



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:10 PM UTC

PDB ID : 4XZ2 / pdb_00004xz2
Title : Human platelet phosphofructokinase in an R-state in complex with ADP and F6P, crystal form I
Authors : Kloos, M.; Strater, N.
Deposited on : 2015-02-03
Resolution : 2.67 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

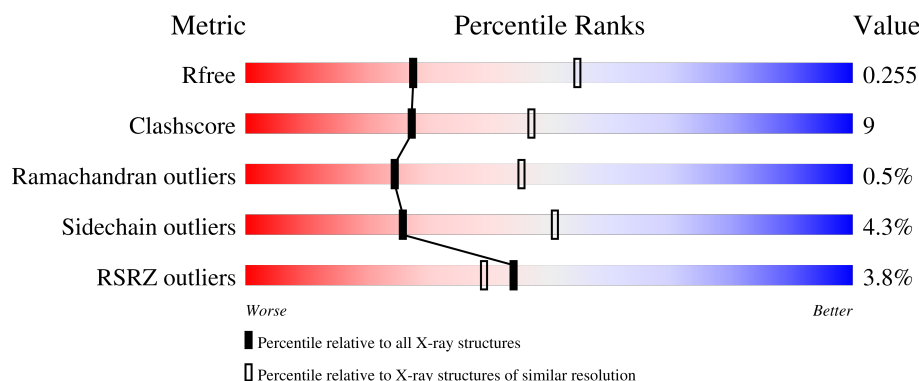
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

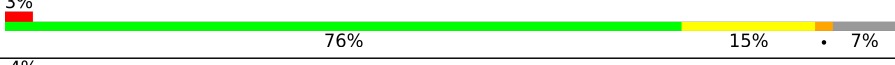
The reported resolution of this entry is 2.67 Å.

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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	761	
1	B	761	
1	C	761	
1	D	761	

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	PO4	C	802	-	-	X	-
5	F6P	B	803	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22132 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 ATP-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	0	0
			5426	3410	961	1018	37			
1	B	728	Total	C	N	O	S	0	0	0
			5568	3496	986	1048	38			
1	C	704	Total	C	N	O	S	0	0	0
			5396	3389	957	1013	37			
1	D	725	Total	C	N	O	S	0	0	0
			5546	3481	983	1044	38			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q01813
A	3	ALA	-	expression tag	UNP Q01813
A	4	SER	-	expression tag	UNP Q01813
A	5	TRP	-	expression tag	UNP Q01813
A	6	SER	-	expression tag	UNP Q01813
A	7	HIS	-	expression tag	UNP Q01813
A	8	PRO	-	expression tag	UNP Q01813
A	9	GLN	-	expression tag	UNP Q01813
A	10	PHE	-	expression tag	UNP Q01813
A	11	GLU	-	expression tag	UNP Q01813
A	12	LYS	-	expression tag	UNP Q01813
A	13	GLY	-	expression tag	UNP Q01813
A	14	ALA	-	expression tag	UNP Q01813
A	15	ASP	-	expression tag	UNP Q01813
A	16	ASP	-	expression tag	UNP Q01813
A	17	ASP	-	expression tag	UNP Q01813
A	18	ASP	-	expression tag	UNP Q01813
A	19	LYS	-	expression tag	UNP Q01813
A	20	VAL	-	expression tag	UNP Q01813
A	21	PRO	-	expression tag	UNP Q01813
A	22	ASP	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

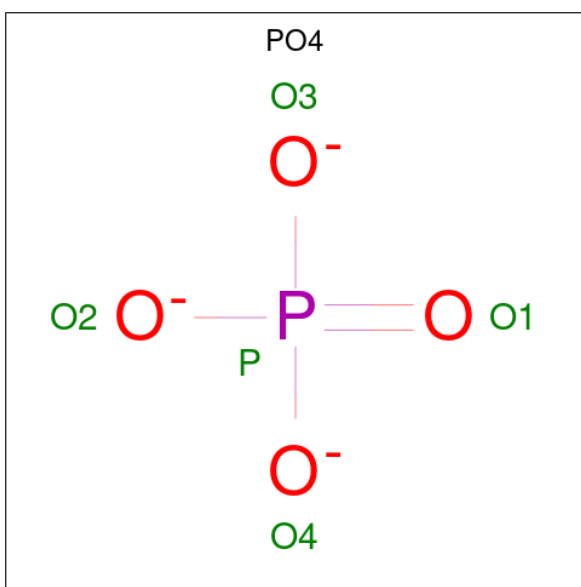
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	PRO	-	expression tag	UNP Q01813
A	24	THR	-	expression tag	UNP Q01813
A	25	SER	-	expression tag	UNP Q01813
B	2	MET	-	initiating methionine	UNP Q01813
B	3	ALA	-	expression tag	UNP Q01813
B	4	SER	-	expression tag	UNP Q01813
B	5	TRP	-	expression tag	UNP Q01813
B	6	SER	-	expression tag	UNP Q01813
B	7	HIS	-	expression tag	UNP Q01813
B	8	PRO	-	expression tag	UNP Q01813
B	9	GLN	-	expression tag	UNP Q01813
B	10	PHE	-	expression tag	UNP Q01813
B	11	GLU	-	expression tag	UNP Q01813
B	12	LYS	-	expression tag	UNP Q01813
B	13	GLY	-	expression tag	UNP Q01813
B	14	ALA	-	expression tag	UNP Q01813
B	15	ASP	-	expression tag	UNP Q01813
B	16	ASP	-	expression tag	UNP Q01813
B	17	ASP	-	expression tag	UNP Q01813
B	18	ASP	-	expression tag	UNP Q01813
B	19	LYS	-	expression tag	UNP Q01813
B	20	VAL	-	expression tag	UNP Q01813
B	21	PRO	-	expression tag	UNP Q01813
B	22	ASP	-	expression tag	UNP Q01813
B	23	PRO	-	expression tag	UNP Q01813
B	24	THR	-	expression tag	UNP Q01813
B	25	SER	-	expression tag	UNP Q01813
C	2	MET	-	initiating methionine	UNP Q01813
C	3	ALA	-	expression tag	UNP Q01813
C	4	SER	-	expression tag	UNP Q01813
C	5	TRP	-	expression tag	UNP Q01813
C	6	SER	-	expression tag	UNP Q01813
C	7	HIS	-	expression tag	UNP Q01813
C	8	PRO	-	expression tag	UNP Q01813
C	9	GLN	-	expression tag	UNP Q01813
C	10	PHE	-	expression tag	UNP Q01813
C	11	GLU	-	expression tag	UNP Q01813
C	12	LYS	-	expression tag	UNP Q01813
C	13	GLY	-	expression tag	UNP Q01813
C	14	ALA	-	expression tag	UNP Q01813
C	15	ASP	-	expression tag	UNP Q01813
C	16	ASP	-	expression tag	UNP Q01813

Continued on next page...

Continued from previous page...

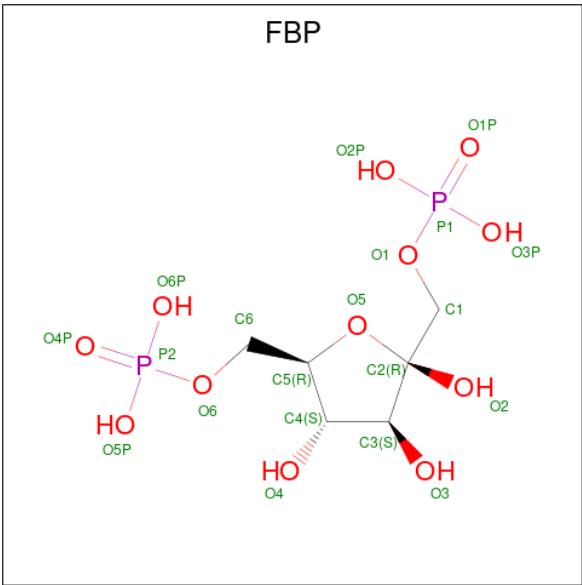
Chain	Residue	Modelled	Actual	Comment	Reference
C	17	ASP	-	expression tag	UNP Q01813
C	18	ASP	-	expression tag	UNP Q01813
C	19	LYS	-	expression tag	UNP Q01813
C	20	VAL	-	expression tag	UNP Q01813
C	21	PRO	-	expression tag	UNP Q01813
C	22	ASP	-	expression tag	UNP Q01813
C	23	PRO	-	expression tag	UNP Q01813
C	24	THR	-	expression tag	UNP Q01813
C	25	SER	-	expression tag	UNP Q01813
D	2	MET	-	initiating methionine	UNP Q01813
D	3	ALA	-	expression tag	UNP Q01813
D	4	SER	-	expression tag	UNP Q01813
D	5	TRP	-	expression tag	UNP Q01813
D	6	SER	-	expression tag	UNP Q01813
D	7	HIS	-	expression tag	UNP Q01813
D	8	PRO	-	expression tag	UNP Q01813
D	9	GLN	-	expression tag	UNP Q01813
D	10	PHE	-	expression tag	UNP Q01813
D	11	GLU	-	expression tag	UNP Q01813
D	12	LYS	-	expression tag	UNP Q01813
D	13	GLY	-	expression tag	UNP Q01813
D	14	ALA	-	expression tag	UNP Q01813
D	15	ASP	-	expression tag	UNP Q01813
D	16	ASP	-	expression tag	UNP Q01813
D	17	ASP	-	expression tag	UNP Q01813
D	18	ASP	-	expression tag	UNP Q01813
D	19	LYS	-	expression tag	UNP Q01813
D	20	VAL	-	expression tag	UNP Q01813
D	21	PRO	-	expression tag	UNP Q01813
D	22	ASP	-	expression tag	UNP Q01813
D	23	PRO	-	expression tag	UNP Q01813
D	24	THR	-	expression tag	UNP Q01813
D	25	SER	-	expression tag	UNP Q01813

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



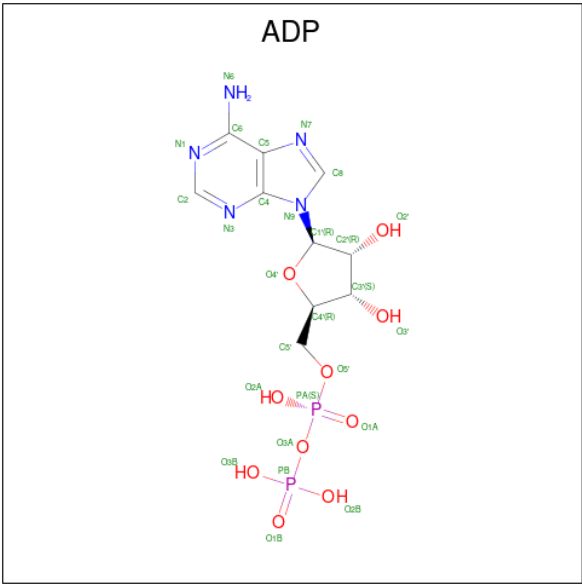
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



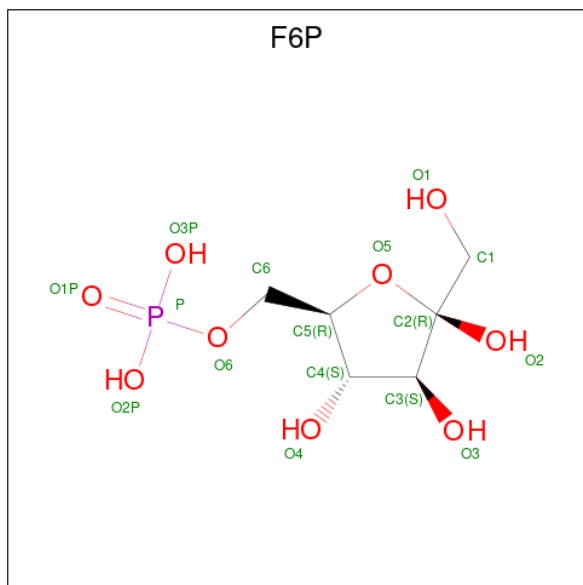
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	B	1	Total	C	O	P	0	0
			20	6	12	2		
3	C	1	Total	C	O	P	0	0
			20	6	12	2		
3	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

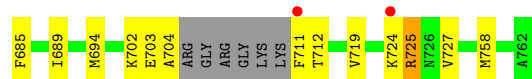


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

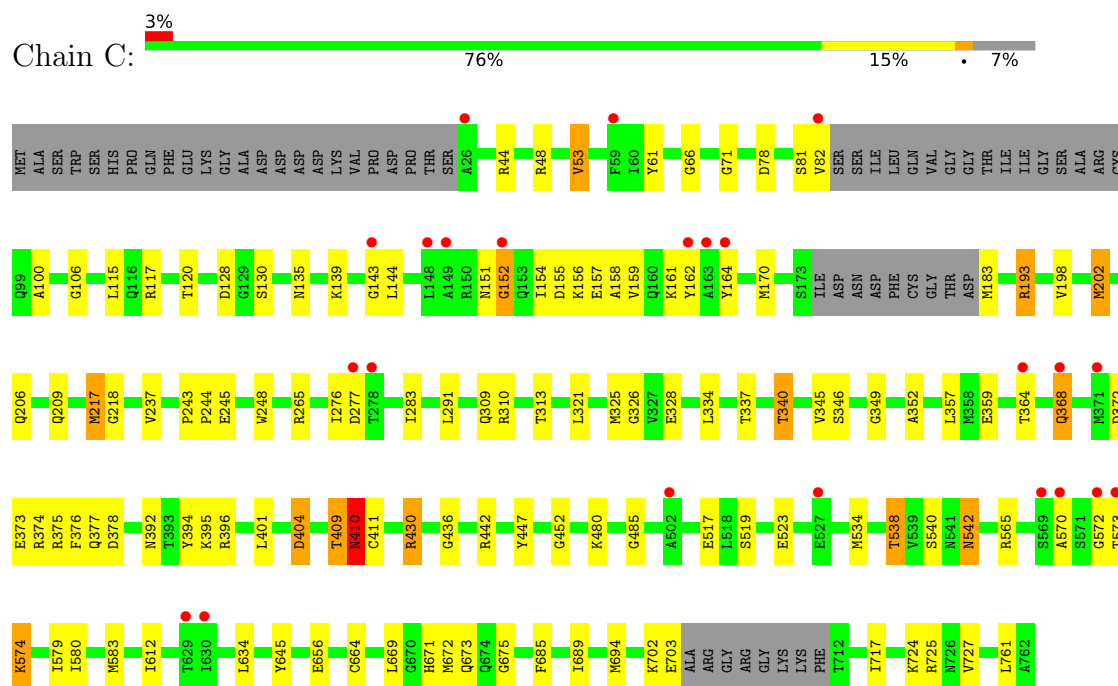
- Molecule 5 is 6-O-phosphono-beta-D-fructofuranose (CCD ID: F6P) (formula: $C_6H_{13}O_9P$).



