



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 03:12 AM BST

PDB ID : 1LLC
Title : STRUCTURE DETERMINATION OF THE ALLOSTERIC L-LACTATE
DEHYDROGENASE FROM LACTOBACILLUS CASEI AT 3.0
ANGSTROMS RESOLUTION
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Deposited on : 1988-11-21
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

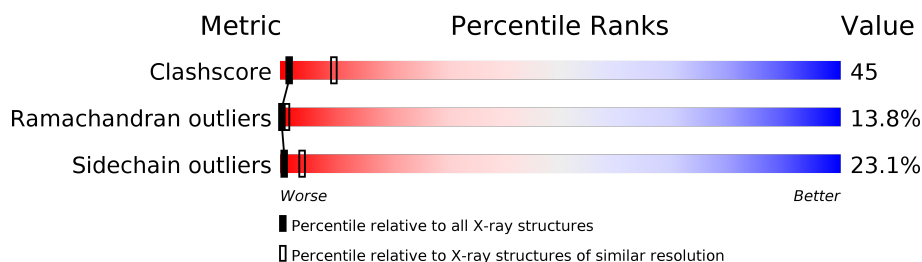
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	325	

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
2	AFP	A	1	-	-	X	-
3	SO4	A	2	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2479 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.

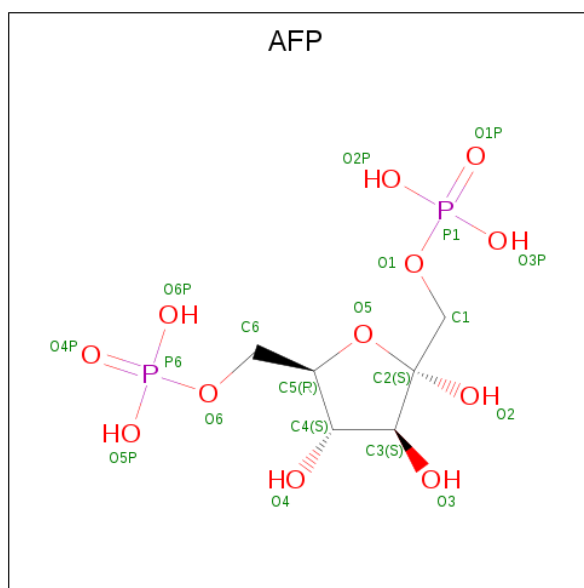
- Molecule 1 is a protein called L-LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	2454	1565	409	474	6	0	0	1

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	PHE	TYR	conflict	UNP P00343
A	102	LYS	GLN	conflict	UNP P00343
A	103	GLN	LYS	conflict	UNP P00343
A	133	LEU	GLY	conflict	UNP P00343
A	281	ILE	LEU	conflict	UNP P00343
A	285	LEU	ILE	conflict	UNP P00343

- Molecule 2 is 1,6-di-O-phosphono-alpha-D-fructofuranose (three-letter code: AFP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

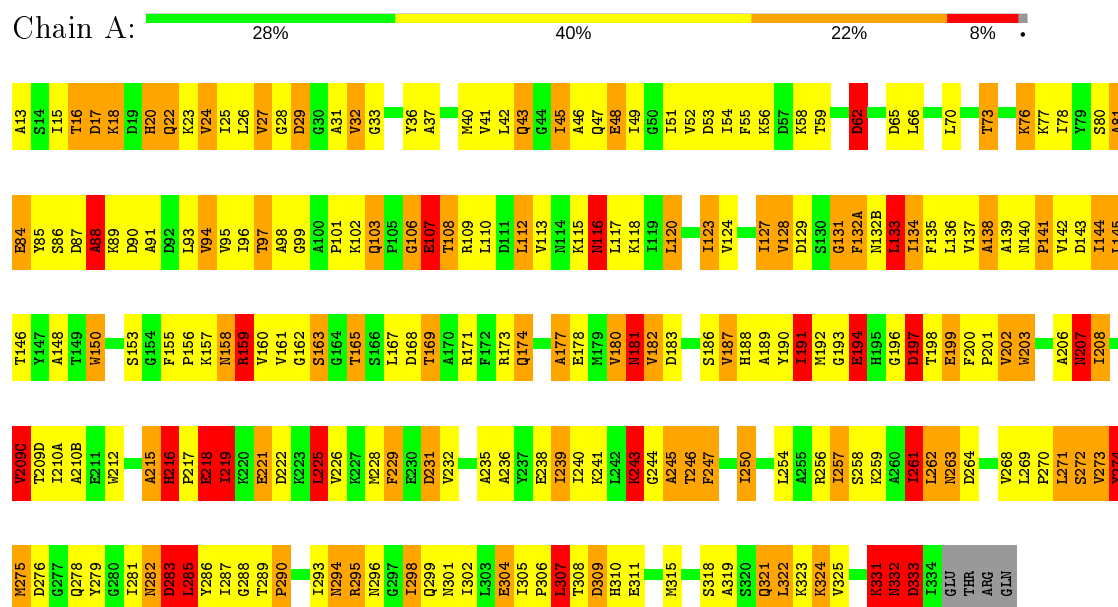


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: L-LACTATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.20 Å 85.38 Å 180.18 Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 42.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.00) 55.3 (42.29-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	EREF	Depositor
R, R_{free}	0.374 , (Not available) 0.474 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.60 , -80.3	EDS
L-test for twinning ¹	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l	Xtriage
F_o, F_c correlation	0.15	EDS
Total number of atoms	2479	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AFP, SO4

