	8.3
1	F	234	PRO	7.4
1	F	126	ILE	6.5
1	F	55	HIS	5.9
1	F	236	ASN	5.6
1	F	269	LYS	5.2
1	A	124	SER	4.8
1	F	235	ASP	4.6
1	F	129	LEU	4.6
1	A	125	ASN	4.3
1	A	126	ILE	3.8
1	A	55	HIS	3.8
1	A	142	ASN	3.7
1	A	234	PRO	3.7
1	A	332	GLN	3.7
1	A	129	LEU	3.6
1	F	54	ALA	3.5
1	F	125	ASN	3.5
1	F	130	VAL	3.5
1	F	142	ASN	3.4
1	A	128	CYS	3.2
1	F	268	LYS	2.8
1	A	54	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	269	LYS	2.7
1	F	143	SER	2.6
1	F	127	ASP	2.6
1	F	144	THR	2.6
1	F	124	SER	2.5
1	A	258	TYR	2.4
1	A	268	LYS	2.4
1	A	123	SER	2.3
1	F	270	SER	2.2
1	A	299	LYS	2.1
1	A	334	HIS	2.1
1	F	128	CYS	2.1
1	A	122	GLY	2.0
1	A	236	ASN	2.0

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)

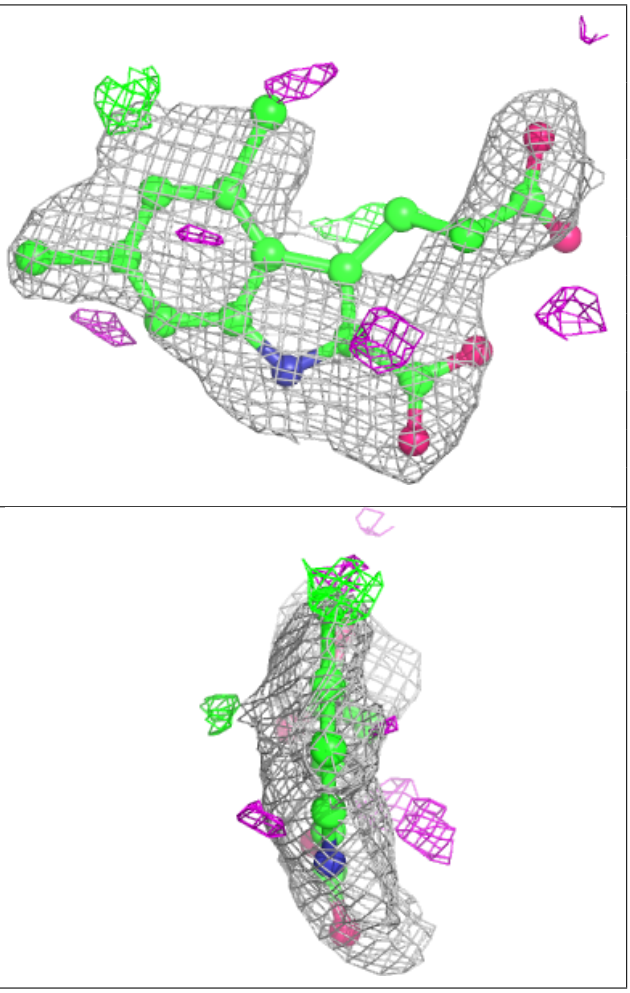
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CLI	F	339	19/19	0.68	0.29	79,82,84,90	0
3	MN	F	343	1/1	0.71	0.10	52,52,52,52	0
4	CLI	A	342	19/19	0.87	0.15	36,48,66,66	0
3	MN	A	341	1/1	0.90	0.10	47,47,47,47	0
3	MN	A	340	1/1	0.94	0.11	38,38,38,38	0
2	F6P	F	338	16/16	0.98	0.07	21,26,34,37	0
2	F6P	A	338	16/16	0.98	0.10	19,23,31,36	0
3	MN	F	342	1/1	0.99	0.08	34,34,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

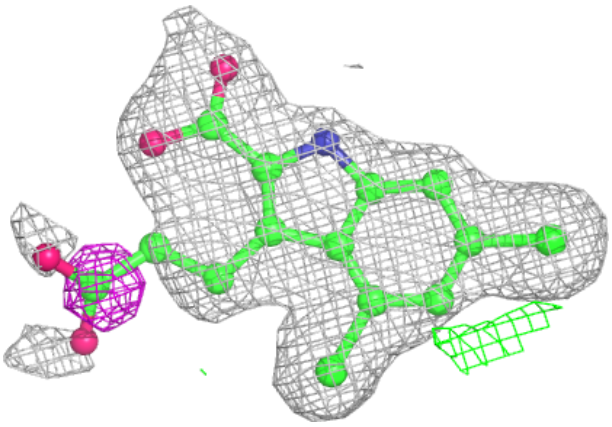
Electron density around CLI F 339:

