



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:16 AM UTC

PDB ID : 7L21 / pdb_00007L21
Title : Pyruvate Kinase M2 mutant-N70D
Authors : Nandi, S.; Dey, M.
Deposited on : 2020-12-16
Resolution : 2.29 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

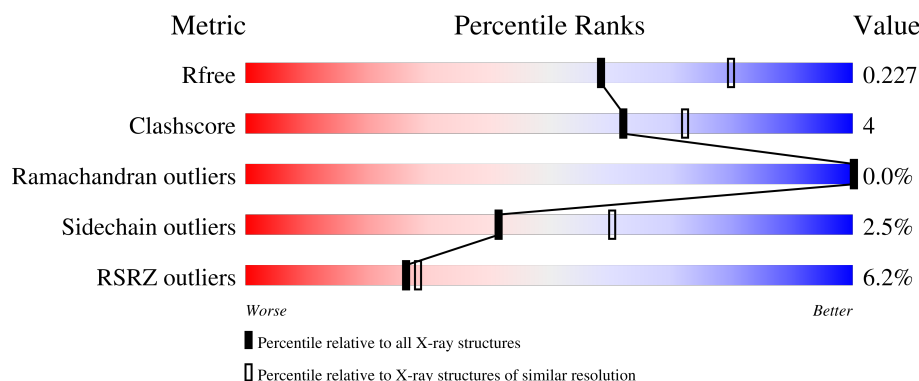
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	550	4% 85% 8% 6%
1	B	550	3% 83% 10% 6%
1	C	550	3% 85% 8% 6%
1	D	550	12% 78% 13% 8%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OXL	A	601	-	X	-	-
2	OXL	B	601	-	X	-	-
2	OXL	C	601	-	X	-	-
2	OXL	D	601	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16070 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 PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	0	0
			3878	2437	686	730	25			
1	B	515	Total	C	N	O	S	0	0	0
			3862	2430	677	730	25			
1	C	518	Total	C	N	O	S	0	0	0
			3886	2441	688	732	25			
1	D	504	Total	C	N	O	S	0	0	0
			3661	2291	659	688	23			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P14618
A	-17	GLY	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	SER	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	HIS	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	SER	-	expression tag	UNP P14618
A	-6	GLY	-	expression tag	UNP P14618
A	-5	LEU	-	expression tag	UNP P14618
A	-4	VAL	-	expression tag	UNP P14618
A	-3	PRO	-	expression tag	UNP P14618
A	-2	ARG	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
A	70	ASP	ASN	engineered mutation	UNP P14618
B	-18	MET	-	initiating methionine	UNP P14618

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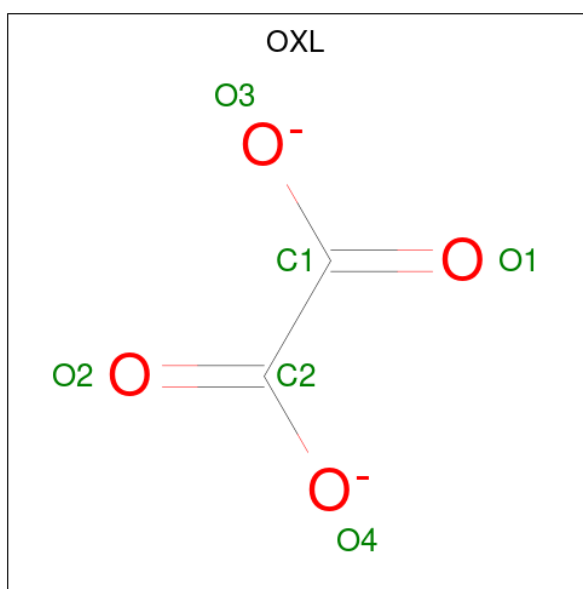
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	expression tag	UNP P14618
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	HIS	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	SER	-	expression tag	UNP P14618
B	-6	GLY	-	expression tag	UNP P14618
B	-5	LEU	-	expression tag	UNP P14618
B	-4	VAL	-	expression tag	UNP P14618
B	-3	PRO	-	expression tag	UNP P14618
B	-2	ARG	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
B	70	ASP	ASN	engineered mutation	UNP P14618
C	-18	MET	-	initiating methionine	UNP P14618
C	-17	GLY	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	SER	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	HIS	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	SER	-	expression tag	UNP P14618
C	-6	GLY	-	expression tag	UNP P14618
C	-5	LEU	-	expression tag	UNP P14618
C	-4	VAL	-	expression tag	UNP P14618
C	-3	PRO	-	expression tag	UNP P14618
C	-2	ARG	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
C	70	ASP	ASN	engineered mutation	UNP P14618
D	-18	MET	-	initiating methionine	UNP P14618
D	-17	GLY	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	VAL	-	expression tag	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	ARG	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618
D	70	ASP	ASN	engineered mutation	UNP P14618

- Molecule 2 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	2	4		
2	B	1	Total	C	O	0	0
			6	2	4		
2	C	1	Total	C	O	0	0
			6	2	4		

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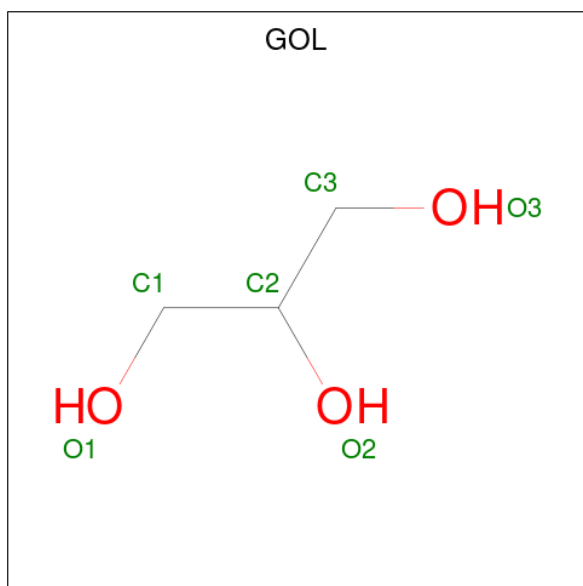
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			6	2	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



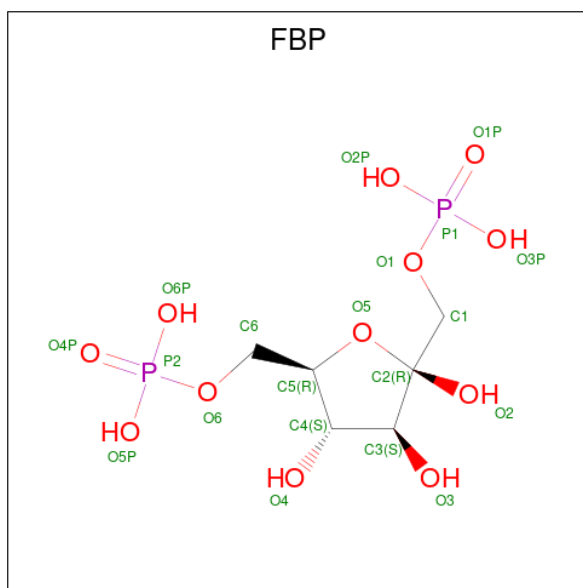
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 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
5	A	1	Total	C	O	P	0	0
			8	2	5	1		
5	B	1	Total	O	P		0	0
			5	4	1			
5	C	1	Total	O	P		0	0
			5	4	1			
5	D	1	Total	C	O	P	0	0
			7	2	4	1		

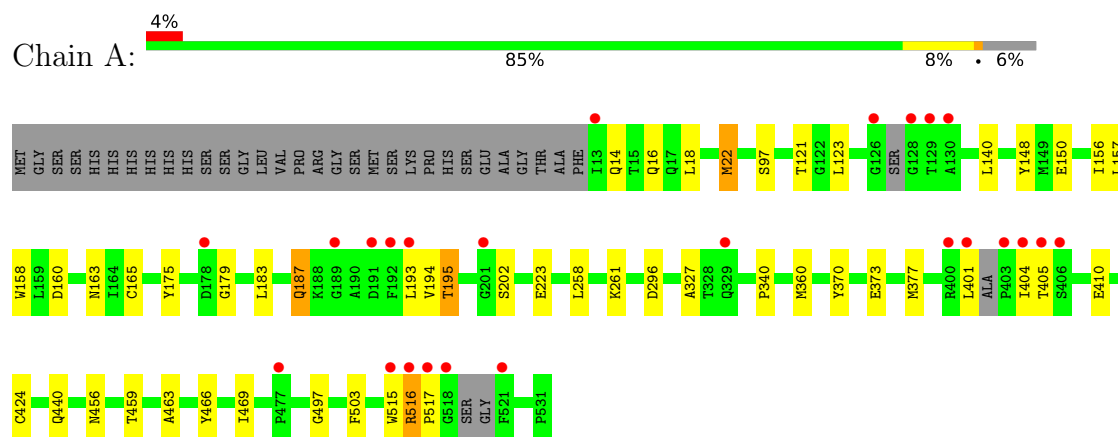
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	191	Total 191	O 191	0	0
6	B	183	Total 183	O 183	0	0
6	C	161	Total 161	O 161	0	0
6	D	129	Total 129	O 129	0	0