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	0.94	3/2498 (0.1%)	1.43	8/3389 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	73

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	TRP	NE1-CE2	-9.26	1.25	1.37
1	A	203	TRP	NE1-CE2	-7.83	1.27	1.37
1	A	212	TRP	NE1-CE2	-7.39	1.27	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	GLN	C-N-CA	6.00	136.69	121.70
1	A	322	LEU	CB-CA-C	-5.92	98.94	110.20
1	A	133	LEU	CB-CA-C	-5.87	99.06	110.20
1	A	116	ASN	CB-CA-C	-5.55	99.30	110.40
1	A	331	LYS	C-N-CA	5.27	134.87	121.70
1	A	16	THR	CA-CB-CG2	5.26	119.76	112.40
1	A	194	GLU	CB-CG-CD	-5.08	100.48	114.20
1	A	194	GLU	OE1-CD-OE2	-5.00	117.30	123.30

There are no chirality outliers.

All (73) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	GLN	Mainchain,Peptide
1	A	106	GLY	Mainchain
1	A	107	GLU	Mainchain
1	A	116	ASN	Sidechain,Mainchain
1	A	127	ILE	Mainchain
1	A	13	ALA	Mainchain
1	A	131	GLY	Mainchain
1	A	133	LEU	Mainchain
1	A	138	ALA	Mainchain
1	A	15	ILE	Mainchain,Peptide
1	A	159	ARG	Mainchain
1	A	16	THR	Mainchain,Peptide
1	A	174	GLN	Mainchain
1	A	181	ASN	Sidechain
1	A	186	SER	Mainchain
1	A	191	ILE	Mainchain
1	A	194	GLU	Sidechain
1	A	197	ASP	Sidechain
1	A	199	GLU	Sidechain
1	A	20	HIS	Mainchain
1	A	207	ASN	Sidechain,Mainchain
1	A	209(C)	VAL	Mainchain
1	A	210(B)	ALA	Mainchain
1	A	215	ALA	Mainchain
1	A	216	HIS	Peptide
1	A	218	GLU	Sidechain
1	A	22	GLN	Sidechain
1	A	221	GLU	Sidechain
1	A	229	PHE	Mainchain
1	A	231	ASP	Mainchain
1	A	238	GLU	Mainchain
1	A	243	LYS	Mainchain
1	A	245	ALA	Mainchain
1	A	246	THR	Mainchain
1	A	261	ILE	Mainchain
1	A	27	VAL	Mainchain
1	A	274	TYR	Sidechain,Mainchain
1	A	282	ASN	Mainchain
1	A	283	ASP	Mainchain
1	A	285	LEU	Mainchain,Peptide
1	A	288	GLY	Mainchain,Peptide
1	A	29	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	A	294	ASN	Sidechain
1	A	304	GLU	Mainchain
1	A	306	PRO	Mainchain
1	A	307	LEU	Mainchain
1	A	321	GLN	Sidechain,Mainchain,Peptide
1	A	324	LYS	Mainchain
1	A	333	ASP	Sidechain
1	A	43	GLN	Mainchain
1	A	46	ALA	Mainchain
1	A	62	ASP	Sidechain
1	A	80	SER	Mainchain,Peptide
1	A	81	ALA	Mainchain,Peptide
1	A	84	GLU	Sidechain,Mainchain
1	A	86	SER	Mainchain,Peptide
1	A	87	ASP	Mainchain
1	A	88	ALA	Mainchain
1	A	99	GLY	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2454	0	2475	222	11
2	A	20	0	7	10	0
3	A	5	0	0	5	0
All	All	2479	0	2482	223	11

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 45.

