



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:22 PM UTC

PDB ID : 4B2D / pdb_00004b2d
Title : human PKM2 with L-serine and FBP bound.
Authors : Chaneton, B.; Hillmann, P.; Zheng, L.; Martin, A.C.L.; Maddocks, O.D.K.; Chokkathukalam, A.; Coyle, J.E.; Jankevics, A.; Holding, F.P.; Vousden, K.H.; Frezza, C.; O'Reilly, M.; Gottlieb, E.
Deposited on : 2012-07-13
Resolution : 2.30 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

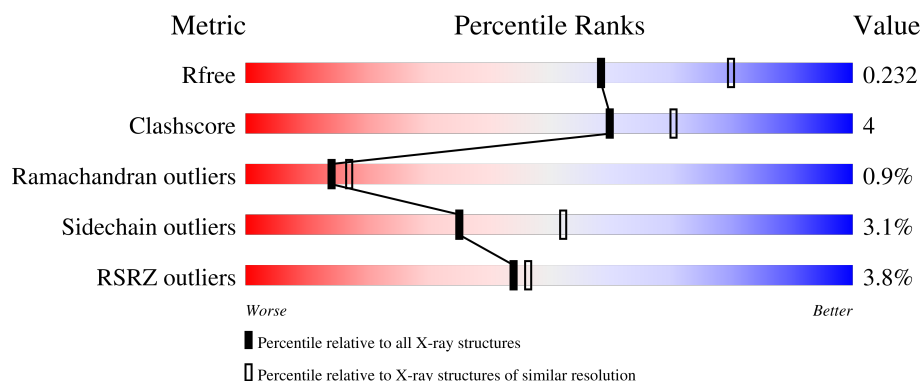
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	548	0% 81% 12% 5%
1	B	548	5% 80% 13% 6%
1	C	548	0% 82% 12% 5%
2	D	548	6% 80% 12% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16980 atoms, of which 28 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 M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3906	2453	695	733	25			
1	B	514	Total	C	N	O	S	0	1	0
			3872	2436	691	721	24			
1	C	518	Total	C	N	O	S	0	0	0
			3907	2460	695	728	24			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	expression tag	UNP P14618
A	-15	GLY	-	expression tag	UNP P14618
A	-14	SER	-	expression tag	UNP P14618
A	-13	SER	-	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	HIS	-	expression tag	UNP P14618
A	-7	HIS	-	expression tag	UNP P14618
A	-6	SER	-	expression tag	UNP P14618
A	-5	SER	-	expression tag	UNP P14618
A	-4	GLY	-	expression tag	UNP P14618
A	-3	LEU	-	expression tag	UNP P14618
A	-2	VAL	-	expression tag	UNP P14618
A	-1	PRO	-	expression tag	UNP P14618
A	0	ARG	-	expression tag	UNP P14618
A	1	GLY	-	expression tag	UNP P14618
B	-16	MET	-	expression tag	UNP P14618
B	-15	GLY	-	expression tag	UNP P14618
B	-14	SER	-	expression tag	UNP P14618
B	-13	SER	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	HIS	-	expression tag	UNP P14618
B	-8	HIS	-	expression tag	UNP P14618
B	-7	HIS	-	expression tag	UNP P14618
B	-6	SER	-	expression tag	UNP P14618
B	-5	SER	-	expression tag	UNP P14618
B	-4	GLY	-	expression tag	UNP P14618
B	-3	LEU	-	expression tag	UNP P14618
B	-2	VAL	-	expression tag	UNP P14618
B	-1	PRO	-	expression tag	UNP P14618
B	0	ARG	-	expression tag	UNP P14618
B	1	GLY	-	expression tag	UNP P14618
C	-16	MET	-	expression tag	UNP P14618
C	-15	GLY	-	expression tag	UNP P14618
C	-14	SER	-	expression tag	UNP P14618
C	-13	SER	-	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	HIS	-	expression tag	UNP P14618
C	-7	HIS	-	expression tag	UNP P14618
C	-6	SER	-	expression tag	UNP P14618
C	-5	SER	-	expression tag	UNP P14618
C	-4	GLY	-	expression tag	UNP P14618
C	-3	LEU	-	expression tag	UNP P14618
C	-2	VAL	-	expression tag	UNP P14618
C	-1	PRO	-	expression tag	UNP P14618
C	0	ARG	-	expression tag	UNP P14618
C	1	GLY	-	expression tag	UNP P14618

- Molecule 2 is a protein called PYRUVATE KINASE ISOZYMES M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	518	Total	C	N	O	S	0	0	0
			3914	2462	692	735	25			

There are 19 discrepancies between the modelled and reference sequences:

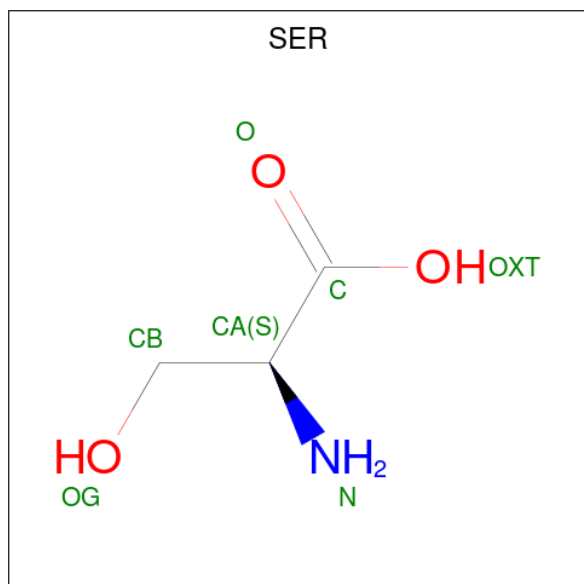
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	MET	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	GLY	-	expression tag	UNP P14618
D	-14	SER	-	expression tag	UNP P14618
D	-13	SER	-	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	HIS	-	expression tag	UNP P14618
D	-7	HIS	-	expression tag	UNP P14618
D	-6	SER	-	expression tag	UNP P14618
D	-5	SER	-	expression tag	UNP P14618
D	-4	GLY	-	expression tag	UNP P14618
D	-3	LEU	-	expression tag	UNP P14618
D	-2	VAL	-	expression tag	UNP P14618
D	-1	PRO	-	expression tag	UNP P14618
D	0	ARG	-	expression tag	UNP P14618
D	1	GLY	-	expression tag	UNP P14618
D	142	LEU	ILE	conflict	UNP P14618

- Molecule 3 is SERINE (CCD ID: SER) (formula: $C_3H_7NO_3$).