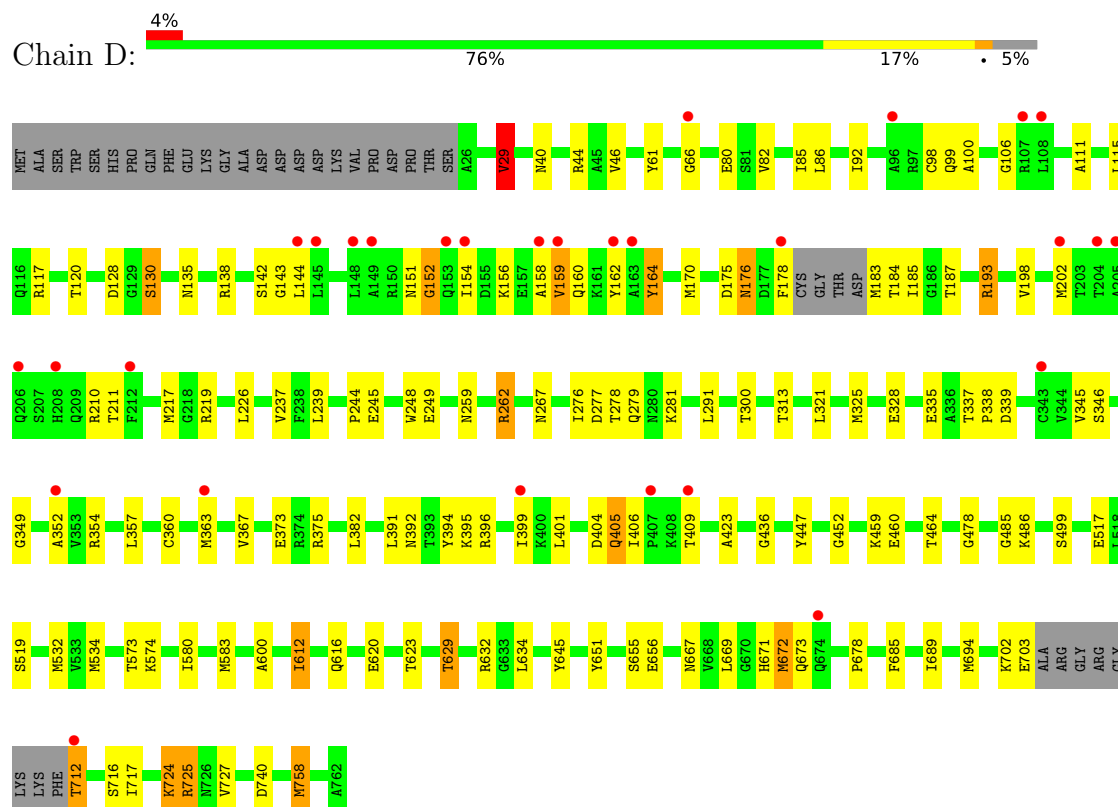
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	P	0	0
			16	6	9	1		
5	D	1	Total	C	O	P	0	0
			16	6	9	1		



- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type



- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.65Å 164.52Å 133.20Å 90.00° 102.96° 90.00°	Depositor
Resolution (Å)	46.03 – 2.67 46.03 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.03-2.67) 99.1 (46.03-2.67)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.216 , 0.255 0.219 , 0.255	Depositor DCC
R_{free} test set	4500 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22132	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F6P, PO4, ADP, FBP

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	0.83	0/5513	0.95	3/7444 (0.0%)
1	B	0.81	0/5657	0.95	6/7640 (0.1%)
1	C	0.76	0/5482	0.94	5/7402 (0.1%)
1	D	0.75	0/5634	0.95	10/7609 (0.1%)
All	All	0.79	0/22286	0.95	24/30095 (0.1%)

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	C	0	1

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	THR	N-CA-C	-11.36	95.53	110.53
1	D	406	ILE	CA-C-N	9.54	129.16	119.24
1	D	406	ILE	C-N-CA	9.54	129.16	119.24
1	B	409	THR	N-CA-C	-9.46	98.78	110.41
1	C	375	ARG	N-CA-C	-7.92	99.67	110.68
1	B	246	GLU	N-CA-C	7.07	119.59	111.11
1	C	409	THR	N-CA-C	-6.90	101.23	110.55
1	D	276	ILE	CA-C-N	6.73	132.25	120.87
1	D	276	ILE	C-N-CA	6.73	132.25	120.87
1	B	255	LYS	CG-CD-CE	6.72	126.75	111.30
1	C	538	THR	CB-CA-C	-6.61	99.34	109.99
1	D	210	ARG	N-CA-C	6.50	119.20	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	164	TYR	N-CA-C	-6.07	105.18	112.59
1	B	308	VAL	CB-CA-C	-5.96	103.35	112.05
1	C	565	ARG	CB-CG-CD	5.72	124.45	111.30
1	D	138	ARG	CB-CG-CD	5.71	124.42	111.30
1	B	406	ILE	N-CA-C	5.66	112.71	107.56
1	A	164	TYR	N-CA-C	-5.43	105.09	112.26
1	B	138	ARG	CB-CG-CD	5.42	123.76	111.30
1	A	507	GLY	N-CA-C	5.29	117.73	110.69
1	D	29	VAL	CB-CA-C	-5.19	102.89	110.62
1	C	410	ASN	N-CA-C	5.16	118.40	112.57
1	D	405	GLN	CA-C-N	-5.10	119.13	122.60
1	D	405	GLN	C-N-CA	-5.10	119.13	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	143	GLY	Peptide

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	5426	0	5453	104	1
1	B	5568	0	5595	107	0
1	C	5396	0	5426	95	1
1	D	5546	0	5576	120	0
2	A	5	0	0	0	0
2	B	10	0	0	2	0
2	C	5	0	0	2	0
2	D	10	0	0	1	0
3	A	20	0	10	1	0
3	B	20	0	10	0	0
3	C	20	0	10	1	0
3	D	20	0	10	3	0
4	B	27	0	12	6	0
4	D	27	0	12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	16	0	11	9	0
5	D	16	0	11	5	0
All	All	22132	0	22136	404	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 9.