All (223) 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)
2:A:1:AFP:O1	2:A:1:AFP:C1	1.66	1.41
1:A:132(A):PHE:HE2	1:A:133:LEU:HD22	1.17	1.06
1:A:188:HIS:HD2	2:A:1:AFP:O2P	1.40	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:HIS:CD2	2:A:1:AFP:O2P	2.12	1.02
1:A:23:LYS:HB3	1:A:91:ALA:HA	1.39	1.01
1:A:101:PRO:HG2	1:A:116:ASN:ND2	1.77	0.99
1:A:118:LYS:HD2	1:A:333:ASP:HB3	1.41	0.98
1:A:102:LYS:HG2	1:A:115:LYS:HE3	1.44	0.95
1:A:27:VAL:HG11	1:A:123:ILE:HD13	1.48	0.93
1:A:132(A):PHE:CE2	1:A:133:LEU:HD22	2.04	0.92
1:A:42:LEU:HA	1:A:73:THR:HG21	1.54	0.90
1:A:216:HIS:HB2	1:A:217:PRO:HD3	1.52	0.89
1:A:103:GLN:HB3	1:A:109:ARG:HH21	1.38	0.89
1:A:112:LEU:HD23	1:A:141:PRO:HD3	1.54	0.88
1:A:52:VAL:HG22	1:A:81:ALA:HB3	1.54	0.88
1:A:257:ILE:HD11	1:A:271:LEU:HD22	1.57	0.86
1:A:37:ALA:HB1	1:A:66:LEU:HD21	1.60	0.82
1:A:268:VAL:O	2:A:1:AFP:O5P	1.98	0.82
1:A:103:GLN:HB2	1:A:112:LEU:HD11	1.62	0.80
1:A:246:THR:HG22	3:A:2:SO4:O1	1.80	0.80
1:A:168:ASP:HB3	1:A:191:ILE:HD13	1.64	0.80
1:A:103:GLN:CB	1:A:112:LEU:HD11	2.13	0.79
1:A:25:ILE:HB	1:A:94:VAL:HG23	1.65	0.78
1:A:113:VAL:CG2	1:A:144:ILE:HD13	2.15	0.77
1:A:101:PRO:CG	1:A:116:ASN:ND2	2.48	0.76
1:A:108:THR:HG21	1:A:322:LEU:HD21	1.67	0.75
1:A:168:ASP:HB2	1:A:191:ILE:HG21	1.69	0.75
1:A:96:ILE:HB	1:A:137:VAL:HG12	1.68	0.74
1:A:298:ILE:HD11	1:A:302:ILE:HG12	1.70	0.74
1:A:246:THR:HG21	3:A:2:SO4:S	2.28	0.73
1:A:103:GLN:HB3	1:A:109:ARG:NH2	2.02	0.73
1:A:101:PRO:CG	1:A:116:ASN:CG	2.57	0.72
1:A:165:THR:HG23	1:A:191:ILE:HG22	1.72	0.72
1:A:108:THR:HG21	1:A:322:LEU:CD2	2.21	0.71
1:A:108:THR:HG23	1:A:144:ILE:HD12	1.73	0.71
1:A:209(C):VAL:HG12	1:A:209(D):THR:H	1.55	0.70
1:A:101:PRO:HG2	1:A:116:ASN:CG	2.13	0.69
1:A:257:ILE:HD11	1:A:271:LEU:CD2	2.23	0.68
1:A:103:GLN:HB2	1:A:112:LEU:CD1	2.23	0.68
1:A:218:GLU:HA	1:A:225:LEU:HD11	1.76	0.68
1:A:269:LEU:HG	2:A:1:AFP:O5P	1.94	0.67
1:A:113:VAL:HG21	1:A:144:ILE:HD13	1.77	0.67
1:A:110:LEU:HA	1:A:325:VAL:HG13	1.76	0.67
1:A:245:ALA:HB1	1:A:247:PHE:HD2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD13	1:A:226:VAL:HG23	1.76	0.66
1:A:40:MET:SD	1:A:45:ILE:HB	2.35	0.66
1:A:281:ILE:HG13	1:A:285:LEU:HD11	1.78	0.65
1:A:245:ALA:HB1	1:A:247:PHE:CD2	2.31	0.65
1:A:132(A):PHE:CE2	1:A:133:LEU:HB2	2.31	0.65
1:A:138:ALA:HB3	1:A:254:LEU:HD21	1.79	0.65
1:A:89:LYS:HG3	1:A:131:GLY:O	1.97	0.64
1:A:285:LEU:HD21	1:A:319:ALA:HB1	1.79	0.64
1:A:48:GLU:HG3	1:A:77:LYS:HG3	1.80	0.64
1:A:173:ARG:HH21	2:A:1:AFP:H11	1.63	0.64
1:A:256:ARG:NE	2:A:1:AFP:O4P	2.31	0.64
1:A:113:VAL:HG22	1:A:144:ILE:HG21	1.80	0.64
1:A:106:GLY:O	1:A:107:GLU:HB3	1.98	0.63
1:A:193:GLY:HA2	1:A:287:ILE:HD11	1.79	0.63
1:A:22:GLN:HB2	1:A:47:GLN:HB2	1.81	0.62
1:A:120:LEU:HD11	1:A:145:LEU:HG	1.80	0.62
1:A:203:TRP:CZ3	1:A:210(A):ILE:HD11	2.34	0.62
1:A:85:TYR:HA	1:A:88:ALA:HB2	1.82	0.62
1:A:246:THR:CG2	3:A:2:SO4:O1	2.48	0.62
1:A:271:LEU:O	1:A:273:VAL:HG13	1.99	0.62
1:A:24:VAL:HG12	1:A:49:ILE:HG12	1.80	0.62
1:A:113:VAL:O	1:A:117:LEU:HB2	2.00	0.62
1:A:275:MET:HG3	1:A:281:ILE:HD11	1.82	0.62
1:A:261:ILE:HG22	1:A:293:ILE:HG12	1.81	0.61
1:A:29:ASP:HB2	1:A:51:ILE:HG22	1.83	0.61
1:A:207:ASN:HB3	1:A:209(C):VAL:O	1.99	0.61
1:A:132(A):PHE:HE2	1:A:133:LEU:CD2	2.02	0.61
1:A:200:PHE:HE2	1:A:307:LEU:CD2	2.12	0.61
1:A:190:TYR:CE1	2:A:1:AFP:O2	2.52	0.60