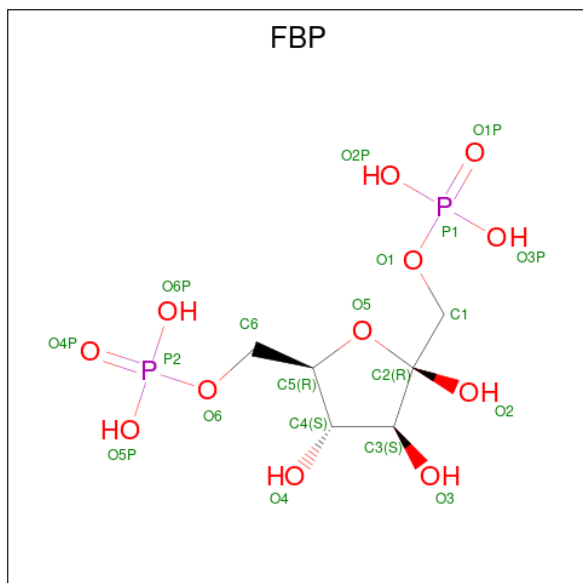
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			14	3	7	1	3		
3	B	1	Total	C	H	N	O	0	0
			14	3	7	1	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	0	0
			14	3	7	1	3		
3	D	1	Total	C	H	N	O	0	0
			14	3	7	1	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

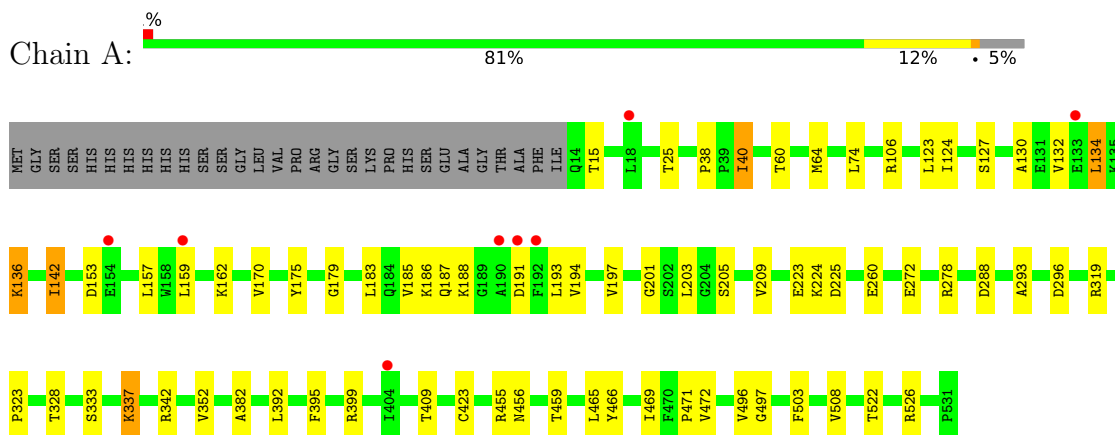
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	395	Total 395	O 395	0	0
6	B	270	Total 270	O 270	0	0
6	C	327	Total 327	O 327	0	0
6	D	251	Total 251	O 251	0	0

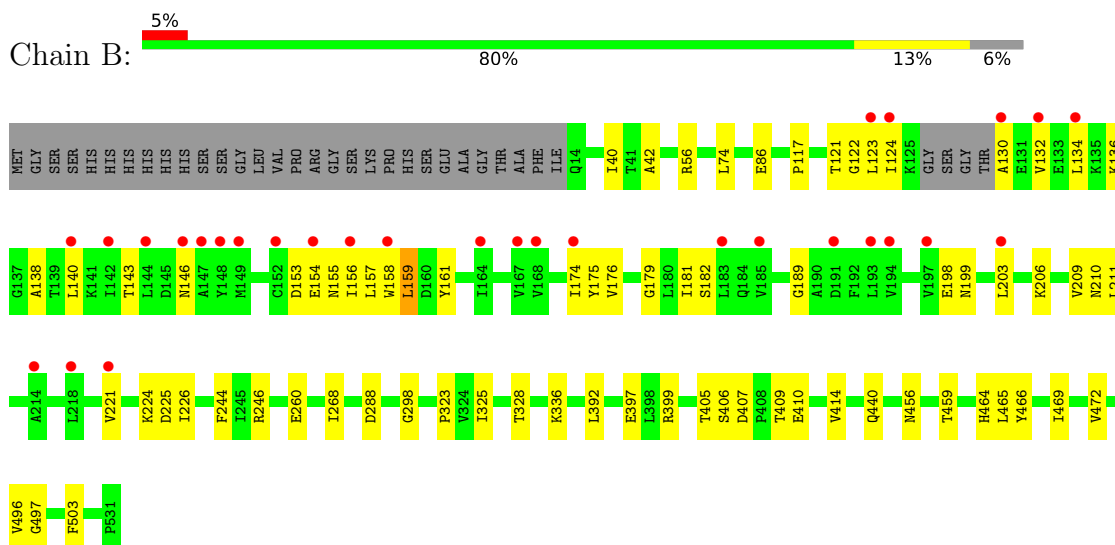
3 Residue-property plots [i](#)

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.

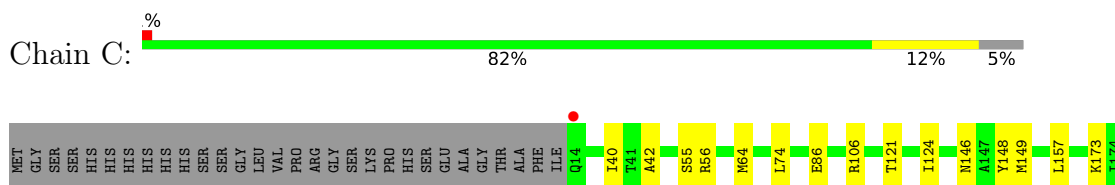
• Molecule 1: PYRUVATE KINASE ISOZYMES M1/M2