All (404) 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:575:ARG:NH1	1:A:631:GLN:NE2	1.62	1.45
1:D:111:ALA:O	1:D:115:LEU:HD12	1.54	1.06
1:A:529:CYS:O	1:A:711:PHE:N	1.88	1.06
1:B:373:GLU:HB3	1:B:375:ARG:HG3	1.34	1.05
1:B:534:MET:HE3	1:B:719:VAL:HG22	1.38	1.04
1:B:534:MET:CE	1:B:719:VAL:HG22	1.93	0.99
1:D:44:ARG:HA	1:D:82:VAL:HG11	1.46	0.97
1:D:40:ASN:HB3	1:D:85:ILE:HG12	1.45	0.96
1:A:417:ASN:CB	1:A:479:THR:HG22	1.97	0.94
1:D:219:ARG:HG3	5:D:803:F6P:O4	1.68	0.92
1:A:417:ASN:HB3	1:A:479:THR:HG22	1.49	0.92
1:B:219:ARG:HG3	5:B:803:F6P:O4	1.70	0.91
1:D:158:ALA:O	1:D:162:TYR:HB2	1.72	0.90
1:B:158:ALA:O	1:B:162:TYR:HB2	1.73	0.89
1:B:515:LEU:HD12	1:B:534:MET:HE2	1.53	0.89
1:A:417:ASN:HB3	1:A:479:THR:CG2	2.02	0.88
1:C:277:ASP:OD1	1:C:283:ILE:HD11	1.72	0.88
1:A:158:ALA:O	1:A:162:TYR:HB2	1.73	0.88
1:B:98:CYS:N	4:B:801:ADP:O3'	2.08	0.87
1:D:80:GLU:OE2	1:D:629:THR:HB	1.77	0.85
1:C:430:ARG:NH1	2:C:802:PO4:O3	2.10	0.85
1:C:158:ALA:O	1:C:162:TYR:HB2	1.78	0.84
1:A:573:THR:HG21	1:B:448:ASP:OD1	1.77	0.82
1:D:178:PHE:CZ	1:D:360:CYS:HB3	2.15	0.81
1:B:40:ASN:HB3	1:B:85:ILE:HG22	1.63	0.80
1:D:111:ALA:O	1:D:115:LEU:CD1	2.32	0.78
1:B:130:SER:OG	4:B:801:ADP:O2B	2.03	0.77
1:D:82:VAL:HG12	1:D:85:ILE:HG21	1.66	0.77
1:D:82:VAL:CG1	1:D:85:ILE:HG21	2.14	0.76
1:A:529:CYS:C	1:A:711:PHE:N	2.42	0.76
1:B:583:MET:H	1:B:673:GLN:HE22	1.34	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ARG:CA	1:D:82:VAL:HG11	2.16	0.76
1:B:373:GLU:HG2	1:B:375:ARG:HE	1.51	0.75
1:D:98:CYS:N	4:D:801:ADP:O3'	2.15	0.75
1:C:436:GLY:HA2	1:C:694:MET:HE2	1.66	0.75
1:D:325:MET:HE1	1:D:345:VAL:O	1.87	0.75
1:D:211:THR:HG22	1:D:267:ASN:HD22	1.50	0.75
1:A:44:ARG:HD2	1:A:82:VAL:HG22	1.68	0.74
1:C:669:LEU:HB3	1:C:672:MET:HE2	1.69	0.74
1:A:244:PRO:O	1:A:245:GLU:HB3	1.87	0.74
1:B:219:ARG:HG3	5:B:803:F6P:HO4	1.49	0.74
1:B:82:VAL:HA	1:B:85:ILE:HD12	1.69	0.74
1:D:29:VAL:CG1	1:D:46:VAL:HG11	2.18	0.74
1:B:535:VAL:HG21	1:B:689:ILE:HG23	1.70	0.74
1:D:335:GLU:OE1	1:D:354:ARG:NH2	2.20	0.73
1:D:436:GLY:HA2	1:D:694:MET:HE2	1.69	0.73
1:D:583:MET:H	1:D:673:GLN:HE22	1.33	0.73
1:D:85:ILE:HD12	1:D:92:ILE:HG21	1.70	0.73
1:A:325:MET:HE1	1:A:345:VAL:O	1.89	0.72
1:C:542:ASN:H	1:C:542:ASN:HD22	1.35	0.72
1:D:82:VAL:O	1:D:85:ILE:HG22	1.89	0.72
1:C:325:MET:HE1	1:C:345:VAL:O	1.90	0.71
1:D:98:CYS:H	4:D:801:ADP:HO3'	1.36	0.71
1:A:403:ASP:OD1	1:A:408:LYS:NZ	2.23	0.70
1:C:183:MET:HE2	1:C:183:MET:HA	1.72	0.70
1:A:575:ARG:HG2	1:A:631:GLN:HB3	1.74	0.69
1:C:368:GLN:O	1:C:372:ASP:OD1	2.10	0.68
1:D:583:MET:HE2	3:D:802:FBP:H3	1.75	0.68
1:D:669:LEU:O	1:D:672:MET:HE3	1.94	0.68
1:A:174:ILE:HD12	1:A:310:ARG:HD3	1.75	0.67
1:A:417:ASN:CB	1:A:479:THR:CG2	2.67	0.67
1:A:573:THR:CG2	1:B:448:ASP:OD1	2.41	0.67
1:C:573:THR:C	1:C:574:LYS:O	2.33	0.67
1:C:409:THR:HG22	1:C:411:CYS:H	1.59	0.67
1:A:301:ARG:NH1	5:B:803:F6P:P	2.68	0.67
1:A:104:ARG:NH1	1:A:146:GLU:OE1	2.28	0.66
1:B:401:LEU:CD2	1:B:405:GLN:OE1	2.42	0.66
1:C:583:MET:H	1:C:673:GLN:HE22	1.43	0.66
1:A:81:SER:O	1:A:82:VAL:HG12	1.96	0.66
1:B:535:VAL:HG21	1:B:689:ILE:CG2	2.26	0.65
1:B:97:ARG:HG3	4:B:801:ADP:H5'1	1.78	0.65
1:C:243:PRO:HG2	1:C:376:PHE:CZ	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:620:GLU:O	1:D:623:THR:HG22	1.97	0.65
1:A:616:GLN:HG3	1:D:612:ILE:HD13	1.77	0.65
1:B:183:MET:HE1	1:B:187:THR:HB	1.78	0.64
1:D:226:LEU:HB2	1:D:239:LEU:HD21	1.78	0.64
1:C:206:GLN:HE21	1:C:265:ARG:HD3	1.62	0.64
1:D:198:VAL:HG12	1:D:202:MET:HE2	1.78	0.64
1:A:198:VAL:HG12	1:A:202:MET:HE2	1.79	0.64
1:B:198:VAL:HG12	1:B:202:MET:HE2	1.79	0.64
1:A:195:ILE:HD12	1:A:680:PRO:HG3	1.80	0.64
1:D:328:GLU:OE2	1:D:354:ARG:NH1	2.30	0.64
1:A:183:MET:HE1	1:A:187:THR:HB	1.80	0.64
1:D:82:VAL:HG12	1:D:82:VAL:O	1.99	0.63
1:D:259:ASN:HA	1:D:262:ARG:HD3	1.79	0.63
1:A:583:MET:SD	3:A:802:FBP:H3	2.38	0.63
1:A:583:MET:H	1:A:673:GLN:HE22	1.46	0.63
1:B:44:ARG:NH1	2:B:805:PO4:O4	2.32	0.63
1:B:401:LEU:HD23	1:B:405:GLN:OE1	1.98	0.63
1:D:130:SER:OG	4:D:801:ADP:O1B	2.17	0.63
1:A:480:LYS:NZ	1:B:573:THR:O	2.31	0.63
1:B:40:ASN:HB3	1:B:85:ILE:CG2	2.28	0.63
1:B:175:ASP:OD2	5:B:803:F6P:H12	1.99	0.63
1:D:183:MET:HE1	1:D:187:THR:HB	1.80	0.63
1:B:522:ARG:NH2	1:B:712:THR:HB	2.14	0.62
1:C:337:THR:H	1:C:340:THR:HB	1.65	0.62
1:B:373:GLU:HB3	1:B:375:ARG:CG	2.21	0.61
1:B:404:ASP:OD1	1:B:404:ASP:N	2.26	0.61
1:C:349:GLY:HA3	1:C:725:ARG:HD3	1.80	0.61
1:A:174:ILE:CG2	1:A:217:MET:HE1	2.31	0.61
1:B:534:MET:HE1	1:B:719:VAL:HG22	1.79	0.61
1:D:175:ASP:OD2	5:D:803:F6P:H11	2.00	0.61
1:C:724:LYS:O	1:C:725:ARG:HB3	2.00	0.61
1:C:409:THR:HG22	1:C:411:CYS:N	2.16	0.61
1:D:82:VAL:HG12	1:D:85:ILE:CG2	2.31	0.60
1:A:417:ASN:HB2	1:A:479:THR:HG22	1.79	0.60
1:A:206:GLN:HE21	1:A:265:ARG:HD3	1.67	0.60
1:B:115:LEU:HD11	1:B:144:LEU:CD2	2.31	0.60
1:A:616:GLN:HG3	1:D:612:ILE:CD1	2.32	0.60
1:C:115:LEU:HD11	1:C:144:LEU:CD2	2.32	0.59
1:C:44:ARG:NH2	1:C:761:LEU:O	2.35	0.59
1:D:259:ASN:OD1	1:D:262:ARG:NH1	2.35	0.59
1:A:115:LEU:HD11	1:A:144:LEU:CD2	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HD12	1:B:680:PRO:HG3	1.83	0.59
1:A:301:ARG:NH1	5:B:803:F6P:O2P	2.33	0.59
1:D:349:GLY:HA3	1:D:725:ARG:HB2	1.83	0.59
1:B:515:LEU:CD1	1:B:534:MET:HE2	2.29	0.59
1:C:154:ILE:HB	1:C:157:GLU:OE1	2.03	0.59
1:B:430:ARG:NH1	2:B:804:PO4:O3	2.36	0.58
1:A:44:ARG:NH2	1:A:761:LEU:O	2.36	0.58
1:C:206:GLN:NE2	1:C:265:ARG:HD3	2.18	0.58
1:B:276:ILE:C	1:B:283:ILE:CD1	2.77	0.58
1:B:442:ARG:NH1	1:B:460:GLU:OE1	2.37	0.58
1:C:349:GLY:CA	1:C:725:ARG:HD3	2.34	0.57
1:A:325:MET:HE1	1:A:345:VAL:C	2.28	0.57
1:C:409:THR:CG2	1:C:411:CYS:SG	2.92	0.57
1:C:583:MET:SD	3:C:801:FBP:H3	2.44	0.57
1:D:583:MET:CE	3:D:802:FBP:H3	2.35	0.57
1:B:724:LYS:O	1:B:725:ARG:HB3	2.05	0.57
1:A:573:THR:HG21	1:B:448:ASP:CG	2.29	0.57
1:A:378:ASP:OD1	1:A:381:ARG:NH2	2.38	0.57
1:B:375:ARG:NH1	1:B:378:ASP:OD2	2.38	0.57
1:C:436:GLY:CA	1:C:694:MET:HE2	2.34	0.57
1:D:325:MET:HE1	1:D:345:VAL:C	2.29	0.56
1:B:535:VAL:HG23	1:B:689:ILE:HG12	1.88	0.56
1:B:611:ASP:OD2	1:B:613:ARG:NH2	2.37	0.56
1:C:325:MET:HE1	1:C:345:VAL:C	2.30	0.56
1:D:436:GLY:CA	1:D:694:MET:HE2	2.35	0.56
1:A:575:ARG:NH1	1:A:631:GLN:CD	2.52	0.56
1:D:244:PRO:O	1:D:245:GLU:HB2	2.06	0.56
1:A:575:ARG:CZ	1:A:631:GLN:NE2	2.59	0.56
1:D:82:VAL:HG13	1:D:85:ILE:HG21	1.88	0.55
1:C:198:VAL:O	1:C:202:MET:HG3	2.06	0.55
1:A:724:LYS:O	1:A:725:ARG:HB3	2.05	0.55
1:A:206:GLN:NE2	1:A:265:ARG:HD3	2.21	0.55
1:D:176:ASN:HD22	1:D:184:THR:HB	1.71	0.55
1:A:301:ARG:HH12	5:B:803:F6P:P	2.29	0.55
1:D:325:MET:HE3	1:D:345:VAL:HG23	1.89	0.55
1:D:632:ARG:NH2	2:D:805:PO4:O4	2.27	0.55
1:D:702:LYS:O	1:D:703:GLU:HG3	2.07	0.55
1:D:712:THR:HG22	1:D:716:SER:OG	2.07	0.55
1:C:340:THR:HG22	1:C:340:THR:O	2.07	0.55
1:C:671:HIS:H	1:D:667:ASN:HD21	1.55	0.54
1:C:573:THR:O	1:C:574:LYS:O	2.25	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:PHE:CE2	1:D:360:CYS:HB3	2.42	0.54
1:C:243:PRO:HG3	1:C:276:ILE:CD1	2.38	0.54
1:C:572:GLY:HA2	1:D:478:GLY:HA2	1.90	0.54
1:D:337:THR:HG22	1:D:338:PRO:HD2	1.90	0.54
1:C:325:MET:HE3	1:C:345:VAL:HG23	1.88	0.54
1:D:277:ASP:OD2	1:D:281:LYS:HB2	2.08	0.54
1:B:276:ILE:C	1:B:283:ILE:HD12	2.33	0.54
1:C:538:THR:HG22	1:C:540:SER:H	1.73	0.54
1:A:204:THR:HG21	1:B:310:ARG:HB2	1.90	0.54
1:C:115:LEU:HD11	1:C:144:LEU:HD21	1.90	0.54
1:A:195:ILE:HD11	1:A:231:ALA:CB	2.38	0.53
1:B:195:ILE:HD11	1:B:231:ALA:CB	2.38	0.53
1:B:115:LEU:HD11	1:B:144:LEU:HD21	1.89	0.53
1:B:195:ILE:HD11	1:B:231:ALA:HB3	1.90	0.53
1:C:702:LYS:O	1:C:703:GLU:HG3	2.07	0.53
1:B:645:TYR:CE2	1:C:656:GLU:HG2	2.44	0.53
1:D:178:PHE:CZ	1:D:360:CYS:CB	2.91	0.53
1:C:373:GLU:O	1:C:373:GLU:HG2	2.08	0.53
1:A:195:ILE:HD11	1:A:231:ALA:HB3	1.91	0.52
1:D:219:ARG:HG3	5:D:803:F6P:HO4	1.71	0.52
1:C:209:GLN:HA	1:C:265:ARG:O	2.10	0.52
1:A:209:GLN:HA	1:A:265:ARG:O	2.10	0.52
1:C:217:MET:HG3	1:C:309:GLN:CD	2.35	0.52
1:A:115:LEU:HD11	1:A:144:LEU:HD21	1.90	0.52
1:D:237:VAL:HG23	1:D:394:TYR:CE2	2.44	0.52
1:C:573:THR:HG22	1:C:574:LYS:O	2.10	0.52
1:D:249:GLU:CG	1:D:291:LEU:HD11	2.39	0.52
1:A:307:HIS:CD2	1:A:310:ARG:NH1	2.78	0.52
1:B:349:GLY:HA3	1:B:725:ARG:HB2	1.92	0.52
1:C:244:PRO:O	1:C:245:GLU:HB2	2.10	0.52
1:D:244:PRO:O	1:D:245:GLU:CB	2.58	0.52
1:A:301:ARG:NH1	5:B:803:F6P:O1P	2.43	0.51
1:B:666:LYS:C	1:B:667:ASN:HD22	2.15	0.51
1:D:237:VAL:HG23	1:D:394:TYR:CZ	2.45	0.51
1:B:702:LYS:C	1:B:704:ALA:H	2.18	0.51
1:D:85:ILE:CD1	1:D:92:ILE:HG21	2.37	0.51
1:C:71:GLY:O	1:C:117:ARG:NH2	2.44	0.51
1:B:207:SER:O	1:B:208:HIS:HB3	2.09	0.51
1:D:40:ASN:CB	1:D:85:ILE:HG12	2.31	0.51
1:D:583:MET:SD	3:D:802:FBP:H3	2.51	0.51
1:A:391:LEU:O	1:A:395:LYS:HG3	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:PHE:N	1:A:711:PHE:CD1	2.78	0.50
1:B:244:PRO:HB2	1:B:248:TRP:CD1	2.46	0.50
1:B:408:LYS:HG2	1:B:409:THR:O	2.11	0.50
1:D:337:THR:CG2	1:D:338:PRO:HD2	2.41	0.50
1:C:183:MET:HA	1:C:183:MET:CE	2.38	0.50
1:C:328:GLU:HG2	1:C:352:ALA:HB1	1.94	0.50
1:A:245:GLU:HG2	1:A:246:GLU:N	2.24	0.50
1:A:711:PHE:N	1:A:711:PHE:HD1	2.10	0.50
1:D:170:MET:CE	1:D:185:ILE:CD1	2.90	0.50
1:D:198:VAL:CG1	1:D:202:MET:HE2	2.41	0.50
1:B:373:GLU:CB	1:B:375:ARG:HG3	2.24	0.49