1:A:200:PHE:HE2	1:A:307:LEU:HD22	1.66	0.60
1:A:187:VAL:HG22	1:A:208:ILE:HG23	1.84	0.60
1:A:102:LYS:HG2	1:A:115:LYS:CE	2.27	0.60
1:A:134:ILE:HD11	1:A:295:ARG:O	2.02	0.60
1:A:113:VAL:HG22	1:A:144:ILE:HD13	1.85	0.59
1:A:246:THR:CG2	3:A:2:SO4:S	2.91	0.59
1:A:236:ALA:O	1:A:240:ILE:HG13	2.03	0.58
1:A:158:ASN:HB3	1:A:298:ILE:HG23	1.84	0.58
1:A:273:VAL:CG1	1:A:298:ILE:HD12	2.33	0.58
1:A:127:ILE:O	1:A:132(A):PHE:HB2	2.03	0.58
1:A:141:PRO:O	1:A:145:LEU:HB2	2.05	0.57
1:A:103:GLN:HB3	1:A:112:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:HB1	1:A:127:ILE:CD1	2.34	0.57
1:A:55:PHE:O	1:A:56:LYS:HG3	2.05	0.57
1:A:243:LYS:HD3	1:A:245:ALA:HB2	1.86	0.56
1:A:174:GLN:HA	1:A:177:ALA:HB2	1.88	0.56
1:A:190:TYR:HB2	1:A:202:VAL:CG2	2.35	0.56
1:A:281:ILE:HD12	1:A:287:ILE:HG21	1.87	0.56
1:A:165:THR:HG23	1:A:191:ILE:CG2	2.35	0.56
1:A:102:LYS:H	1:A:115:LYS:HZ1	1.53	0.56
1:A:101:PRO:HG3	1:A:116:ASN:HA	1.86	0.56
1:A:285:LEU:HD13	1:A:287:ILE:HG22	1.87	0.56
1:A:257:ILE:CD1	1:A:271:LEU:HD22	2.32	0.55
1:A:167:LEU:O	1:A:171:ARG:HG3	2.06	0.55
1:A:89:LYS:HG2	1:A:90:ASP:H	1.72	0.55
1:A:273:VAL:HG12	1:A:298:ILE:HD12	1.88	0.55
1:A:228:MET:O	1:A:232:VAL:HG13	2.07	0.54
1:A:113:VAL:HG21	1:A:325:VAL:HG12	1.89	0.54
1:A:139:ALA:HB3	1:A:145:LEU:HD22	1.89	0.54
1:A:182:VAL:HG21	1:A:208:ILE:HG21	1.88	0.54
1:A:36:TYR:CZ	1:A:95:VAL:HG21	2.43	0.53
1:A:281:ILE:HD12	1:A:287:ILE:CG2	2.38	0.53
1:A:180:VAL:HG12	1:A:181:ASN:H	1.74	0.53
1:A:304:GLU:HA	1:A:305:ILE:HD12	1.91	0.53
1:A:89:LYS:CG	1:A:90:ASP:H	2.21	0.53
1:A:132(A):PHE:HE1	1:A:135:PHE:CE1	2.27	0.53
1:A:101:PRO:HB3	1:A:115:LYS:HE2	1.91	0.52
1:A:153:SER:HB2	1:A:155:PHE:CD2	2.45	0.52
1:A:305:ILE:O	1:A:307:LEU:HD12	2.09	0.52
1:A:108:THR:HG23	1:A:144:ILE:CD1	2.38	0.52
1:A:200:PHE:CE2	1:A:307:LEU:HD22	2.43	0.52
1:A:88:ALA:HB1	1:A:127:ILE:HD13	1.91	0.51
1:A:93:LEU:N	1:A:133:LEU:HD23	2.25	0.51
1:A:174:GLN:HA	1:A:177:ALA:CB	2.40	0.51
1:A:168:ASP:CB	1:A:191:ILE:HG21	2.38	0.51
1:A:231:ASP:O	1:A:235:ALA:HB2	2.11	0.51
1:A:161:VAL:HG13	1:A:271:LEU:HD13	1.93	0.51
1:A:198:THR:HB	1:A:318:SER:OG	2.11	0.51
1:A:218:GLU:O	1:A:219:ILE:HB	2.09	0.51
1:A:91:ALA:C	1:A:133:LEU:HD21	2.32	0.50
1:A:101:PRO:HG3	1:A:116:ASN:CA	2.41	0.50
1:A:143:ASP:HB3	1:A:286:TYR:O	2.12	0.50
1:A:307:LEU:O	1:A:311:GLU:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HB	1:A:97:THR:HG22	1.92	0.50
1:A:102:LYS:H	1:A:115:LYS:CE	2.25	0.50
1:A:24:VAL:CG2	1:A:93:LEU:HB3	2.42	0.50
1:A:108:THR:CG2	1:A:144:ILE:HD12	2.41	0.50
1:A:158:ASN:CB	1:A:298:ILE:HG23	2.42	0.50
1:A:24:VAL:HG23	1:A:93:LEU:HB3	1.93	0.50
1:A:298:ILE:HD11	1:A:302:ILE:CG1	2.40	0.50
1:A:216:HIS:HB2	1:A:217:PRO:CD	2.30	0.49
1:A:91:ALA:O	1:A:133:LEU:HD11	2.12	0.49
1:A:203:TRP:HZ3	1:A:210(A):ILE:HD11	1.76	0.49
1:A:259:LYS:O	1:A:263:ASN:HB2	2.11	0.49
1:A:134:ILE:HG22	1:A:161:VAL:HG23	1.95	0.49
1:A:218:GLU:HA	1:A:225:LEU:CD1	2.42	0.49
1:A:27:VAL:CG1	1:A:123:ILE:HD13	2.31	0.49
1:A:165:THR:HB	1:A:270:PRO:HB2	1.95	0.48
1:A:123:ILE:O	1:A:127:ILE:HG22	2.13	0.48
1:A:173:ARG:NH2	2:A:1:AFP:H11	2.28	0.48
1:A:29:ASP:HB2	1:A:51:ILE:CG2	2.43	0.48
1:A:110:LEU:HA	1:A:325:VAL:CG1	2.43	0.48
1:A:28:GLY:O	1:A:33:GLY:HA3	2.13	0.48
1:A:162:GLY:HA3	1:A:272:SER:OG	2.14	0.48
1:A:37:ALA:O	1:A:41:VAL:HG23	2.13	0.48