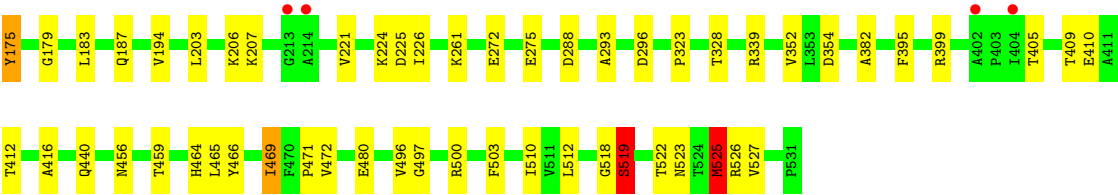


• Molecule 1: PYRUVATE KINASE ISOZYMES M1/M2

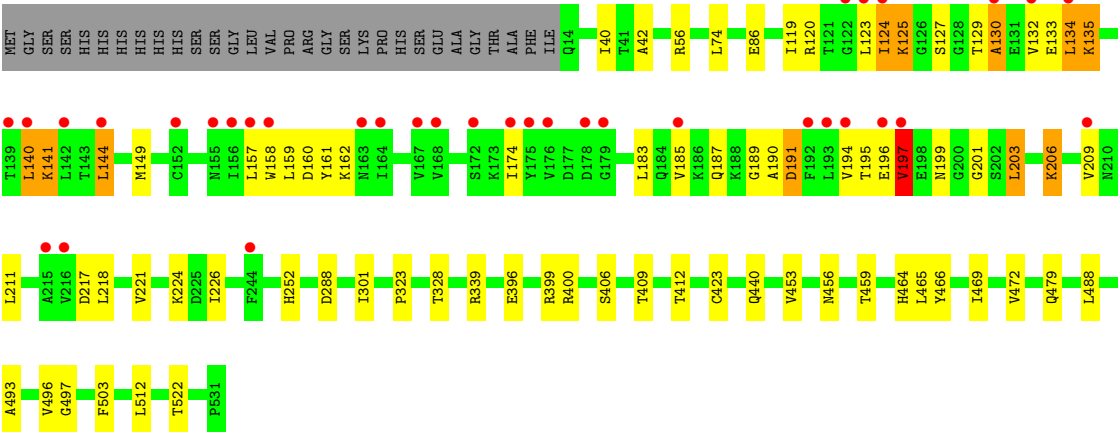
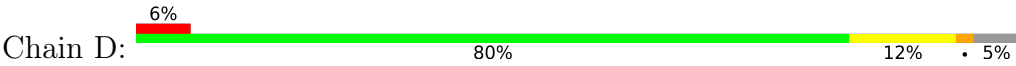


• Molecule 1: PYRUVATE KINASE ISOZYMES M1/M2





● Molecule 2: PYRUVATE KINASE ISOZYMES M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.61Å 151.10Å 91.79Å 90.00° 102.01° 90.00°	Depositor
Resolution (Å)	78.85 – 2.30 78.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (78.85-2.30) 97.9 (78.85-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.173 , 0.226 0.179 , 0.232	Depositor DCC
R_{free} test set	4702 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16980	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: MG, FBP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.98	1/3970 (0.0%)	1.22	6/5370 (0.1%)
1	B	0.98	0/3937	1.24	13/5326 (0.2%)
1	C	0.92	2/3971 (0.1%)	1.19	8/5370 (0.1%)
2	D	0.94	2/3978 (0.1%)	1.23	9/5379 (0.2%)
All	All	0.96	5/15856 (0.0%)	1.22	36/21445 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	525	MET	SD-CE	-7.30	1.61	1.79
2	D	301	ILE	CA-C	6.34	1.57	1.52
1	A	508	VAL	CA-C	-5.10	1.46	1.52
2	D	197	VAL	CA-C	5.05	1.58	1.52
1	C	175	TYR	CA-C	-5.04	1.46	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	134	LEU	CA-C-N	6.77	133.88	121.70
2	D	134	LEU	C-N-CA	6.77	133.88	121.70
2	D	183	LEU	N-CA-C	6.65	119.54	109.23
1	A	225	ASP	CA-C-N	6.22	128.40	120.56
1	A	225	ASP	C-N-CA	6.22	128.40	120.56
1	B	123	LEU	N-CA-C	6.16	119.07	109.52
1	C	207	LYS	CA-C-N	6.00	125.67	119.92
1	C	207	LYS	C-N-CA	6.00	125.67	119.92
1	B	260	GLU	CB-CG-CD	5.95	122.72	112.60
1	B	123	LEU	CA-C-N	5.90	128.56	122.96
1	B	123	LEU	C-N-CA	5.90	128.56	122.96
1	B	189	GLY	CA-C-N	5.83	132.19	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	GLY	C-N-CA	5.83	132.19	121.70
1	C	480	GLU	CB-CG-CD	5.77	122.41	112.60
1	B	225	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	414	VAL	CA-C-N	5.68	126.28	119.98
1	B	414	VAL	C-N-CA	5.68	126.28	119.98
1	B	161	TYR	CA-C-N	5.56	127.66	120.44
1	B	161	TYR	C-N-CA	5.56	127.66	120.44
1	C	148	TYR	CA-C-N	5.47	127.93	120.54
1	C	148	TYR	C-N-CA	5.47	127.93	120.54
1	C	469	ILE	N-CA-CB	5.44	117.69	111.39
2	D	140	LEU	CA-C-N	5.41	131.44	121.70
2	D	140	LEU	C-N-CA	5.41	131.44	121.70
1	C	354	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	337	LYS	CG-CD-CE	5.28	123.44	111.30
1	A	260	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	124	ILE	N-CA-CB	5.22	117.05	111.46
1	C	225	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	156	ILE	N-CA-C	5.13	115.66	108.17
2	D	130	ALA	CA-C-N	5.08	128.88	121.31
2	D	130	ALA	C-N-CA	5.08	128.88	121.31
1	A	153	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	153	ASP	CA-CB-CG	5.05	117.65	112.60
2	D	196	GLU	CA-C-N	5.02	129.09	122.51
2	D	196	GLU	C-N-CA	5.02	129.09	122.51

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	3906	0	3924	34	0
1	B	3872	0	3889	35	0
1	C	3907	0	3944	34	0
2	D	3914	0	3946	39	0
3	A	7	7	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	7	4	1	0
3	C	7	7	4	1	0
3	D	7	7	4	1	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	1	0	0	0	0
5	C	1	0	0	0	0
6	A	395	0	0	1	0
6	B	270	0	0	5	0
6	C	327	0	0	1	0
6	D	251	0	0	2	0
All	All	16952	28	15759	134	0

