



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:33 PM UTC

PDB ID : 4IP7 / pdb_00004ip7
Title : Structure of the S12D variant of human liver pyruvate kinase in complex with citrate and FBP.
Authors : Holyoak, T.; Fenton, A.W.
Deposited on : 2013-01-09
Resolution : 1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

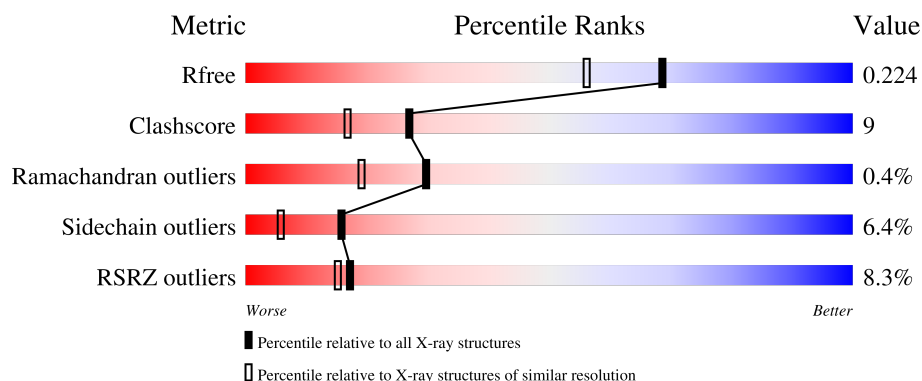
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	543	4% 73% 17% • 7%
1	B	543	8% 73% 15% • • 7%
1	C	543	7% 73% 17% • 8%
1	D	543	11% 73% 16% • • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	B	602	-	-	X	-
6	PEG	A	606	-	-	X	-
8	1PE	C	605	-	X	-	-
8	1PE	C	606	-	X	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17146 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 Pyruvate kinase isozymes L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	S	0	19	0
			3944	2485	706	733	20			
1	B	505	Total	C	N	O	S	0	11	0
			3882	2449	695	718	20			
1	C	500	Total	C	N	O	S	0	11	2
			3831	2412	686	714	19			
1	D	507	Total	C	N	O	S	0	12	0
			3920	2469	709	723	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ASP	SER	engineered mutation	UNP P30613
B	12	ASP	SER	engineered mutation	UNP P30613
C	12	ASP	SER	engineered mutation	UNP P30613
D	12	ASP	SER	engineered mutation	UNP P30613

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

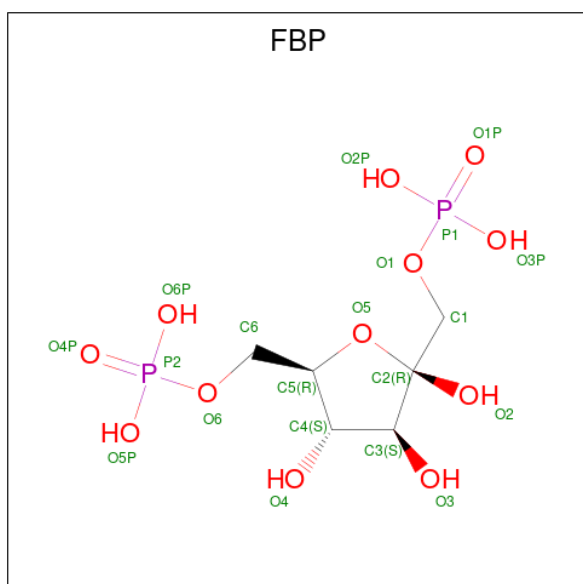
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



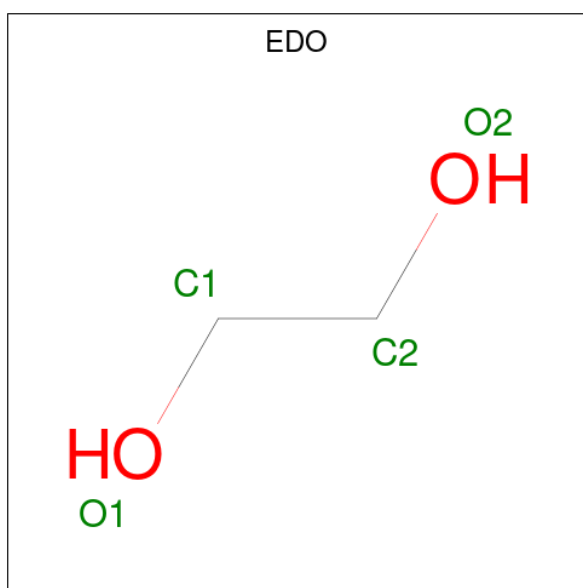
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 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
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

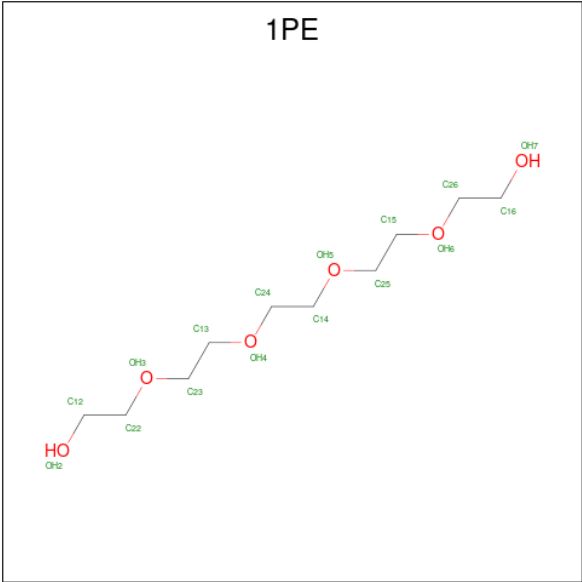


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

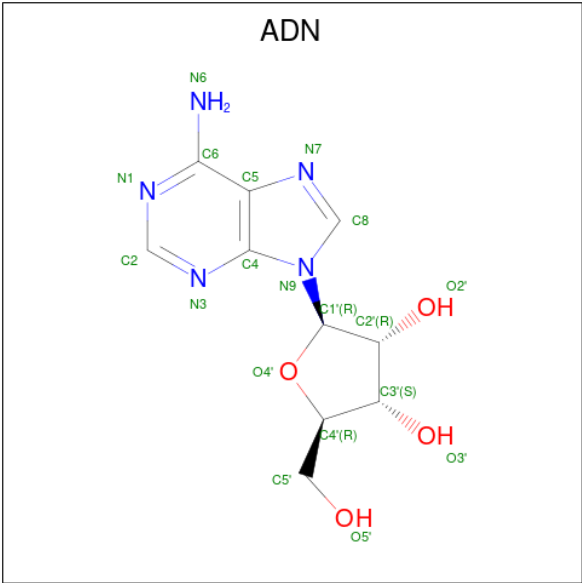
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Na	0	0
			1	1		
7	B	1	Total	Na	0	0
			1	1		
7	C	1	Total	Na	0	0
			1	1		
7	D	1	Total	Na	0	0
			1	1		

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			10	6	4		
8	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is ADENOSINE (CCD ID: ADN) (formula: C₁₀H₁₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	N	O	0	1
			38	20	10	8		

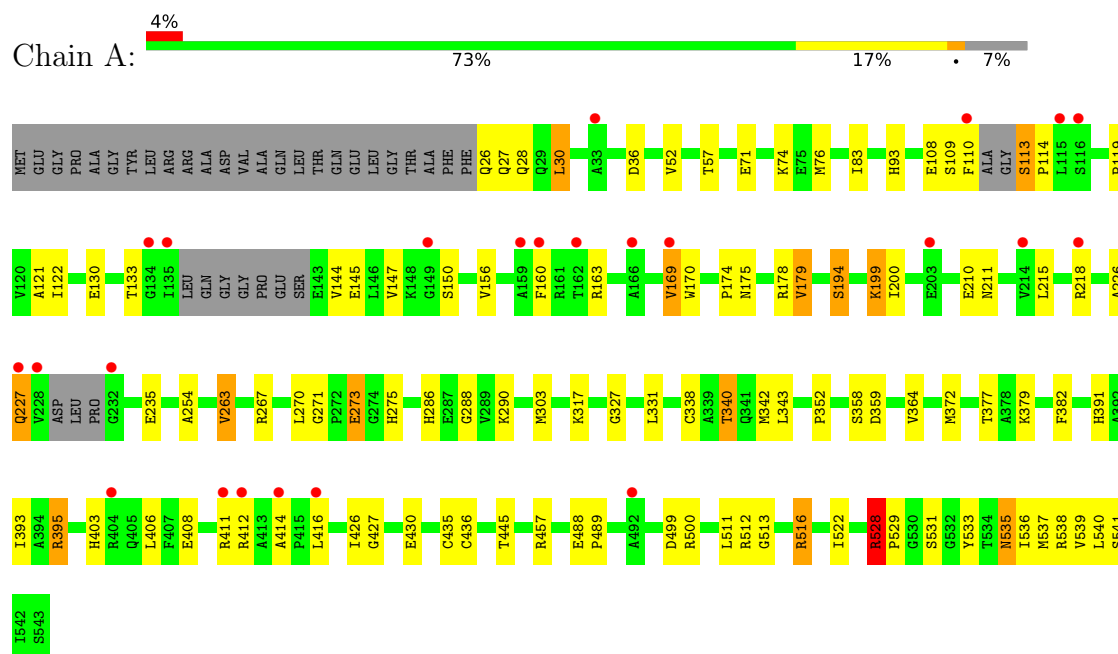
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	361	Total 361	O 361	0	0
10	B	324	Total 324	O 324	0	0
10	C	333	Total 333	O 333	0	0
10	D	306	Total 306	O 306	0	0

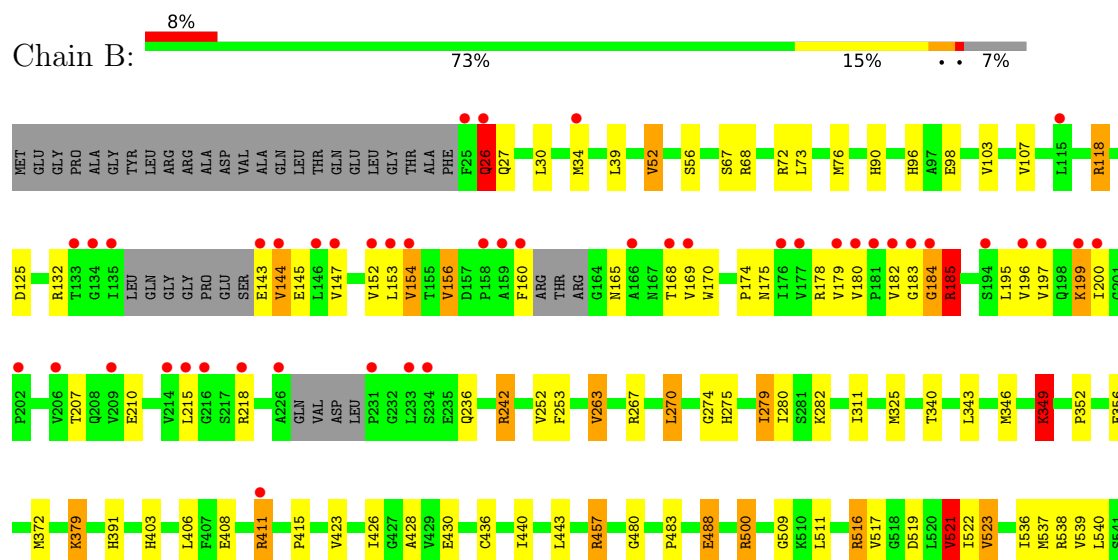
3 Residue-property plots

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 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: Pyruvate kinase isozymes L



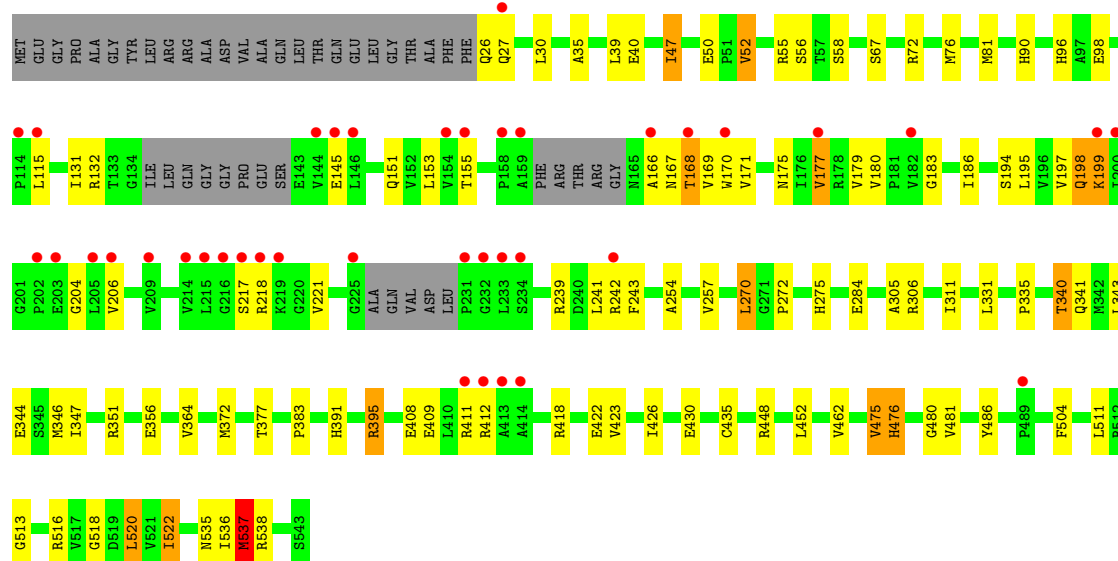
• Molecule 1: Pyruvate kinase isozymes L