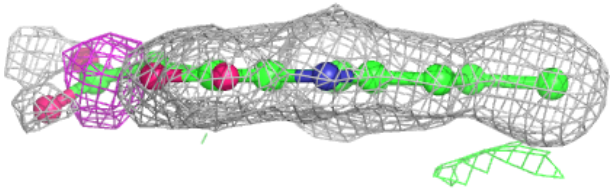
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

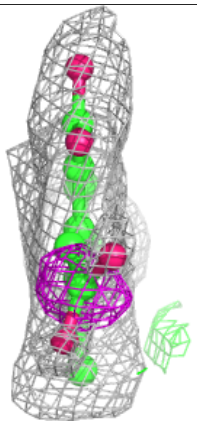


Electron density around CLI A 342:

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

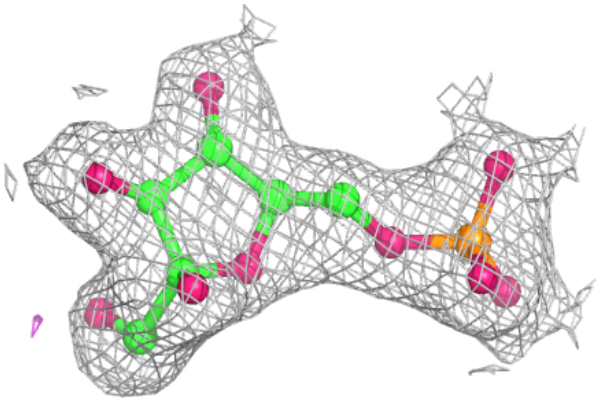


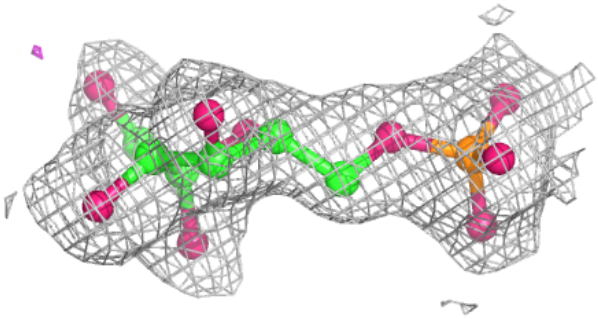


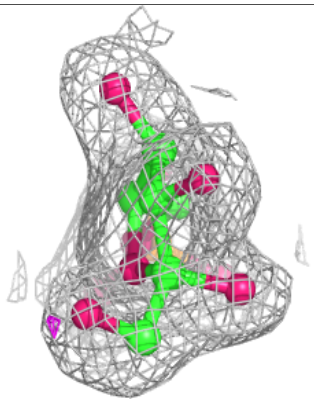


Electron density around F6P F 338:

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

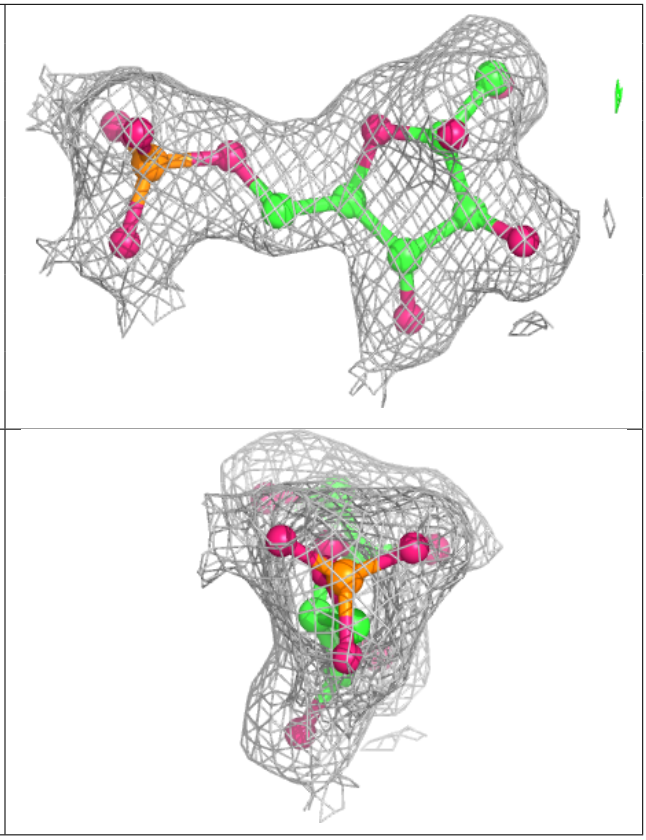






Electron density around F6P A 338:

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



6.5 Other polymers (i)

There are no such residues in this entry.