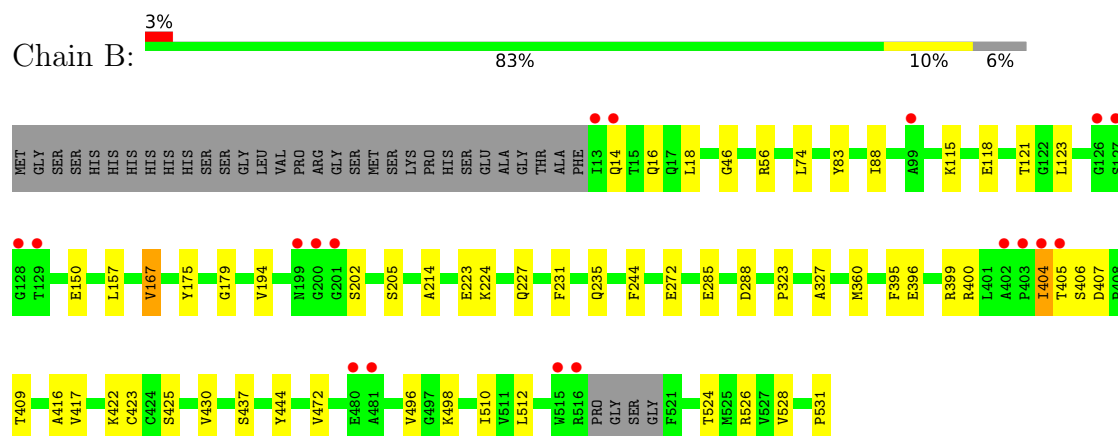
3 Residue-property plots [i](#)

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

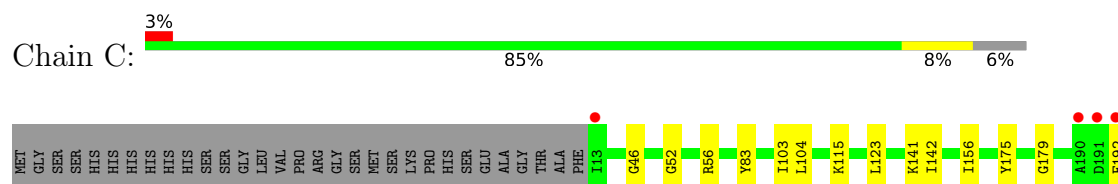
• Molecule 1: Pyruvate kinase PKM

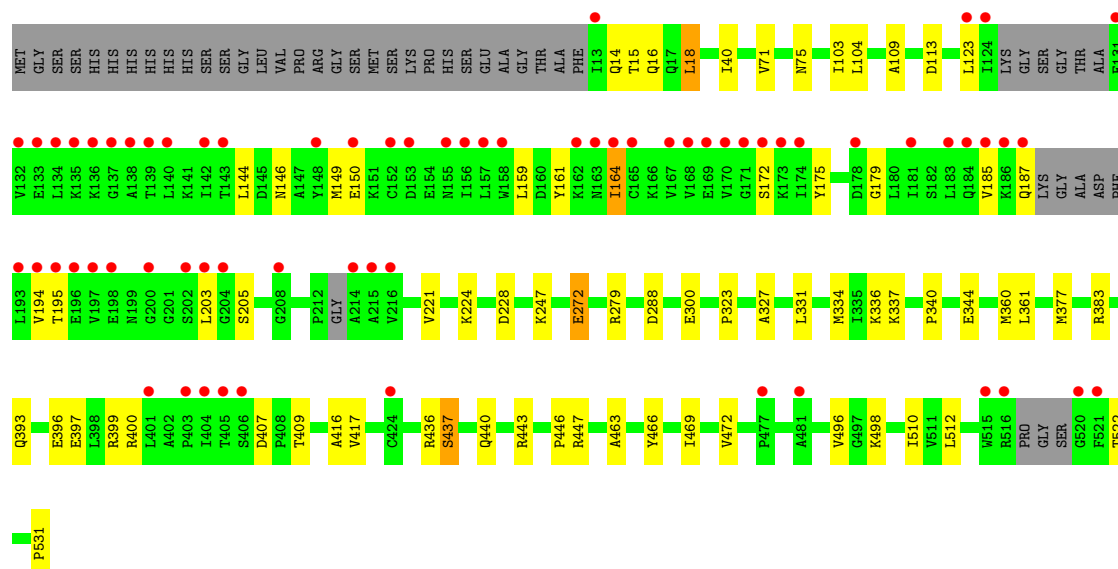


• Molecule 1: Pyruvate kinase PKM



• Molecule 1: Pyruvate kinase PKM





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	139.34Å 158.30Å 241.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.81 – 2.29 63.81 – 2.29	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.81-2.29) 100.0 (63.81-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.18 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.183 , 0.229 0.184 , 0.227	Depositor DCC
R_{free} test set	5906 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16070	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: FBP, OXL, GOL, MG

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	0.37	0/3935	0.63	5/5320 (0.1%)
1	B	0.35	0/3921	0.55	0/5308
1	C	0.34	0/3944	0.55	1/5335 (0.0%)
1	D	0.31	0/3714	0.50	2/5034 (0.0%)
All	All	0.34	0/15514	0.56	8/20997 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	ARG	CA-C-N	-10.45	106.78	119.84
1	A	516	ARG	C-N-CA	-10.45	106.78	119.84
1	A	515	TRP	O-C-N	-7.40	114.39	122.38
1	A	516	ARG	N-CA-C	-7.13	93.93	109.11
1	A	516	ARG	CA-C-O	-6.45	113.56	119.62
1	C	488	LEU	CB-CA-C	-5.95	98.57	110.42
1	D	361	LEU	CA-C-N	-5.30	115.23	121.90
1	D	361	LEU	C-N-CA	-5.30	115.23	121.90

There are no chirality outliers.

There are no planarity outliers.

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	3878	0	3888	24	2
1	B	3862	0	3867	32	2
1	C	3886	0	3898	28	0
1	D	3661	0	3503	42	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	16	1	0
4	B	18	0	24	6	0
4	C	18	0	24	3	0
4	D	18	0	24	0	0
5	A	8	0	2	0	0
5	B	5	0	0	1	0
5	C	5	0	0	0	0
5	D	7	0	2	1	0
6	A	191	0	0	2	0
6	B	183	0	0	2	0
6	C	161	0	0	0	0
6	D	129	0	0	2	0
All	All	16070	0	15248	127	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 4.