1:A:133:LEU:HB3	1:A:134:ILE:H	1.45	0.47
1:A:142:VAL:HG11	1:A:163:SER:HB3	1.96	0.47
1:A:254:LEU:O	1:A:258:SER:HB2	2.15	0.47
1:A:250:ILE:O	1:A:254:LEU:HD12	2.14	0.47
1:A:107:GLU:HB2	1:A:197:ASP:OD2	2.15	0.47
1:A:132(A):PHE:HB3	1:A:155:PHE:HZ	1.78	0.47
1:A:157:LYS:HB3	1:A:274:TYR:HD1	1.78	0.47
1:A:218:GLU:HB3	1:A:226:VAL:CG2	2.45	0.47
1:A:262:LEU:H	1:A:295:ARG:HA	1.79	0.47
1:A:181:ASN:HD22	1:A:181:ASN:HA	1.32	0.47
1:A:91:ALA:CB	1:A:133:LEU:HD21	2.45	0.47
1:A:102:LYS:H	1:A:115:LYS:NZ	2.13	0.46
1:A:132(A):PHE:HE2	1:A:133:LEU:HB2	1.79	0.46
1:A:101:PRO:HG3	1:A:116:ASN:CG	2.34	0.46
1:A:144:ILE:HG13	1:A:322:LEU:HD22	1.97	0.46
1:A:192:MET:HB2	1:A:200:PHE:CZ	2.51	0.46
1:A:190:TYR:CD1	1:A:270:PRO:HG3	2.50	0.46
1:A:285:LEU:CD2	1:A:319:ALA:HB1	2.46	0.46
1:A:37:ALA:CB	1:A:66:LEU:HD21	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:THR:HG23	1:A:290:PRO:HD2	1.97	0.46
1:A:103:GLN:NE2	1:A:112:LEU:HD12	2.30	0.45
1:A:146:THR:HG23	1:A:286:TYR:CD2	2.50	0.45
1:A:165:THR:CG2	1:A:270:PRO:HB2	2.46	0.45
1:A:143:ASP:OD2	1:A:287:ILE:HA	2.16	0.45
1:A:93:LEU:CD1	1:A:261:ILE:HD11	2.46	0.45
1:A:66:LEU:HB3	1:A:78:ILE:HD13	1.98	0.45
1:A:194:GLU:OE2	1:A:322:LEU:HG	2.16	0.45
1:A:256:ARG:CD	2:A:1:AFP:O4P	2.65	0.45
1:A:109:ARG:O	1:A:325:VAL:HG11	2.16	0.45
1:A:239:ILE:C	1:A:241:LYS:H	2.19	0.45
1:A:203:TRP:CE3	1:A:210(A):ILE:HD11	2.51	0.45
1:A:250:ILE:HG13	1:A:254:LEU:CD1	2.46	0.45
1:A:182:VAL:HG11	1:A:208:ILE:HG22	2.00	0.44
1:A:45:ILE:HD12	1:A:259:LYS:HB2	1.99	0.44
1:A:26:LEU:HD21	1:A:33:GLY:CA	2.47	0.44
1:A:321:GLN:O	1:A:325:VAL:HG23	2.17	0.44
1:A:120:LEU:O	1:A:124:VAL:HB	2.18	0.44
1:A:26:LEU:HD23	1:A:51:ILE:HG23	1.99	0.44
1:A:24:VAL:HG22	1:A:93:LEU:HD23	1.99	0.44
1:A:145:LEU:O	1:A:148:ALA:HB3	2.18	0.44
1:A:193:GLY:HA2	1:A:287:ILE:CD1	2.46	0.44
1:A:89:LYS:HG2	1:A:90:ASP:N	2.31	0.44
1:A:134:ILE:HG21	1:A:261:ILE:HD12	1.99	0.43
1:A:32:VAL:HG21	1:A:98:ALA:HB2	2.00	0.43
1:A:269:LEU:HB3	1:A:271:LEU:HD23	2.00	0.43
1:A:42:LEU:HD23	1:A:73:THR:HG21	1.99	0.43
1:A:76:LYS:HB2	1:A:77:LYS:H	1.67	0.43
1:A:128:VAL:HG22	1:A:155:PHE:HE2	1.84	0.43
1:A:37:ALA:HB1	1:A:66:LEU:CD2	2.39	0.43
1:A:136:LEU:HD21	1:A:257:ILE:CG2	2.48	0.43
1:A:324:LYS:HB3	1:A:324:LYS:HE3	1.81	0.43
1:A:331:LYS:N	1:A:331:LYS:HD3	2.34	0.42
1:A:273:VAL:O	1:A:274:TYR:HB2	2.19	0.42
1:A:58:LYS:O	1:A:62:ASP:HB2	2.19	0.42
1:A:261:ILE:HD13	1:A:261:ILE:HG21	1.67	0.42
1:A:51:ILE:O	1:A:59:THR:HG21	2.19	0.42
1:A:332:ASN:C	1:A:332:ASN:HD22	2.23	0.42
1:A:156:PRO:O	1:A:160:VAL:HG22	2.19	0.42
1:A:93:LEU:CA	1:A:133:LEU:HD23	2.50	0.42
1:A:169:THR:HG22	1:A:191:ILE:HG22	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HG13	1:A:254:LEU:HD12	2.01	0.41
1:A:275:MET:CG	1:A:281:ILE:HD11	2.47	0.41
1:A:134:ILE:HG23	1:A:159:ARG:HA	2.02	0.41
1:A:88:ALA:HB1	1:A:127:ILE:HD12	2.02	0.41
1:A:257:ILE:HG23	1:A:257:ILE:HD12	1.66	0.41
1:A:196:GLY:H	1:A:199:GLU:CD	2.23	0.41
1:A:287:ILE:HD13	1:A:315:MET:HE3	2.02	0.41
1:A:163:SER:O	1:A:271:LEU:HA	2.21	0.41
1:A:134:ILE:HG13	1:A:261:ILE:HD11	2.03	0.41
1:A:246:THR:HG21	3:A:2:SO4:O2	2.21	0.40
1:A:84:GLU:HB3	1:A:85:TYR:H	1.54	0.40
1:A:150:TRP:HA	1:A:160:VAL:HG11	2.02	0.40
1:A:210(A):ILE:HG21	1:A:210(A):ILE:HD13	1.75	0.40
1:A:285:LEU:O	1:A:285:LEU:HD12	2.22	0.40
1:A:49:ILE:O	1:A:78:ILE:HA	2.22	0.40