1:C:237:VAL:HG23	1:C:394:TYR:CE2	2.47	0.49
1:C:244:PRO:O	1:C:245:GLU:CB	2.60	0.49
1:D:373:GLU:CD	1:D:375:ARG:HH11	2.20	0.49
1:A:174:ILE:CD1	1:A:310:ARG:HD3	2.42	0.49
1:B:580:ILE:CD1	1:B:634:LEU:HD11	2.43	0.49
1:A:244:PRO:HB2	1:A:248:TRP:CD1	2.47	0.49
1:D:337:THR:HG22	1:D:339:ASP:H	1.78	0.49
1:C:447:TYR:O	1:C:452:GLY:HA3	2.13	0.49
1:A:198:VAL:CG1	1:A:202:MET:HE2	2.42	0.49
1:D:120:THR:HB	1:D:164:TYR:O	2.13	0.49
1:D:193:ARG:NH2	1:D:313:THR:O	2.46	0.49
1:B:198:VAL:CG1	1:B:202:MET:HE2	2.42	0.48
1:D:61:TYR:O	1:D:66:GLY:HA3	2.13	0.48
1:B:447:TYR:O	1:B:452:GLY:HA3	2.13	0.48
1:A:368:GLN:O	1:A:368:GLN:NE2	2.46	0.48
1:B:193:ARG:NH2	1:B:313:THR:O	2.47	0.48
1:C:243:PRO:HG3	1:C:276:ILE:HD12	1.94	0.48
1:D:29:VAL:HG13	1:D:46:VAL:HG11	1.94	0.48
1:D:447:TYR:O	1:D:452:GLY:HA3	2.13	0.48
1:D:82:VAL:O	1:D:85:ILE:CG2	2.58	0.48
1:D:724:LYS:O	1:D:725:ARG:HB3	2.14	0.48
1:B:127:GLY:HA3	4:B:801:ADP:O3B	2.13	0.48
1:B:277:ASP:N	1:B:283:ILE:CD1	2.76	0.48
1:C:325:MET:HE1	1:C:346:SER:HA	1.96	0.48
1:D:219:ARG:CG	5:D:803:F6P:O4	2.53	0.48
1:D:391:LEU:O	1:D:395:LYS:HG3	2.14	0.48
1:C:61:TYR:O	1:C:66:GLY:HA3	2.14	0.48
1:A:656:GLU:HG2	1:D:645:TYR:CE2	2.49	0.48
1:D:532:MET:HE3	1:D:717:ILE:HD13	1.95	0.48
1:B:373:GLU:CG	1:B:375:ARG:HE	2.25	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:CG	4:B:801:ADP:H5'1	2.43	0.47
1:B:170:MET:CE	1:B:185:ILE:CD1	2.92	0.47
1:C:120:THR:HB	1:C:164:TYR:O	2.14	0.47
1:A:447:TYR:O	1:A:452:GLY:HA3	2.13	0.47
1:A:328:GLU:HG2	1:A:352:ALA:HB1	1.96	0.47
1:B:328:GLU:HG2	1:B:352:ALA:HB1	1.97	0.47
1:D:328:GLU:HG2	1:D:352:ALA:HB1	1.96	0.47
1:C:193:ARG:NH2	1:C:313:THR:O	2.48	0.47
1:C:237:VAL:HG23	1:C:394:TYR:CZ	2.50	0.47
1:A:120:THR:HB	1:A:164:TYR:O	2.15	0.47
1:D:321:LEU:O	1:D:325:MET:HG2	2.14	0.47
1:B:612:ILE:HD11	1:C:612:ILE:HD11	1.97	0.47
1:C:349:GLY:HA3	1:C:725:ARG:HB2	1.96	0.47
1:D:325:MET:HE1	1:D:346:SER:HA	1.96	0.47
1:A:573:THR:HB	1:B:478:GLY:HA3	1.96	0.46
1:A:713:THR:HB	1:A:715:ASP:OD1	2.15	0.46
1:B:151:ASN:O	1:B:152:GLY:C	2.58	0.46
1:B:321:LEU:O	1:B:325:MET:HG2	2.16	0.46
1:A:430:ARG:HD3	1:A:470:THR:HG22	1.97	0.46
1:B:656:GLU:HG2	1:C:645:TYR:CE2	2.51	0.46
1:D:178:PHE:CD1	1:D:178:PHE:C	2.92	0.46
1:A:325:MET:HE1	1:A:346:SER:HA	1.97	0.46
1:B:522:ARG:CZ	1:B:712:THR:HB	2.45	0.46
1:D:135:ASN:HB2	1:D:357:LEU:HD21	1.96	0.46
1:B:685:PHE:O	1:B:689:ILE:HG22	2.15	0.46
1:D:44:ARG:CB	1:D:82:VAL:HG11	2.46	0.46
1:D:357:LEU:C	1:D:357:LEU:HD23	2.40	0.46
1:A:195:ILE:HD12	1:A:680:PRO:CG	2.45	0.46
1:A:645:TYR:CE2	1:D:656:GLU:HG2	2.50	0.46
1:B:61:TYR:O	1:B:66:GLY:HA3	2.15	0.46
1:A:685:PHE:O	1:A:689:ILE:HG22	2.16	0.46
1:D:580:ILE:CD1	1:D:634:LEU:HD11	2.45	0.46
1:B:310:ARG:HD3	5:B:803:F6P:O2	2.15	0.46
1:B:115:LEU:HD23	1:B:161:LYS:HG3	1.98	0.46
1:C:151:ASN:O	1:C:152:GLY:C	2.59	0.46
1:A:151:ASN:O	1:A:152:GLY:C	2.59	0.45
1:C:155:ASP:OD1	1:C:156:LYS:N	2.49	0.45
1:A:485:GLY:N	1:A:517:GLU:OE1	2.49	0.45
1:A:575:ARG:NH1	1:A:631:GLN:HG2	2.31	0.45
1:C:430:ARG:NH1	2:C:802:PO4:P	2.89	0.45
1:B:711:PHE:HD1	1:B:711:PHE:O	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TYR:O	1:A:66:GLY:HA3	2.16	0.45
1:A:349:GLY:HA3	1:A:725:ARG:HB2	1.97	0.45
1:D:151:ASN:O	1:D:152:GLY:C	2.59	0.45
1:B:535:VAL:CG2	1:B:689:ILE:CG2	2.95	0.45
1:C:243:PRO:HG2	1:C:376:PHE:CE2	2.52	0.45
1:A:193:ARG:NH2	1:A:313:THR:O	2.48	0.45
1:B:363:MET:HE3	1:B:363:MET:HB3	1.87	0.45
1:C:580:ILE:CD1	1:C:634:LEU:HD11	2.47	0.45
1:D:217:MET:SD	5:D:803:F6P:O3	2.75	0.45
1:D:373:GLU:CD	1:D:375:ARG:NH1	2.75	0.45
1:A:321:LEU:O	1:A:325:MET:HG2	2.17	0.45
1:B:178:PHE:CE2	1:B:360:CYS:HB3	2.52	0.45
1:B:193:ARG:HA	1:B:193:ARG:HD3	1.63	0.45
1:C:485:GLY:N	1:C:517:GLU:OE1	2.49	0.45
1:D:176:ASN:HD22	1:D:184:THR:CB	2.30	0.45
1:D:244:PRO:HB2	1:D:248:TRP:CD1	2.52	0.45
1:B:195:ILE:HD12	1:B:680:PRO:CG	2.47	0.45
1:C:321:LEU:O	1:C:325:MET:HG2	2.17	0.45
1:D:29:VAL:HG11	1:D:46:VAL:HG11	1.96	0.45
1:D:651:TYR:O	1:D:655:SER:HB3	2.17	0.45
1:D:685:PHE:O	1:D:689:ILE:HG22	2.17	0.45
1:D:485:GLY:N	1:D:517:GLU:OE1	2.50	0.44
1:C:357:LEU:C	1:C:357:LEU:HD23	2.42	0.44
1:C:685:PHE:O	1:C:689:ILE:HG22	2.17	0.44
1:C:48:ARG:NH1	1:C:761:LEU:O	2.50	0.44
1:D:144:LEU:HD12	1:D:162:TYR:HD1	1.83	0.44
1:D:249:GLU:HG2	1:D:291:LEU:HD11	1.98	0.44
1:A:156:LYS:O	1:A:159:VAL:HG12	2.18	0.44
1:B:534:MET:HE2	1:B:534:MET:HB3	1.85	0.44
1:C:372:ASP:OD1	1:C:372:ASP:N	2.51	0.44
1:A:406:ILE:O	1:A:408:LYS:HE3	2.18	0.44
1:C:672:MET:O	1:C:675:GLY:HA2	2.18	0.44
1:D:85:ILE:CD1	1:D:92:ILE:CG2	2.95	0.44
1:A:193:ARG:HA	1:A:193:ARG:HD3	1.67	0.44
1:A:144:LEU:HD12	1:A:162:TYR:HD1	1.81	0.44
1:A:580:ILE:CD1	1:A:634:LEU:HD11	2.48	0.44
1:D:198:VAL:O	1:D:202:MET:HG3	2.17	0.44
1:A:667:ASN:HD21	1:B:672:MET:H	1.65	0.44
1:B:144:LEU:HD12	1:B:162:TYR:HD1	1.83	0.43
1:C:276:ILE:HD12	1:C:276:ILE:O	2.18	0.43
1:C:724:LYS:O	1:C:725:ARG:CB	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LYS:O	1:D:159:VAL:HG12	2.18	0.43
1:D:392:ASN:O	1:D:396:ARG:HG3	2.18	0.43
1:B:392:ASN:O	1:B:396:ARG:HG3	2.18	0.43
1:D:193:ARG:HD3	1:D:193:ARG:HA	1.63	0.43
1:A:569:SER:HB3	1:B:675:GLY:O	2.18	0.43
1:C:135:ASN:HB2	1:C:357:LEU:HD21	2.01	0.43
1:A:115:LEU:HD23	1:A:161:LYS:HG3	1.99	0.43
1:A:616:GLN:OE1	1:D:616:GLN:OE1	2.35	0.43
1:C:115:LEU:HD23	1:C:161:LYS:HG3	1.99	0.43
1:C:193:ARG:HA	1:C:193:ARG:HD3	1.66	0.43
1:C:244:PRO:HB2	1:C:248:TRP:CD1	2.54	0.43
1:A:198:VAL:O	1:A:202:MET:HG3	2.18	0.43
1:B:325:MET:HE2	1:B:325:MET:HA	2.01	0.43
1:B:485:GLY:N	1:B:517:GLU:OE1	2.51	0.43
1:A:307:HIS:CD2	1:A:310:ARG:HH12	2.37	0.42
1:D:237:VAL:CG2	1:D:394:TYR:CZ	3.02	0.42
1:B:277:ASP:N	1:B:283:ILE:HD11	2.34	0.42
1:B:645:TYR:CZ	1:C:656:GLU:HG2	2.54	0.42
1:C:154:ILE:HG22	1:C:156:LYS:H	1.84	0.42
1:C:276:ILE:HD12	1:C:276:ILE:C	2.44	0.42
1:D:337:THR:HG22	1:D:338:PRO:CD	2.49	0.42
1:A:217:MET:H	1:A:309:GLN:HE22	1.65	0.42
1:A:329:ALA:HA	1:A:345:VAL:HG21	2.01	0.42
1:A:423:ALA:HB1	1:A:678:PRO:HB3	2.01	0.42
1:B:198:VAL:O	1:B:202:MET:HG3	2.18	0.42
1:D:532:MET:HE3	1:D:717:ILE:CD1	2.50	0.42
1:A:217:MET:HB3	1:A:217:MET:HE2	1.79	0.42
1:D:277:ASP:HB3	1:D:279:GLN:H	1.84	0.42
1:C:53:VAL:HG11	1:C:334:LEU:HD11	2.02	0.42
1:C:392:ASN:O	1:C:396:ARG:HG3	2.20	0.42
1:C:570:ALA:C	1:C:572:GLY:H	2.28	0.41
1:C:373:GLU:C	1:C:374:ARG:HG3	2.45	0.41
1:D:423:ALA:HB1	1:D:678:PRO:HB3	2.02	0.41
1:A:170:MET:CE	1:A:326:GLY:HA2	2.49	0.41
1:B:97:ARG:HA	4:B:801:ADP:O3'	2.21	0.41
1:C:78:ASP:OD1	1:C:81:SER:N	2.53	0.41
1:D:367:VAL:HG22	1:D:382:LEU:HB3	2.01	0.41
1:A:99:GLN:CG	1:A:100:ALA:H	2.33	0.41
1:A:174:ILE:HG21	1:A:217:MET:HE1	2.02	0.41
1:A:574:LYS:HG3	1:A:575:ARG:N	2.34	0.41
1:B:42:ALA:CB	1:B:170:MET:HE1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLN:CG	1:A:100:ALA:N	2.84	0.41
1:A:160:GLN:O	1:A:164:TYR:HD2	2.03	0.41
1:B:673:GLN:O	1:B:674:GLN:C	2.60	0.41
1:C:170:MET:CE	1:C:326:GLY:HA2	2.51	0.41
1:A:469:TRP:O	1:A:470:THR:C	2.64	0.41
1:B:277:ASP:HB3	1:B:283:ILE:HD11	2.03	0.41
1:B:758:MET:HE3	1:B:758:MET:HB2	1.96	0.41
1:C:154:ILE:HB	1:C:157:GLU:CD	2.45	0.41
1:C:519:SER:HB2	1:C:717:ILE:HD12	2.03	0.41
1:D:154:ILE:HG22	1:D:156:LYS:H	1.86	0.41
1:D:176:ASN:HD21	1:D:184:THR:H	1.68	0.41
1:A:174:ILE:HG23	1:A:190:ALA:CB	2.51	0.41
1:A:392:ASN:O	1:A:396:ARG:HG3	2.21	0.41
1:A:713:THR:CB	1:A:715:ASP:OD1	2.68	0.41
1:B:206:GLN:O	1:B:208:HIS:O	2.40	0.41
1:B:420:ALA:HB2	1:B:481:ARG:NH1	2.35	0.41
1:B:529:CYS:C	1:B:712:THR:HG21	2.45	0.41
1:C:480:LYS:NZ	1:D:573:THR:O	2.53	0.41
1:C:542:ASN:HD22	1:C:542:ASN:N	2.09	0.41
1:D:100:ALA:O	1:D:106:GLY:HA3	2.21	0.41
1:D:363:MET:HE3	1:D:363:MET:HB3	1.88	0.41
1:D:600:ALA:HB3	1:D:758:MET:HE1	2.03	0.41
1:D:740:ASP:C	1:D:740:ASP:OD1	2.64	0.41
1:A:115:LEU:CD2	1:A:161:LYS:HG3	2.51	0.40
1:A:402:PRO:O	1:A:405:GLN:HB2	2.21	0.40
1:B:42:ALA:HB1	1:B:170:MET:HE1	2.03	0.40
1:B:175:ASP:OD2	5:B:803:F6P:C1	2.68	0.40
1:B:580:ILE:HD12	1:B:634:LEU:HD11	2.02	0.40
1:C:115:LEU:CD2	1:C:161:LYS:HG3	2.51	0.40
1:D:160:GLN:O	1:D:164:TYR:HD2	2.03	0.40
1:A:154:ILE:N	1:A:157:GLU:OE2	2.55	0.40
1:B:32:SER:HB3	1:B:130:SER:HB3	2.03	0.40
1:B:724:LYS:O	1:B:725:ARG:CB	2.67	0.40
1:D:211:THR:OG1	1:D:300:THR:HG23	2.21	0.40
1:B:100:ALA:O	1:B:106:GLY:HA3	2.22	0.40
1:B:154:ILE:HG22	1:B:156:LYS:H	1.86	0.40
1:C:579:ILE:CD1	1:C:664:CYS:HB3	2.51	0.40
1:C:702:LYS:C	1:C:703:GLU:HG3	2.46	0.40
1:D:519:SER:HB2	1:D:717:ILE:HD12	2.04	0.40
1:C:409:THR:HG22	1:C:410:ASN:N	2.37	0.40
1:A:204:THR:HA	1:B:35:ASP:OD2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:GLY:H	1:B:568:GLN:NE2	2.19	0.40
1:C:100:ALA:O	1:C:106:GLY:HA3	2.22	0.40
1:C:404:ASP:OD1	1:C:404:ASP:N	2.54	0.40
1:D:170:MET:HE3	1:D:185:ILE:HD11	2.03	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:372:ASP:OD2	1:C:139:LYS:NZ[1_554]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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	700/761 (92%)	686 (98%)	11 (2%)	3 (0%)	30	51
1	B	722/761 (95%)	698 (97%)	20 (3%)	4 (1%)	21	41
1	C	696/761 (92%)	682 (98%)	11 (2%)	3 (0%)	30	51
1	D	719/761 (94%)	695 (97%)	20 (3%)	4 (1%)	21	41
All	All	2837/3044 (93%)	2761 (97%)	62 (2%)	14 (0%)	24	45