All (127) 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:C:488:LEU:O	1:C:488:LEU:HD22	1.53	1.06
1:C:488:LEU:O	1:C:488:LEU:CD2	2.21	0.89
1:C:341:THR:HG22	1:C:344:GLU:H	1.40	0.84
1:B:285:GLU:OE2	6:B:701:HOH:O	2.01	0.79
1:D:144:LEU:HD11	1:D:164:ILE:HD11	1.65	0.79
1:D:185:VAL:HA	1:D:195:THR:HG22	1.64	0.78
1:D:123:LEU:HB2	1:D:150:GLU:HA	1.69	0.74
1:A:183:LEU:HD13	1:A:195:THR:HG21	1.70	0.72
1:D:14:GLN:OE1	6:D:701:HOH:O	2.13	0.66
1:C:498:LYS:NZ	1:C:531:PRO:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:HB3	1:A:195:THR:HG23	1.80	0.63
1:D:123:LEU:HA	1:D:205:SER:HB2	1.79	0.63
1:D:399:ARG:NH2	6:D:704:HOH:O	2.34	0.59
1:A:516:ARG:O	1:A:517:PRO:C	2.41	0.59
1:B:167:VAL:HG13	1:B:214:ALA:HB1	1.85	0.59
1:B:123:LEU:HD23	1:B:205:SER:HB3	1.84	0.59
1:C:142:ILE:HB	1:C:193:LEU:HB3	1.86	0.58
1:D:498:LYS:NZ	1:D:531:PRO:O	2.31	0.58
1:D:103:ILE:HG22	1:D:104:LEU:HD22	1.85	0.57
1:C:487:ASP:O	1:C:488:LEU:HB3	2.05	0.56
1:D:247:LYS:HB3	1:D:279:ARG:HE	1.69	0.56
1:B:498:LYS:NZ	1:B:531:PRO:O	2.38	0.56
1:D:437:SER:OG	5:D:606:FBP:O5P	2.23	0.56
1:B:327:ALA:HB1	1:B:360:MET:HE2	1.89	0.55
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.89	0.55
1:D:159:LEU:HD11	1:D:164:ILE:HD13	1.88	0.55
1:D:327:ALA:HB1	1:D:360:MET:HE2	1.89	0.55
1:B:244:PHE:HZ	4:B:603:GOL:H31	1.71	0.54
1:B:405:THR:OG1	1:B:406:SER:N	2.38	0.54
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.42	0.54
1:D:161:TYR:O	1:D:164:ILE:HG12	2.06	0.54
1:C:46:GLY:HA2	4:C:603:GOL:H2	1.89	0.54
1:D:224:LYS:NZ	1:D:228:ASP:OD2	2.37	0.53
1:D:14:GLN:HG3	1:D:15:THR:H	1.72	0.53
1:A:121:THR:HB	1:A:157:LEU:HD11	1.91	0.52
1:D:417:VAL:HG13	1:D:446:PRO:HB3	1.91	0.52
1:D:14:GLN:HG2	1:D:18:LEU:HB2	1.92	0.52
1:D:175:TYR:HB3	1:D:179:GLY:HA2	1.92	0.51
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.91	0.51
1:C:341:THR:HG23	1:C:343:ALA:H	1.74	0.51
1:A:14:GLN:HB3	6:A:839:HOH:O	2.10	0.51
1:D:340:PRO:HG3	1:D:377:MET:HG2	1.92	0.51
1:C:330:MET:HB3	1:C:347:ASP:OD2	2.11	0.50
1:B:56:ARG:HD2	1:B:83:TYR:OH	2.10	0.50
1:B:396:GLU:O	1:B:400:ARG:HG3	2.11	0.50
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.93	0.50
1:A:327:ALA:HB1	1:A:360:MET:HE2	1.92	0.50
1:B:118:GLU:HG2	4:B:603:GOL:H2	1.93	0.50
1:B:526:ARG:HB3	1:B:528:VAL:HG13	1.93	0.50
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.92	0.50
1:A:123:LEU:HD12	1:A:150:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:NZ	6:B:708:HOH:O	2.44	0.49
1:C:52:GLY:O	1:C:56:ARG:HG3	2.12	0.49
4:B:605:GOL:O3	4:B:605:GOL:O1	2.18	0.49
1:A:148:TYR:CE1	1:A:156:ILE:HD13	2.48	0.49
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.95	0.48
1:C:464:HIS:ND1	4:C:603:GOL:O2	2.37	0.48
1:C:46:GLY:CA	4:C:603:GOL:H2	2.43	0.48
1:D:407:ASP:OD2	1:D:436:ARG:NH2	2.46	0.48
1:D:40:ILE:O	1:D:383:ARG:HD2	2.13	0.48
1:A:296:ASP:OD1	4:A:603:GOL:H31	2.14	0.47
1:D:161:TYR:CD2	1:D:164:ILE:HG23	2.49	0.47
1:B:16:GLN:HG3	1:B:18:LEU:HG	1.96	0.47
1:A:183:LEU:HB3	1:A:195:THR:CG2	2.44	0.47
1:A:22:MET:HE2	1:A:22:MET:HB3	1.58	0.47
1:C:123:LEU:HD23	1:C:205:SER:HB3	1.96	0.47
1:A:187:GLN:HG3	1:A:194:VAL:HB	1.97	0.47
1:B:223:GLU:O	1:B:227:GLN:HG2	2.15	0.46
1:C:487:ASP:C	1:C:489:ARG:H	2.24	0.46
1:D:409:THR:HG23	1:D:522:THR:HB	1.97	0.46
1:D:16:GLN:OE1	1:D:447:ARG:HD2	2.15	0.46
1:B:231:PHE:CE2	1:B:235:GLN:HG3	2.51	0.46
1:D:334:MET:HA	1:D:337:LYS:O	2.15	0.46
1:A:16:GLN:HG3	1:A:18:LEU:HG	1.97	0.45
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.97	0.45
1:A:165:CYS:SG	6:A:867:HOH:O	2.55	0.45
1:C:56:ARG:HD2	1:C:83:TYR:OH	2.16	0.45
1:A:410:GLU:OE2	1:A:440:GLN:NE2	2.50	0.45
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.52	0.45
1:D:159:LEU:HD12	1:D:161:TYR:H	1.80	0.45
1:B:244:PHE:CZ	4:B:603:GOL:H31	2.51	0.45
1:D:463:ALA:HB1	1:D:469:ILE:HG21	1.99	0.45
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.98	0.44
1:A:340:PRO:HG3	1:A:377:MET:HG2	1.98	0.44
1:B:121:THR:HB	1:B:157:LEU:HD11	1.99	0.44
1:A:140:LEU:O	1:A:195:THR:HB	2.18	0.44
1:D:336:LYS:HA	1:D:336:LYS:HD2	1.74	0.44
1:B:423:CYS:SG	1:B:425:SER:HB3	2.58	0.44
1:C:330:MET:O	1:C:331:LEU:HD23	2.17	0.44
1:B:405:THR:HB	1:B:407:ASP:H	1.83	0.43
1:B:437:SER:OG	5:B:606:FBP:O4P	2.25	0.43
1:D:187:GLN:CB	1:D:194:VAL:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:HD3	1:B:224:LYS:HE3	2.00	0.43
1:C:417:VAL:HG21	1:C:444:TYR:HB2	2.01	0.43
1:D:146:ASN:O	1:D:149:MET:HG2	2.18	0.43
1:C:141:LYS:HE2	1:C:192:PHE:CB	2.48	0.43
1:B:288:ASP:O	1:B:323:PRO:HD2	2.19	0.43
1:A:370:TYR:HB3	1:A:373:GLU:HB2	2.01	0.43
1:B:46:GLY:HA2	4:B:604:GOL:H2	2.01	0.43
1:D:18:LEU:HD12	1:D:18:LEU:HA	1.89	0.43
1:D:272:GLU:O	1:D:300:GLU:HG3	2.19	0.43
1:C:327:ALA:HB1	1:C:360:MET:HE2	2.01	0.42
1:A:456:ASN:HB3	1:A:459:THR:HB	2.01	0.42
1:B:46:GLY:CA	4:B:604:GOL:H2	2.48	0.42
1:B:123:LEU:HD12	1:B:150:GLU:HG2	2.00	0.42
1:B:404:ILE:HD13	1:B:404:ILE:HA	1.84	0.42
1:D:71:VAL:HG22	1:D:109:ALA:HB3	2.01	0.42
1:B:395:PHE:O	1:B:399:ARG:HG3	2.20	0.42
1:C:340:PRO:HG3	1:C:377:MET:HG2	2.01	0.42
1:C:445:ARG:HA	1:C:445:ARG:HD3	1.82	0.42
1:D:396:GLU:O	1:D:400:ARG:HG3	2.19	0.42
1:D:416:ALA:HB2	1:D:512:LEU:HD21	2.02	0.42
1:A:158:TRP:CH2	1:A:160:ASP:HB3	2.55	0.41
1:C:323:PRO:HB3	1:C:465:LEU:O	2.21	0.41
1:C:104:LEU:HD23	1:C:104:LEU:HA	1.89	0.41
1:D:331:LEU:HD23	1:D:344:GLU:HB3	2.02	0.41
1:B:416:ALA:HB2	1:B:512:LEU:HD11	2.03	0.41
1:D:75:ASN:HA	1:D:113:ASP:HB3	2.02	0.41
1:B:74:LEU:HD21	1:B:88:ILE:HG13	2.02	0.41
1:D:393:GLN:O	1:D:397:GLU:HG3	2.20	0.41
1:B:417:VAL:HG21	1:B:444:TYR:HB2	2.03	0.40
1:C:115:LYS:HD3	1:C:224:LYS:HD2	2.03	0.40
1:D:288:ASP:O	1:D:323:PRO:HD2	2.22	0.40
1:C:103:ILE:HD13	1:C:492:PHE:HE1	1.86	0.40
1:D:440:GLN:O	1:D:443:ARG:HG2	2.20	0.40
1:C:175:TYR:HB3	1:C:179:GLY:HA2	2.04	0.40
1:C:297:LEU:O	1:C:301:ILE:HG12	2.21	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)
1:A:404:ILE:CB	1:B:422:LYS:O[3_654]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ILE:CA	1:B:422:LYS:O[3_654]	2.15	0.05