1542
S543

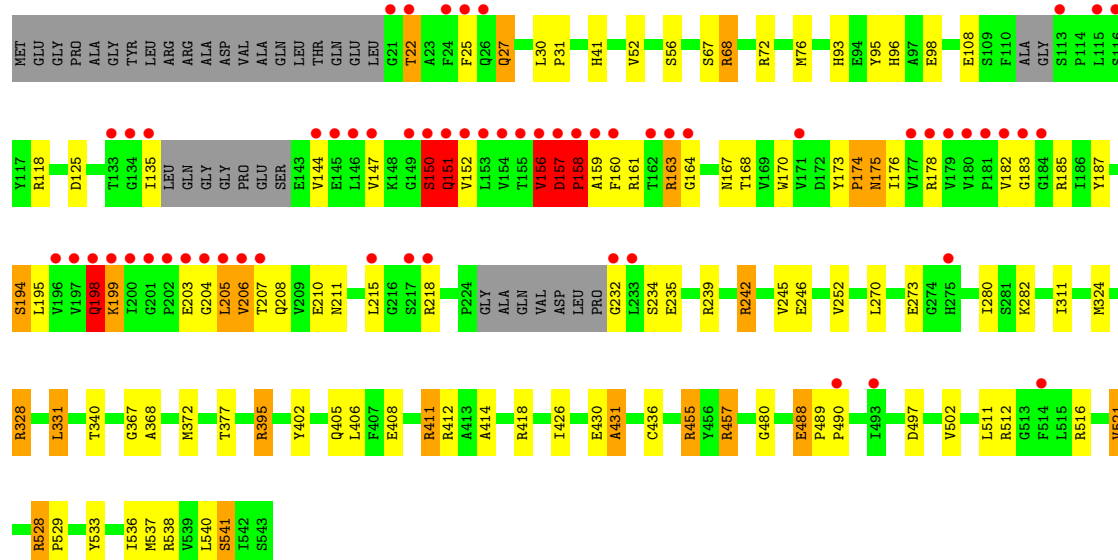
• Molecule 1: Pyruvate kinase isozymes L

Chain C: 



• Molecule 1: Pyruvate kinase isozymes L

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.14Å 205.08Å 83.91Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	37.53 – 1.80 37.53 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (37.53-1.80) 97.5 (37.53-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.226 0.186 , 0.224	Depositor DCC
R_{free} test set	11896 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17146	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: FLC, NA, PEG, EDO, ADN, MN, FBP, 1PE

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	1.50	25/4061 (0.6%)	1.37	23/5494 (0.4%)
1	B	1.37	11/3976 (0.3%)	1.29	17/5380 (0.3%)
1	C	1.42	17/3924 (0.4%)	1.25	14/5313 (0.3%)
1	D	1.58	41/4018 (1.0%)	1.38	45/5436 (0.8%)
All	All	1.47	94/15979 (0.6%)	1.32	99/21623 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	174	PRO	C-N	14.39	1.55	1.33
1	D	156	VAL	CA-C	14.20	1.70	1.52
1	D	204	GLY	C-N	13.11	1.52	1.33
1	D	203	GLU	CD-OE1	12.81	1.49	1.25
1	D	198	GLN	CD-NE2	12.32	1.59	1.33
1	D	151	GLN	CA-C	11.00	1.65	1.53
1	D	164	GLY	C-O	10.61	1.38	1.23
1	D	158	PRO	N-CA	9.75	1.59	1.47
1	D	167	ASN	C-N	9.41	1.45	1.33
1	D	157	ASP	CA-C	8.77	1.62	1.52
1	D	167	ASN	C-O	8.72	1.35	1.24
1	D	205	LEU	C-N	8.35	1.41	1.33
1	D	203	GLU	CD-OE2	7.98	1.40	1.25
1	A	119	PRO	C-O	7.94	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	483	PRO	C-O	7.64	1.32	1.23
1	D	204	GLY	C-O	7.56	1.33	1.23
1	C	167	ASN	CG-ND2	7.29	1.48	1.33
1	D	159	ALA	C-N	7.03	1.42	1.33
1	D	207	THR	C-N	6.99	1.43	1.33
1	D	207	THR	CA-CB	6.99	1.65	1.53
1	A	122	ILE	C-O	6.85	1.31	1.24
1	C	47	ILE	N-CA	6.76	1.54	1.46
1	B	352	PRO	N-CA	6.61	1.52	1.46
1	D	182	VAL	C-O	6.61	1.31	1.24
1	D	311	ILE	C-O	-6.39	1.17	1.23
1	D	156	VAL	CA-CB	6.36	1.61	1.54
1	D	157	ASP	C-O	6.36	1.32	1.24
1	A	391	HIS	ND1-CE1	6.34	1.38	1.32
1	D	457	ARG	N-CA	6.31	1.50	1.46
1	D	205	LEU	C-O	6.26	1.31	1.24
1	C	347	ILE	N-CA	6.26	1.53	1.46
1	A	352	PRO	N-CA	6.16	1.52	1.46
1	A	254	ALA	N-CA	6.15	1.53	1.46
1	C	335	PRO	C-O	6.15	1.30	1.23
1	C	391	HIS	ND1-CE1	6.12	1.38	1.32
1	A	93	HIS	CE1-NE2	6.06	1.38	1.32
1	A	340	THR	N-CA	6.05	1.53	1.46
1	D	150	SER	CA-C	6.02	1.60	1.52
1	D	367	GLY	N-CA	5.97	1.54	1.45
1	B	428	ALA	N-CA	5.96	1.53	1.46
1	B	279	ILE	C-O	5.90	1.30	1.24
1	D	206	VAL	C-O	5.79	1.30	1.23
1	A	342	MET	N-CA	5.77	1.53	1.46
1	A	57	THR	N-CA	5.76	1.53	1.46
1	C	167	ASN	CG-OD1	5.74	1.34	1.23
1	A	150	SER	N-CA	5.73	1.53	1.45
1	C	462	VAL	C-O	5.68	1.30	1.24
1	D	96	HIS	CE1-NE2	5.66	1.38	1.32
1	D	175	ASN	C-N	5.64	1.40	1.34
1	A	489	PRO	CA-C	5.64	1.57	1.52
1	C	257	VAL	N-CA	5.62	1.52	1.46
1	A	539	VAL	C-O	-5.58	1.18	1.24
1	D	234	SER	N-CA	5.53	1.52	1.45
1	D	41	HIS	CE1-NE2	5.49	1.38	1.32
1	B	90	HIS	CG-CD2	5.46	1.41	1.35
1	A	130	GLU	CA-C	-5.46	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	90	HIS	CG-CD2	5.46	1.41	1.35
1	C	486	TYR	CA-C	-5.45	1.46	1.52
1	D	252	VAL	C-O	5.44	1.29	1.24
1	D	98	GLU	CA-C	5.44	1.59	1.52
1	A	288	GLY	CA-C	5.35	1.58	1.52
1	D	93	HIS	ND1-CE1	5.34	1.37	1.32
1	A	93	HIS	CG-CD2	5.33	1.41	1.35
1	C	520	LEU	CA-C	-5.33	1.46	1.52
1	A	303	MET	C-O	5.32	1.30	1.24
1	D	457	ARG	CA-CB	5.30	1.56	1.52
1	A	528	ARG	CD-NE	-5.28	1.38	1.46
1	D	152	VAL	N-CA	5.28	1.52	1.46
1	D	158	PRO	C-O	5.28	1.30	1.24
1	D	96	HIS	CG-CD2	5.24	1.41	1.35
1	A	403	HIS	CE1-NE2	5.21	1.37	1.32
1	C	171	VAL	N-CA	5.20	1.52	1.46
1	A	215	LEU	N-CA	5.20	1.52	1.46
1	C	96	HIS	CG-CD2	5.19	1.41	1.35
1	B	391	HIS	CE1-NE2	5.18	1.37	1.32
1	D	206	VAL	C-N	5.18	1.40	1.33
1	A	358	SER	CB-OG	-5.16	1.31	1.42
1	B	539	VAL	N-CA	-5.15	1.40	1.46
1	C	476	HIS	ND1-CE1	5.14	1.37	1.32
1	B	96	HIS	ND1-CE1	5.14	1.37	1.32
1	A	364	VAL	C-O	5.14	1.29	1.24
1	D	521	VAL	N-CA	-5.14	1.40	1.46
1	C	254	ALA	N-CA	5.13	1.52	1.46
1	B	523	VAL	N-CA	5.08	1.52	1.46
1	A	359	ASP	C-O	-5.08	1.18	1.24
1	A	144	VAL	N-CA	5.08	1.51	1.46
1	C	346	MET	N-CA	5.06	1.52	1.46
1	B	415	PRO	CA-C	5.05	1.58	1.52
1	B	252	VAL	C-O	5.04	1.29	1.24
1	D	368	ALA	N-CA	5.04	1.52	1.46
1	A	338	CYS	C-O	5.04	1.30	1.24
1	A	93	HIS	ND1-CE1	5.03	1.37	1.32
1	C	476	HIS	CG-CD2	5.02	1.41	1.35
1	D	164	GLY	C-N	5.01	1.39	1.33

All (99) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	ALA	CA-C-N	-12.76	103.89	119.84
1	A	414	ALA	C-N-CA	-12.76	103.89	119.84
1	D	151	GLN	CA-C-N	-11.51	107.53	122.37
1	D	151	GLN	C-N-CA	-11.51	107.53	122.37
1	D	158	PRO	N-CA-CB	-9.01	93.79	103.25
1	D	537	MET	CG-SD-CE	-8.94	81.23	100.90
1	D	52	VAL	N-CA-C	-8.91	104.64	112.12
1	B	311	ILE	N-CA-C	-8.89	104.70	111.90
1	D	156	VAL	N-CA-C	-8.18	104.90	112.43
1	D	198	GLN	CG-CD-OE1	7.94	136.67	120.80
1	C	52	VAL	N-CA-C	-7.31	105.98	112.12
1	A	271	GLY	CA-C-N	7.30	128.96	119.84
1	A	271	GLY	C-N-CA	7.30	128.96	119.84
1	C	522	ILE	N-CA-C	-7.28	97.91	108.11
1	D	198	GLN	OE1-CD-NE2	-7.21	115.39	122.60
1	D	174	PRO	O-C-N	7.18	131.49	122.22
1	D	152	VAL	N-CA-C	7.14	118.86	108.58
1	A	113	SER	CA-C-N	6.93	126.53	119.19
1	A	113	SER	C-N-CA	6.93	126.53	119.19
1	C	537	MET	CG-SD-CE	-6.91	85.71	100.90
1	D	68	ARG	NE-CZ-NH2	-6.90	112.99	119.20
1	D	151	GLN	O-C-N	-6.84	114.82	122.55
1	D	156	VAL	CA-C-O	6.83	126.19	119.97
1	D	311	ILE	N-CA-C	-6.82	106.38	111.90
1	D	150	SER	N-CA-C	6.68	119.44	110.35
1	D	280	ILE	N-CA-C	-6.68	98.11	107.80
1	D	198	GLN	CG-CD-NE2	-6.64	106.44	116.40
1	A	427	GLY	N-CA-C	-6.63	104.81	112.50
1	D	151	GLN	CA-C-O	6.61	129.60	122.13
1	A	226	ALA	N-CA-C	6.40	118.79	110.53
1	D	151	GLN	CA-CB-CG	-6.33	101.44	114.10
1	A	395	ARG	NE-CZ-NH1	6.30	127.80	121.50
1	D	395	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	B	349	LYS	CD-CE-NZ	-6.28	91.81	111.90
1	D	414	ALA	CA-C-N	-6.27	114.31	120.52
1	D	414	ALA	C-N-CA	-6.27	114.31	120.52
1	D	157	ASP	O-C-N	6.25	127.53	121.28
1	B	154	VAL	N-CA-CB	6.23	118.11	111.00
1	A	178	ARG	CA-C-N	-6.20	115.17	122.36
1	A	178	ARG	C-N-CA	-6.20	115.17	122.36
1	B	52	VAL	N-CA-C	-6.08	107.01	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	ARG	N-CA-C	-5.96	104.86	111.36
1	A	382	PHE	CA-C-N	-5.92	112.91	119.19
1	A	382	PHE	C-N-CA	-5.92	112.91	119.19
1	C	409	GLU	N-CA-C	5.76	117.24	111.07
1	B	185	ARG	N-CA-C	5.75	119.19	109.76
1	C	311	ILE	N-CA-C	-5.75	106.87	111.81
1	A	263	VAL	CG1-CB-CG2	5.74	123.44	110.80
1	B	325	MET	CA-CB-CG	-5.70	102.71	114.10
1	A	436	CYS	CB-CA-C	-5.69	103.81	111.89
1	D	203	GLU	N-CA-C	-5.68	106.39	113.38
1	B	521	VAL	N-CA-CB	-5.68	101.30	111.92
1	A	436	CYS	CA-C-O	-5.66	115.28	121.84
1	D	22	THR	N-CA-C	5.66	117.53	111.36
1	D	183	GLY	N-CA-C	-5.64	101.53	111.80
1	D	488	GLU	N-CA-C	5.64	116.99	109.83
1	B	26	GLN	N-CA-C	-5.63	104.29	113.19
1	C	475	VAL	CG1-CB-CG2	5.62	123.16	110.80
1	D	206	VAL	CA-C-N	-5.61	112.99	123.03
1	D	206	VAL	C-N-CA	-5.61	112.99	123.03
1	A	169	VAL	N-CA-CB	5.60	118.92	111.64
1	D	232	GLY	CA-C-N	5.53	129.41	121.50
1	D	232	GLY	C-N-CA	5.53	129.41	121.50
1	D	125	ASP	CA-C-O	-5.53	114.24	120.32
1	C	344	GLU	N-CA-C	5.51	117.73	111.11
1	A	395	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	C	448	ARG	N-CA-C	5.50	116.96	111.07
1	B	236	GLN	N-CA-C	-5.49	105.22	111.14
1	D	173	TYR	CA-C-N	5.48	125.31	119.28
1	D	173	TYR	C-N-CA	5.48	125.31	119.28
1	A	393	ILE	N-CA-C	-5.45	105.22	110.72
1	B	509	GLY	N-CA-C	-5.40	106.10	112.64
1	B	457	ARG	CA-C-N	-5.40	114.22	119.78
1	B	457	ARG	C-N-CA	-5.40	114.22	119.78
1	D	156	VAL	O-C-N	-5.38	116.23	122.09
1	D	328	ARG	CB-CG-CD	5.30	123.50	111.30
1	C	364	VAL	N-CA-C	-5.30	105.55	110.53
1	A	528	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	D	502	VAL	N-CA-C	-5.26	105.59	110.53
1	D	395	ARG	NE-CZ-NH1	5.23	126.73	121.50
1	A	36	ASP	N-CA-C	5.22	117.87	111.82
1	B	263	VAL	CB-CA-C	5.21	119.42	112.22
1	D	436	CYS	CB-CA-C	-5.21	104.33	111.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	306	ARG	N-CA-C	5.20	118.89	112.54
1	D	27	GLN	N-CA-C	5.20	117.23	110.53
1	D	431	ALA	N-CA-C	-5.17	105.73	111.36
1	C	243	PHE	CA-C-N	5.13	125.64	119.94
1	C	243	PHE	C-N-CA	5.13	125.64	119.94
1	B	379	LYS	CB-CA-C	5.12	115.77	109.16
1	B	263	VAL	N-CA-C	5.11	115.88	110.72
1	B	488	GLU	CA-C-N	5.10	125.63	120.38
1	B	488	GLU	C-N-CA	5.10	125.63	120.38
1	C	335	PRO	CB-CA-C	-5.09	104.89	111.46
1	A	528	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	D	204	GLY	CA-C-O	-5.07	114.73	121.12
1	D	245	VAL	N-CA-C	5.03	115.25	110.42
1	A	179	VAL	CB-CA-C	5.03	115.68	110.70
1	D	489	PRO	CA-C-N	5.01	125.29	119.93
1	D	489	PRO	C-N-CA	5.01	125.29	119.93