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	152	GLY
1	A	152	GLY
1	B	152	GLY
1	C	574	LYS
1	D	152	GLY
1	D	724	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	724	LYS
1	B	703	GLU
1	D	574	LYS
1	B	574	LYS
1	A	143	GLY
1	B	143	GLY
1	C	218	GLY
1	D	143	GLY

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	571/614 (93%)	549 (96%)	22 (4%)	28	54
1	B	587/614 (96%)	567 (97%)	20 (3%)	32	59
1	C	568/614 (92%)	542 (95%)	26 (5%)	24	48
1	D	585/614 (95%)	554 (95%)	31 (5%)	20	43
All	All	2311/2456 (94%)	2212 (96%)	99 (4%)	26	51

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	VAL
1	A	142	SER
1	A	159	VAL
1	A	193	ARG
1	A	242	SER
1	A	266	LEU
1	A	291	LEU
1	A	373	GLU
1	A	377	GLN
1	A	399	ILE
1	A	401	LEU
1	A	404	ASP
1	A	486	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	534	MET
1	A	573	THR
1	A	574	LYS
1	A	667	ASN
1	A	694	MET
1	A	713	THR
1	A	717	ILE
1	A	725	ARG
1	A	727	VAL
1	B	86	LEU
1	B	99	GLN
1	B	117	ARG
1	B	130	SER
1	B	159	VAL
1	B	193	ARG
1	B	242	SER
1	B	291	LEU
1	B	359	GLU
1	B	373	GLU
1	B	399	ILE
1	B	401	LEU
1	B	404	ASP
1	B	448	ASP
1	B	534	MET
1	B	568	GLN
1	B	671	HIS
1	B	694	MET
1	B	725	ARG
1	B	727	VAL
1	C	53	VAL
1	C	82	VAL
1	C	128	ASP
1	C	130	SER
1	C	159	VAL
1	C	193	ARG
1	C	202	MET
1	C	217	MET
1	C	291	LEU
1	C	310	ARG
1	C	340	THR
1	C	359	GLU
1	C	364	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	368	GLN
1	C	377	GLN
1	C	378	ASP
1	C	395	LYS
1	C	401	LEU
1	C	404	ASP
1	C	410	ASN
1	C	430	ARG
1	C	442	ARG
1	C	523	GLU
1	C	534	MET
1	C	542	ASN
1	C	727	VAL
1	D	29	VAL
1	D	86	LEU
1	D	99	GLN
1	D	117	ARG
1	D	128	ASP
1	D	130	SER
1	D	142	SER
1	D	159	VAL
1	D	176	ASN
1	D	193	ARG
1	D	262	ARG
1	D	278	THR
1	D	399	ILE
1	D	401	LEU
1	D	404	ASP
1	D	405	GLN
1	D	409	THR
1	D	459	LYS
1	D	460	GLU
1	D	464	THR
1	D	486	LYS
1	D	499	SER
1	D	534	MET
1	D	612	ILE
1	D	629	THR
1	D	671	HIS
1	D	672	MET
1	D	712	THR
1	D	725	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	727	VAL
1	D	758	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	116	GLN
1	A	121	ASN
1	A	153	GLN
1	A	166	ASN
1	A	192	HIS
1	A	206	GLN
1	A	220	HIS
1	A	309	GLN
1	A	368	GLN
1	A	498	HIS
1	A	525	HIS
1	A	568	GLN
1	A	644	ASN
1	A	652	GLN
1	A	673	GLN
1	A	738	GLN
1	B	65	GLN
1	B	116	GLN
1	B	121	ASN
1	B	153	GLN
1	B	166	ASN
1	B	220	HIS
1	B	251	GLN
1	B	267	ASN
1	B	279	GLN
1	B	351	HIS
1	B	368	GLN
1	B	417	ASN
1	B	498	HIS
1	B	568	GLN
1	B	638	ASN
1	B	644	ASN
1	B	652	GLN
1	B	671	HIS
1	B	673	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	730	GLN
1	B	738	GLN
1	C	73	ASN
1	C	116	GLN
1	C	121	ASN
1	C	166	ASN
1	C	206	GLN
1	C	307	HIS
1	C	392	ASN
1	C	498	HIS
1	C	525	HIS
1	C	542	ASN
1	C	568	GLN
1	C	616	GLN
1	C	638	ASN
1	C	652	GLN
1	C	673	GLN
1	D	73	ASN
1	D	116	GLN
1	D	153	GLN
1	D	166	ASN
1	D	176	ASN
1	D	220	HIS
1	D	259	ASN
1	D	267	ASN
1	D	307	HIS
1	D	362	GLN
1	D	368	GLN
1	D	392	ASN
1	D	501	ASN
1	D	525	HIS
1	D	616	GLN
1	D	644	ASN
1	D	667	ASN
1	D	673	GLN
1	D	738	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 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	PO4	B	805	-	4,4,4	1.17	0	6,6,6	0.79	0
2	PO4	D	804	-	4,4,4	0.86	0	6,6,6	0.89	0
2	PO4	C	802	-	4,4,4	1.40	0	6,6,6	0.72	0
3	FBP	B	802	-	18,20,20	1.19	1 (5%)	21,32,32	1.11	1 (4%)
3	FBP	A	802	-	18,20,20	1.30	1 (5%)	21,32,32	1.56	1 (4%)
5	F6P	B	803	-	15,16,16	0.78	1 (6%)	16,25,25	1.36	1 (6%)
4	ADP	D	801	-	28,29,29	1.41	4 (14%)	43,45,45	2.02	13 (30%)
2	PO4	D	805	-	4,4,4	0.99	0	6,6,6	0.69	0
3	FBP	C	801	-	18,20,20	1.12	1 (5%)	21,32,32	1.42	2 (9%)
2	PO4	A	801	-	4,4,4	1.16	0	6,6,6	0.79	0
4	ADP	B	801	-	28,29,29	1.64	5 (17%)	43,45,45	2.07	12 (27%)
2	PO4	B	804	-	4,4,4	1.22	0	6,6,6	0.71	0
5	F6P	D	803	-	15,16,16	0.81	1 (6%)	16,25,25	1.18	1 (6%)
3	FBP	D	802	-	18,20,20	0.97	1 (5%)	21,32,32	0.97	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FBP	B	802	-	-	6/13/32/32	0/1/1/1
3	FBP	A	802	-	-	5/13/32/32	0/1/1/1
5	F6P	B	803	-	-	3/9/28/28	0/1/1/1
4	ADP	D	801	-	-	4/16/32/32	0/3/3/3
3	FBP	C	801	-	-	3/13/32/32	0/1/1/1
4	ADP	B	801	-	-	0/16/32/32	0/3/3/3
5	F6P	D	803	-	-	4/9/28/28	0/1/1/1
3	FBP	D	802	-	-	4/13/32/32	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	ADP	PA-O3A	4.84	1.64	1.59
4	D	801	ADP	C5-C4	4.69	1.47	1.39
4	B	801	ADP	C5-C4	4.20	1.46	1.39
3	A	802	FBP	O2-C2	3.95	1.47	1.40
3	B	802	FBP	O2-C2	3.01	1.45	1.40
3	D	802	FBP	O2-C2	2.94	1.45	1.40
4	B	801	ADP	C5-C6	2.80	1.48	1.41
3	C	801	FBP	O5-C2	-2.50	1.39	1.43
4	D	801	ADP	C8-N7	2.49	1.36	1.31
4	B	801	ADP	C4-N9	-2.40	1.32	1.37
4	D	801	ADP	C5-C6	2.29	1.47	1.41
4	D	801	ADP	C5-N7	-2.17	1.35	1.39
5	B	803	F6P	O2-C2	2.16	1.44	1.40
5	D	803	F6P	O2-C2	2.02	1.44	1.40
4	B	801	ADP	C5-N7	-2.01	1.35	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	ADP	C5-C4-N3	-5.90	118.59	126.72
4	D	801	ADP	C5-C4-N3	-5.86	118.65	126.72
3	A	802	FBP	O2-C2-O5	5.32	119.55	109.33
4	D	801	ADP	N3-C4-N9	5.16	135.94	127.17
4	B	801	ADP	N3-C4-N9	4.98	135.65	127.17
4	B	801	ADP	C2-N3-C4	4.06	121.74	111.83
4	B	801	ADP	N3-C2-N1	-3.76	122.88	128.58
4	D	801	ADP	C2-N3-C4	3.72	120.92	111.83
4	D	801	ADP	N3-C2-N1	-3.58	123.16	128.58
4	B	801	ADP	C4-N9-C8	3.40	109.31	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	801	ADP	C4-N9-C8	3.39	109.30	105.74
5	B	803	F6P	O1-C1-C2	3.26	118.89	111.67
4	B	801	ADP	C4-C5-N7	-2.87	107.30	110.58
4	D	801	ADP	C4-C5-N7	-2.85	107.32	110.58
3	C	801	FBP	O2P-P1-O1	2.85	114.10	106.67
3	C	801	FBP	O2-C2-O5	2.78	114.66	109.33
4	B	801	ADP	O2B-PB-O1B	2.64	121.12	110.83
3	B	802	FBP	O6-P2-O4P	2.58	113.41	106.44
4	D	801	ADP	C5-N7-C8	2.52	107.42	103.45
4	B	801	ADP	O3B-PB-O2B	2.48	117.10	107.80
4	B	801	ADP	C2'-C3'-C4'	2.44	107.33	102.61
4	B	801	ADP	N9-C8-N7	-2.44	110.47	113.94
4	D	801	ADP	N9-C8-N7	-2.39	110.54	113.94
4	B	801	ADP	C5-N7-C8	2.36	107.16	103.45
4	D	801	ADP	C2'-C3'-C4'	2.21	106.89	102.61
4	D	801	ADP	N6-C6-N1	2.21	123.29	118.38
4	D	801	ADP	C3'-C2'-C1'	2.19	105.60	101.46
4	B	801	ADP	C2'-C1'-N9	-2.18	107.90	113.30
3	D	802	FBP	O2-C2-O5	2.08	113.31	109.33
4	D	801	ADP	C5-C6-N6	-2.08	118.15	123.29
5	D	803	F6P	O3P-P-O2P	2.06	115.55	107.80
4	D	801	ADP	O3A-PA-O1A	-2.05	104.53	110.70

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	FBP	O1-C1-C2-O2
3	A	802	FBP	O1-C1-C2-C3
3	A	802	FBP	O1-C1-C2-O5
3	B	802	FBP	O1-C1-C2-O2
3	B	802	FBP	O1-C1-C2-O5
3	C	801	FBP	O5-C5-C6-O6
3	D	802	FBP	O1-C1-C2-O2
3	D	802	FBP	O1-C1-C2-C3
3	D	802	FBP	O5-C5-C6-O6
4	D	801	ADP	PA-O3A-PB-O2B
4	D	801	ADP	PA-O3A-PB-O3B
5	B	803	F6P	O1-C1-C2-O2
5	D	803	F6P	C6-O6-P-O1P
3	A	802	FBP	C4-C5-C6-O6
3	A	802	FBP	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	801	FBP	C4-C5-C6-O6
3	D	802	FBP	C4-C5-C6-O6
5	D	803	F6P	O1-C1-C2-O5
3	B	802	FBP	C1-O1-P1-O1P
5	B	803	F6P	O1-C1-C2-C3
5	D	803	F6P	O1-C1-C2-C3
3	B	802	FBP	C4-C5-C6-O6
5	B	803	F6P	O1-C1-C2-O5
3	B	802	FBP	O5-C5-C6-O6
4	D	801	ADP	O4'-C4'-C5'-O5'
4	D	801	ADP	C3'-C4'-C5'-O5'
3	B	802	FBP	C6-O6-P2-O6P
3	C	801	FBP	C6-O6-P2-O4P
5	D	803	F6P	C6-O6-P-O2P

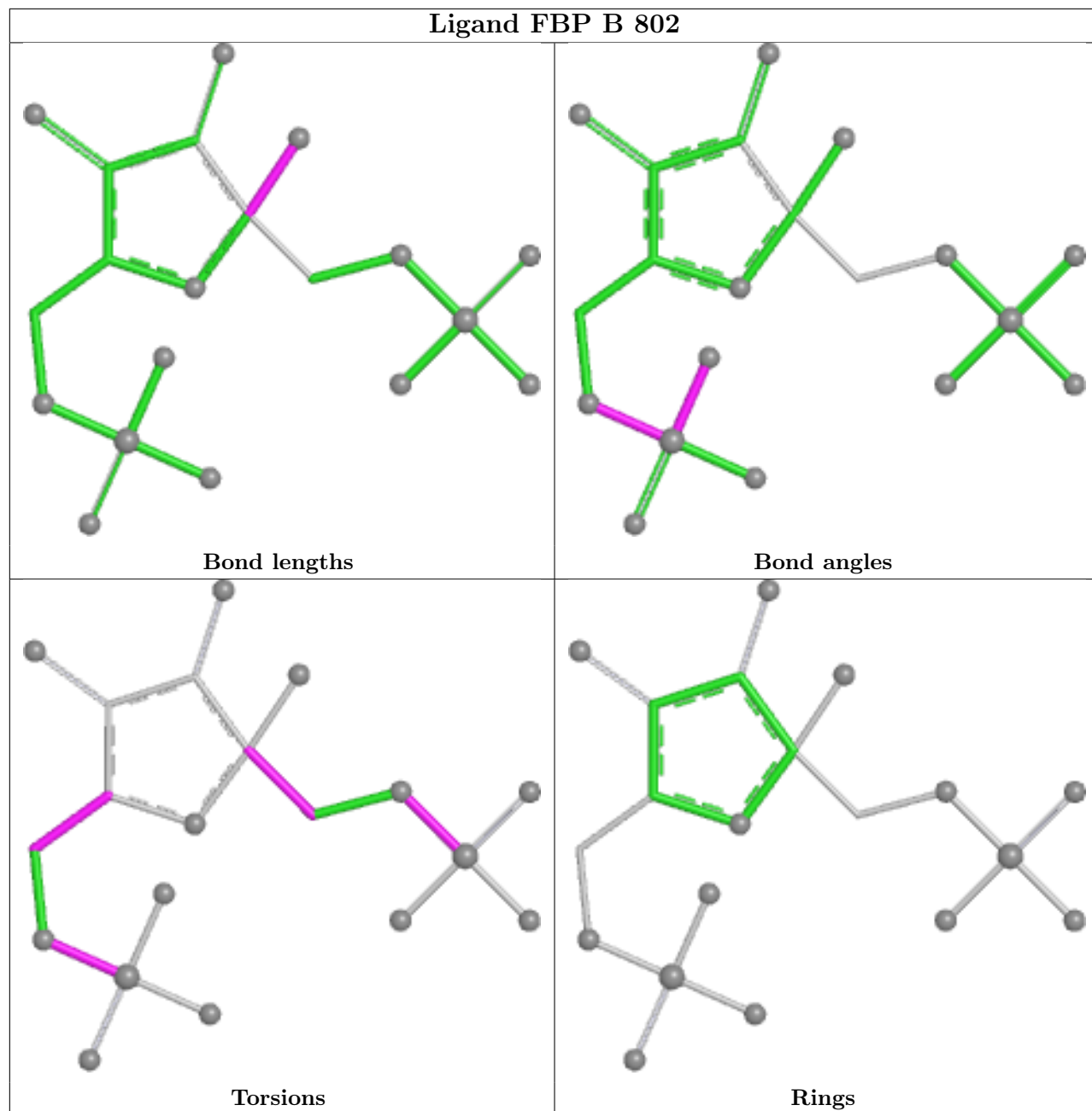
There are no ring outliers.

11 monomers are involved in 33 short contacts:

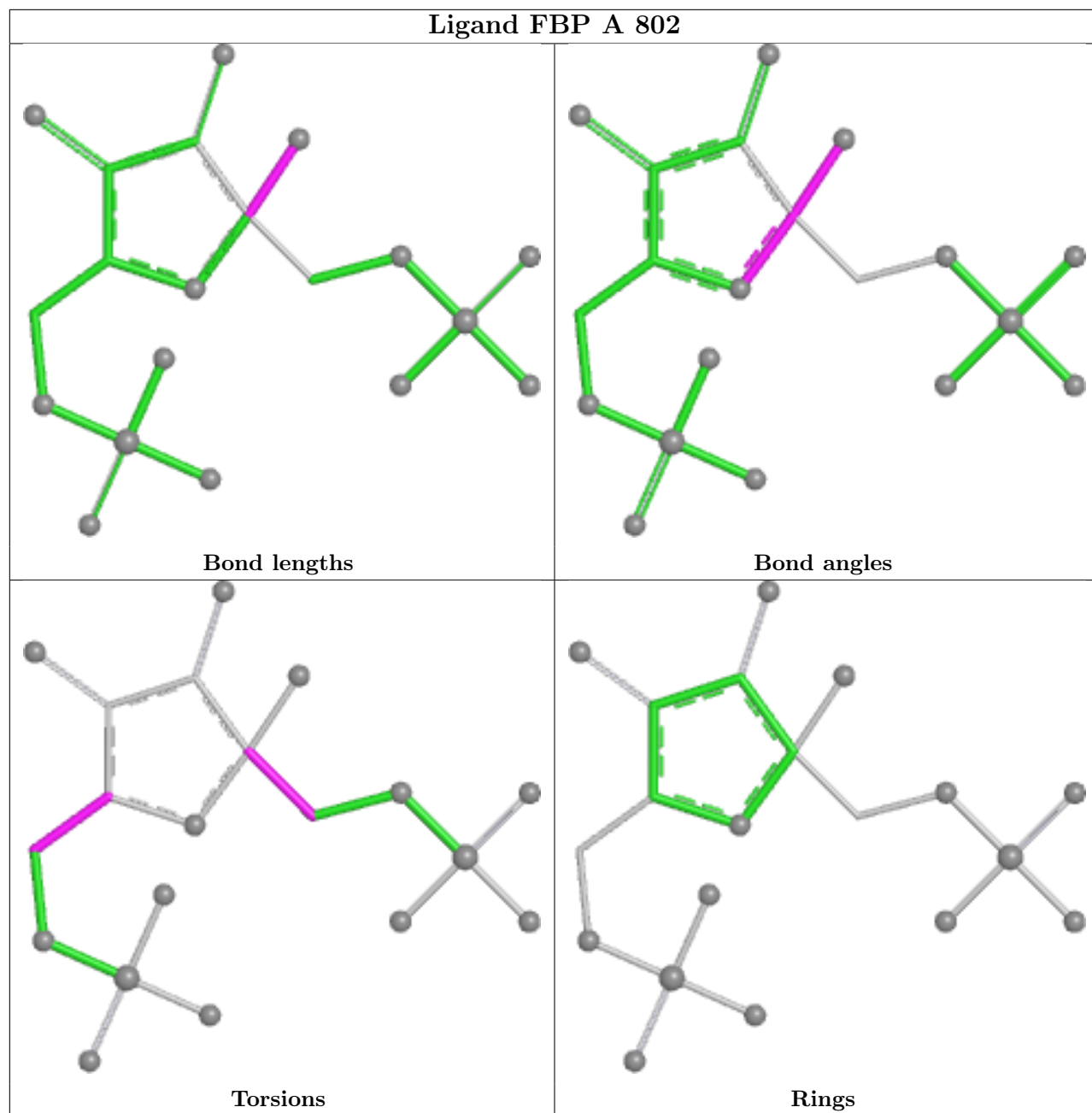
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	805	PO4	1	0
2	C	802	PO4	2	0
3	A	802	FBP	1	0
5	B	803	F6P	9	0
4	D	801	ADP	3	0
2	D	805	PO4	1	0
3	C	801	FBP	1	0
4	B	801	ADP	6	0
2	B	804	PO4	1	0
5	D	803	F6P	5	0
3	D	802	FBP	3	0