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	507/550 (92%)	493 (97%)	14 (3%)	0	100	100
1	B	511/550 (93%)	496 (97%)	15 (3%)	0	100	100
1	C	514/550 (94%)	501 (98%)	12 (2%)	1 (0%)	43	55
1	D	494/550 (90%)	480 (97%)	14 (3%)	0	100	100
All	All	2026/2200 (92%)	1970 (97%)	55 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	481	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	404/452 (89%)	391 (97%)	13 (3%)	34	51
1	B	402/452 (89%)	392 (98%)	10 (2%)	42	60
1	C	403/452 (89%)	395 (98%)	8 (2%)	48	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	352/452 (78%)	344 (98%)	8 (2%)	44 63
All	All	1561/1808 (86%)	1522 (98%)	39 (2%)	42 60

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	MET
1	A	97	SER
1	A	163	ASN
1	A	187	GLN
1	A	193	LEU
1	A	195	THR
1	A	202	SER
1	A	223	GLU
1	A	258	LEU
1	A	261	LYS
1	A	401	LEU
1	A	405	THR
1	A	424	CYS
1	B	14	GLN
1	B	167	VAL
1	B	194	VAL
1	B	202	SER
1	B	272	GLU
1	B	404	ILE
1	B	409	THR
1	B	430	VAL
1	B	510	ILE
1	B	524	THR
1	C	156	ILE
1	C	202	SER
1	C	258	LEU
1	C	272	GLU
1	C	330	MET
1	C	341	THR
1	C	346	SER
1	C	488	LEU
1	D	18	LEU
1	D	164	ILE
1	D	172	SER
1	D	203	LEU
1	D	221	VAL

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Mol	Chain	Res	Type
1	D	272	GLU
1	D	437	SER
1	D	510	ILE

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	378	GLN
1	A	440	GLN
1	A	458	GLN
1	B	14	GLN
1	B	199	ASN
1	B	458	GLN
1	C	44	ASN
1	C	78	HIS
1	C	227	GLN
1	C	391	HIS
1	D	14	GLN
1	D	378	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	604	-	5,5,5	0.39	0	5,5,5	1.28	0
4	GOL	C	605	-	5,5,5	0.90	0	5,5,5	1.21	1 (20%)
2	OXL	B	601	3	5,5,5	1.44	0	6,6,6	2.68	4 (66%)
5	FBP	B	606	-	4,4,20	2.07	1 (25%)	6,6,32	0.44	0
4	GOL	B	605	-	5,5,5	0.81	0	5,5,5	1.37	1 (20%)
2	OXL	C	601	3	5,5,5	1.43	0	6,6,6	3.07	4 (66%)
5	FBP	A	605	-	7,7,20	1.72	2 (28%)	9,9,32	0.89	1 (11%)
4	GOL	C	604	-	5,5,5	1.30	0	5,5,5	0.80	0
5	FBP	C	606	-	4,4,20	3.33	1 (25%)	6,6,32	0.63	0
4	GOL	A	603	-	5,5,5	0.67	0	5,5,5	1.16	0
4	GOL	D	605	-	5,5,5	0.96	0	5,5,5	1.04	0
4	GOL	C	603	-	5,5,5	1.17	0	5,5,5	1.02	0
5	FBP	D	606	-	6,6,20	1.03	0	7,8,32	0.89	0
4	GOL	B	603	-	5,5,5	0.53	0	5,5,5	1.53	1 (20%)
2	OXL	A	601	3	5,5,5	1.36	0	6,6,6	2.69	4 (66%)
4	GOL	D	604	-	5,5,5	0.81	0	5,5,5	1.17	0
4	GOL	A	604	-	5,5,5	1.21	1 (20%)	5,5,5	1.08	0
4	GOL	D	603	-	5,5,5	1.00	0	5,5,5	1.11	0
2	OXL	D	601	3	5,5,5	1.30	0	6,6,6	2.64	4 (66%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	603	-	-	3/4/4/4	-
4	GOL	B	604	-	-	3/4/4/4	-
4	GOL	B	605	-	-	0/4/4/4	-
4	GOL	C	605	-	-	2/4/4/4	-
4	GOL	D	605	-	-	2/4/4/4	-
2	OXL	C	601	3	-	4/4/4/4	-
2	OXL	B	601	3	-	4/4/4/4	-
5	FBP	A	605	-	-	1/5/5/32	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	603	-	-	4/4/4/4	-
4	GOL	A	604	-	-	4/4/4/4	-
4	GOL	D	603	-	-	0/4/4/4	-
5	FBP	D	606	-	-	2/4/4/32	-
4	GOL	B	603	-	-	1/4/4/4	-
4	GOL	C	604	-	-	4/4/4/4	-
2	OXL	A	601	3	-	4/4/4/4	-
4	GOL	D	604	-	-	4/4/4/4	-
2	OXL	D	601	3	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	606	FBP	P2-O4P	6.47	1.65	1.50
5	B	606	FBP	P2-O6	3.91	1.66	1.54
5	A	605	FBP	O5-C5	3.89	1.61	1.42
4	A	604	GOL	C3-C2	2.39	1.60	1.51
5	A	605	FBP	P2-O6	2.14	1.67	1.60

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	OXL	O4-C2-C1	5.13	122.78	112.83
2	A	601	OXL	O4-C2-C1	4.38	121.32	112.83
2	D	601	OXL	O3-C1-C2	4.31	121.19	112.83
2	B	601	OXL	O4-C2-C1	4.25	121.08	112.83
2	C	601	OXL	O3-C1-C2	4.14	120.86	112.83
2	D	601	OXL	O4-C2-C1	3.81	120.22	112.83
2	B	601	OXL	O3-C1-C2	3.80	120.20	112.83
2	A	601	OXL	O3-C1-C2	3.23	119.10	112.83
4	B	603	GOL	C3-C2-C1	-2.81	101.50	111.80
2	C	601	OXL	O3-C1-O1	-2.64	117.61	123.90
2	A	601	OXL	O4-C2-O2	-2.59	117.73	123.90
2	A	601	OXL	O3-C1-O1	-2.43	118.10	123.90
4	B	605	GOL	C3-C2-C1	-2.39	103.04	111.80
2	B	601	OXL	O3-C1-O1	-2.37	118.25	123.90
5	A	605	FBP	O6P-P2-O6	2.35	112.80	106.67
2	C	601	OXL	O4-C2-O2	-2.22	118.60	123.90
2	B	601	OXL	O4-C2-O2	-2.19	118.68	123.90
2	D	601	OXL	O3-C1-O1	-2.15	118.79	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	605	GOL	C3-C2-C1	-2.09	104.15	111.80
2	D	601	OXL	O4-C2-O2	-2.01	119.12	123.90

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	OXL	O1-C1-C2-O2
2	D	601	OXL	O1-C1-C2-O4
2	D	601	OXL	O3-C1-C2-O4
4	A	603	GOL	C1-C2-C3-O3
4	B	604	GOL	O1-C1-C2-C3
4	C	603	GOL	O1-C1-C2-O2
4	C	603	GOL	O1-C1-C2-C3
4	C	604	GOL	O1-C1-C2-C3
4	C	604	GOL	C1-C2-C3-O3
4	C	605	GOL	C1-C2-C3-O3
4	C	605	GOL	O2-C2-C3-O3
4	D	604	GOL	O1-C1-C2-C3
4	D	605	GOL	C1-C2-C3-O3
5	D	606	FBP	C6-O6-P2-O5P
5	D	606	FBP	C6-O6-P2-O6P
2	D	601	OXL	O3-C1-C2-O2
2	A	601	OXL	O1-C1-C2-O2
4	C	604	GOL	O2-C2-C3-O3
4	D	605	GOL	O2-C2-C3-O3
4	A	604	GOL	O1-C1-C2-C3
4	A	604	GOL	C1-C2-C3-O3
4	B	603	GOL	C1-C2-C3-O3
4	C	603	GOL	C1-C2-C3-O3
4	D	604	GOL	C1-C2-C3-O3
4	A	604	GOL	O1-C1-C2-O2
4	B	604	GOL	O1-C1-C2-O2
4	D	604	GOL	O1-C1-C2-O2
4	D	604	GOL	O2-C2-C3-O3
2	A	601	OXL	O3-C1-C2-O4
2	A	601	OXL	O1-C1-C2-O4
2	A	601	OXL	O3-C1-C2-O2
4	A	604	GOL	O2-C2-C3-O3
4	C	604	GOL	O1-C1-C2-O2
2	B	601	OXL	O1-C1-C2-O2
2	B	601	OXL	O3-C1-C2-O4