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	151	GLN	Mainchain
1	D	157	ASP	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	3944	0	4061	69	1
1	B	3882	0	3990	78	0
1	C	3831	0	3928	79	0
1	D	3920	0	4026	79	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	4	4	0
3	C	13	0	4	1	0
3	D	13	0	4	2	0
4	A	20	0	10	0	0
4	B	20	0	10	0	0
4	C	20	0	10	0	0
4	D	20	0	10	0	0
5	A	8	0	12	0	0
5	B	8	0	12	1	0
5	C	8	0	12	1	0
5	D	12	0	18	0	0
6	A	7	0	10	9	0
6	B	7	0	10	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	C	17	0	22	22	0
9	D	38	0	26	3	0
10	A	361	0	0	13	1
10	B	324	0	0	6	0
10	C	333	0	0	12	0
10	D	306	0	0	11	0
All	All	17146	0	16183	294	2

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 (294) 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)
8:C:606:1PE:H232	10:C:734:HOH:O	1.45	1.17
1:C:58:SER:N	8:C:606:1PE:H131	1.66	1.09
1:D:455:ARG:HG3	1:D:455:ARG:HH11	1.10	1.09
1:B:156:VAL:HG21	1:B:174:PRO:HA	1.34	1.08
1:C:476:HIS:ND1	8:C:606:1PE:H122	1.70	1.06
8:C:605:1PE:H221	8:C:605:1PE:H241	1.34	1.05
1:B:516:ARG:HG3	1:B:516:ARG:NH1	1.61	1.02
1:B:185:ARG:HG2	1:B:185:ARG:HH11	1.22	1.02
1:B:516:ARG:HH11	1:B:516:ARG:CG	1.74	0.99
1:B:185:ARG:HH11	1:B:185:ARG:CG	1.77	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ARG:HG3	1:D:163:ARG:O	1.62	0.97
1:B:516:ARG:HG3	1:B:516:ARG:HH11	0.81	0.96
1:C:56:SER:O	8:C:606:1PE:H132	1.67	0.93
1:D:160:PHE:HD2	1:D:163:ARG:HG2	1.35	0.90
1:D:242[B]:ARG:HG2	1:D:242[B]:ARG:HH11	1.35	0.89
1:C:408:GLU:HG3	10:C:704:HOH:O	1.72	0.89
1:A:267[B]:ARG:HD2	10:A:800:HOH:O	1.74	0.88
1:D:455:ARG:HG3	1:D:455:ARG:NH1	1.88	0.88
1:A:430:GLU:OE2	1:B:430[B]:GLU:OE1	1.93	0.87
1:A:411:ARG:HH12	6:A:606:PEG:H41	1.41	0.85
1:A:528:ARG:HD2	1:A:533:TYR:CD1	2.13	0.83
1:A:327:GLY:O	1:A:331[B]:LEU:HD13	1.79	0.83
1:B:185:ARG:HD2	1:B:196:VAL:HG22	1.61	0.82
8:C:605:1PE:H241	8:C:605:1PE:C22	2.10	0.81
1:D:418:ARG:NH1	10:D:954:HOH:O	2.11	0.81
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.61	0.81
1:D:147:VAL:O	1:D:150:SER:HB2	1.79	0.80
1:C:58:SER:H	8:C:606:1PE:H131	1.41	0.80
1:A:488[B]:GLU:OE1	1:A:500:ARG:NH2	2.14	0.80
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.65	0.79
1:A:227:GLN:HB2	10:A:883:HOH:O	1.82	0.78
1:C:72:ARG:NH1	10:C:998:HOH:O	1.88	0.78
1:A:331[A]:LEU:HD22	10:A:979:HOH:O	1.83	0.77
1:D:108:GLU:HG2	10:D:858:HOH:O	1.83	0.77
1:C:218:ARG:NH1	1:C:218:ARG:HB3	1.99	0.77
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.66	0.77
1:B:185:ARG:HG2	1:B:185:ARG:NH1	1.89	0.76
1:D:68:ARG:NH2	1:D:95:TYR:O	2.18	0.75
1:D:118[A]:ARG:HG2	10:D:747:HOH:O	1.86	0.75
6:A:606:PEG:H12	10:B:748:HOH:O	1.87	0.75
10:C:832:HOH:O	1:D:411:ARG:HD2	1.84	0.75
1:A:411:ARG:NH1	6:A:606:PEG:H41	2.00	0.75
1:C:58:SER:OG	8:C:606:1PE:H221	1.87	0.75
8:C:606:1PE:H121	10:C:734:HOH:O	1.86	0.74
1:C:430[A]:GLU:OE2	1:D:411:ARG:HD3	1.88	0.74
1:B:175:ASN:OD1	1:B:178:ARG:HD3	1.88	0.74
1:D:528:ARG:HD2	1:D:533:TYR:CD1	2.23	0.74
1:B:178:ARG:HB3	1:B:178:ARG:NH1	2.03	0.73
1:D:418:ARG:HG2	1:D:418:ARG:HH11	1.53	0.73
1:A:199:LYS:HG3	1:A:200:ILE:H	1.54	0.72
1:C:476:HIS:CE1	8:C:606:1PE:H122	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:HE3	1:A:109:SER:OG	1.89	0.71
1:C:56:SER:O	8:C:606:1PE:C23	2.38	0.71
1:B:185:ARG:HH11	1:B:185:ARG:CB	2.03	0.71
1:B:67:SER:HB2	1:B:76[B]:MET:SD	2.31	0.71
1:C:218:ARG:HB3	1:C:218:ARG:HH11	1.55	0.70
1:A:512:ARG:HD3	10:A:887:HOH:O	1.91	0.70
1:A:538:ARG:HG2	1:B:536:ILE:HG12	1.73	0.70
1:B:521:VAL:HB	1:B:542[A]:ILE:HD11	1.72	0.70
1:B:183:GLY:HA2	1:B:197:VAL:O	1.92	0.69
1:D:411:ARG:HG3	1:D:426:ILE:HD11	1.73	0.69
1:B:523:VAL:HG21	1:B:540[A]:LEU:HD12	1.73	0.69
1:A:331[B]:LEU:HD11	1:C:39:LEU:HD11	1.75	0.68
1:D:163:ARG:O	1:D:163:ARG:CG	2.40	0.68
1:D:194:SER:HB2	1:D:211:ASN:HB2	1.74	0.68
1:A:411:ARG:HH22	6:A:606:PEG:H41	1.59	0.68
1:D:160:PHE:CD2	1:D:163:ARG:HG2	2.25	0.68
1:D:242[B]:ARG:HH11	1:D:242[B]:ARG:CG	2.04	0.68
9:D:604[B]:ADN:O5'	9:D:604[B]:ADN:H2'	1.94	0.68
1:D:198:GLN:HE22	1:D:208:GLN:HB3	1.58	0.68
1:C:56:SER:O	8:C:606:1PE:H231	1.94	0.67
1:A:331[A]:LEU:HD21	10:A:981:HOH:O	1.94	0.67
1:C:56:SER:O	8:C:606:1PE:C13	2.41	0.67
1:C:27:GLN:HE21	1:C:50:GLU:H	1.42	0.67
1:B:197:VAL:HG22	1:B:207:THR:HG22	1.77	0.67
1:C:177:VAL:HG21	1:C:204:GLY:HA2	1.76	0.67
1:B:519:ASP:O	1:B:542[A]:ILE:HD13	1.94	0.66
1:A:74:LYS:CE	1:A:109:SER:OG	2.43	0.66
1:C:198:GLN:HG3	10:C:907:HOH:O	1.95	0.66
1:A:199:LYS:HG3	1:A:200:ILE:N	2.10	0.66
1:B:156:VAL:CG2	1:B:174:PRO:HA	2.20	0.66
1:A:108:GLU:HG2	10:A:783:HOH:O	1.96	0.66
1:B:372:MET:HE1	3:B:602:FLC:OA2	1.96	0.66
1:A:327:GLY:O	1:A:331[B]:LEU:CD1	2.44	0.65
1:C:67:SER:HB2	1:C:76[B]:MET:SD	2.37	0.65
1:C:411:ARG:HH21	1:C:412:ARG:HH11	1.45	0.65
1:A:499[B]:ASP:OD1	10:A:1039:HOH:O	2.15	0.65
1:B:185:ARG:CG	1:B:185:ARG:NH1	2.47	0.63
1:D:156:VAL:CG2	1:D:176:ILE:HG22	2.28	0.63
1:D:175:ASN:OD1	1:D:178:ARG:HD3	1.98	0.63
1:B:488:GLU:HG3	1:B:500:ARG:HH21	1.63	0.63
1:B:27:GLN:OE1	1:B:52:VAL:HG21	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:ARG:HG3	1:D:516:ARG:HH11	1.64	0.62
1:D:541:SER:HB3	10:D:874:HOH:O	1.99	0.62
1:A:411:ARG:NH2	6:A:606:PEG:H41	2.14	0.62
1:A:194:SER:HB3	1:A:211:ASN:HB2	1.80	0.61
1:A:331[B]:LEU:CD1	1:C:39:LEU:HD11	2.31	0.61
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.82	0.61
1:B:178:ARG:HB3	1:B:178:ARG:HH11	1.64	0.61
1:D:273:GLU:HG2	10:D:721:HOH:O	1.99	0.61
1:D:418:ARG:NH1	1:D:418:ARG:HG2	2.15	0.61
1:A:156:VAL:HG11	1:A:174:PRO:HA	1.84	0.60
1:C:199:LYS:HA	1:C:199:LYS:HZ3	1.66	0.59
1:C:58:SER:CA	8:C:606:1PE:H131	2.32	0.58
1:D:27:GLN:HG2	10:D:957:HOH:O	2.02	0.58
1:D:528:ARG:HD2	1:D:533:TYR:CE1	2.39	0.58
1:D:455:ARG:NH1	1:D:455:ARG:CG	2.57	0.58
1:C:518:GLY:O	1:D:418:ARG:NH2	2.37	0.58
1:A:411:ARG:HG3	1:A:426:ILE:HD11	1.85	0.57
1:C:58:SER:OG	8:C:606:1PE:C13	2.52	0.57
1:D:157:ASP:O	1:D:158:PRO:C	2.48	0.57
1:A:267[B]:ARG:HD2	10:A:869:HOH:O	2.03	0.57
1:B:267[B]:ARG:HD2	1:B:279:ILE:HD12	1.87	0.57
1:D:455:ARG:HH11	1:D:455:ARG:CG	1.93	0.57
1:C:26:GLN:HG2	10:C:805:HOH:O	2.04	0.56
1:D:282:LYS:HE3	3:D:602:FLC:OA2	2.05	0.56
1:C:183:GLY:HA2	1:C:197:VAL:O	2.04	0.56
1:D:160:PHE:HD2	1:D:163:ARG:CG	2.13	0.56
1:A:331[B]:LEU:HD11	1:C:39:LEU:CD1	2.36	0.56
1:C:27:GLN:NE2	1:C:50:GLU:H	2.04	0.56
1:D:156:VAL:CG1	1:D:174:PRO:HA	2.36	0.56
1:C:56:SER:HB2	1:C:480:GLY:CA	2.35	0.56
1:D:198:GLN:HE22	1:D:208:GLN:CB	2.19	0.56
1:A:528:ARG:HD3	1:A:529:PRO:O	2.06	0.55
8:C:606:1PE:C23	10:C:734:HOH:O	2.23	0.55
1:D:324:MET:SD	1:D:328:ARG:HD3	2.46	0.55
1:B:156:VAL:HG21	1:B:174:PRO:CA	2.23	0.55
1:B:56:SER:HB2	1:B:480:GLY:CA	2.36	0.55
1:B:67:SER:HA	1:B:72:ARG:HG2	1.86	0.55
1:C:177:VAL:CG2	1:C:204:GLY:HA2	2.36	0.55
1:D:194:SER:HB3	1:D:210:GLU:HB3	1.89	0.55
1:A:331[A]:LEU:CD2	10:A:981:HOH:O	2.54	0.54
1:A:445:THR:HB	1:A:531[B]:SER:OG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:VAL:HG21	1:D:176:ILE:HG22	1.89	0.54
1:B:517:VAL:HG23	10:B:922:HOH:O	2.06	0.54
1:C:58:SER:N	8:C:606:1PE:C13	2.57	0.54
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.89	0.54
1:B:516:ARG:NH1	1:B:516:ARG:CG	2.43	0.54
1:C:536:ILE:HG12	1:D:538[A]:ARG:HG2	1.89	0.53
1:D:175:ASN:HB2	10:D:999:HOH:O	2.07	0.53
1:A:411:ARG:CZ	6:A:606:PEG:H41	2.37	0.53
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.91	0.53
1:A:537[B]:MET:HE3	1:B:537[B]:MET:HE3	1.89	0.53
1:A:411:ARG:HH22	6:A:606:PEG:C4	2.21	0.53
1:C:343:LEU:HD23	1:C:356:GLU:HB3	1.91	0.53
1:C:55:ARG:HB2	1:C:395:ARG:HG3	1.91	0.52
1:D:156:VAL:HG11	1:D:174:PRO:HA	1.91	0.52
1:B:343:LEU:HD23	1:B:356:GLU:HB3	1.91	0.52
1:B:118[A]:ARG:HG2	10:B:702:HOH:O	2.10	0.52
1:A:267[B]:ARG:CD	10:A:869:HOH:O	2.57	0.52
1:B:196:VAL:HG23	1:B:210:GLU:HB2	1.92	0.52
1:A:513:GLY:HA2	1:A:516:ARG:HH21	1.74	0.52
1:A:535:ASN:OD1	1:A:536:ILE:HG13	2.09	0.52
1:B:160:PHE:HB2	1:B:170:TRP:CD1	2.45	0.52
1:B:523:VAL:HG21	1:B:540[A]:LEU:CD1	2.38	0.51
1:A:372:MET:HE1	3:A:602:FLC:OA1	2.10	0.51
1:C:52:VAL:HG22	10:C:886:HOH:O	2.08	0.51
1:C:522:ILE:HG23	1:C:537:MET:HE3	1.92	0.51
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.75	0.51
1:A:416:LEU:HD13	1:B:436:CYS:SG	2.51	0.51
1:C:411:ARG:HD2	1:D:430[A]:GLU:OE2	2.10	0.51
1:D:185:ARG:HH21	1:D:210:GLU:CD	2.18	0.51
1:D:490:PRO:HA	1:D:497:ASP:OD1	2.10	0.51
9:D:604[B]:ADN:H1'	10:D:756:HOH:O	2.11	0.51
1:C:67:SER:HA	1:C:72:ARG:HG2	1.93	0.50
1:B:267[B]:ARG:HD2	1:B:279:ILE:CD1	2.41	0.50
1:B:372:MET:CE	3:B:602:FLC:OA2	2.60	0.50
1:D:372:MET:HE1	3:D:602:FLC:OA1	2.11	0.50
1:A:163:ARG:HG2	1:A:163:ARG:NH1	2.27	0.49
1:A:331[B]:LEU:HD11	1:C:39:LEU:CG	2.41	0.49
1:A:76[B]:MET:HE1	1:A:377:THR:CG2	2.42	0.49
1:A:522:ILE:HG23	1:A:537[A]:MET:HE3	1.92	0.49
1:B:178:ARG:HH11	1:B:178:ARG:CB	2.25	0.49
1:D:170:TRP:HZ3	1:D:218:ARG:HH22	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:TRP:HZ3	1:D:218:ARG:NH2	2.10	0.49
1:D:235:GLU:HG2	1:D:239:ARG:NH1	2.28	0.49
1:C:58:SER:OG	8:C:606:1PE:H131	2.12	0.48
1:B:68:ARG:NH2	1:B:98:GLU:HB2	2.28	0.48
1:C:153:LEU:HB3	1:C:168:THR:HG23	1.94	0.48
1:B:98:GLU:HG3	10:B:859:HOH:O	2.14	0.48
1:C:58:SER:H	8:C:606:1PE:C13	2.19	0.48
1:A:537[A]:MET:HG2	1:B:537[A]:MET:HE2	1.95	0.47
1:B:132:ARG:HD2	1:B:218:ARG:HH21	1.79	0.47
1:C:155:THR:O	1:C:170:TRP:HA	2.15	0.47
1:D:235:GLU:HG2	1:D:239:ARG:HH12	1.79	0.47
1:D:402:TYR:CD2	1:D:405[A]:GLN:HB3	2.49	0.47
9:D:604[B]:ADN:O5'	9:D:604[B]:ADN:C2'	2.62	0.47
1:A:435:CYS:HB3	1:B:423:VAL:CG2	2.45	0.47
1:B:185:ARG:NH1	1:B:185:ARG:CB	2.74	0.47
1:D:147:VAL:O	1:D:150:SER:CB	2.57	0.47
1:A:194:SER:OG	1:A:210:GLU:OE1	2.32	0.47
1:B:488:GLU:HG3	1:B:500:ARG:NH2	2.30	0.47
1:C:435:CYS:HB2	1:C:520:LEU:HD12	1.96	0.47
1:C:151:GLN:HE22	1:C:206:VAL:HG12	1.79	0.47
1:B:103:VAL:O	1:B:107:VAL:HG23	2.15	0.47
1:A:275[A]:HIS:CD2	10:A:800:HOH:O	2.68	0.46
1:D:198:GLN:N	1:D:206:VAL:O	2.26	0.46
1:C:377:THR:HA	1:C:383:PRO:HB3	1.97	0.46
6:A:606:PEG:H11	1:B:403:HIS:HB2	1.97	0.46
1:C:58:SER:CB	8:C:606:1PE:H131	2.46	0.46
1:C:284:GLU:HG2	1:C:305:ALA:HB3	1.97	0.46
1:D:25:PHE:O	1:D:31:PRO:HD3	2.15	0.46
1:D:406:LEU:HD21	1:D:457:ARG:HG3	1.97	0.46
1:B:406:LEU:HD21	1:B:457:ARG:HG3	1.98	0.46
1:B:516:ARG:NH1	10:B:946:HOH:O	2.47	0.46
1:C:175:ASN:HB2	10:C:836:HOH:O	2.15	0.46
1:A:199:LYS:HE2	1:A:200:ILE:H	1.80	0.46
1:B:267[B]:ARG:NH2	1:B:274:GLY:O	2.48	0.46
1:D:488:GLU:H	1:D:488:GLU:HG2	1.62	0.46
1:A:113:SER:HA	1:A:114:PRO:HD3	1.77	0.45
1:B:408:GLU:HA	1:B:411:ARG:HH21	1.81	0.45
1:D:56:SER:HB2	1:D:480:GLY:CA	2.46	0.45
1:C:199:LYS:HA	1:C:199:LYS:NZ	2.32	0.45
1:B:39:LEU:HD21	1:D:331:LEU:CD1	2.47	0.45
1:B:282:LYS:HE3	3:B:602:FLC:OA1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ILE:HB	1:C:221:VAL:HB	1.98	0.45
1:A:199:LYS:CG	1:A:200:ILE:H	2.28	0.45
1:D:118[A]:ARG:HH12	1:D:512:ARG:HD3	1.81	0.45
1:A:286:HIS:CE1	1:A:290:LYS:HG3	2.51	0.45
1:C:372:MET:HE1	3:C:603:FLC:OA2	2.17	0.45
1:D:412:ARG:HB2	10:D:995:HOH:O	2.15	0.45
1:D:408:GLU:HA	1:D:411:ARG:HH21	1.81	0.45
1:B:267[A]:ARG:NH1	10:B:942:HOH:O	2.42	0.45
1:C:186:ILE:O	1:C:194:SER:HA	2.17	0.45
1:C:481:VAL:O	8:C:606:1PE:H121	2.17	0.44
1:A:28:GLN:HG2	1:A:30:LEU:HD22	2.00	0.44
1:A:411:ARG:HH12	6:A:606:PEG:C4	2.20	0.44
1:B:56:SER:O	5:B:606:EDO:O1	2.33	0.44
1:D:194:SER:O	1:D:195:LEU:HD23	2.17	0.44
1:D:516:ARG:HG3	1:D:516:ARG:NH1	2.30	0.44
1:B:199:LYS:HG3	1:B:200:ILE:N	2.31	0.44
1:B:26:GLN:CD	1:B:26:GLN:C	2.86	0.44
1:B:125:ASP:OD2	3:B:602:FLC:OA1	2.35	0.44
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.99	0.44
1:C:272:PRO:HA	1:C:275[B]:HIS:CD2	2.53	0.44
1:A:435:CYS:HB3	1:B:423:VAL:HG21	2.00	0.43
1:B:144:VAL:HG21	1:B:165:ASN:HA	2.00	0.43
1:C:81:MET:HE2	1:C:81:MET:HB3	1.91	0.43
1:D:67:SER:HA	1:D:72:ARG:HG2	1.99	0.43
1:C:535:ASN:OD1	1:C:536:ILE:HG13	2.17	0.43
8:C:605:1PE:H242	8:C:605:1PE:H231	1.71	0.43
1:A:133:THR:HA	1:A:170:TRP:O	2.17	0.43
1:C:513:GLY:HA2	10:C:821:HOH:O	2.18	0.43
1:A:110:PHE:HB2	10:A:867:HOH:O	2.18	0.43
1:C:241:LEU:HD22	1:C:270[A]:LEU:HD11	2.00	0.43
1:D:161:ARG:HA	1:D:170:TRP:CD2	2.54	0.43
1:D:161:ARG:HA	1:D:170:TRP:CG	2.53	0.43
1:A:406:LEU:HD21	1:A:457:ARG:HG3	2.00	0.43
1:A:83:ILE:HG12	1:A:121:ALA:HB3	2.01	0.43
1:C:199:LYS:HA	1:C:199:LYS:CE	2.49	0.43
1:B:26:GLN:C	1:B:26:GLN:NE2	2.77	0.43
1:A:331[B]:LEU:HD11	1:C:39:LEU:HG	1.99	0.43
1:A:160:PHE:HA	1:A:163:ARG:HD2	2.01	0.42
1:A:71[A]:GLU:HG3	10:A:773:HOH:O	2.18	0.42
1:C:35:ALA:HB1	1:C:40[A]:GLU:HB3	2.01	0.42
1:B:267[B]:ARG:NH2	1:B:275:HIS:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242[A]:ARG:NH2	1:D:270:LEU:O	2.52	0.42
1:D:516:ARG:NH1	1:D:516:ARG:CG	2.80	0.42
1:B:242:ARG:NH2	1:B:270:LEU:O	2.52	0.42
1:D:218:ARG:HD2	10:D:925:HOH:O	2.17	0.42
1:B:440:ILE:HA	1:B:522:ILE:O	2.20	0.42
1:C:67:SER:CB	1:C:76[B]:MET:SD	3.08	0.42
1:A:317:LYS:HD3	1:C:47:ILE:O	2.20	0.41
1:B:346:MET:HA	1:B:349:LYS:O	2.21	0.41
1:C:331:LEU:HD23	1:C:331:LEU:HA	1.83	0.41
1:C:408:GLU:OE1	1:D:408:GLU:OE2	2.38	0.41
1:B:519:ASP:C	1:B:542[A]:ILE:HD13	2.45	0.41
1:D:185:ARG:CD	1:D:187:TYR:CE1	3.03	0.41
1:D:528:ARG:HD3	1:D:529:PRO:O	2.21	0.41
1:D:242[B]:ARG:CG	1:D:242[B]:ARG:NH1	2.71	0.41
1:A:408[B]:GLU:OE1	1:A:412:ARG:HD3	2.20	0.41
1:C:340:THR:HG22	1:C:341:GLN:HG3	2.01	0.41
1:C:408:GLU:O	1:C:412:ARG:HB2	2.21	0.41
1:C:422[A]:GLU:HG2	1:C:452:LEU:HD13	2.01	0.41
1:A:528:ARG:CD	1:A:529:PRO:O	2.67	0.41
1:D:118[B]:ARG:NE	10:D:973:HOH:O	2.09	0.41
1:C:418:ARG:HD2	10:C:803:HOH:O	2.21	0.41
1:A:163:ARG:HH11	1:A:163:ARG:CG	2.33	0.40
1:B:253:PHE:HD1	1:B:280:ILE:HB	1.87	0.40
1:C:351:ARG:HB2	5:C:601:EDO:H21	2.03	0.40
1:A:273:GLU:H	1:A:273:GLU:HG2	1.54	0.40
1:B:132:ARG:HD2	1:B:218:ARG:NH2	2.35	0.40
1:B:183:GLY:O	1:B:197:VAL:HB	2.21	0.40
1:D:76[B]:MET:HE1	1:D:377:THR:CG2	2.51	0.40
1:D:198:GLN:HB3	1:D:199:LYS:H	1.63	0.40
6:B:605:PEG:H41	6:B:605:PEG:H21	1.89	0.40
1:C:115:LEU:HD23	1:C:504:PHE:CE1	2.57	0.40
1:C:423:VAL:HG12	1:D:431:ALA:HB1	2.03	0.40
1:B:183:GLY:O	1:B:184:GLY:O	2.39	0.40
1:C:132:ARG:HD2	1:C:218:ARG:HH12	1.86	0.40