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 (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLN:HB2	1:A:194:VAL:HB	1.58	0.85
1:C:510:ILE:HG23	1:C:525:MET:HE3	1.61	0.83
1:C:518:GLY:O	1:C:519:SER:HB2	1.79	0.80
2:D:134:LEU:HA	2:D:135:LYS:HB2	1.65	0.76
1:A:106:ARG:NH2	1:A:471:PRO:O	2.18	0.75
1:C:464:HIS:HD1	3:C:1532:SER:N	1.88	0.71
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.71	0.70
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.74	0.70
1:C:410:GLU:HG2	1:C:440:GLN:HE21	1.57	0.69
1:C:187:GLN:HB3	1:C:194:VAL:HB	1.74	0.67
2:D:140:LEU:HD13	2:D:197:VAL:HG21	1.79	0.65
1:B:410:GLU:HG3	1:B:440:GLN:HE21	1.60	0.65
2:D:464:HIS:HD1	3:D:1532:SER:N	1.96	0.64
1:B:440:GLN:HG2	6:B:2211:HOH:O	1.98	0.63
1:C:146:ASN:O	1:C:149:MET:HB2	1.99	0.62
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.82	0.61
2:D:124:ILE:HD13	2:D:130:ALA:HB3	1.83	0.60
1:B:336:LYS:HG2	6:B:2186:HOH:O	2.01	0.59
2:D:56:ARG:NH2	2:D:86:GLU:HB3	2.19	0.58
1:A:319:ARG:HD2	6:B:2016:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:GLY:HA3	6:B:2097:HOH:O	2.03	0.57
1:B:121:THR:HB	1:B:157:LEU:HD11	1.86	0.57
1:A:142:ILE:HA	1:A:157:LEU:O	2.04	0.57
1:C:55:SER:HB2	1:C:64:MET:HE2	1.87	0.57
1:B:464:HIS:HD1	3:B:1532:SER:N	2.02	0.56
1:B:134:LEU:CD1	1:B:181:ILE:HG12	2.36	0.56
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.86	0.56
1:B:175:TYR:HB2	1:B:210:ASN:HB2	1.88	0.56
2:D:174:ILE:HG23	2:D:209:VAL:HG22	1.87	0.56
2:D:125:LYS:HA	2:D:129:THR:HG22	1.88	0.55
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.88	0.54
2:D:141:LYS:HB2	2:D:195:THR:HG21	1.89	0.54
2:D:409:THR:HG23	2:D:522:THR:HB	1.89	0.54
1:B:56:ARG:NH2	1:B:86:GLU:HB3	2.21	0.54
2:D:412:THR:HG22	2:D:512:LEU:HD22	1.90	0.54
2:D:409:THR:HG21	2:D:440:GLN:HE22	1.73	0.53
1:B:410:GLU:HG2	6:B:2229:HOH:O	2.07	0.53
2:D:174:ILE:HD12	2:D:185:VAL:HG21	1.91	0.53
2:D:409:THR:CG2	2:D:440:GLN:NE2	2.72	0.53
2:D:149:MET:HE2	2:D:158:TRP:HE1	1.75	0.52
2:D:466:TYR:HB2	2:D:469:ILE:HD12	1.91	0.52
2:D:472:VAL:HG11	2:D:496:VAL:HG11	1.92	0.52
1:C:395:PHE:CE2	1:C:399:ARG:HD2	2.45	0.52
1:C:412:THR:HG22	1:C:512:LEU:HD22	1.92	0.52
1:B:288:ASP:O	1:B:323:PRO:HD2	2.10	0.52
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.92	0.51
1:B:407:ASP:OD1	1:B:409[B]:THR:OG1	2.23	0.51
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.92	0.51
2:D:409:THR:CG2	2:D:440:GLN:HE22	2.23	0.51
1:B:399:ARG:HH12	2:D:399:ARG:CD	2.23	0.51
1:A:132:VAL:HG23	1:A:203:LEU:HB3	1.92	0.50
1:A:423:CYS:HA	1:C:405:THR:O	2.11	0.50
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.46	0.50
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.47	0.50
1:C:121:THR:O	1:C:206:LYS:HA	2.12	0.49
1:A:123:LEU:HA	1:A:205:SER:HB3	1.93	0.49
2:D:120:ARG:HD2	2:D:206:LYS:HB3	1.94	0.49
2:D:288:ASP:O	2:D:323:PRO:HD2	2.12	0.49
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.94	0.49
1:C:352:VAL:HG21	1:C:382:ALA:HA	1.95	0.49
1:A:409:THR:HG23	1:A:522:THR:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ARG:HE	1:B:298:GLY:HA3	1.78	0.48
1:A:60:THR:O	1:A:64:MET:HG2	2.14	0.48
2:D:497:GLY:HA3	2:D:503:PHE:CZ	2.48	0.48
1:B:182:SER:HB3	1:B:198:GLU:HB2	1.96	0.48
1:C:272:GLU:HB3	1:C:293:ALA:HB3	1.95	0.48
1:A:288:ASP:O	1:A:323:PRO:HD2	2.13	0.47
1:A:395:PHE:CE2	1:A:399:ARG:HD2	2.48	0.47
1:B:134:LEU:HD13	1:B:181:ILE:HG12	1.95	0.47
1:A:15:THR:HG22	1:A:38:PRO:HG2	1.95	0.47
1:C:409:THR:HG23	1:C:522:THR:HB	1.97	0.47
1:B:399:ARG:HH21	2:D:396:GLU:HG2	1.79	0.47
1:B:132:VAL:HG22	1:B:203:LEU:HB3	1.97	0.47
1:C:157:LEU:HD13	1:C:203:LEU:HD21	1.96	0.47
2:D:144:LEU:HD12	2:D:187:GLN:HE22	1.80	0.47
1:C:323:PRO:HB3	1:C:465:LEU:O	2.15	0.46
2:D:323:PRO:HB3	2:D:465:LEU:O	2.14	0.46
1:A:456:ASN:HB3	1:A:459:THR:HB	1.98	0.46
1:A:455:ARG:HD2	6:A:2359:HOH:O	2.16	0.46
1:B:176:VAL:HB	1:B:181:ILE:HB	1.98	0.46
2:D:134:LEU:HA	2:D:135:LYS:CB	2.40	0.46
2:D:479:GLN:HG2	2:D:488:LEU:HD22	1.97	0.46
1:A:159:LEU:HD22	1:A:209:VAL:HG21	1.97	0.45
2:D:409:THR:HG22	2:D:440:GLN:NE2	2.31	0.45
1:C:288:ASP:O	1:C:323:PRO:HD2	2.17	0.45
2:D:453:VAL:CG2	2:D:493:ALA:HB2	2.47	0.45
2:D:40:ILE:HD12	2:D:42:ALA:HB3	1.98	0.45
1:A:272:GLU:HB3	1:A:293:ALA:HB3	1.98	0.45
1:B:159:LEU:HD11	1:B:209:VAL:HG21	1.99	0.45
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.99	0.45
2:D:132:VAL:O	2:D:134:LEU:N	2.49	0.45
1:A:188:LYS:HA	1:A:193:LEU:HD23	1.99	0.44
1:B:405:THR:O	2:D:423:CYS:HA	2.17	0.44
2:D:339:ARG:NH1	6:D:2171:HOH:O	2.49	0.44
2:D:456:ASN:HB3	2:D:459:THR:HB	1.98	0.44
1:B:323:PRO:HB3	1:B:465:LEU:O	2.17	0.44
1:A:136:LYS:HD3	1:A:136:LYS:H	1.83	0.44
1:C:272:GLU:HB2	1:C:296:ASP:HB2	1.98	0.44
1:A:526:ARG:HA	1:C:523:ASN:O	2.17	0.44
1:A:127:SER:HB3	1:A:130:ALA:HB2	1.99	0.44
1:B:268:ILE:HG21	1:B:325:ILE:HD12	2.00	0.44
1:C:106:ARG:NH2	1:C:471:PRO:O	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:VAL:HG12	1:C:226:ILE:HG13	1.99	0.44
1:C:526:ARG:HD3	6:C:2320:HOH:O	2.18	0.43
1:C:124:ILE:HD11	1:C:203:LEU:HG	2.00	0.43
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.53	0.43
1:A:323:PRO:HB3	1:A:465:LEU:O	2.19	0.43
1:C:525:MET:HE1	1:C:527:VAL:CG2	2.48	0.43
1:B:456:ASN:HB3	1:B:459:THR:HB	2.01	0.43
1:A:134:LEU:HB2	1:A:201:GLY:O	2.18	0.43
1:B:174:ILE:HG12	1:B:211:LEU:HD22	2.01	0.43
1:C:40:ILE:HD12	1:C:42:ALA:HB3	2.01	0.43
1:B:122:GLY:O	1:B:206:LYS:N	2.51	0.43
1:A:272:GLU:HB2	1:A:296:ASP:HB2	2.01	0.43
1:B:117:PRO:HG3	1:B:246:ARG:NH2	2.34	0.43
1:C:56:ARG:NH2	1:C:86:GLU:HB2	2.34	0.43
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.00	0.42
1:A:134:LEU:HD22	1:A:203:LEU:HB2	2.01	0.42
1:A:25:THR:HB	1:B:397:GLU:CD	2.45	0.42
1:B:40:ILE:HD12	1:B:42:ALA:HB3	2.02	0.42
1:C:456:ASN:HB3	1:C:459:THR:HB	2.01	0.42
2:D:161:TYR:CD1	2:D:218:LEU:HD21	2.54	0.42
2:D:119:ILE:HG12	2:D:161:TYR:HB3	2.01	0.42
2:D:221:VAL:HG12	2:D:226:ILE:HG13	2.01	0.42
1:B:124:ILE:HG21	1:B:130:ALA:HA	2.02	0.41
1:A:352:VAL:HG21	1:A:382:ALA:HA	2.03	0.41
2:D:129:THR:OG1	2:D:203:LEU:HB3	2.21	0.41
1:A:183:LEU:HD23	1:A:197:VAL:HA	2.03	0.40
1:A:399:ARG:HH12	1:C:399:ARG:CZ	2.33	0.40
2:D:252:HIS:HE1	6:D:2127:HOH:O	2.04	0.40
1:A:333:SER:HB2	1:A:337:LYS:HE3	2.04	0.40
1:C:173:LYS:HA	1:C:183:LEU:O	2.22	0.40
1:B:221:VAL:HG12	1:B:226:ILE:HG13	2.03	0.40
2:D:189:GLY:C	2:D:191:ASP:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	516/548 (94%)	499 (97%)	14 (3%)	3 (1%)	21	27
1	B	511/548 (93%)	489 (96%)	16 (3%)	6 (1%)	10	12
1	C	516/548 (94%)	502 (97%)	12 (2%)	2 (0%)	30	38
2	D	516/548 (94%)	461 (89%)	47 (9%)	8 (2%)	7	7
All	All	2059/2192 (94%)	1951 (95%)	89 (4%)	19 (1%)	14	17