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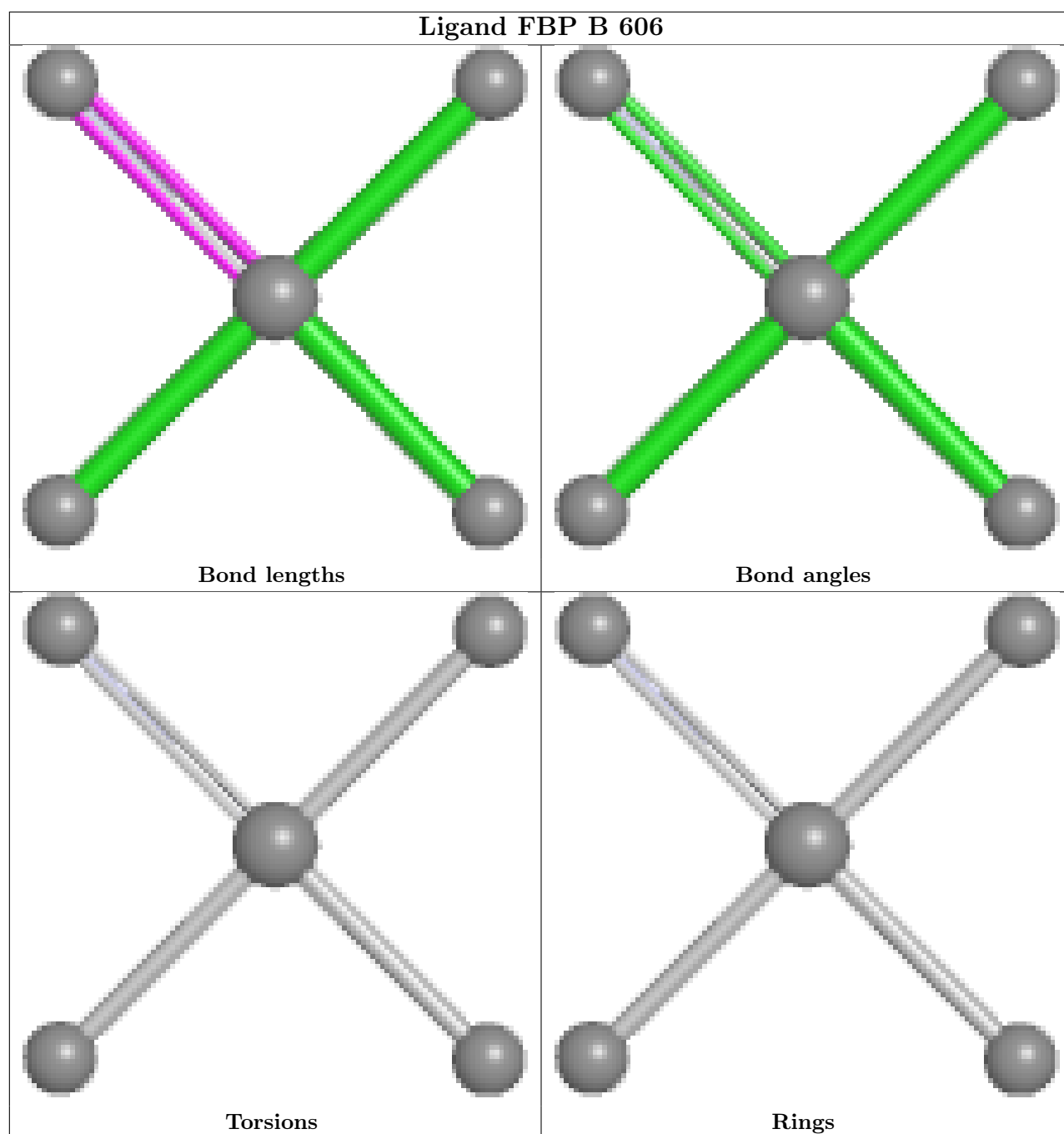
Mol	Chain	Res	Type	Atoms
4	A	603	GOL	O2-C2-C3-O3
4	C	603	GOL	O2-C2-C3-O3
5	A	605	FBP	O5-C5-C6-O6
2	C	601	OXL	O3-C1-C2-O4
2	B	601	OXL	O1-C1-C2-O4
2	C	601	OXL	O1-C1-C2-O2
2	B	601	OXL	O3-C1-C2-O2
4	A	603	GOL	O1-C1-C2-O2
4	B	604	GOL	C1-C2-C3-O3
2	C	601	OXL	O1-C1-C2-O4
2	C	601	OXL	O3-C1-C2-O2