All (2) 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)
10:A:994:HOH:O	10:A:1017:HOH:O[1_455]	1.83	0.37
1:A:74:LYS:NZ	1:D:246:GLU:OE1[2_645]	2.13	0.07

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	517/543 (95%)	504 (98%)	11 (2%)	2 (0%)	30	19
1	B	508/543 (94%)	491 (97%)	15 (3%)	2 (0%)	30	19
1	C	503/543 (93%)	492 (98%)	9 (2%)	2 (0%)	30	19
1	D	511/543 (94%)	494 (97%)	16 (3%)	1 (0%)	43	31
All	All	2039/2172 (94%)	1981 (97%)	51 (2%)	7 (0%)	30	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	GLY
1	D	340	THR
1	B	340	THR
1	C	340	THR
1	A	535	ASN
1	A	340	THR
1	C	166	ALA

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	426/433 (98%)	400 (94%)	26 (6%)	17	6
1	B	415/433 (96%)	378 (91%)	37 (9%)	9	2
1	C	412/433 (95%)	393 (95%)	19 (5%)	24	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	420/433 (97%)	394 (94%)	26 (6%)	16	6
All	All	1673/1732 (97%)	1565 (94%)	108 (6%)	16	5

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	GLN
1	A	30	LEU
1	A	52	VAL
1	A	145	GLU
1	A	147	VAL
1	A	169	VAL
1	A	175	ASN
1	A	179	VAL
1	A	194	SER
1	A	199	LYS
1	A	218	ARG
1	A	227	GLN
1	A	235	GLU
1	A	263	VAL
1	A	270	LEU
1	A	273	GLU
1	A	343	LEU
1	A	379	LYS
1	A	395	ARG
1	A	511	LEU
1	A	516	ARG
1	A	528	ARG
1	A	540	LEU
1	A	541[A]	SER
1	A	541[B]	SER
1	B	26	GLN
1	B	30	LEU
1	B	34	MET
1	B	73	LEU
1	B	118[A]	ARG
1	B	118[B]	ARG
1	B	143	GLU
1	B	144	VAL
1	B	145	GLU
1	B	147	VAL

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Mol	Chain	Res	Type
1	B	152	VAL
1	B	153	LEU
1	B	154	VAL
1	B	156	VAL
1	B	168	THR
1	B	169	VAL
1	B	179	VAL
1	B	180	VAL
1	B	182	VAL
1	B	185	ARG
1	B	195	LEU
1	B	199	LYS
1	B	215	LEU
1	B	242	ARG
1	B	263	VAL
1	B	270	LEU
1	B	349	LYS
1	B	379	LYS
1	B	411	ARG
1	B	443	LEU
1	B	500	ARG
1	B	511	LEU
1	B	516	ARG
1	B	521	VAL
1	B	542[A]	ILE
1	B	542[B]	ILE
1	B	543	SER
1	C	30	LEU
1	C	145	GLU
1	C	168	THR
1	C	169	VAL
1	C	177	VAL
1	C	179	VAL
1	C	180	VAL
1	C	195	LEU
1	C	198	GLN
1	C	199	LYS
1	C	217	SER
1	C	242	ARG
1	C	270[A]	LEU
1	C	270[B]	LEU
1	C	395	ARG