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	B	138	ALA
1	C	519	SER
1	B	154	GLU
2	D	135	LYS
1	A	328	THR
1	B	155	ASN
2	D	162	LYS
2	D	190	ALA
2	D	206	LYS
2	D	328	THR
1	B	136	LYS
1	B	328	THR
1	C	328	THR
2	D	133	GLU
1	A	185	VAL
1	B	146	ASN
2	D	127	SER
2	D	201	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	409/450 (91%)	396 (97%)	13 (3%)	34	51
1	B	402/450 (89%)	392 (98%)	10 (2%)	42	60
1	C	408/450 (91%)	400 (98%)	8 (2%)	48	67
2	D	411/450 (91%)	392 (95%)	19 (5%)	24	36
All	All	1630/1800 (91%)	1580 (97%)	50 (3%)	35	52

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	74	LEU
1	A	134	LEU
1	A	136	LYS
1	A	142	ILE
1	A	162	LYS
1	A	170	VAL
1	A	186	LYS
1	A	191	ASP
1	A	223	GLU
1	A	224	LYS
1	A	278	ARG
1	A	392	LEU
1	B	74	LEU
1	B	140	LEU
1	B	143	THR
1	B	158	TRP
1	B	159	LEU
1	B	199	ASN
1	B	224	LYS
1	B	244	PHE
1	B	392	LEU
1	B	406	SER
1	C	74	LEU
1	C	224	LYS
1	C	261	LYS
1	C	275	GLU
1	C	339	ARG
1	C	500	ARG
1	C	519	SER
1	C	525	MET
2	D	74	LEU
2	D	123	LEU

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Mol	Chain	Res	Type
2	D	124	ILE
2	D	125	LYS
2	D	141	LYS
2	D	144	LEU
2	D	157	LEU
2	D	159	LEU
2	D	160	ASP
2	D	191	ASP
2	D	194	VAL
2	D	197	VAL
2	D	199	ASN
2	D	203	LEU
2	D	211	LEU
2	D	217	ASP
2	D	224	LYS
2	D	400	ARG
2	D	406	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	146	ASN
1	A	187	GLN
1	A	199	ASN
1	A	252	HIS
1	A	274	HIS
1	A	458	GLN
1	B	252	HIS
1	B	273	ASN
1	B	440	GLN
1	B	458	GLN
1	C	44	ASN
1	C	199	ASN
1	C	391	HIS
1	C	393	GLN
1	C	440	GLN
1	C	458	GLN
2	D	146	ASN
2	D	187	GLN
2	D	199	ASN
2	D	252	HIS

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Mol	Chain	Res	Type
2	D	391	HIS
2	D	393	GLN
2	D	439	HIS
2	D	440	GLN
2	D	458	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	FBP	B	600	-	18,20,20	1.03	2 (11%)	21,32,32	0.68	0
3	SER	B	1532	-	4,6,6	1.09	0	2,7,7	0.50	0
3	SER	C	1532	-	4,6,6	1.05	0	2,7,7	0.66	0
3	SER	A	1532	-	4,6,6	1.03	0	2,7,7	0.47	0
4	FBP	A	600	-	18,20,20	0.86	0	21,32,32	0.65	0
4	FBP	D	600	-	18,20,20	0.74	0	21,32,32	0.66	0
3	SER	D	1532	-	4,6,6	0.96	0	2,7,7	0.41	0
4	FBP	C	600	-	18,20,20	0.86	1 (5%)	21,32,32	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FBP	B	600	-	-	2/13/32/32	0/1/1/1
3	SER	B	1532	-	-	0/6/6/6	-
3	SER	C	1532	-	-	2/6/6/6	-
3	SER	A	1532	-	-	0/6/6/6	-
4	FBP	A	600	-	-	2/13/32/32	0/1/1/1
4	FBP	D	600	-	-	2/13/32/32	0/1/1/1
3	SER	D	1532	-	-	0/6/6/6	-
4	FBP	C	600	-	-	2/13/32/32	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	FBP	O5-C2	2.90	1.48	1.43
4	C	600	FBP	O5-C2	2.47	1.47	1.43
4	B	600	FBP	O2-C2	2.27	1.44	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