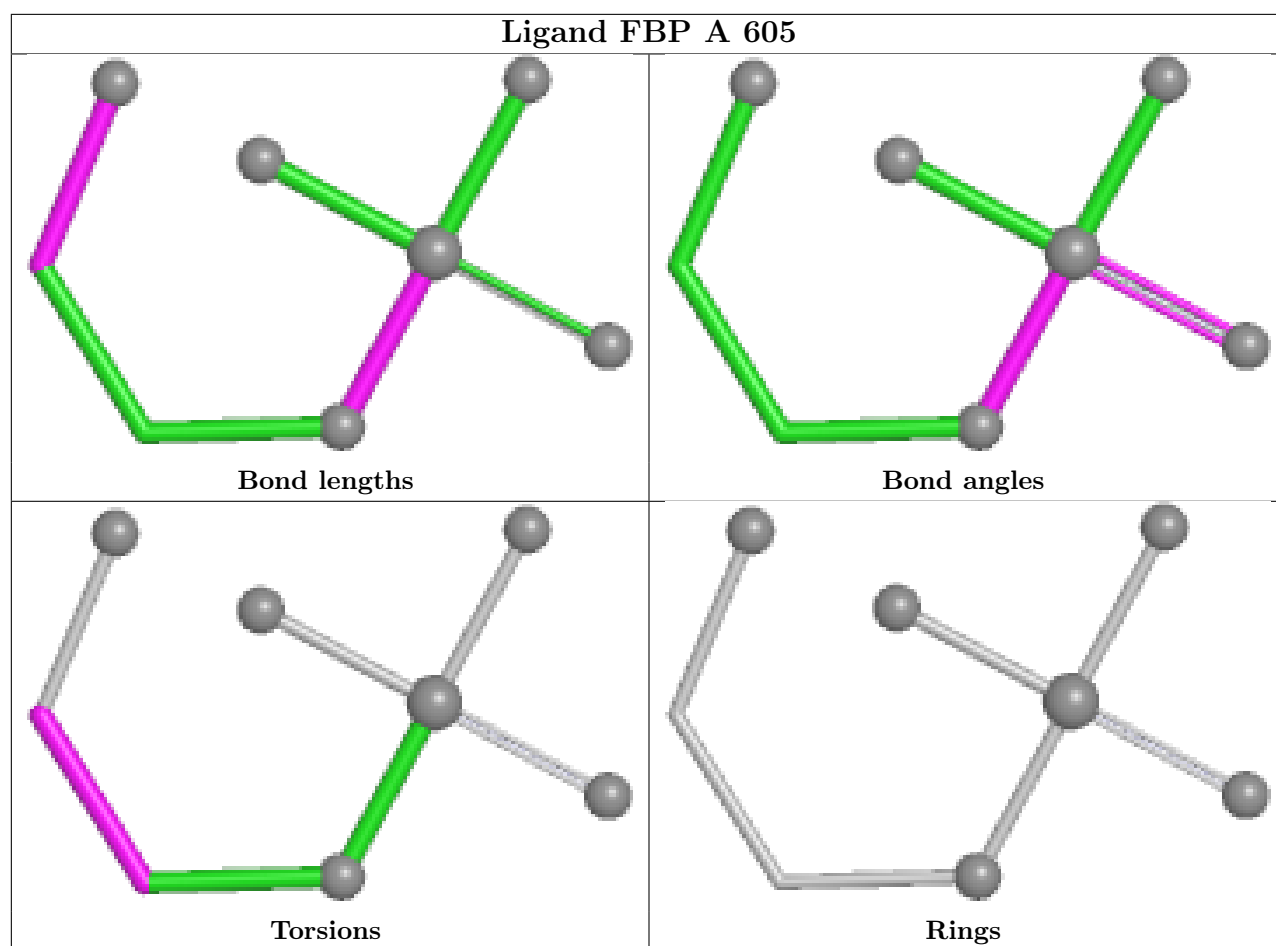
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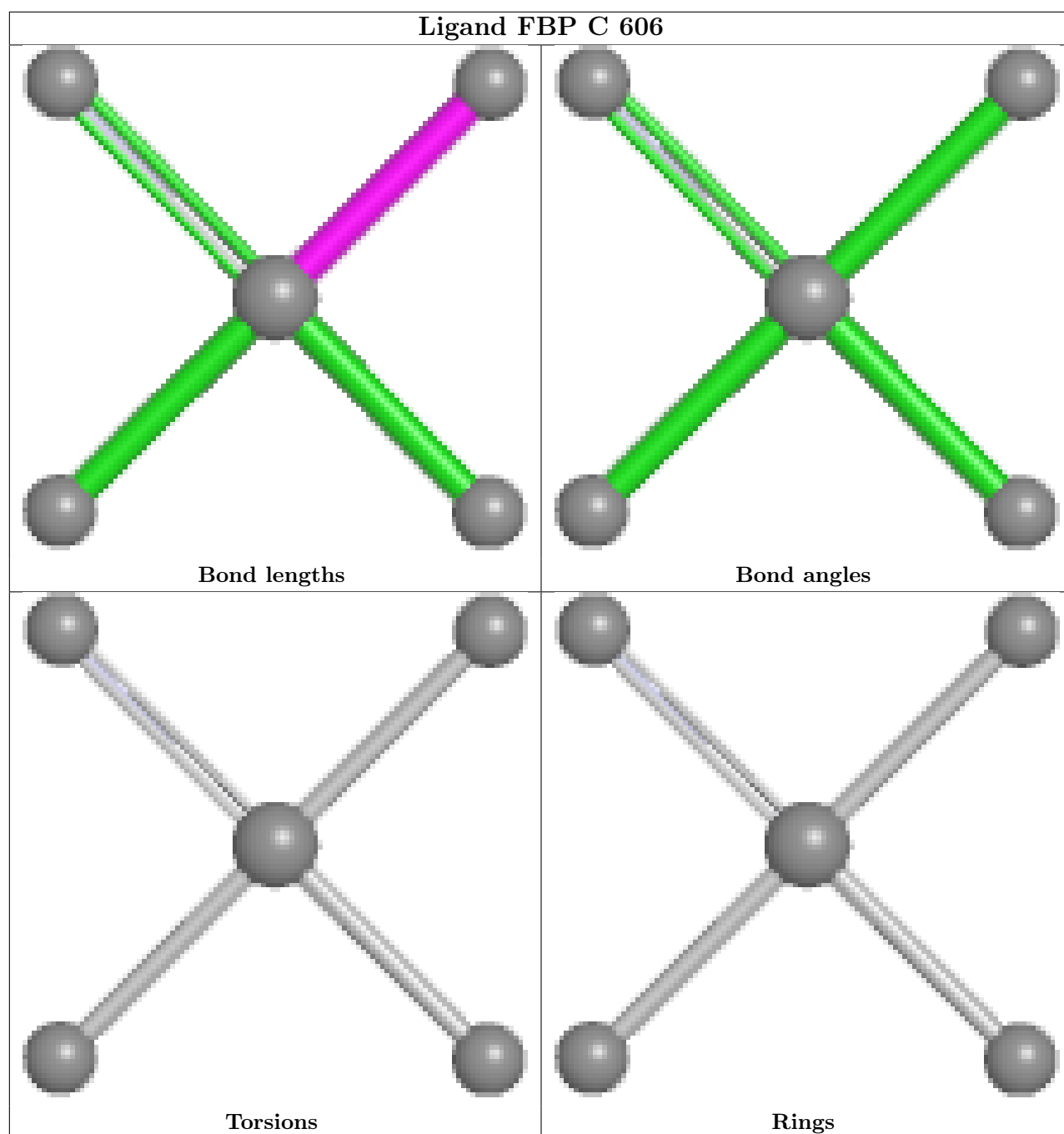
7 monomers are involved in 12 short contacts:

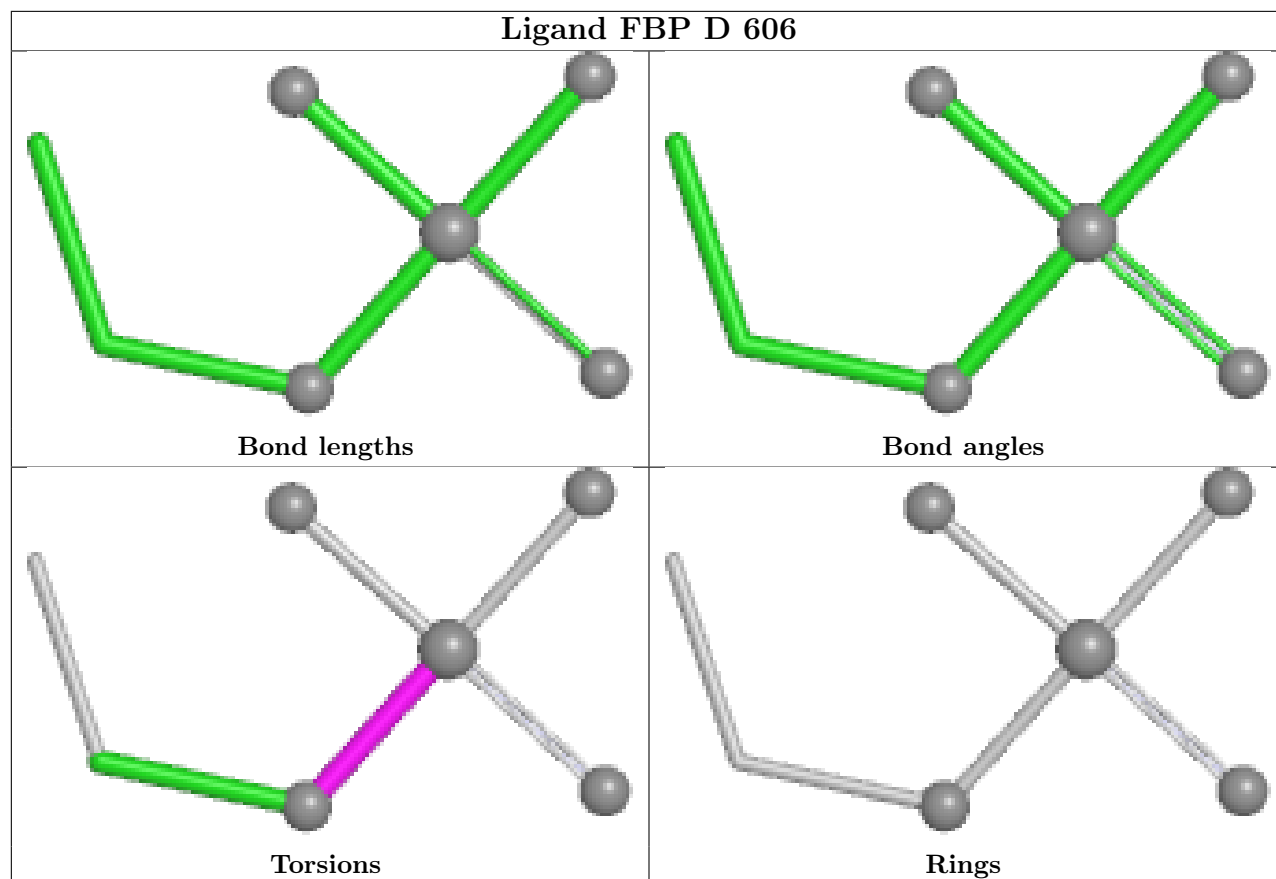
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	604	GOL	2	0
5	B	606	FBP	1	0
4	B	605	GOL	1	0
4	A	603	GOL	1	0
4	C	603	GOL	3	0
5	D	606	FBP	1	0
4	B	603	GOL	3	0

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.