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Mol	Chain	Res	Type
1	C	475	VAL
1	C	511	LEU
1	C	516	ARG
1	C	537	MET
1	D	22	THR
1	D	30	LEU
1	D	135	ILE
1	D	144	VAL
1	D	150	SER
1	D	151	GLN
1	D	156	VAL
1	D	158	PRO
1	D	163	ARG
1	D	168	THR
1	D	194	SER
1	D	198	GLN
1	D	199	LYS
1	D	205	LEU
1	D	215	LEU
1	D	242[A]	ARG
1	D	242[B]	ARG
1	D	331	LEU
1	D	395	ARG
1	D	411	ARG
1	D	455	ARG
1	D	511	LEU
1	D	521	VAL
1	D	528	ARG
1	D	540	LEU
1	D	541	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	222	ASN
1	B	28	GLN
1	B	211	ASN
1	B	222	ASN
1	B	236	GLN
1	B	275	HIS
1	C	27	GLN

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Mol	Chain	Res	Type
1	C	151	GLN
1	C	167	ASN
1	D	198	GLN
1	D	211	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 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$
8	1PE	C	605	-	9,9,15	2.11	5 (55%)	8,8,14	1.72	2 (25%)
4	FBP	A	603	-	18,20,20	1.13	2 (11%)	21,32,32	1.64	5 (23%)
5	EDO	A	605	-	3,3,3	0.70	0	2,2,2	0.55	0
9	ADN	D	604[B]	-	21,21,21	1.58	3 (14%)	31,31,31	2.39	13 (41%)
3	FLC	B	602	2	12,12,12	1.28	1 (8%)	17,17,17	1.60	2 (11%)
5	EDO	D	607	-	3,3,3	1.10	0	2,2,2	0.27	0
6	PEG	B	605	-	6,6,6	0.93	0	5,5,5	0.56	0
3	FLC	D	602	2	12,12,12	1.74	4 (33%)	17,17,17	1.63	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ADN	D	604[A]	-	21,21,21	1.60	3 (14%)	31,31,31	2.22	12 (38%)
5	EDO	D	605	-	3,3,3	0.95	0	2,2,2	0.69	0
5	EDO	D	606	-	3,3,3	0.77	0	2,2,2	1.11	0
5	EDO	B	606	-	3,3,3	1.55	1 (33%)	2,2,2	0.62	0
4	FBP	B	603	-	18,20,20	1.15	3 (16%)	21,32,32	1.64	3 (14%)
4	FBP	C	604	-	18,20,20	0.94	1 (5%)	21,32,32	1.29	3 (14%)
5	EDO	C	601	-	3,3,3	0.85	0	2,2,2	1.04	0
5	EDO	A	604	-	3,3,3	0.68	0	2,2,2	0.87	0
4	FBP	D	603	-	18,20,20	1.54	4 (22%)	21,32,32	1.69	7 (33%)
5	EDO	C	607	-	3,3,3	0.80	0	2,2,2	0.29	0
3	FLC	A	602	2	12,12,12	1.76	2 (16%)	17,17,17	2.09	5 (29%)
5	EDO	B	604	-	3,3,3	0.73	0	2,2,2	0.77	0
3	FLC	C	603	2	12,12,12	1.85	3 (25%)	17,17,17	1.84	4 (23%)
8	1PE	C	606	-	6,6,15	2.66	2 (33%)	5,5,14	4.14	3 (60%)
6	PEG	A	606	-	6,6,6	0.68	0	5,5,5	1.53	2 (40%)

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
8	1PE	C	605	-	-	5/7/7/13	-
4	FBP	A	603	-	-	3/13/32/32	0/1/1/1
5	EDO	A	605	-	-	0/1/1/1	-
9	ADN	D	604[B]	-	-	3/6/22/22	0/3/3/3
3	FLC	B	602	2	-	8/16/16/16	-
5	EDO	D	607	-	-	0/1/1/1	-
6	PEG	B	605	-	-	3/4/4/4	-
3	FLC	D	602	2	-	2/16/16/16	-
9	ADN	D	604[A]	-	-	5/6/22/22	0/3/3/3
5	EDO	D	605	-	-	1/1/1/1	-
5	EDO	D	606	-	-	1/1/1/1	-
5	EDO	B	606	-	-	0/1/1/1	-
4	FBP	B	603	-	-	2/13/32/32	0/1/1/1
4	FBP	C	604	-	-	2/13/32/32	0/1/1/1
5	EDO	C	601	-	-	0/1/1/1	-
5	EDO	A	604	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FBP	D	603	-	-	2/13/32/32	0/1/1/1
5	EDO	C	607	-	-	1/1/1/1	-
3	FLC	A	602	2	-	3/16/16/16	-
5	EDO	B	604	-	-	0/1/1/1	-
3	FLC	C	603	2	-	2/16/16/16	-
8	1PE	C	606	-	-	2/4/4/13	-
6	PEG	A	606	-	-	3/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	606	1PE	OH3-C23	4.88	1.63	1.42
9	D	604[A]	ADN	C5-C4	4.83	1.47	1.39
9	D	604[B]	ADN	C5-C4	4.82	1.47	1.39
3	A	602	FLC	CG-CB	4.25	1.59	1.54
3	C	603	FLC	CG-CB	3.95	1.58	1.54
8	C	606	1PE	OH4-C13	3.66	1.60	1.42
8	C	605	1PE	OH4-C24	3.10	1.55	1.42
9	D	604[B]	ADN	C5-C6	2.99	1.49	1.41
8	C	605	1PE	OH3-C23	2.95	1.54	1.42
3	C	603	FLC	OHB-CB	2.95	1.48	1.43
9	D	604[A]	ADN	C5-C6	2.83	1.48	1.41
4	D	603	FBP	O5-C2	2.79	1.48	1.43
3	A	602	FLC	CA-CB	2.75	1.57	1.54
3	B	602	FLC	OG1-CGC	2.70	1.30	1.22
9	D	604[B]	ADN	C8-N7	2.60	1.36	1.31
3	D	602	FLC	CB-CBC	2.59	1.56	1.53
3	D	602	FLC	OHB-CB	2.59	1.48	1.43
3	D	602	FLC	CA-CB	2.57	1.57	1.54
4	A	603	FBP	O4-C4	2.49	1.49	1.43
8	C	605	1PE	C23-C13	2.44	1.61	1.49
3	D	602	FLC	OG1-CGC	2.38	1.29	1.22
3	C	603	FLC	CB-CBC	-2.35	1.51	1.53
4	D	603	FBP	O2-C2	2.31	1.44	1.40
9	D	604[A]	ADN	C8-N7	2.30	1.36	1.31
4	D	603	FBP	O4-C4	2.28	1.48	1.43
4	B	603	FBP	P2-O4P	2.26	1.57	1.50
8	C	605	1PE	OH3-C22	2.16	1.51	1.42
4	B	603	FBP	O2-C2	2.12	1.44	1.40
4	D	603	FBP	P1-O1	2.11	1.67	1.60
5	B	606	EDO	O1-C1	2.10	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	FBP	P1-O1	2.09	1.66	1.60
4	A	603	FBP	P1-O1P	2.06	1.56	1.50
4	C	604	FBP	O5-C2	-2.03	1.40	1.43
8	C	605	1PE	OH4-C13	2.02	1.50	1.42

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	606	1PE	OH3-C23-C13	6.59	139.17	110.11
9	D	604[B]	ADN	C5-C4-N3	-5.78	118.75	126.72
8	C	606	1PE	OH4-C13-C23	5.28	142.93	111.82
9	D	604[A]	ADN	C5-C4-N3	-5.12	119.67	126.72
3	B	602	FLC	OB2-CBC-CB	4.85	122.45	113.14
4	A	603	FBP	O6P-P2-O5P	4.54	124.81	107.80
3	C	603	FLC	OB2-CBC-CB	4.39	121.55	113.14
9	D	604[B]	ADN	C2-N3-C4	4.29	122.32	111.83
9	D	604[B]	ADN	N3-C4-N9	4.24	134.38	127.17
9	D	604[A]	ADN	N3-C4-N9	4.24	134.37	127.17
9	D	604[B]	ADN	C4-C5-N7	-4.07	105.92	110.58
3	A	602	FLC	OHB-CB-CBC	4.06	114.72	108.96
9	D	604[B]	ADN	N3-C2-N1	-4.06	122.44	128.58
3	A	602	FLC	CG-CB-CA	3.83	119.14	109.31
3	D	602	FLC	CG-CB-CBC	-3.78	101.67	110.03
9	D	604[A]	ADN	C4-C5-N7	-3.76	106.28	110.58
4	B	603	FBP	O1-P1-O1P	-3.75	96.30	106.44
4	C	604	FBP	O1-P1-O1P	-3.72	96.39	106.44
3	A	602	FLC	OB2-CBC-CB	3.70	120.24	113.14
8	C	606	1PE	C23-OH3-C22	-3.63	97.37	113.26
3	D	602	FLC	OB2-CBC-CB	3.38	119.62	113.14
3	C	603	FLC	CG-CB-CBC	-3.36	102.61	110.03
4	D	603	FBP	O2-C2-O5	3.32	115.70	109.33
9	D	604[A]	ADN	O2'-C2'-C3'	3.29	122.37	111.82
9	D	604[A]	ADN	N3-C2-N1	-3.28	123.61	128.58
9	D	604[A]	ADN	C2-N3-C4	3.24	119.73	111.83
4	B	603	FBP	O6P-P2-O5P	3.23	119.92	107.80
3	A	602	FLC	CG-CB-CBC	-3.22	102.90	110.03
9	D	604[A]	ADN	C5-N7-C8	3.21	108.50	103.45
9	D	604[A]	ADN	C4-N9-C8	3.20	109.10	105.74
9	D	604[B]	ADN	C2'-C3'-C4'	-3.17	96.48	102.61
8	C	605	1PE	OH3-C22-C12	3.08	123.67	110.11
4	D	603	FBP	O1-P1-O1P	-3.07	98.13	106.44
9	D	604[B]	ADN	C5-N7-C8	2.85	107.92	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	604[B]	ADN	C6-C5-N7	2.82	137.52	132.09
9	D	604[B]	ADN	O2'-C2'-C3'	2.74	120.59	111.82
9	D	604[A]	ADN	O2'-C2'-C1'	2.70	119.42	110.10
4	D	603	FBP	O6P-P2-O5P	2.68	117.84	107.80
9	D	604[A]	ADN	N9-C8-N7	-2.67	110.15	113.94
8	C	605	1PE	OH4-C24-C14	2.65	121.77	110.11
3	D	602	FLC	OB1-CBC-CB	-2.62	117.01	122.09
9	D	604[B]	ADN	C4-N9-C8	2.60	108.47	105.74
4	A	603	FBP	O3P-P1-O1P	2.42	120.27	110.83
9	D	604[B]	ADN	C2'-C1'-N9	-2.36	107.44	113.30
4	B	603	FBP	O3P-P1-O1P	2.34	119.96	110.83
9	D	604[A]	ADN	O4'-C1'-C2'	-2.31	101.67	106.62
6	A	606	PEG	O2-C2-C1	-2.28	100.08	110.11
4	D	603	FBP	O5P-P2-O6	-2.27	100.75	106.67
9	D	604[B]	ADN	N9-C8-N7	-2.24	110.76	113.94
9	D	604[A]	ADN	C2-N1-C6	2.22	122.37	118.73
3	C	603	FLC	OHB-CB-CG	2.21	114.42	109.38
4	C	604	FBP	O3P-P1-O1P	2.21	119.43	110.83
4	D	603	FBP	O6P-P2-O6	2.17	112.32	106.67
6	A	606	PEG	O2-C3-C4	-2.12	100.76	110.11
4	D	603	FBP	O3P-P1-O1P	2.12	119.08	110.83
3	D	602	FLC	CG-CB-CA	2.09	114.69	109.31
9	D	604[B]	ADN	C2-N1-C6	2.09	122.17	118.73
4	D	603	FBP	O6-P2-O4P	-2.08	100.82	106.44
3	B	602	FLC	CG-CB-CA	2.07	114.62	109.31
3	A	602	FLC	CA-CB-CBC	-2.07	105.47	110.03
4	C	604	FBP	O3P-P1-O1	2.03	111.96	106.67
4	A	603	FBP	O3-C3-C4	2.02	120.37	113.25
3	C	603	FLC	OG1-CGC-CG	-2.02	117.23	122.95
4	A	603	FBP	O5P-P2-O6	-2.02	101.41	106.67
4	A	603	FBP	O6P-P2-O6	2.02	111.92	106.67

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	604[A]	ADN	C2'-C1'-N9-C8
8	C	605	1PE	C23-C13-OH4-C24
9	D	604[A]	ADN	C3'-C4'-C5'-O5'
9	D	604[A]	ADN	O4'-C4'-C5'-O5'
4	B	603	FBP	C4-C5-C6-O6
4	C	604	FBP	C4-C5-C6-O6