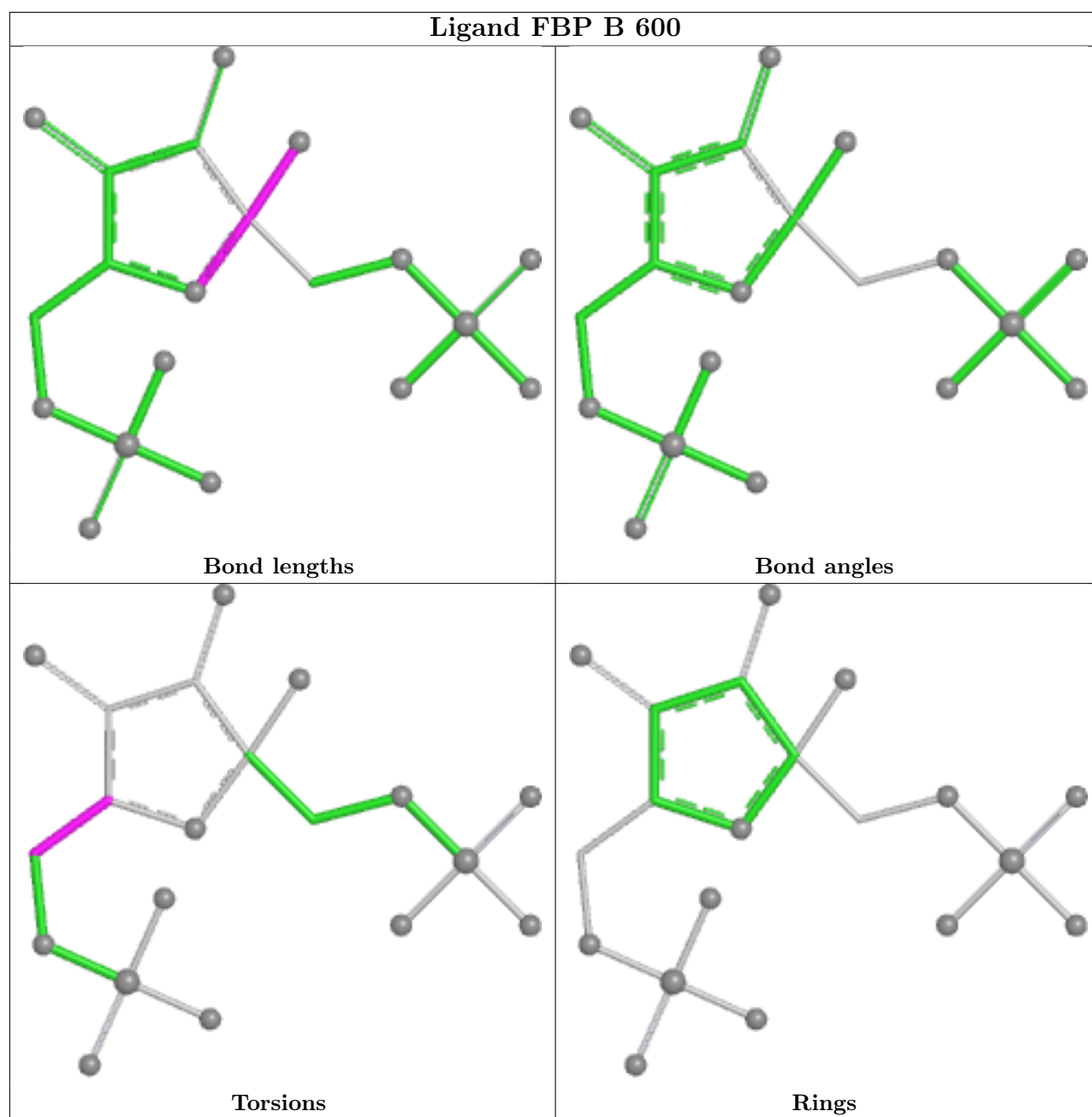
Mol	Chain	Res	Type	Atoms
3	C	1532	SER	N-CA-CB-OG
4	A	600	FBP	C4-C5-C6-O6
4	B	600	FBP	C4-C5-C6-O6
4	C	600	FBP	C4-C5-C6-O6
4	D	600	FBP	C4-C5-C6-O6
4	C	600	FBP	O5-C5-C6-O6
4	B	600	FBP	O5-C5-C6-O6
4	D	600	FBP	O5-C5-C6-O6
4	A	600	FBP	O5-C5-C6-O6
3	C	1532	SER	C-CA-CB-OG

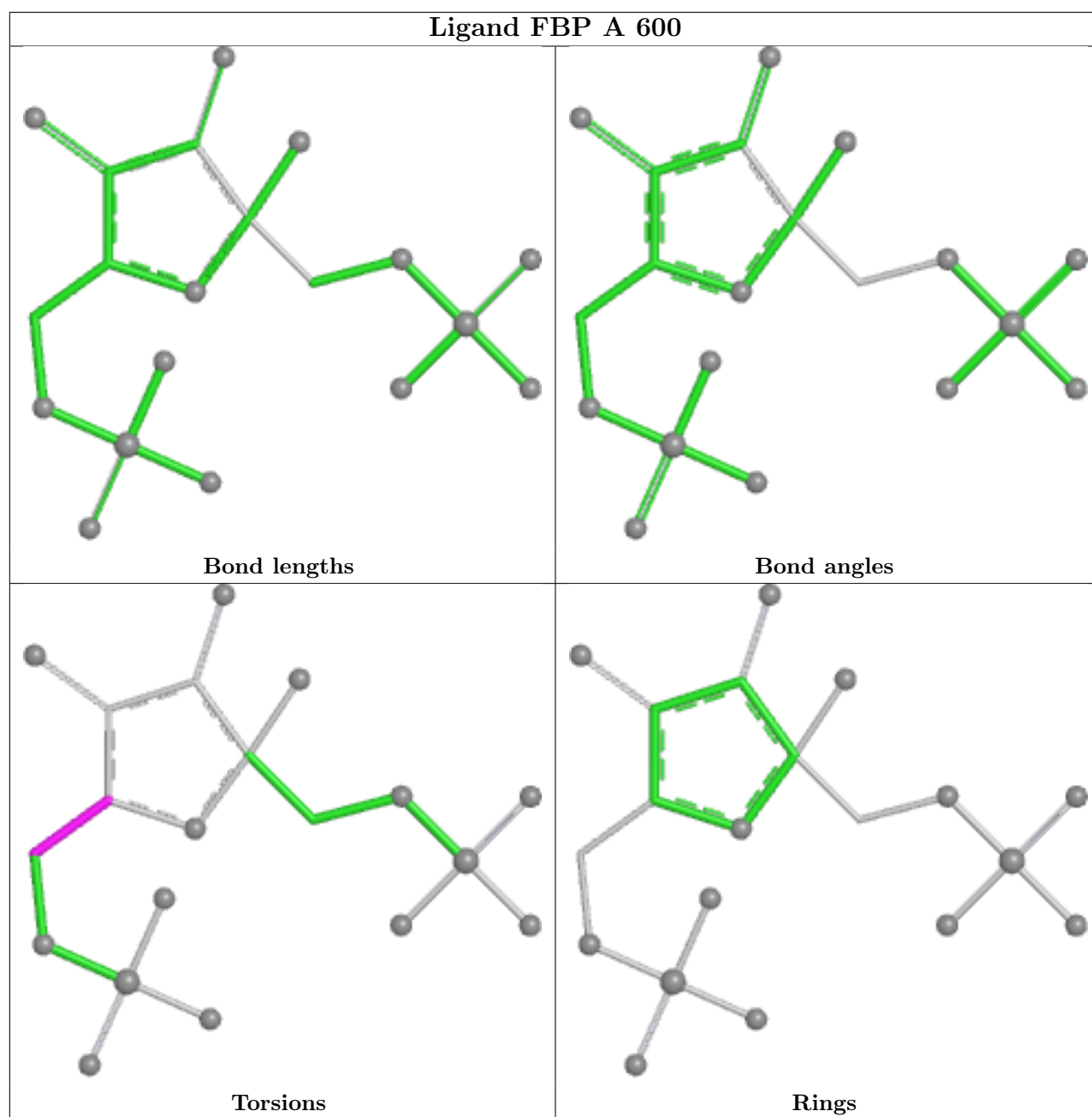
There are no ring outliers.