All (11) 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:18:LYS:CG	1:A:264:ASP:OD1[2_555]	0.69	1.51
1:A:18:LYS:CG	1:A:264:ASP:CG[2_555]	0.93	1.27
1:A:18:LYS:CD	1:A:264:ASP:CG[2_555]	1.38	0.82
1:A:18:LYS:CG	1:A:264:ASP:OD2[2_555]	1.52	0.68
1:A:18:LYS:CD	1:A:264:ASP:OD2[2_555]	1.59	0.61
1:A:18:LYS:CE	1:A:264:ASP:CA[2_555]	1.69	0.51
1:A:18:LYS:CB	1:A:264:ASP:OD2[2_555]	1.90	0.30
1:A:18:LYS:CB	1:A:264:ASP:OD1[2_555]	1.98	0.22
1:A:18:LYS:CD	1:A:264:ASP:OD1[2_555]	1.99	0.21
1:A:18:LYS:CE	1:A:264:ASP:CG[2_555]	2.08	0.12
1:A:18:LYS:CE	1:A:264:ASP:CB[2_555]	2.10	0.10

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	319/325 (98%)	211 (66%)	64 (20%)	44 (14%)	0 1

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	54	ILE
1	A	159	ARG
1	A	165	THR
1	A	177	ALA
1	A	178	GLU
1	A	187	VAL
1	A	216	HIS
1	A	219	ILE
1	A	243	LYS
1	A	262	LEU
1	A	274	TYR
1	A	279	TYR
1	A	308	THR
1	A	332	ASN
1	A	48	GLU
1	A	53	ASP
1	A	108	THR
1	A	163	SER
1	A	189	ALA
1	A	197	ASP
1	A	206	ALA
1	A	222	ASP
1	A	275	MET
1	A	282	ASN
1	A	88	ALA
1	A	107	GLU
1	A	225	LEU
1	A	272	SER
1	A	283	ASP
1	A	323	LYS
1	A	333	ASP
1	A	18	LYS
1	A	31	ALA
1	A	183	ASP

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Mol	Chain	Res	Type
1	A	209(C)	VAL
1	A	221	GLU
1	A	301	ASN
1	A	215	ALA
1	A	309	ASP
1	A	290	PRO
1	A	70	LEU
1	A	244	GLY
1	A	180	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	264/269 (98%)	203 (77%)	61 (23%)	1 4

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	20	HIS
1	A	24	VAL
1	A	32	VAL
1	A	43	GLN
1	A	45	ILE
1	A	62	ASP
1	A	65	ASP
1	A	73	THR
1	A	76	LYS
1	A	94	VAL
1	A	97	THR
1	A	112	LEU
1	A	120	LEU
1	A	123	ILE
1	A	128	VAL
1	A	129	ASP