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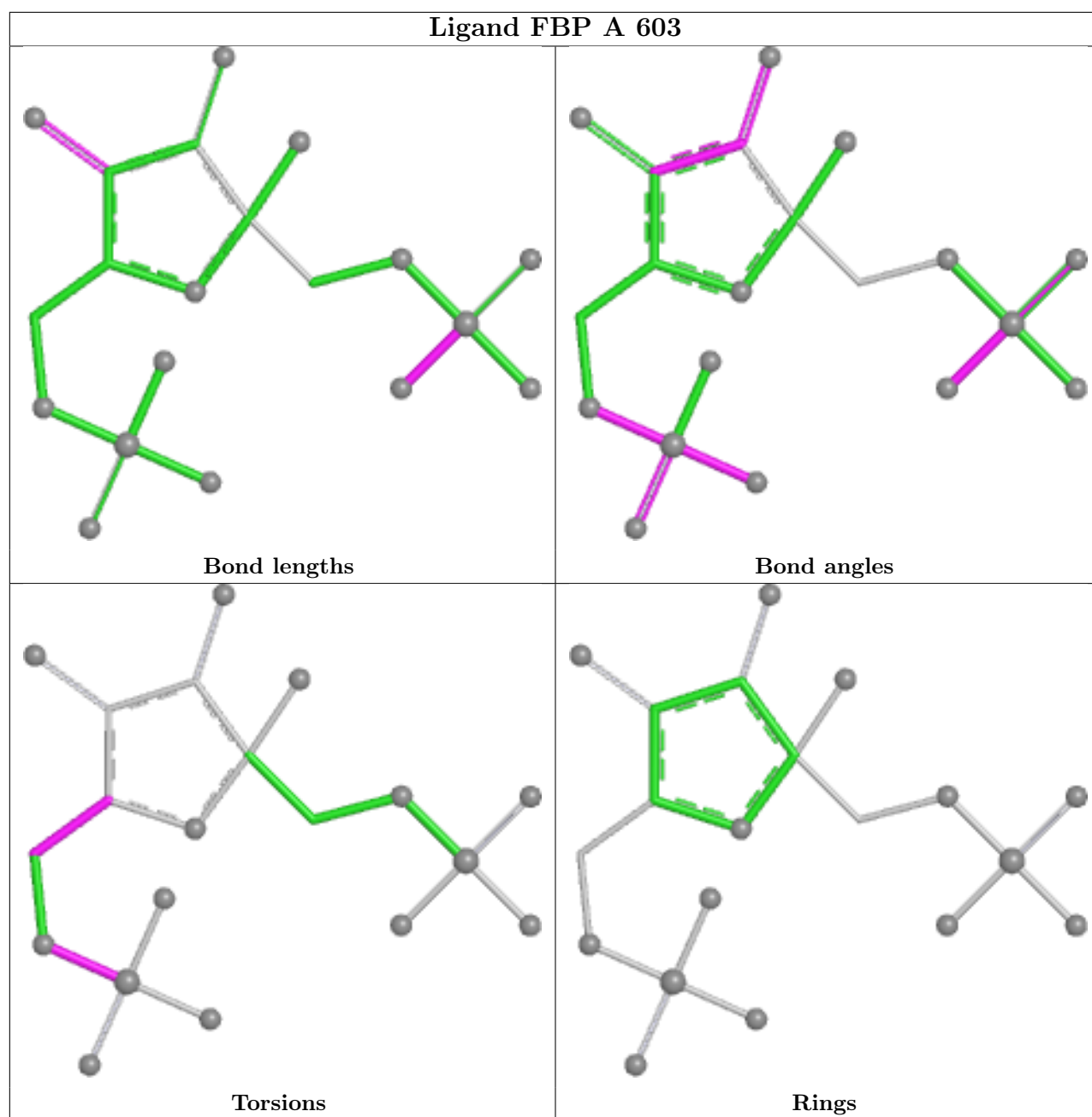
Mol	Chain	Res	Type	Atoms
4	D	603	FBP	C4-C5-C6-O6
4	A	603	FBP	C4-C5-C6-O6
6	A	606	PEG	O2-C3-C4-O4
6	B	605	PEG	O2-C3-C4-O4
9	D	604[A]	ADN	C2'-C1'-N9-C4
6	B	605	PEG	O1-C1-C2-O2
3	B	602	FLC	CG-CB-CBC-OB2
4	B	603	FBP	O5-C5-C6-O6
5	C	607	EDO	O1-C1-C2-O2
6	B	605	PEG	C4-C3-O2-C2
6	A	606	PEG	O1-C1-C2-O2
4	A	603	FBP	O5-C5-C6-O6
4	C	604	FBP	O5-C5-C6-O6
4	D	603	FBP	O5-C5-C6-O6
8	C	606	1PE	OH4-C13-C23-OH3
9	D	604[B]	ADN	C2'-C1'-N9-C8
8	C	605	1PE	C12-C22-OH3-C23
8	C	605	1PE	OH5-C14-C24-OH4
5	D	606	EDO	O1-C1-C2-O2
4	A	603	FBP	C6-O6-P2-O4P
3	B	602	FLC	OHB-CB-CBC-OB2
3	B	602	FLC	CA-CB-CBC-OB2
8	C	605	1PE	OH2-C12-C22-OH3
3	A	602	FLC	CG-CB-CBC-OB2
3	B	602	FLC	CA-CB-CBC-OB1
3	B	602	FLC	CG-CB-CBC-OB1
8	C	606	1PE	C13-C23-OH3-C22
8	C	605	1PE	C13-C23-OH3-C22
9	D	604[B]	ADN	O4'-C1'-N9-C8
5	D	605	EDO	O1-C1-C2-O2
3	A	602	FLC	OHB-CB-CBC-OB1
3	B	602	FLC	OHB-CB-CBC-OB1
3	C	603	FLC	CB-CG-CGC-OG1
3	D	602	FLC	CB-CG-CGC-OG2
3	A	602	FLC	CG-CB-CBC-OB1
9	D	604[A]	ADN	O4'-C1'-N9-C8
3	B	602	FLC	CB-CG-CGC-OG2
3	C	603	FLC	CB-CG-CGC-OG2
9	D	604[B]	ADN	C2'-C1'-N9-C4
3	D	602	FLC	CB-CG-CGC-OG1
3	B	602	FLC	CB-CG-CGC-OG1
6	A	606	PEG	C1-C2-O2-C3

There are no ring outliers.

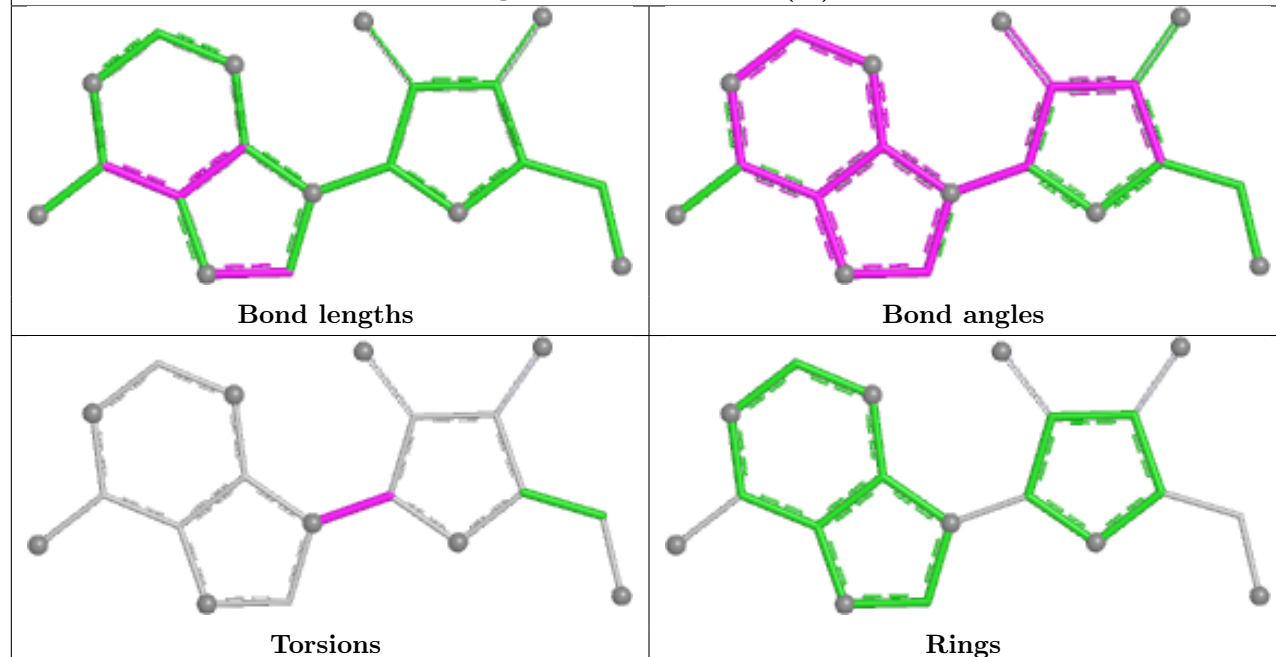
11 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	605	1PE	3	0
9	D	604[B]	ADN	3	0
3	B	602	FLC	4	0
6	B	605	PEG	1	0
3	D	602	FLC	2	0
5	B	606	EDO	1	0
5	C	601	EDO	1	0
3	A	602	FLC	1	0
3	C	603	FLC	1	0
8	C	606	1PE	19	0
6	A	606	PEG	9	0

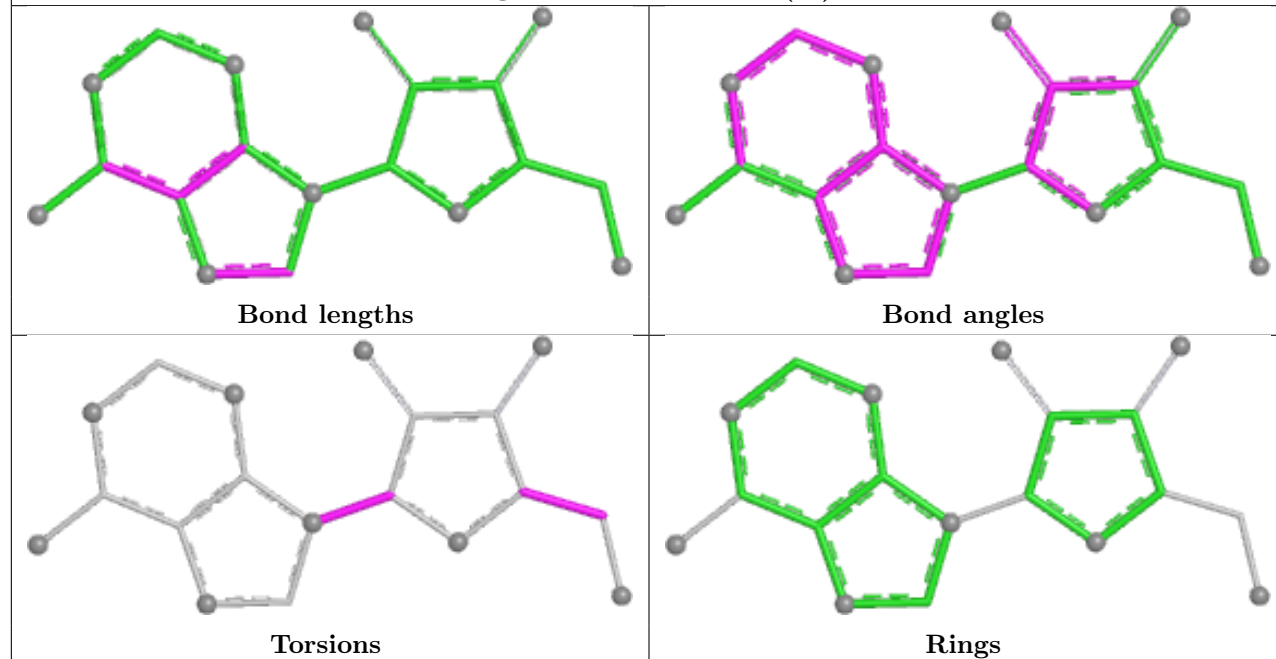
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



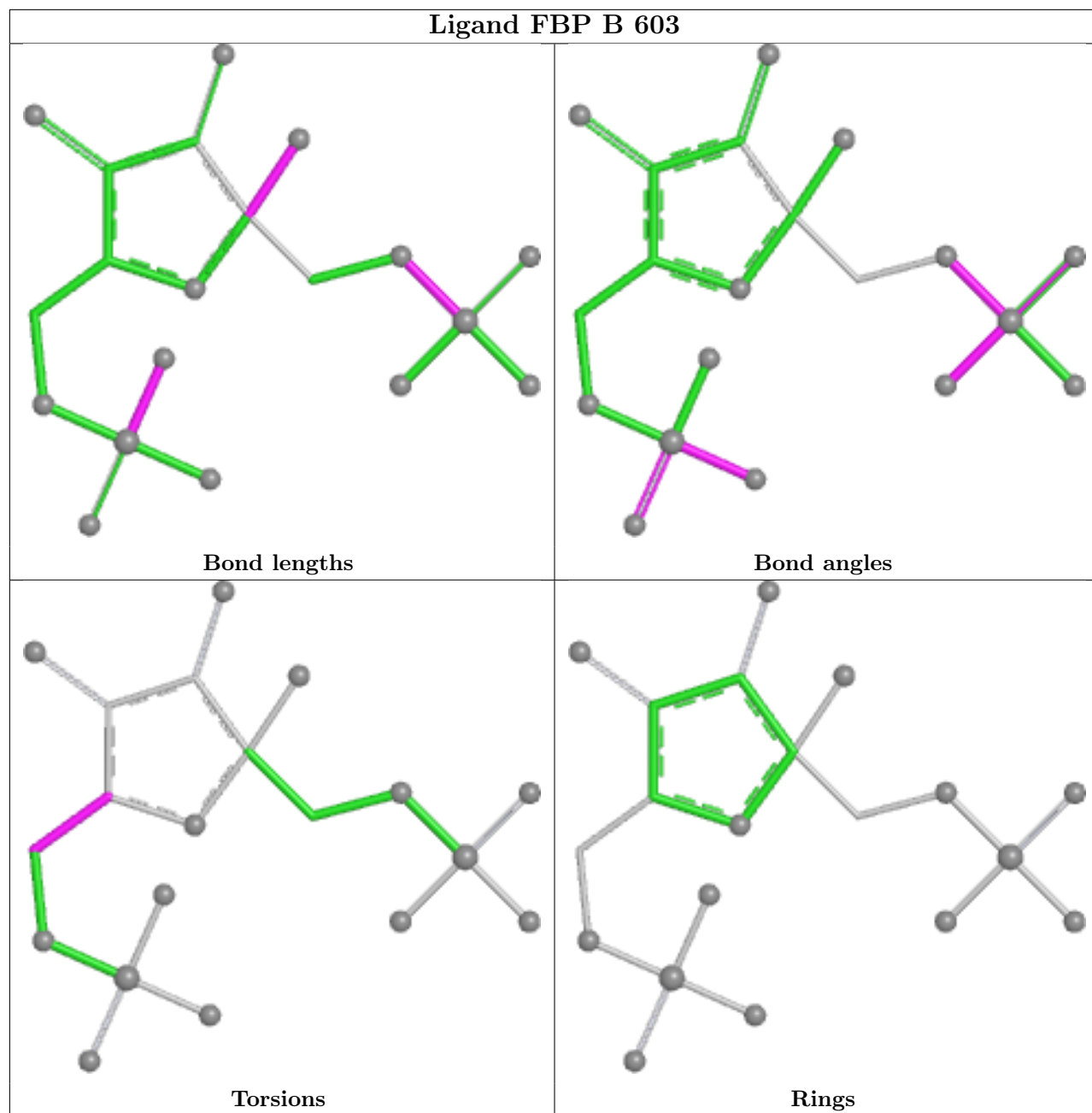
Ligand ADN D 604 (B)