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

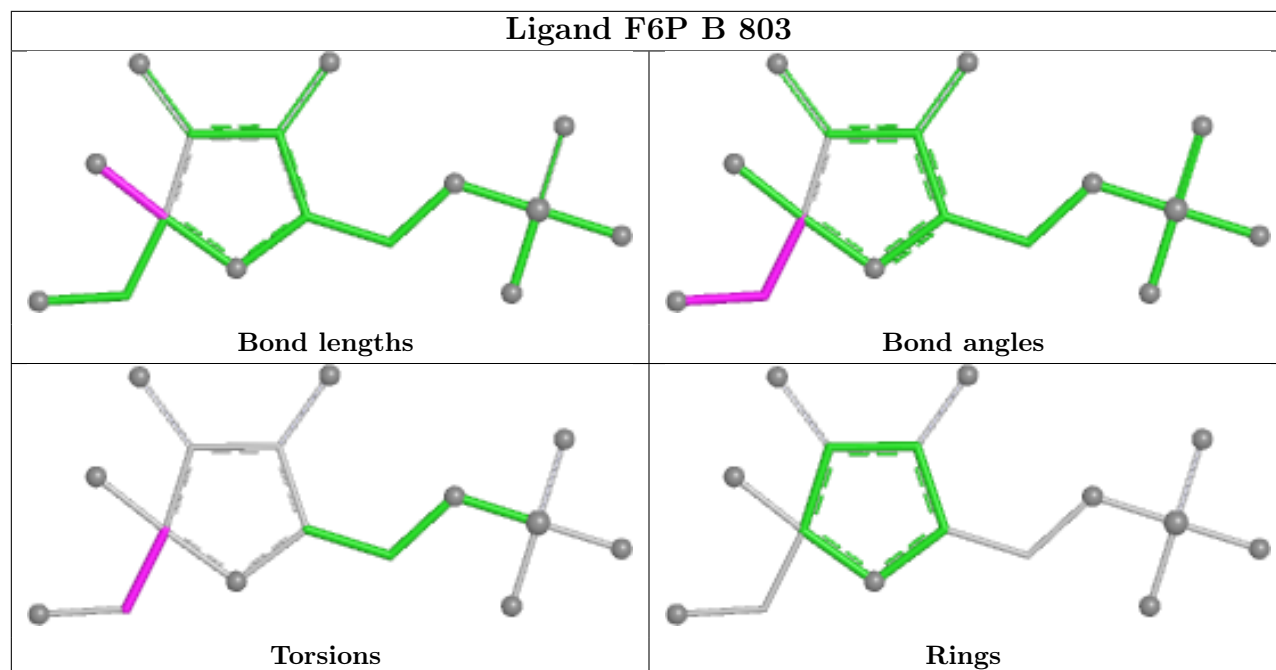
equivalents in the CSD to analyse the geometry.



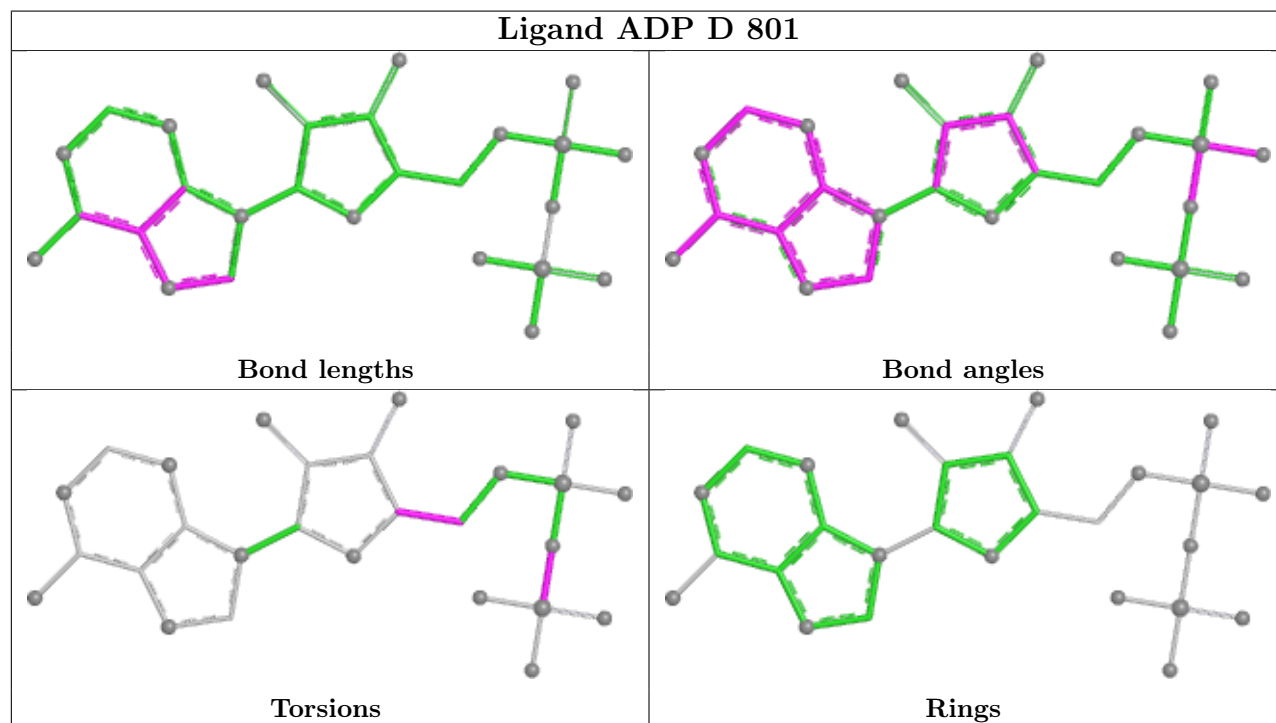
Ligand FBP A 802

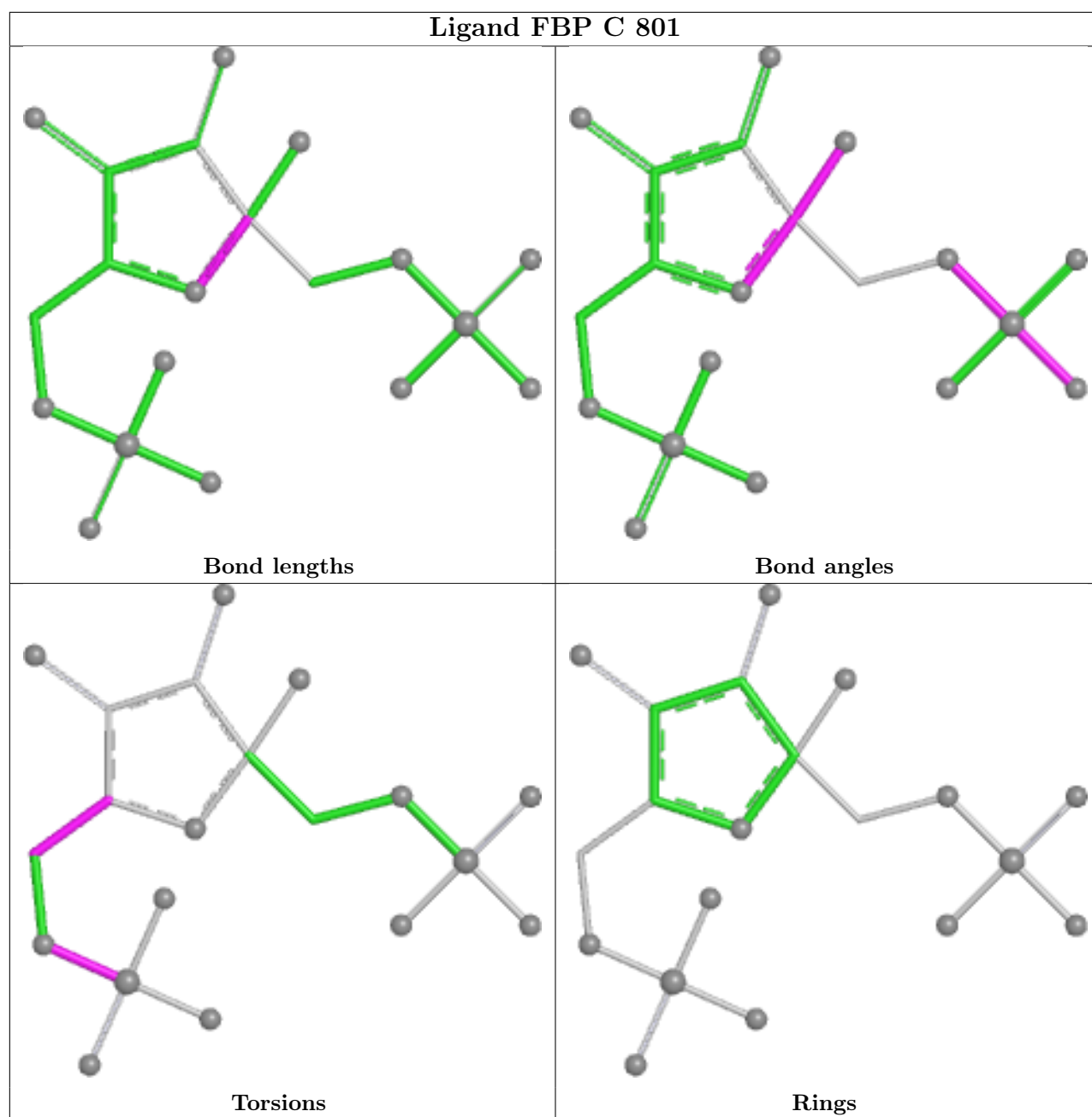


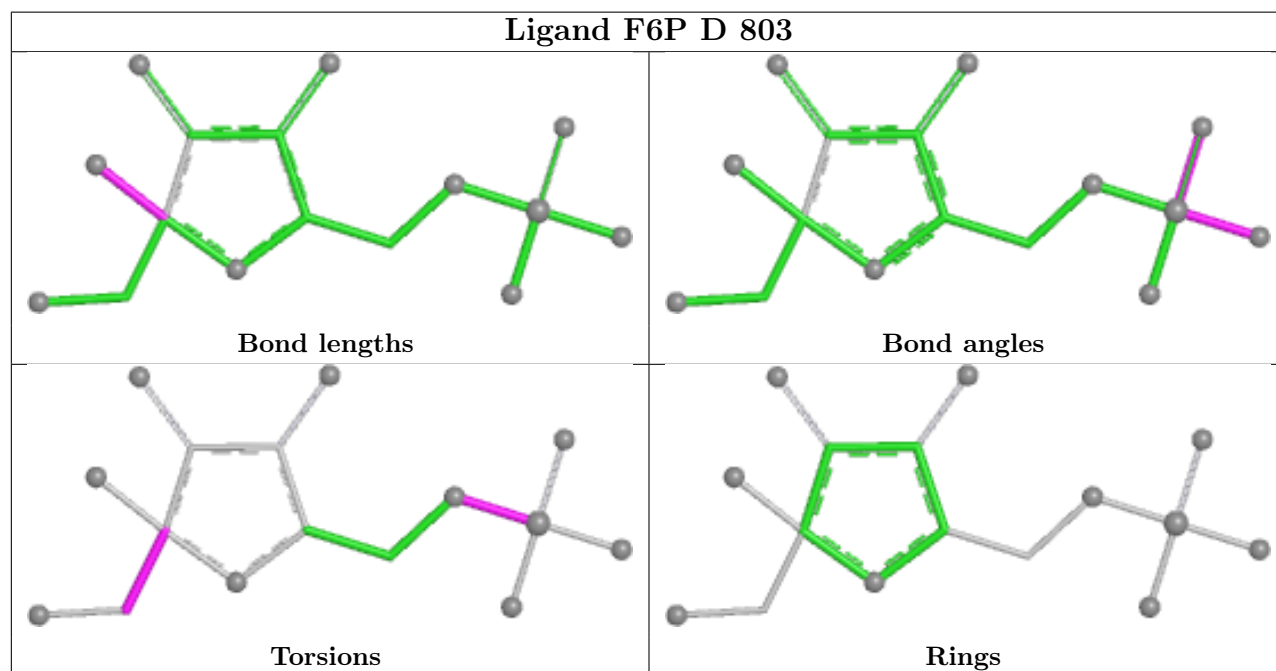
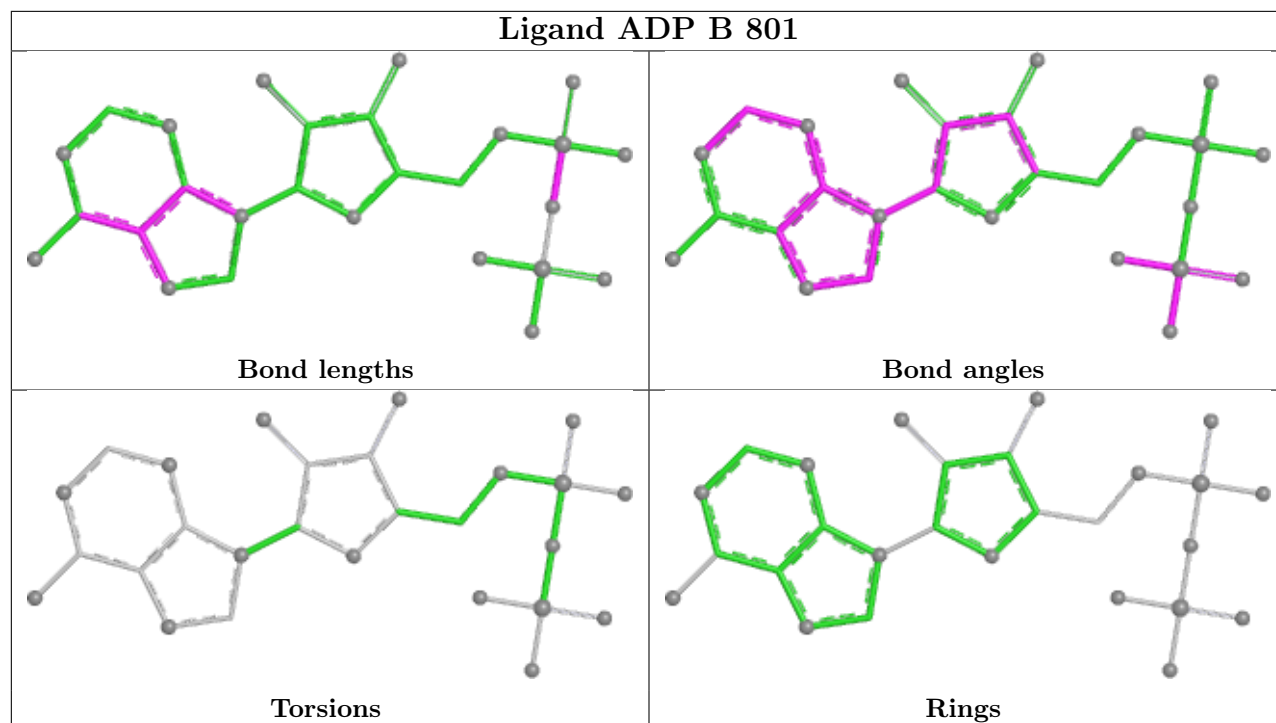
Ligand F6P B 803