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Mol	Chain	Res	Type
1	A	132(A)	PHE
1	A	132(B)	ASN
1	A	133	LEU
1	A	134	ILE
1	A	140	ASN
1	A	141	PRO
1	A	144	ILE
1	A	145	LEU
1	A	158	ASN
1	A	169	THR
1	A	181	ASN
1	A	182	VAL
1	A	191	ILE
1	A	201	PRO
1	A	202	VAL
1	A	207	ASN
1	A	208	ILE
1	A	216	HIS
1	A	218	GLU
1	A	219	ILE
1	A	225	LEU
1	A	229	PHE
1	A	239	ILE
1	A	247	PHE
1	A	250	ILE
1	A	257	ILE
1	A	261	ILE
1	A	263	ASN
1	A	271	LEU
1	A	273	VAL
1	A	276	ASP
1	A	283	ASP
1	A	285	LEU
1	A	294	ASN
1	A	295	ARG
1	A	296	ASN
1	A	298	ILE
1	A	299	GLN
1	A	307	LEU
1	A	309	ASP
1	A	310	HIS
1	A	331	LYS

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Mol	Chain	Res	Type
1	A	332	ASN
1	A	333	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	43	GLN
1	A	103	GLN
1	A	116	ASN
1	A	140	ASN
1	A	174	GLN
1	A	181	ASN
1	A	188	HIS
1	A	296	ASN
1	A	310	HIS
1	A	332	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](#)

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	AFP	A	1	-	18,20,20	2.65	5 (27%)	23,32,32	1.22	3 (13%)
3	SO4	A	2	-	4,4,4	0.78	0	6,6,6	0.12	0

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	AFP	A	1	-	-	11/13/32/32	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	AFP	P1-O1	7.42	1.84	1.60
2	A	1	AFP	O1-C1	6.90	1.66	1.43
2	A	1	AFP	O5-C2	-2.37	1.39	1.43
2	A	1	AFP	O2-C2	2.28	1.44	1.40
2	A	1	AFP	P1-O3P	2.10	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	AFP	P1-O1-C1	3.63	128.28	118.30
2	A	1	AFP	O2-C2-O5	-2.31	105.04	109.50
2	A	1	AFP	O3P-P1-O1	2.03	112.15	106.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	AFP	C1-O1-P1-O1P
2	A	1	AFP	C1-O1-P1-O3P
2	A	1	AFP	O1-C1-C2-O2
2	A	1	AFP	O1-C1-C2-C3
2	A	1	AFP	O1-C1-C2-O5
2	A	1	AFP	C4-C5-C6-O6
2	A	1	AFP	O5-C5-C6-O6

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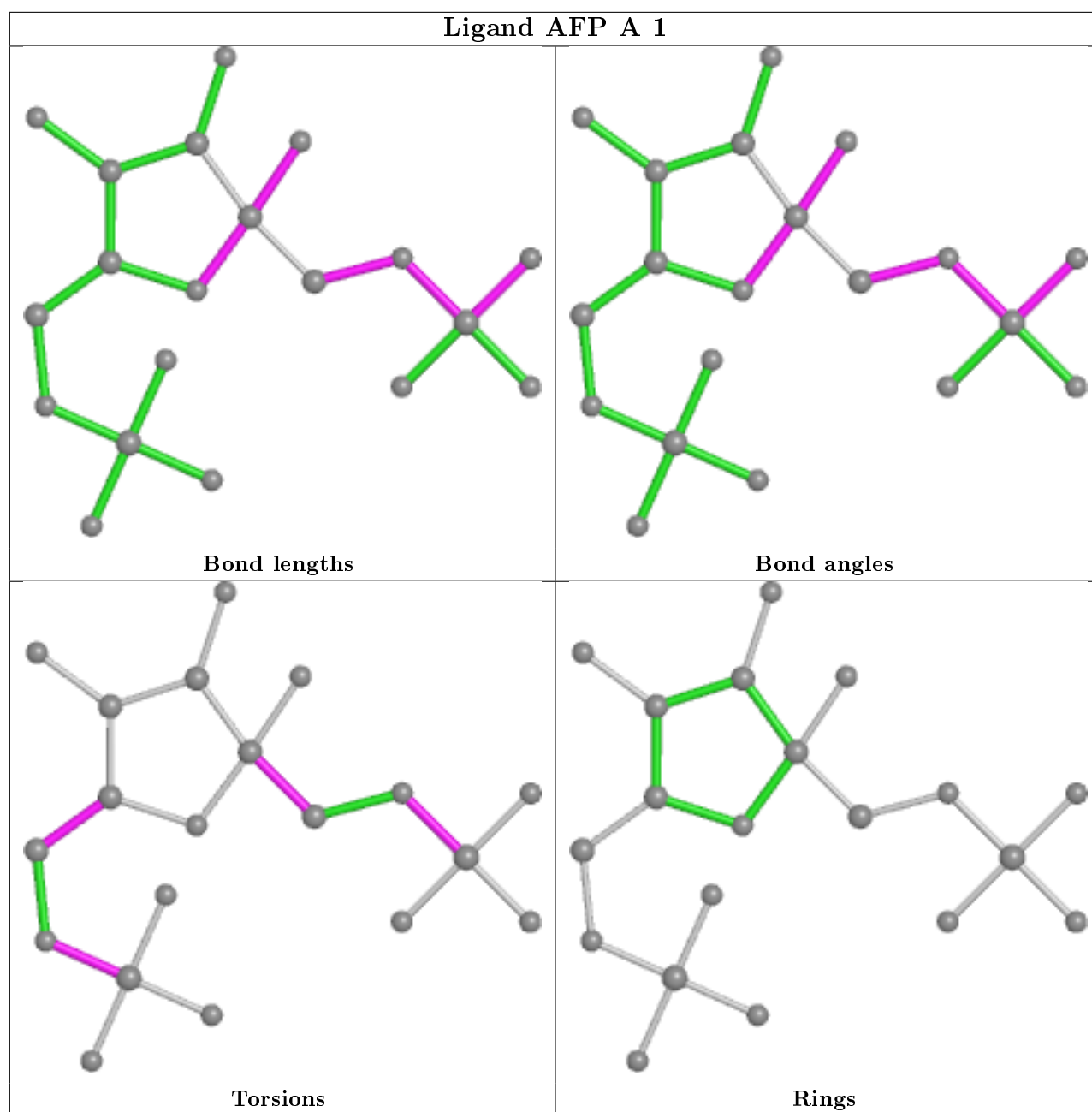
Mol	Chain	Res	Type	Atoms
2	A	1	AFP	C6-O6-P6-O5P
2	A	1	AFP	C6-O6-P6-O6P
2	A	1	AFP	C1-O1-P1-O2P
2	A	1	AFP	C6-O6-P6-O4P