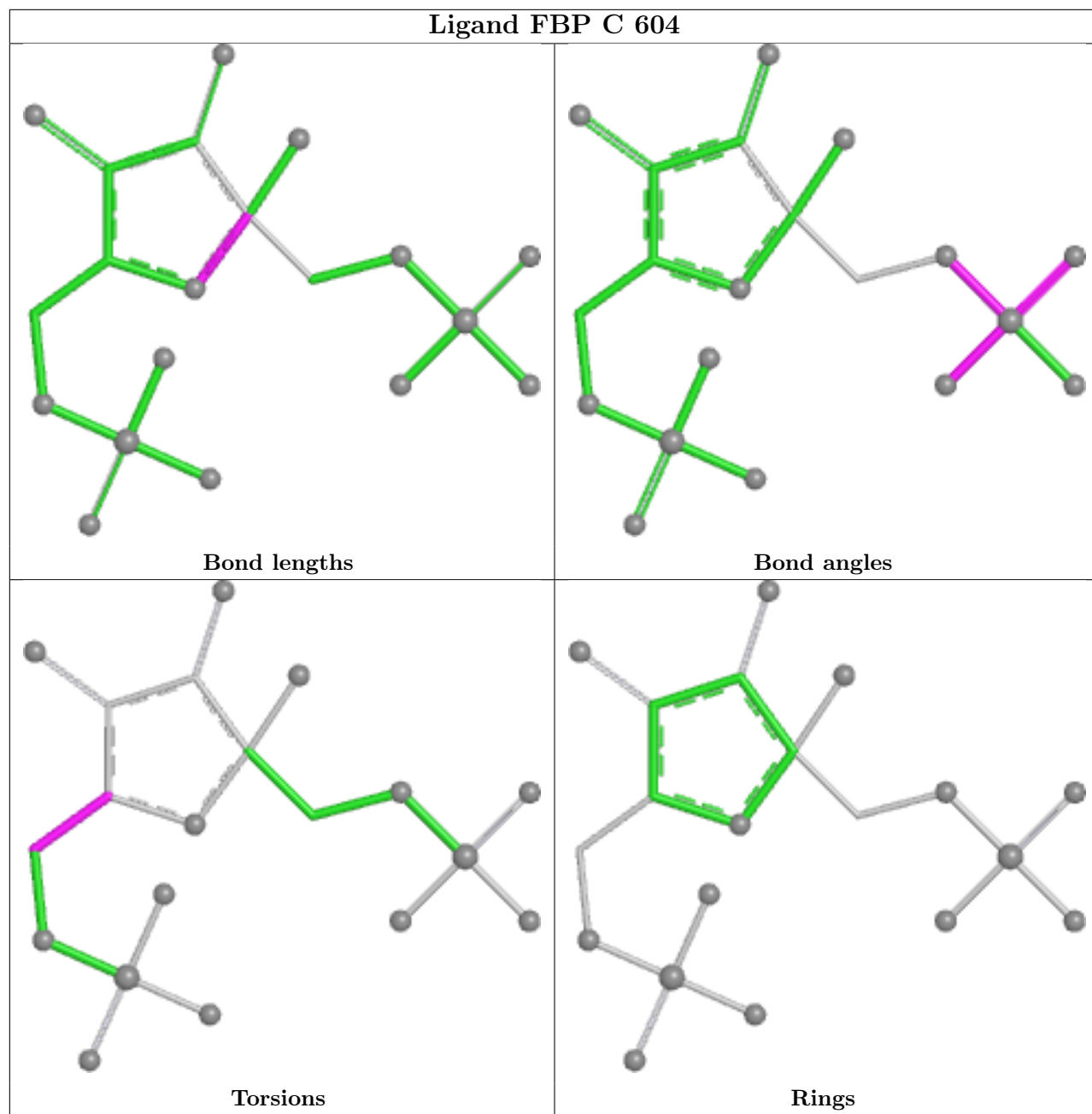


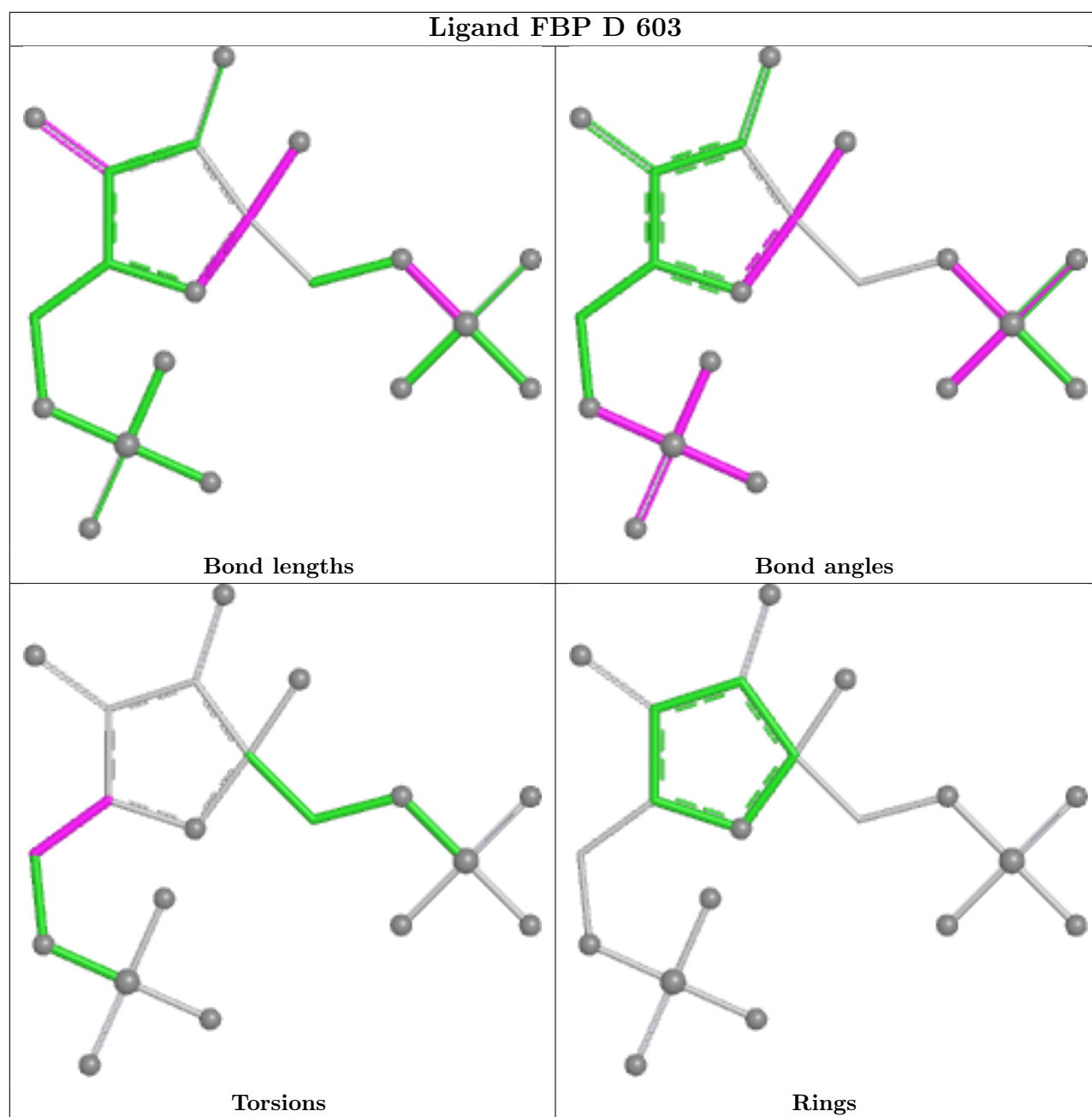
Ligand ADN D 604 (A)



Ligand FBP B 603







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

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	506/543 (93%)	0.01	24 (4%)	36	35	15, 31, 73, 103	19 (3%)
1	B	505/543 (93%)	0.22	45 (8%)	15	13	16, 33, 96, 125	11 (2%)
1	C	500/543 (92%)	0.22	39 (7%)	19	17	16, 34, 95, 120	12 (2%)
1	D	507/543 (93%)	0.27	60 (11%)	9	7	16, 34, 115, 197	12 (2%)
All	All	2018/2172 (92%)	0.18	168 (8%)	17	15	15, 33, 96, 197	54 (2%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	VAL	8.8
1	B	135	ILE	6.3
1	C	233	LEU	6.3
1	D	160	PHE	6.0
1	D	21	GLY	5.6
1	D	135	ILE	5.5
1	D	200	ILE	5.0
1	A	135	ILE	5.0
1	C	159	ALA	4.9
1	D	203	GLU	4.9
1	D	199	LYS	4.9
1	B	25	PHE	4.9
1	B	144	VAL	4.9
1	C	231	PRO	4.9
1	B	160	PHE	4.8
1	B	214	VAL	4.7
1	D	202	PRO	4.7
1	D	182	VAL	4.6
1	C	144	VAL	4.5
1	B	226	ALA	4.4
1	B	233	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	202	PRO	4.3
1	C	234	SER	4.3
1	C	232	GLY	4.2
1	B	146	LEU	4.2
1	B	159	ALA	4.1
1	B	231	PRO	4.1
1	D	205	LEU	4.1
1	B	182	VAL	4.0
1	D	177	VAL	4.0
1	B	177	VAL	3.9
1	C	182	VAL	3.9
1	B	215	LEU	3.8
1	D	204	GLY	3.8
1	B	200	ILE	3.8
1	B	147	VAL	3.8
1	C	217	SER	3.8
1	B	26	GLN	3.7
1	B	202	PRO	3.7
1	B	166	ALA	3.6
1	D	201	GLY	3.5
1	B	181	PRO	3.4
1	B	199	LYS	3.4
1	B	216	GLY	3.4
1	D	206	VAL	3.4
1	D	22	THR	3.3
1	C	166	ALA	3.3
1	C	177	VAL	3.3
1	D	490	PRO	3.3
1	A	232	GLY	3.2
1	D	178	ARG	3.2
1	D	493	ILE	3.2
1	D	25	PHE	3.2
1	B	218	ARG	3.2
1	B	196	VAL	3.1
1	D	183	GLY	3.1
1	D	158	PRO	3.0
1	C	413	ALA	3.0
1	C	206	VAL	3.0
1	D	116[A]	SER	3.0
1	D	151	GLN	3.0
1	B	133	THR	2.9
1	C	216	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	115	LEU	2.9
1	C	215	LEU	2.9
1	D	171	VAL	2.8
1	A	218	ARG	2.8
1	D	154	VAL	2.8
1	D	156	VAL	2.8
1	D	179	VAL	2.8
1	D	196	VAL	2.8
1	A	411	ARG	2.8
1	C	214	VAL	2.8
1	D	152	VAL	2.8
1	D	133	THR	2.8
1	D	153	LEU	2.8
1	D	232	GLY	2.7
1	B	115	LEU	2.7
1	D	233	LEU	2.7
1	B	134	GLY	2.7
1	B	184	GLY	2.7
1	B	209	VAL	2.7
1	D	184	GLY	2.6
1	C	155	THR	2.6
1	D	24	PHE	2.6
1	B	143	GLU	2.6
1	D	159	ALA	2.6
1	D	197	VAL	2.6
1	D	144	VAL	2.5
1	D	115	LEU	2.5
1	D	149	GLY	2.5
1	A	414	ALA	2.5
1	B	180	VAL	2.5
1	D	181	PRO	2.5
1	A	149	GLY	2.4
1	B	411	ARG	2.4
1	D	163	ARG	2.4
1	D	218	ARG	2.4
1	B	179	VAL	2.4
1	C	225	GLY	2.4
1	D	150	SER	2.4
1	C	199	LYS	2.4
1	D	157	ASP	2.4
1	D	162	THR	2.4
1	C	414	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	234	SER	2.4
1	A	115	LEU	2.4
1	C	200	ILE	2.4
1	C	158	PRO	2.4
1	D	134	GLY	2.4
1	A	116	SER	2.4
1	C	170	TRP	2.4
1	B	176	ILE	2.3
1	C	242	ARG	2.3
1	D	164	GLY	2.3
1	A	214	VAL	2.3
1	D	147	VAL	2.3
1	C	203	GLU	2.3
1	A	227	GLN	2.3
1	C	168	THR	2.3
1	D	275[A]	HIS	2.3
1	B	158	PRO	2.3
1	B	206	VAL	2.3
1	D	180	VAL	2.3
1	A	492	ALA	2.2
1	C	27	GLN	2.2
1	B	153	LEU	2.2
1	D	146	LEU	2.2
1	A	159	ALA	2.2
1	C	218	ARG	2.2
1	C	209	VAL	2.2
1	D	26	GLN	2.2
1	C	114	PRO	2.2
1	A	110	PHE	2.2
1	B	168	THR	2.2
1	A	416	LEU	2.2
1	A	160	PHE	2.1
1	D	145	GLU	2.1
1	B	152	VAL	2.1
1	B	154	VAL	2.1
1	B	169	VAL	2.1
1	D	207	THR	2.1
1	A	404	ARG	2.1
1	C	205	LEU	2.1
1	C	145	GLU	2.1
1	B	194	SER	2.1
1	A	134	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	169	VAL	2.1
1	D	215	LEU	2.1
1	A	33	ALA	2.1
1	A	412	ARG	2.1
1	A	162	THR	2.1
1	D	155[A]	THR	2.1
1	B	183	GLY	2.1
1	B	34	MET	2.1
1	C	154	VAL	2.1
1	C	489	PRO	2.1
1	C	412	ARG	2.1
1	C	219	LYS	2.0
1	D	198	GLN	2.0
1	C	146	LEU	2.0
1	A	166	ALA	2.0
1	C	411	ARG	2.0
1	A	203	GLU	2.0
1	D	113	SER	2.0
1	D	217	SER	2.0
1	D	514	PHE	2.0
1	B	197	VAL	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
6	PEG	B	605	7/7	0.77	0.16	42,50,59,60	0
8	1PE	C	605	10/16	0.81	0.14	41,46,48,49	0