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	515/550 (93%)	-0.15	24 (4%) 36 38	13, 25, 45, 76	0
1	B	515/550 (93%)	-0.11	18 (3%) 47 49	12, 27, 48, 67	0
1	C	518/550 (94%)	-0.12	17 (3%) 49 51	14, 27, 50, 66	0
1	D	504/550 (91%)	0.39	68 (13%) 7 8	14, 32, 70, 89	0
All	All	2052/2200 (93%)	0.00	127 (6%) 26 28	12, 27, 58, 89	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	PRO	8.7
1	A	404	ILE	7.0
1	A	518	GLY	7.0
1	A	192	PHE	6.1
1	D	515	TRP	6.0
1	D	170	VAL	6.0
1	B	13	ILE	5.9
1	C	404	ILE	5.9
1	A	517	PRO	5.8
1	A	405	THR	5.7
1	C	519	SER	5.6
1	D	137	GLY	5.6
1	D	165	CYS	5.5
1	D	124	ILE	5.1
1	C	403	PRO	4.9
1	D	13	ILE	4.9
1	A	516	ARG	4.9
1	D	138	ALA	4.9
1	D	153	ASP	4.9
1	A	13	ILE	4.7
1	D	171	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	404	ILE	4.4
1	A	129	THR	4.4
1	D	520	GLY	4.4
1	D	157	LEU	4.3
1	D	194	VAL	4.3
1	D	403	PRO	4.2
1	A	193	LEU	4.2
1	D	123	LEU	4.2
1	D	193	LEU	4.2
1	D	152	CYS	4.1
1	A	329	GLN	4.1
1	D	156	ILE	4.1
1	C	520	GLY	4.0
1	D	215	ALA	4.0
1	B	14	GLN	4.0
1	D	195	THR	3.9
1	A	401	LEU	3.9
1	B	403	PRO	3.9
1	D	183	LEU	3.8
1	D	169	GLU	3.8
1	B	201	GLY	3.8
1	A	521	PHE	3.7
1	A	191	ASP	3.7
1	C	517	PRO	3.7
1	D	134	LEU	3.7
1	D	143	THR	3.6
1	D	162	LYS	3.6
1	D	148	TYR	3.6
1	B	200	GLY	3.6
1	C	13	ILE	3.5
1	C	191	ASP	3.5
1	D	516	ARG	3.5
1	D	139	THR	3.5
1	D	406	SER	3.5
1	D	132	VAL	3.4
1	C	515	TRP	3.4
1	D	187	GLN	3.4
1	D	405	THR	3.3
1	D	136	LYS	3.3
1	B	126	GLY	3.3
1	D	186	LYS	3.2
1	A	128	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	174	ILE	3.1
1	D	155	ASN	3.1
1	D	184	GLN	3.1
1	B	127	SER	3.0
1	D	163	ASN	3.0
1	D	150	GLU	3.0
1	B	516	ARG	2.9
1	D	202	SER	2.9
1	B	515	TRP	2.9
1	D	198	GLU	2.9
1	C	488	LEU	2.9
1	D	168	VAL	2.9
1	D	477	PRO	2.8
1	B	404	ILE	2.8
1	C	516	ARG	2.8
1	A	406	SER	2.8
1	B	99	ALA	2.8
1	A	515	TRP	2.8
1	C	521	PHE	2.8
1	C	481	ALA	2.7
1	D	140	LEU	2.7
1	A	130	ALA	2.7
1	B	129	THR	2.7
1	D	173	LYS	2.6
1	D	200	GLY	2.6
1	D	197	VAL	2.6
1	D	181	ILE	2.6
1	B	481	ALA	2.6
1	D	164	ILE	2.6
1	B	402	ALA	2.5
1	C	192	PHE	2.5
1	D	167	VAL	2.5
1	A	126	GLY	2.5
1	D	521	PHE	2.5
1	D	178	ASP	2.5
1	A	201	GLY	2.5
1	C	480	GLU	2.4
1	D	196	GLU	2.4
1	D	172	SER	2.4
1	D	158	TRP	2.4
1	C	190	ALA	2.4
1	D	142	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	203	LEU	2.4
1	B	128	GLY	2.3
1	D	214	ALA	2.3
1	A	400	ARG	2.3
1	B	405	THR	2.3
1	D	131	GLU	2.3
1	D	216	VAL	2.3
1	D	204	GLY	2.3
1	C	213	GLY	2.2
1	D	185	VAL	2.2
1	D	133	GLU	2.2
1	A	189	GLY	2.2
1	D	208	GLY	2.2
1	D	401	LEU	2.1
1	D	135	LYS	2.1
1	A	477	PRO	2.1
1	B	199	ASN	2.1
1	C	477	PRO	2.1
1	D	424	CYS	2.1
1	B	480	GLU	2.1
1	A	178	ASP	2.1
1	D	481	ALA	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(Å ²)	Q<0.9
4	GOL	D	603	6/6	0.76	0.18	27,31,35,36	0

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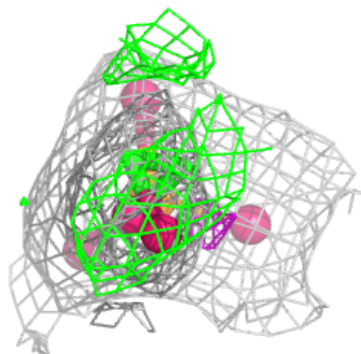
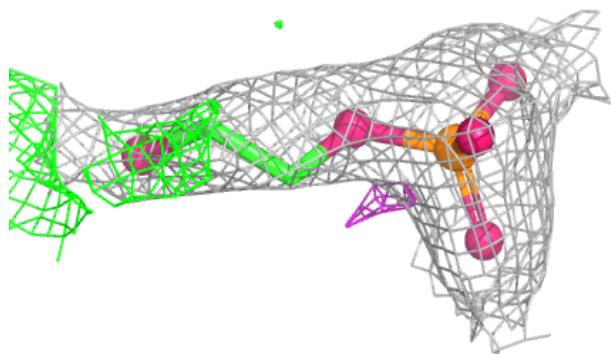
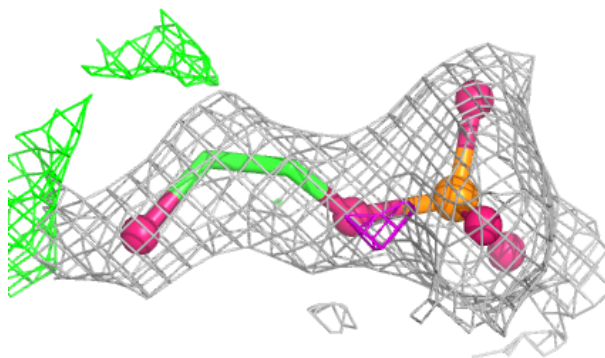
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	C	604	6/6	0.84	0.14	38,39,43,44	0
5	FBP	A	605	8/20	0.84	0.16	27,33,39,43	8
5	FBP	D	606	7/20	0.85	0.17	33,44,48,51	7
4	GOL	B	604	6/6	0.86	0.18	26,27,30,30	0
4	GOL	C	603	6/6	0.87	0.18	27,31,34,34	0
4	GOL	A	603	6/6	0.88	0.14	24,28,34,41	0
4	GOL	B	603	6/6	0.88	0.14	24,29,31,38	0
4	GOL	D	604	6/6	0.89	0.12	33,38,40,50	0
4	GOL	B	605	6/6	0.90	0.18	35,39,42,42	0
4	GOL	D	605	6/6	0.91	0.15	40,40,44,46	0
5	FBP	C	606	5/20	0.92	0.09	32,32,43,44	5
4	GOL	A	604	6/6	0.92	0.15	29,31,34,35	0
3	MG	D	602	1/1	0.93	0.08	35,35,35,35	0
2	OXL	B	601	6/6	0.94	0.08	21,22,30,31	0
2	OXL	D	601	6/6	0.94	0.08	25,31,35,42	0
4	GOL	C	605	6/6	0.94	0.08	23,34,36,40	0
5	FBP	B	606	5/20	0.95	0.07	24,29,37,41	5
2	OXL	C	601	6/6	0.96	0.09	21,23,29,36	0
2	OXL	A	601	6/6	0.96	0.07	22,24,32,33	0
3	MG	C	602	1/1	0.98	0.03	19,19,19,19	0
3	MG	B	602	1/1	0.99	0.02	24,24,24,24	0
3	MG	A	602	1/1	0.99	0.03	23,23,23,23	0