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	AFP	10	0
3	A	2	SO4	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

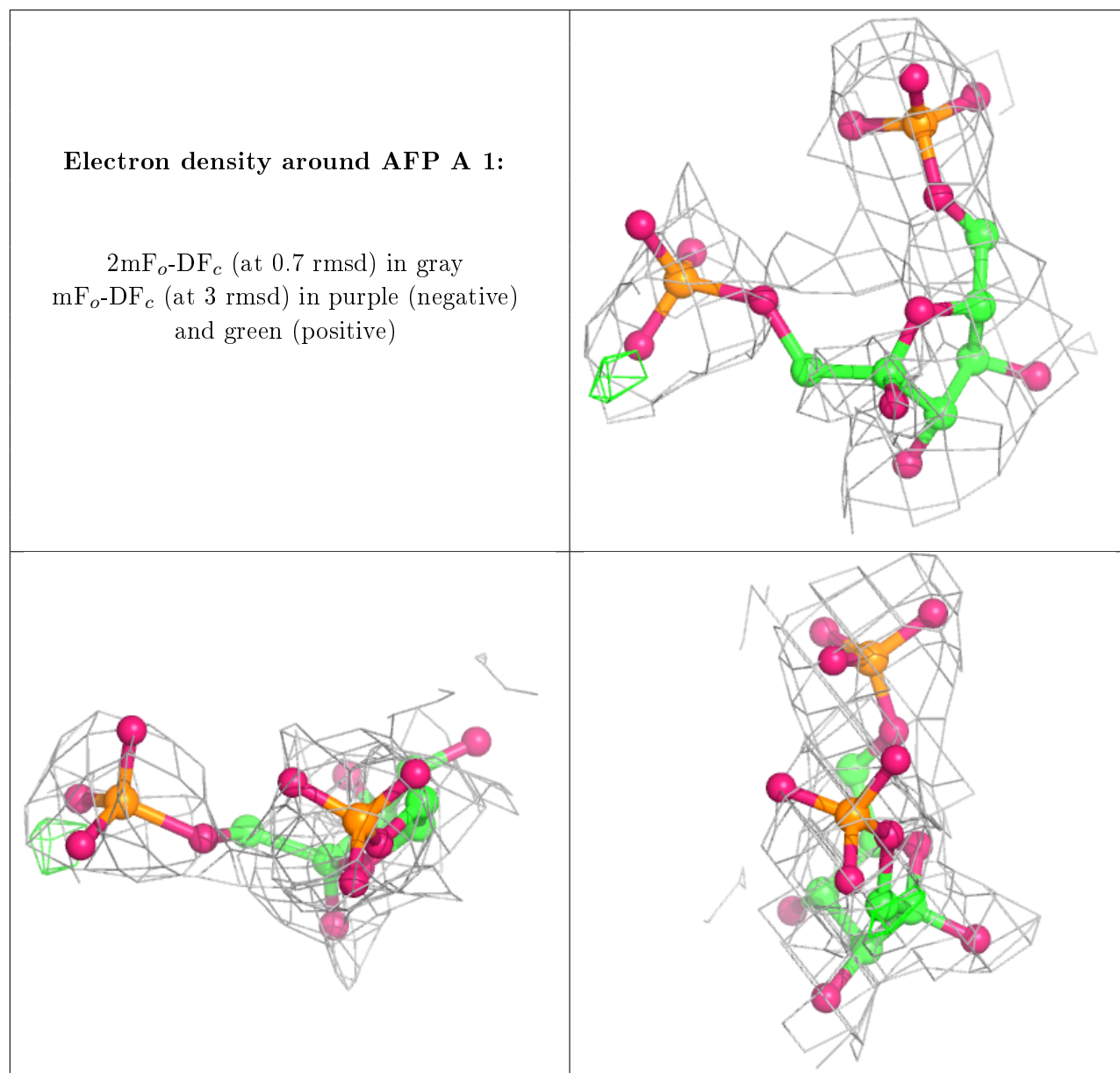
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.