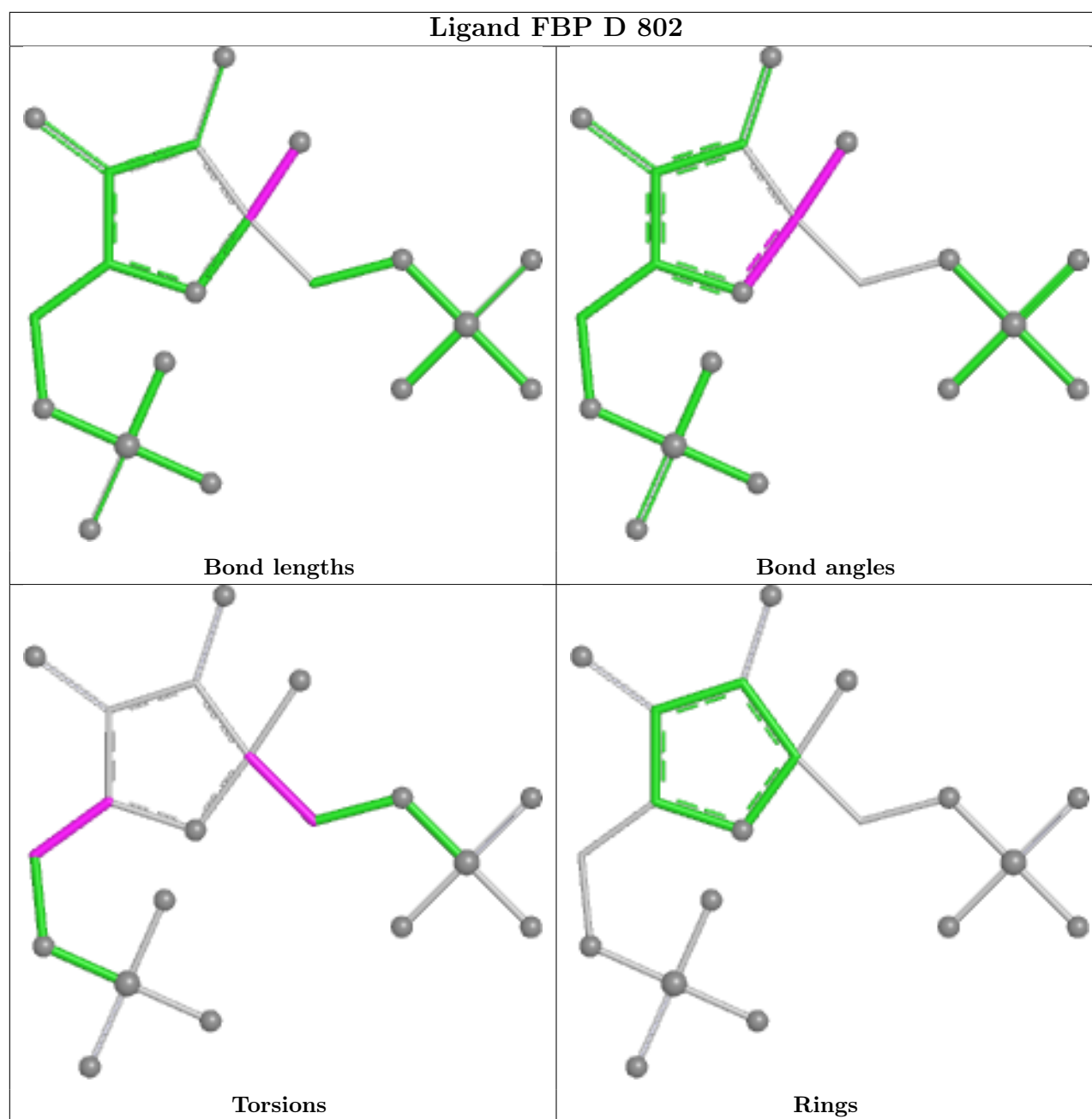


Ligand ADP D 801









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	708/761 (93%)	0.05	29 (4%)	41	36	27, 48, 94, 158	0
1	B	728/761 (95%)	0.11	28 (3%)	44	39	30, 51, 100, 194	0
1	C	704/761 (92%)	0.36	23 (3%)	49	44	35, 66, 108, 138	0
1	D	725/761 (95%)	0.34	29 (4%)	42	37	35, 66, 115, 174	0
All	All	2865/3044 (94%)	0.21	109 (3%)	44	39	27, 57, 108, 194	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	205	ALA	6.6
1	A	162	TYR	5.5
1	B	162	TYR	5.2
1	B	163	ALA	5.0
1	C	570	ALA	4.7
1	C	162	TYR	4.5
1	C	163	ALA	4.5
1	A	174	ILE	4.4
1	A	163	ALA	4.3
1	D	162	TYR	4.3
1	B	711	PHE	4.2
1	C	277	ASP	4.2
1	B	159	VAL	4.0
1	A	82	VAL	3.9
1	B	164	TYR	3.8
1	C	629	THR	3.8
1	C	573	THR	3.7
1	D	148	LEU	3.7
1	B	148	LEU	3.6
1	B	149	ALA	3.5
1	B	145	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	157	GLU	3.4
1	C	569	SER	3.3
1	B	147	GLU	3.3
1	C	148	LEU	3.2
1	B	96	ALA	3.2
1	C	572	GLY	3.2
1	B	154	ILE	3.2
1	D	202	MET	3.1
1	D	178	PHE	3.1
1	C	371	MET	3.1
1	C	143	GLY	3.1
1	A	630	ILE	3.1
1	A	632	ARG	3.1
1	B	115	LEU	3.0
1	C	502	ALA	3.0
1	A	158	ALA	3.0
1	D	149	ALA	3.0
1	D	204	THR	2.9
1	D	145	LEU	2.9
1	B	153	GLN	2.9
1	A	148	LEU	2.9
1	A	143	GLY	2.9
1	B	156	LYS	2.8
1	A	149	ALA	2.8
1	A	364	THR	2.8
1	D	158	ALA	2.8
1	D	154	ILE	2.8
1	A	351	HIS	2.8
1	D	208	HIS	2.8
1	C	364	THR	2.8
1	A	128	ASP	2.7
1	D	107	ARG	2.7
1	D	153	GLN	2.7
1	D	206	GLN	2.6
1	C	152	GLY	2.6
1	C	149	ALA	2.6
1	B	144	LEU	2.5
1	D	96	ALA	2.5
1	D	163	ALA	2.5
1	D	144	LEU	2.5
1	B	363	MET	2.5
1	D	212	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	352	ALA	2.5
1	A	343	CYS	2.5
1	A	154	ILE	2.5
1	D	363	MET	2.5
1	B	158	ALA	2.5
1	D	712	THR	2.4
1	A	108	LEU	2.4
1	A	628	THR	2.4
1	A	629	THR	2.4
1	B	724	LYS	2.4
1	D	674	GLN	2.4
1	D	407	PRO	2.3
1	D	66	GLY	2.3
1	A	150	ARG	2.3
1	A	349	GLY	2.3
1	D	343	CYS	2.3
1	A	153	GLN	2.3
1	B	401	LEU	2.3
1	C	82	VAL	2.3
1	C	527	GLU	2.2
1	C	368	GLN	2.2
1	C	59	PHE	2.2
1	B	205	ALA	2.2
1	B	203	THR	2.2
1	C	164	TYR	2.2
1	D	108	LEU	2.2
1	D	159	VAL	2.2
1	B	151	ASN	2.1
1	A	152	GLY	2.1
1	B	535	VAL	2.1
1	A	59	PHE	2.1
1	D	409	THR	2.1
1	A	759	LYS	2.1
1	B	161	LYS	2.1
1	A	367	VAL	2.1
1	C	26	ALA	2.1
1	B	671	HIS	2.1
1	A	159	VAL	2.1
1	B	105	GLU	2.0
1	B	110	ALA	2.0
1	C	278	THR	2.0
1	A	561	ASP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	724	LYS	2.0
1	C	630	ILE	2.0
1	D	399	ILE	2.0
1	A	164	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

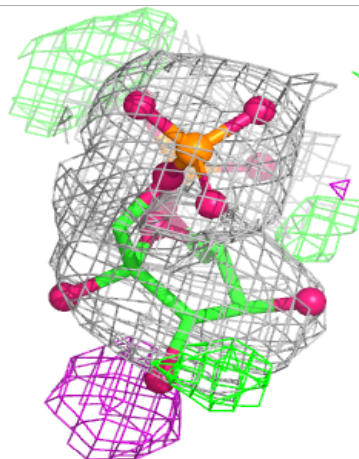
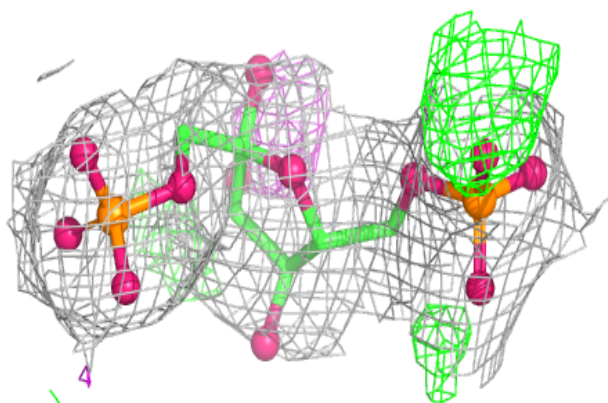
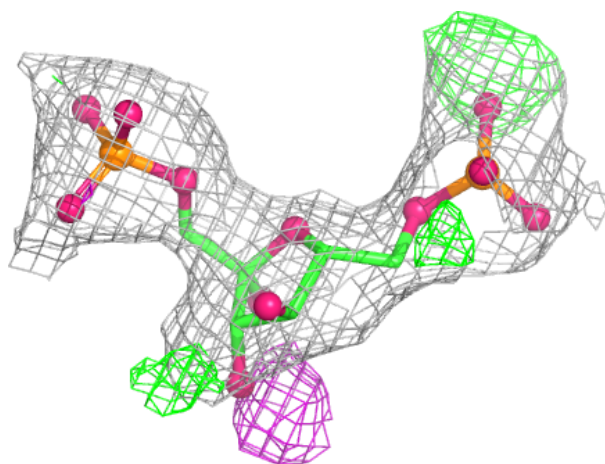
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FBP	B	802	20/20	0.78	0.14	70,89,99,100	0
2	PO4	D	804	5/5	0.87	0.09	62,72,76,76	0
4	ADP	B	801	27/27	0.87	0.10	59,69,78,81	0
3	FBP	D	802	20/20	0.88	0.11	65,84,105,119	0
4	ADP	D	801	27/27	0.88	0.09	84,89,96,102	0
5	F6P	D	803	16/16	0.90	0.09	65,72,77,77	0
3	FBP	C	801	20/20	0.92	0.10	38,54,61,70	0
5	F6P	B	803	16/16	0.94	0.08	43,54,61,69	0
2	PO4	B	804	5/5	0.95	0.06	49,49,51,54	0
3	FBP	A	802	20/20	0.96	0.07	36,43,44,46	0
2	PO4	C	802	5/5	0.96	0.05	54,55,59,61	0
2	PO4	D	805	5/5	0.97	0.06	48,54,57,59	0
2	PO4	B	805	5/5	0.98	0.04	39,39,40,42	0
2	PO4	A	801	5/5	0.99	0.04	33,33,34,36	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.