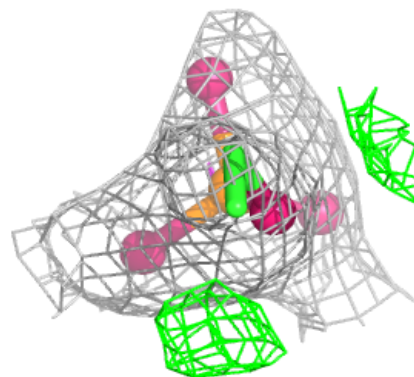
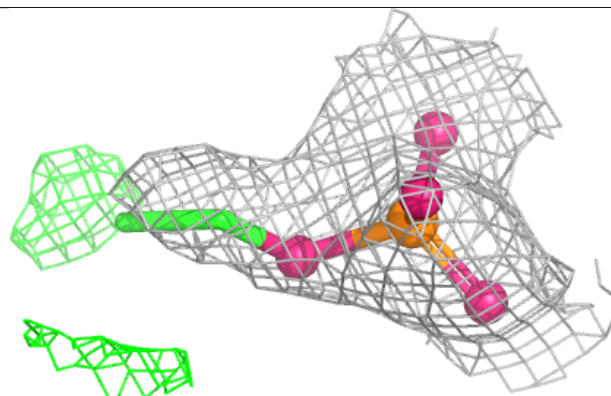
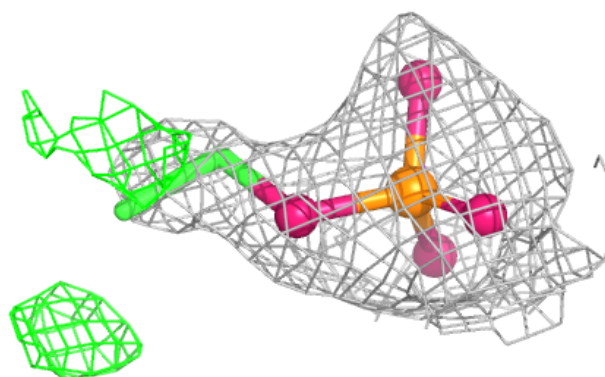
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP A 605:

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

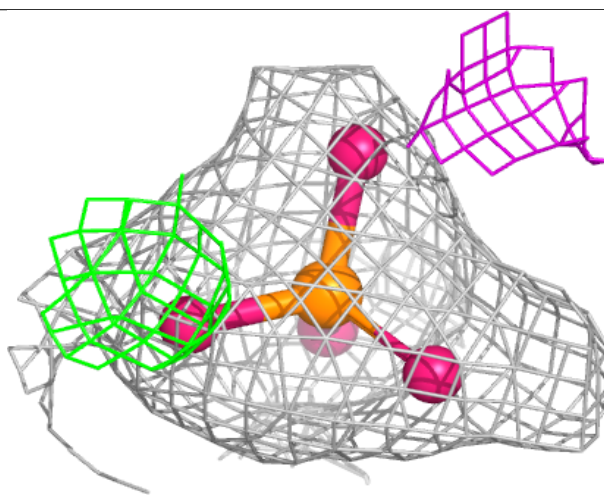
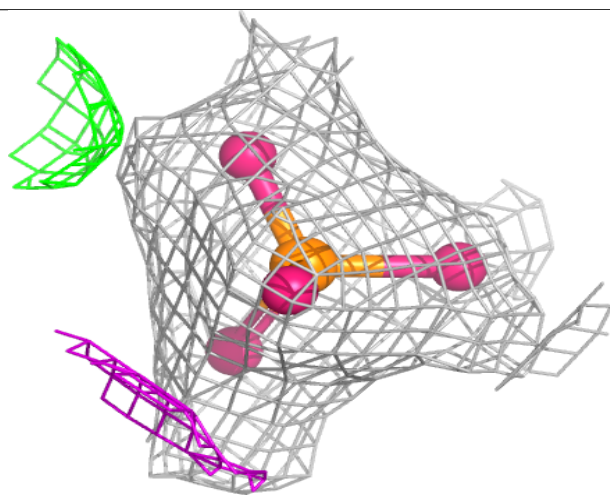
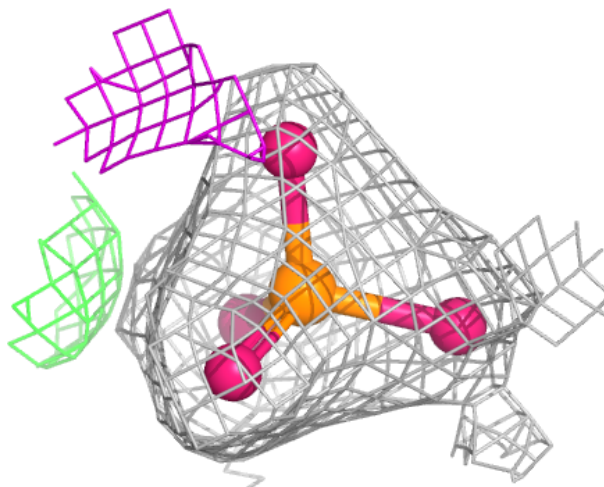
**Electron density around FBP D 606:**

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



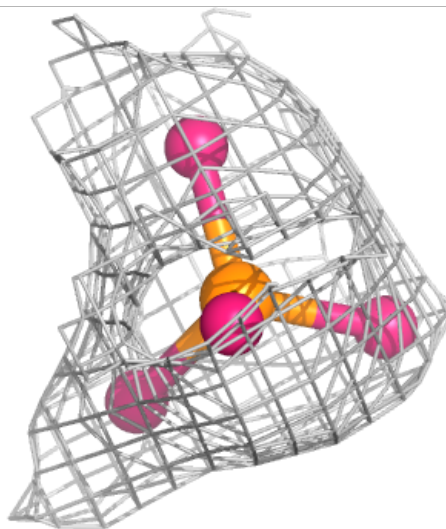
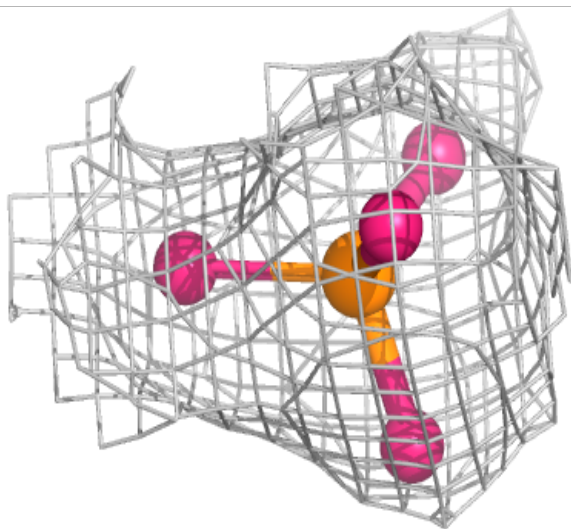
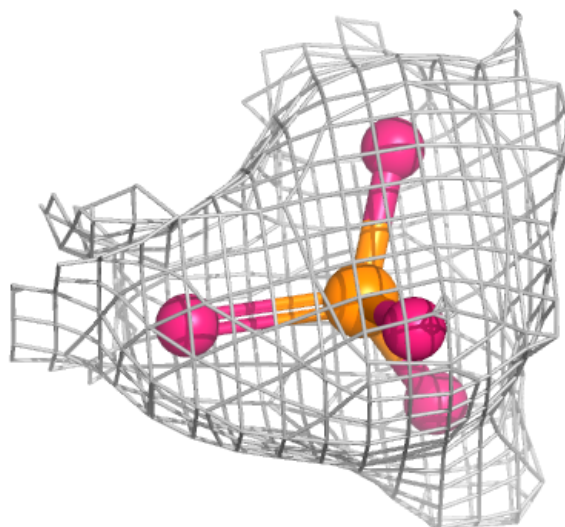
Electron density around FBP C 606:

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



Electron density around FBP B 606:

$2mF_o-DF_c$ (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.