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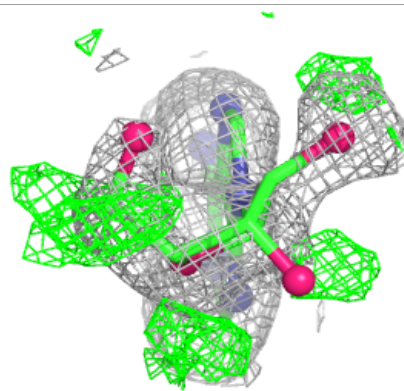
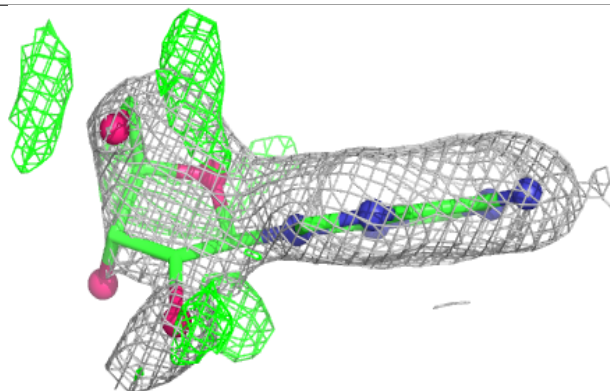
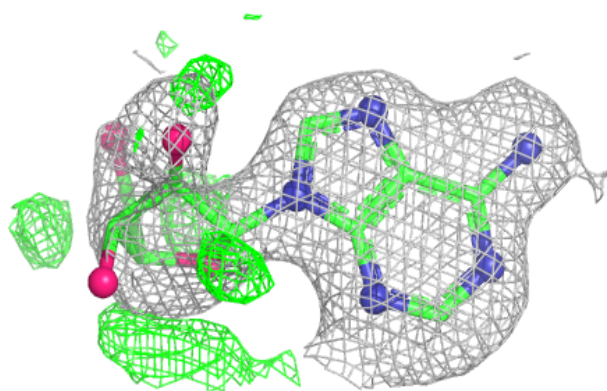
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	C	607	4/4	0.82	0.13	44,52,55,56	0
9	ADN	D	604[A]	19/19	0.82	0.14	26,30,41,43	19
9	ADN	D	604[B]	19/19	0.82	0.14	26,30,47,49	19
6	PEG	A	606	7/7	0.84	0.14	37,42,47,48	0
5	EDO	B	606	4/4	0.87	0.19	32,36,36,44	0
5	EDO	D	606	4/4	0.89	0.13	42,43,52,55	0
8	1PE	C	606	7/16	0.91	0.11	29,32,41,42	0
7	NA	C	608	1/1	0.92	0.10	41,41,41,41	0
7	NA	B	607	1/1	0.93	0.10	37,37,37,37	0
3	FLC	B	602	13/13	0.94	0.07	26,30,42,44	0
5	EDO	A	605	4/4	0.94	0.08	30,35,36,38	0
5	EDO	D	605	4/4	0.94	0.11	27,29,32,38	0
3	FLC	D	602	13/13	0.95	0.08	25,32,42,42	0
7	NA	A	607	1/1	0.95	0.11	40,40,40,40	0
5	EDO	C	601	4/4	0.95	0.09	35,35,37,38	0
3	FLC	C	603	13/13	0.95	0.07	24,31,41,47	0
5	EDO	A	604	4/4	0.96	0.07	25,27,28,34	0
3	FLC	A	602	13/13	0.96	0.06	21,27,36,39	0
5	EDO	D	607	4/4	0.96	0.07	31,35,36,38	0
5	EDO	B	604	4/4	0.96	0.07	27,32,34,37	0
7	NA	D	608	1/1	0.97	0.10	38,38,38,38	0
4	FBP	D	603	20/20	0.98	0.05	26,28,32,32	0
4	FBP	C	604	20/20	0.98	0.05	23,27,29,30	0
2	MN	C	602	1/1	0.99	0.05	28,28,28,28	0
4	FBP	A	603	20/20	0.99	0.04	22,25,28,28	0
4	FBP	B	603	20/20	0.99	0.04	23,26,29,30	0
2	MN	A	601	1/1	0.99	0.02	26,26,26,26	0
2	MN	D	601	1/1	1.00	0.02	28,28,28,28	0
2	MN	B	601	1/1	1.00	0.04	27,27,27,27	0

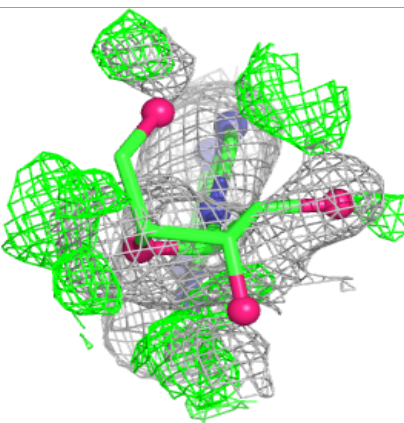
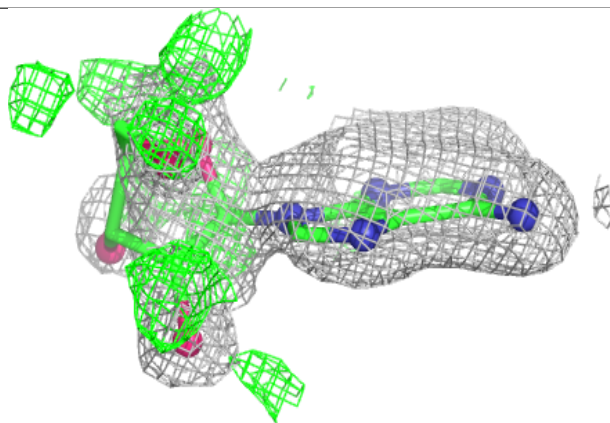
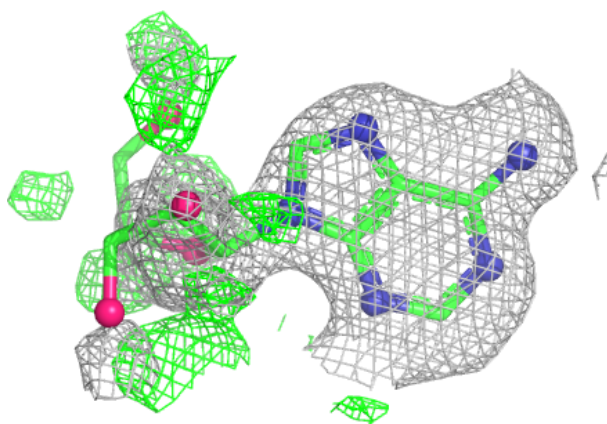
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADN D 604 (A):

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

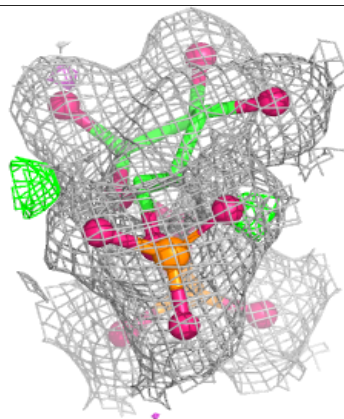
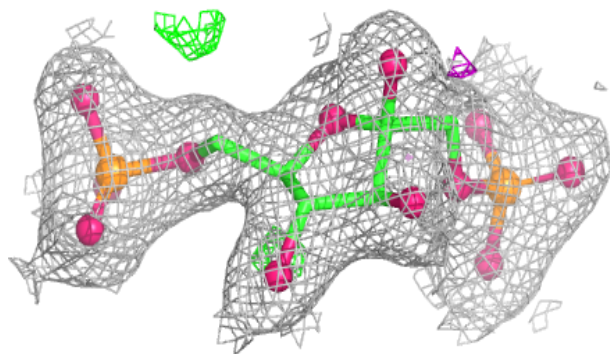
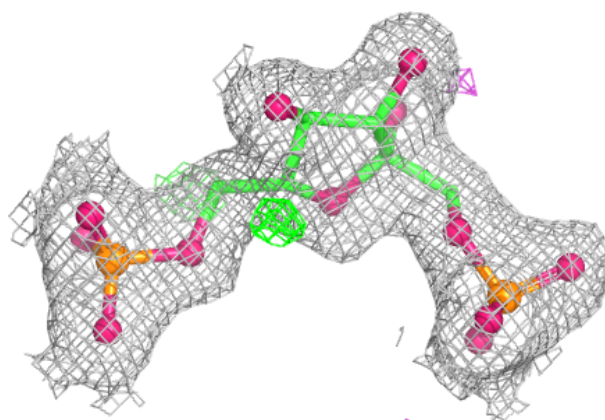
**Electron density around ADN D 604 (B):**

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



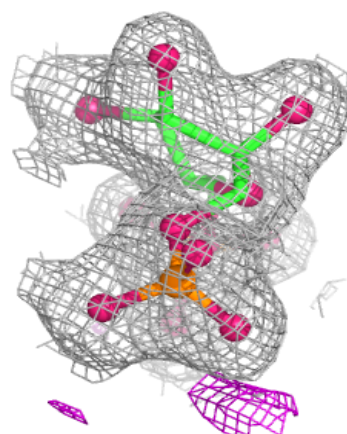
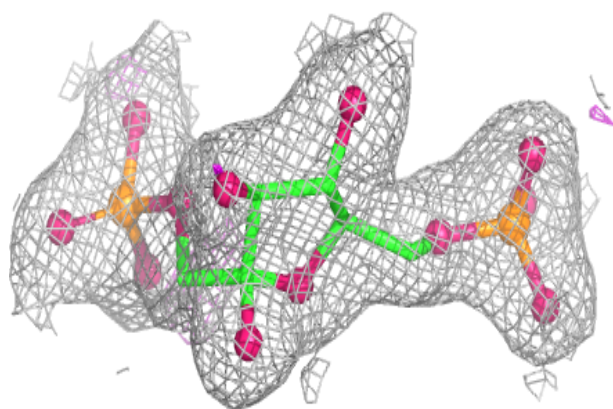
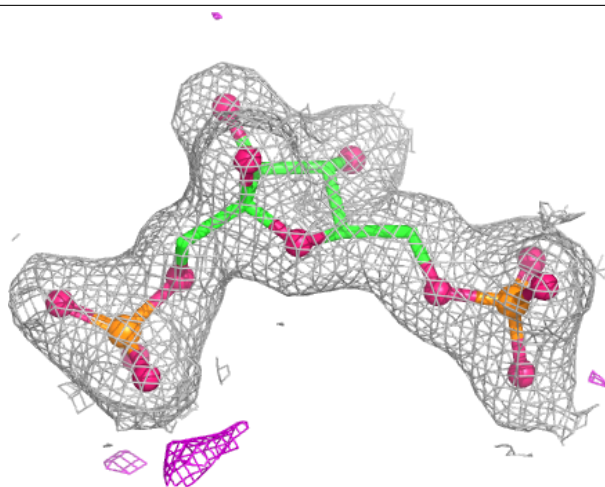
Electron density around FBP D 603:

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



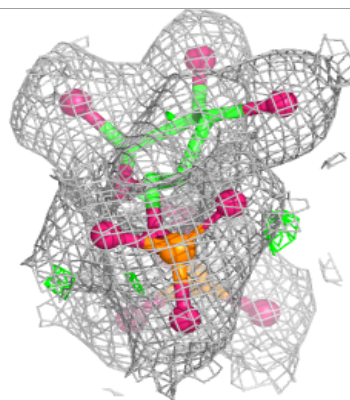
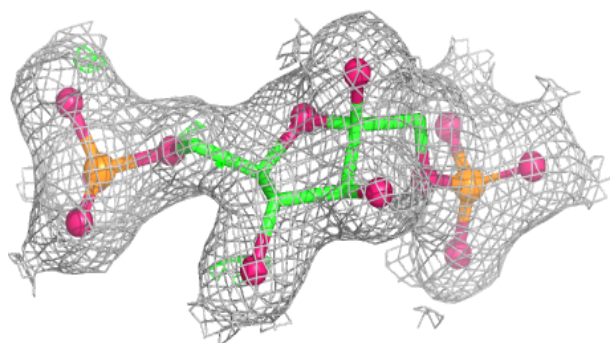
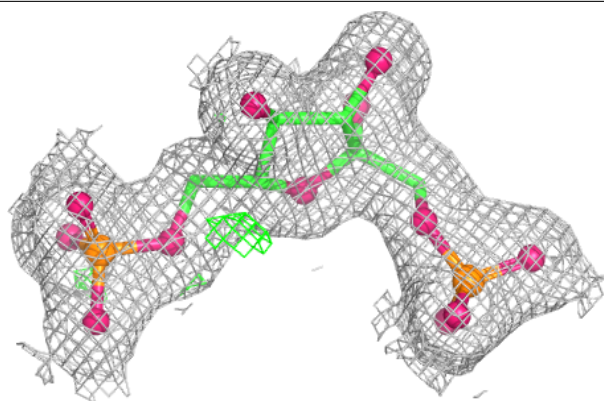
Electron density around FBP C 604:

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

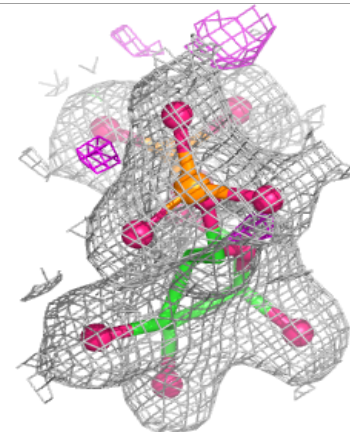
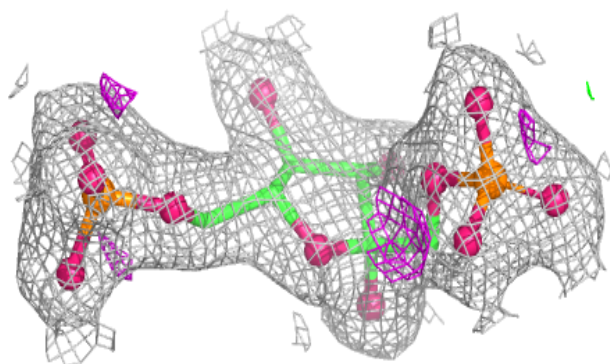
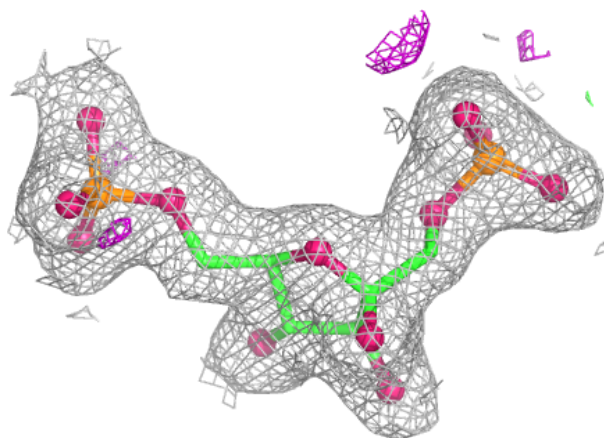


Electron density around FBP A 603:

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

**Electron density around FBP B 603:**

$2mF_o-DF_c$ (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.