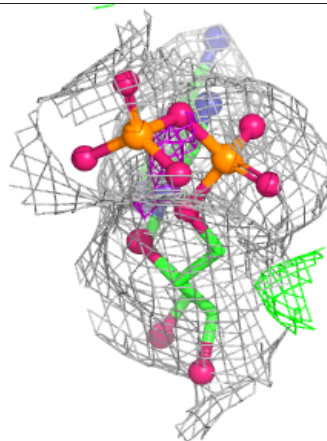
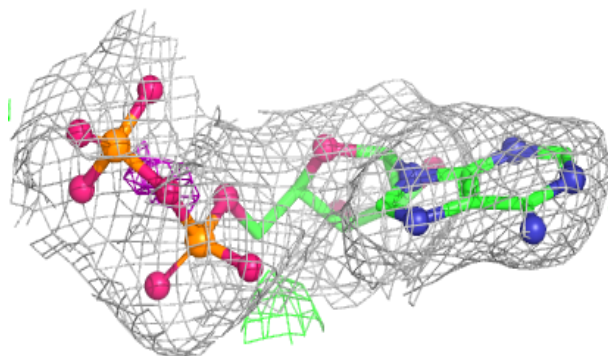
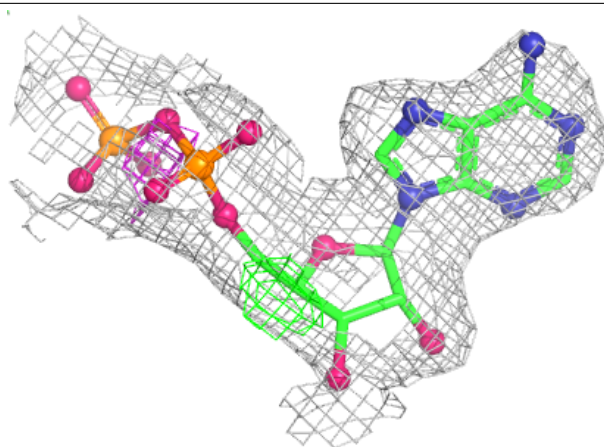
Electron density around FBP B 802:

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



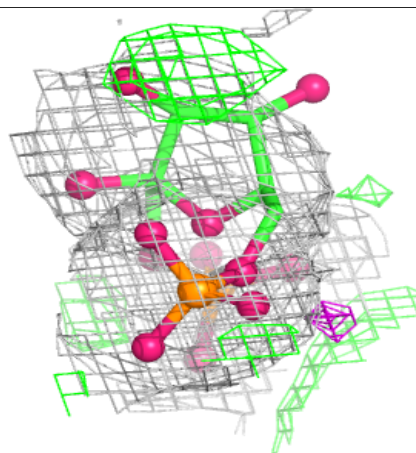
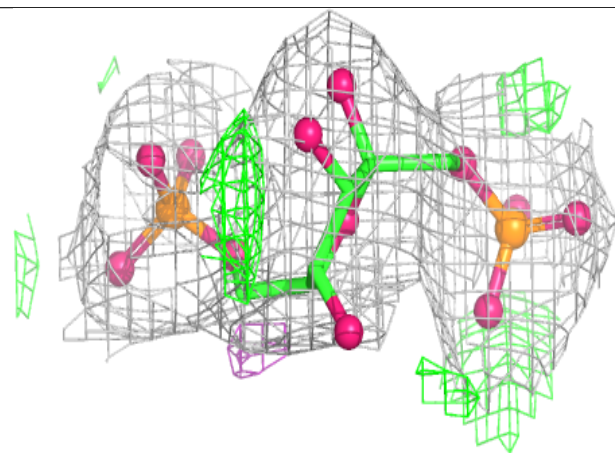
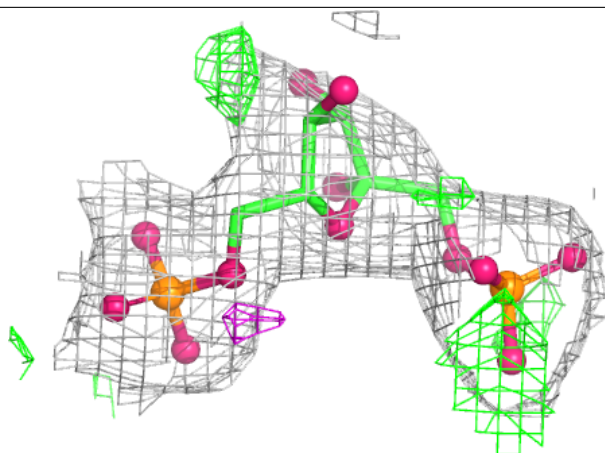
Electron density around ADP B 801:

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



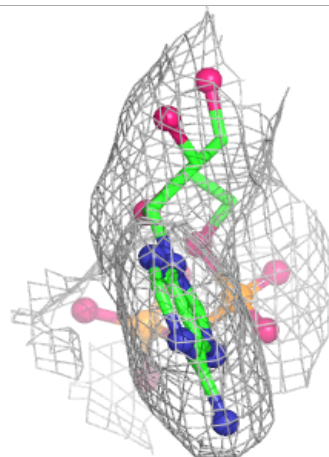
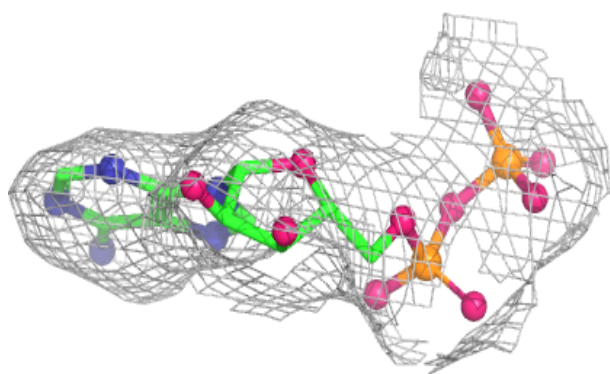
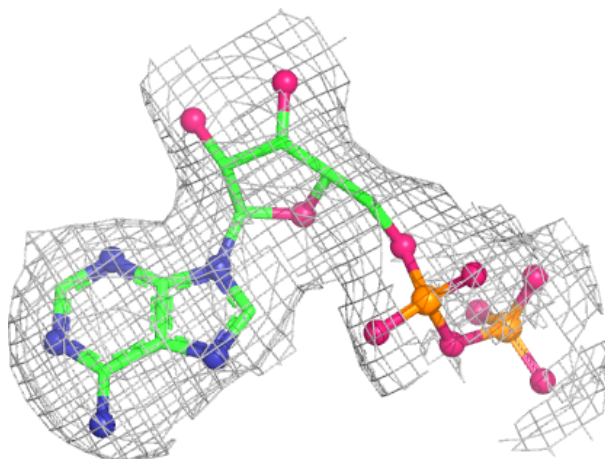
Electron density around FBP D 802:

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



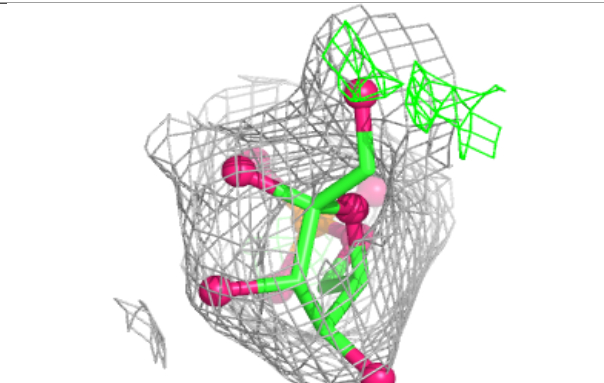
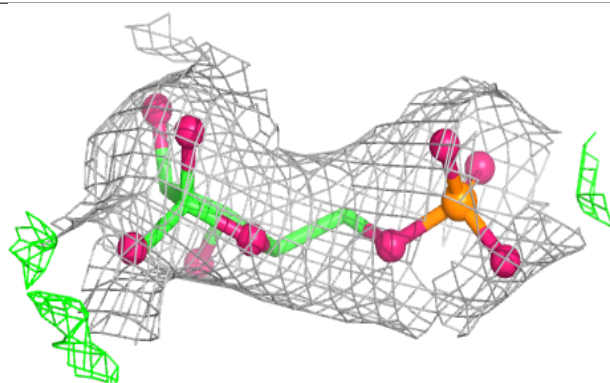
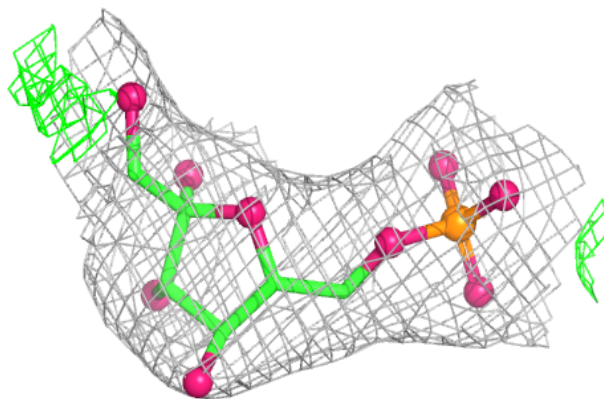
Electron density around ADP D 801:

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

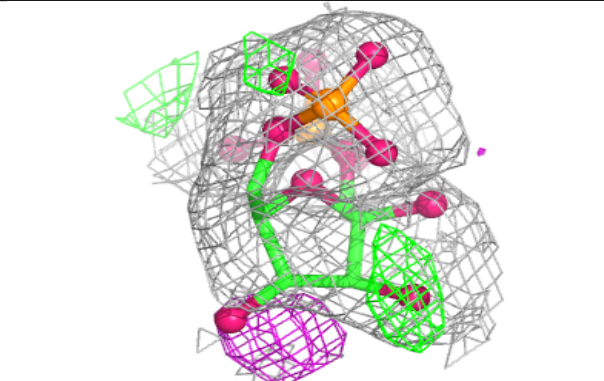
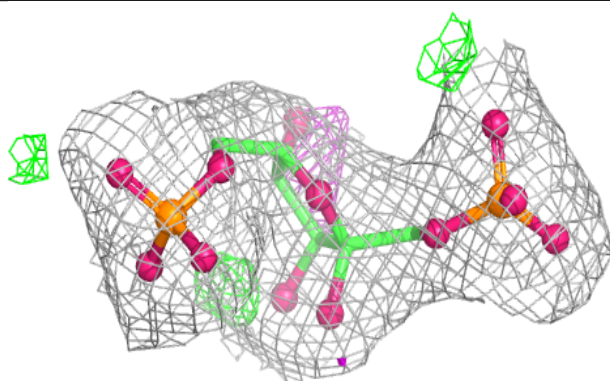
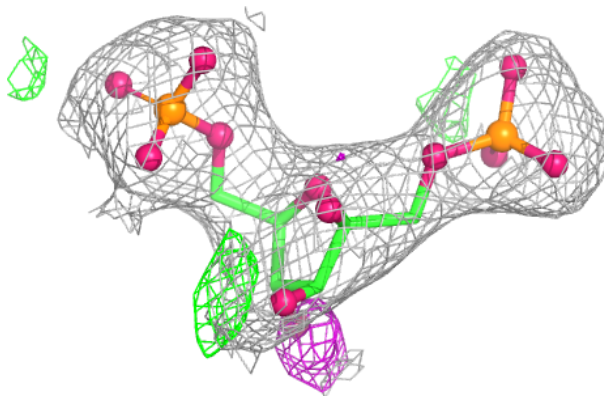


Electron density around F6P D 803:

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

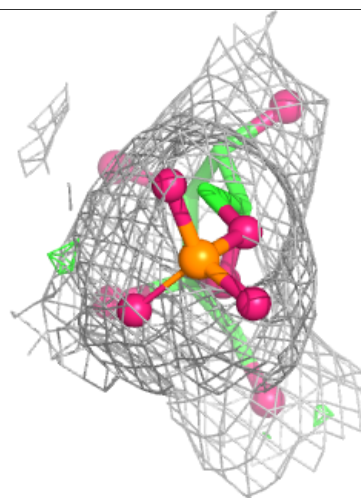
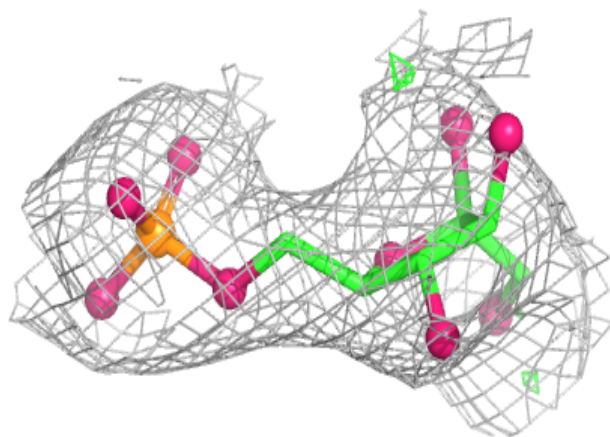
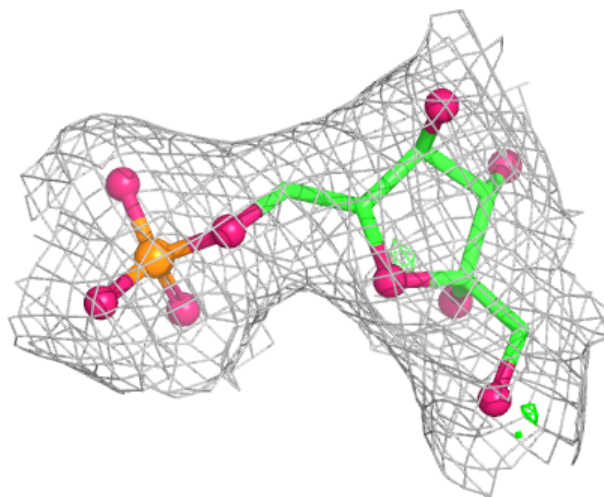
**Electron density around FBP C 801:**

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



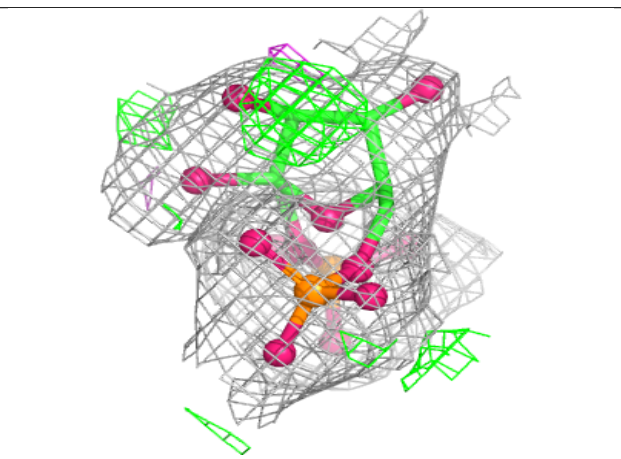
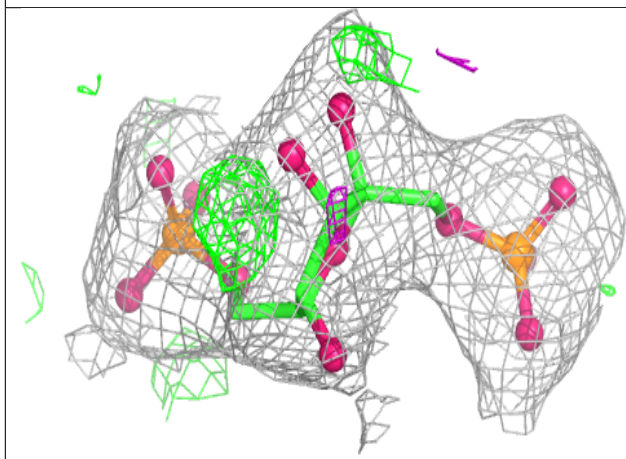
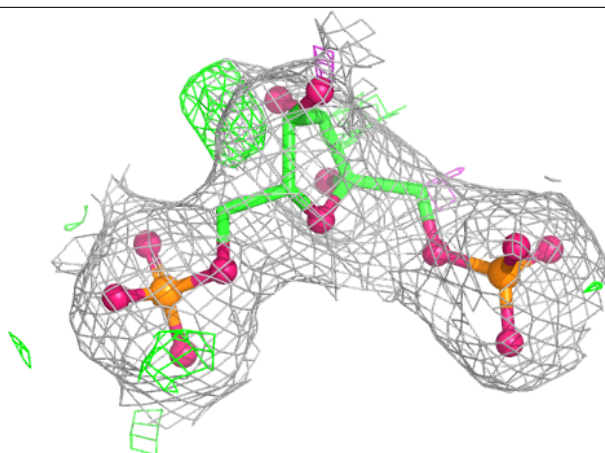
Electron density around F6P B 803:

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



Electron density around FBP A 802:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.