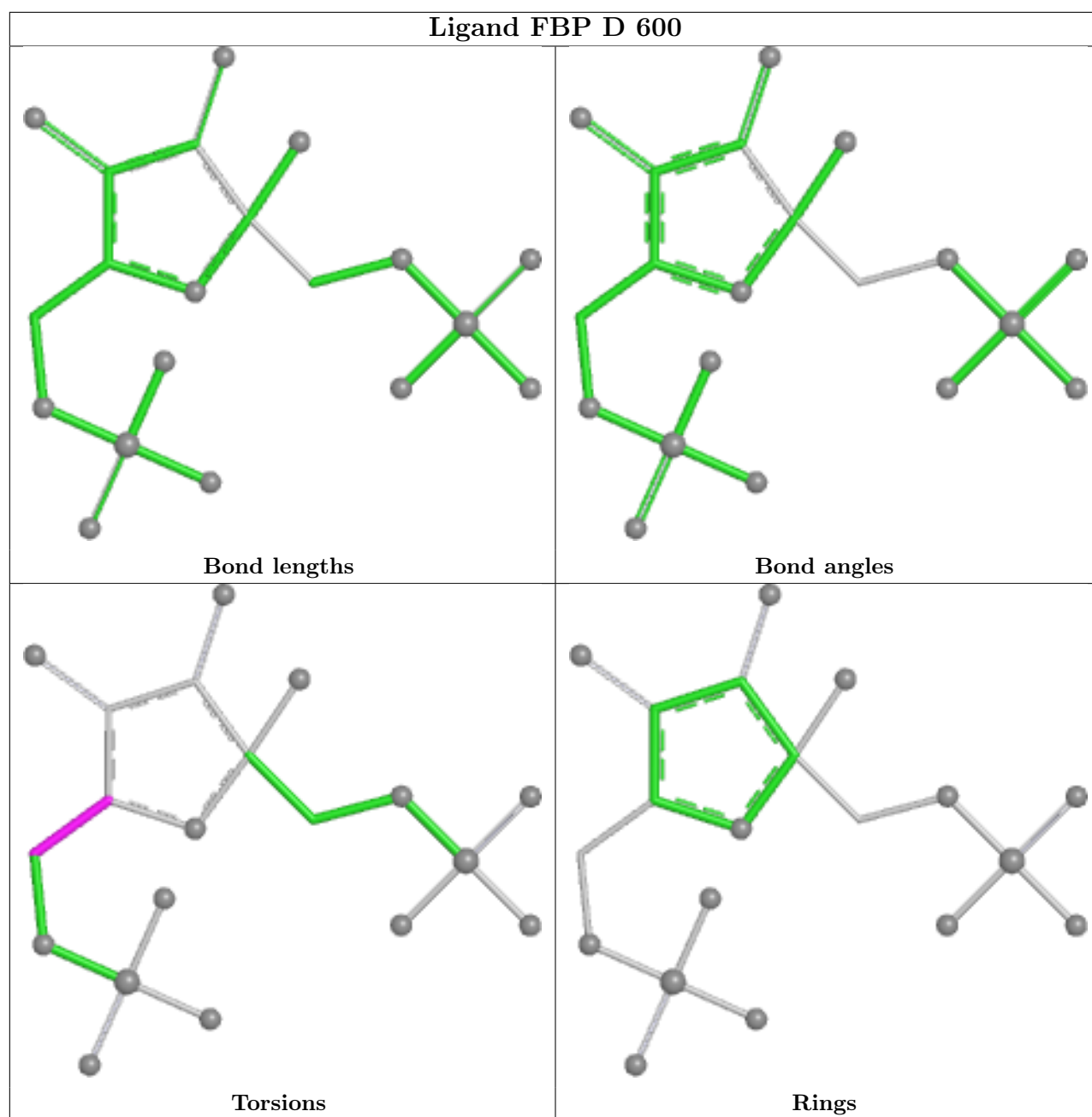
3 monomers are involved in 3 short contacts:

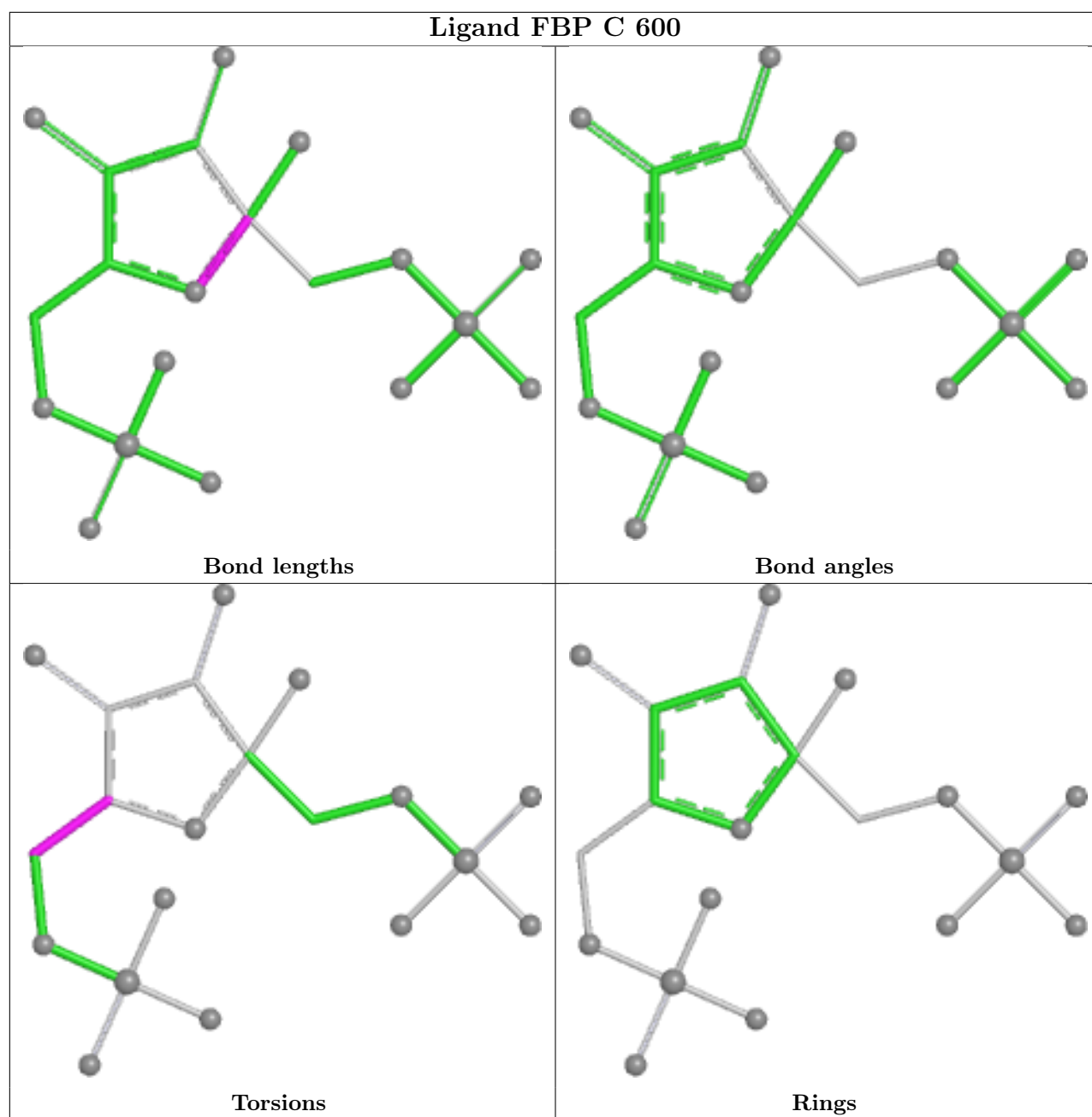
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1532	SER	1	0
3	C	1532	SER	1	0
3	D	1532	SER	1	0

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	518/548 (94%)	-0.04	8 (1%) 72 73	33, 45, 83, 110	0
1	B	514/548 (93%)	0.19	30 (5%) 29 31	30, 50, 145, 173	1 (0%)
1	C	518/548 (94%)	-0.10	5 (0%) 79 80	37, 47, 66, 90	0
2	D	518/548 (94%)	0.30	35 (6%) 23 25	39, 54, 161, 173	0
All	All	2068/2192 (94%)	0.09	78 (3%) 44 46	30, 50, 140, 173	1 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	ILE	4.8
2	D	140	LEU	4.3
1	B	130	ALA	3.9
2	D	123	LEU	3.9
2	D	164	ILE	3.8
2	D	178	ASP	3.8
2	D	157	LEU	3.7
2	D	194	VAL	3.7
2	D	174	ILE	3.5
1	B	134	LEU	3.5
2	D	144	LEU	3.5
2	D	167	VAL	3.4
1	A	18	LEU	3.4
1	B	132	VAL	3.4
2	D	132	VAL	3.3
2	D	163	ASN	3.2
1	A	190	ALA	3.2
2	D	175	TYR	3.1
1	C	404	ILE	3.0
2	D	185	VAL	3.0
2	D	193	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	172	SER	3.0
1	B	221	VAL	2.9
2	D	124	ILE	2.9
1	C	214	ALA	2.8
1	B	123	LEU	2.8
2	D	179	GLY	2.8
1	B	152	CYS	2.8
2	D	142	LEU	2.8
2	D	152	CYS	2.7
2	D	130	ALA	2.7
1	C	213	GLY	2.6
1	B	193	LEU	2.5
2	D	158	TRP	2.5
2	D	215	ALA	2.5
1	B	168	VAL	2.5
1	B	174	ILE	2.5
1	B	197	VAL	2.4
1	B	164	ILE	2.4
1	A	133	GLU	2.4
2	D	244	PHE	2.4
1	B	183	LEU	2.4
2	D	176	VAL	2.4
1	B	191	ASP	2.3
1	B	156	ILE	2.3
2	D	168	VAL	2.3
2	D	196	GLU	2.3
2	D	156	ILE	2.3
1	B	140	LEU	2.3
1	B	167	VAL	2.3
1	B	185	VAL	2.3
1	B	194	VAL	2.3
2	D	134	LEU	2.3
1	A	154	GLU	2.3
1	C	14	GLN	2.3
1	A	159	LEU	2.2
2	D	197	VAL	2.3
1	B	146	ASN	2.2
1	B	147	ALA	2.2
1	B	154	GLU	2.2
1	C	402	ALA	2.2
2	D	139	THR	2.2
1	B	158	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	192	PHE	2.2
1	B	142	ILE	2.2
1	A	192	PHE	2.2
1	B	149	MET	2.2
1	B	203	LEU	2.1
1	A	191	ASP	2.1
1	B	144	LEU	2.1
2	D	216	VAL	2.1
1	B	218	LEU	2.1
1	B	148	TYR	2.1
2	D	209	VAL	2.1
1	B	214	ALA	2.1
2	D	155	ASN	2.0
2	D	122	GLY	2.0
1	A	404	ILE	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
5	MG	C	700	1/1	0.77	0.23	52,52,52,52	0
5	MG	A	700	1/1	0.78	0.28	53,53,53,53	0
3	SER	D	1532	7/7	0.95	0.09	36,45,47,47	14
3	SER	C	1532	7/7	0.97	0.05	27,36,44,44	0
3	SER	B	1532	7/7	0.97	0.05	39,41,43,44	0
4	FBP	C	600	20/20	0.98	0.05	38,44,47,48	0
4	FBP	D	600	20/20	0.98	0.05	41,46,49,49	0
3	SER	A	1532	7/7	0.98	0.05	26,36,43,43	14

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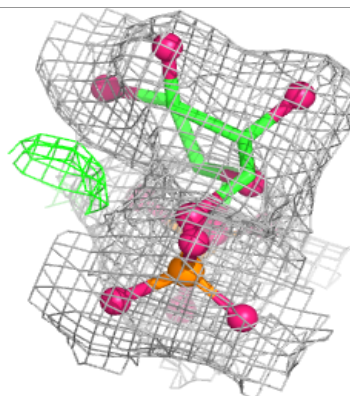
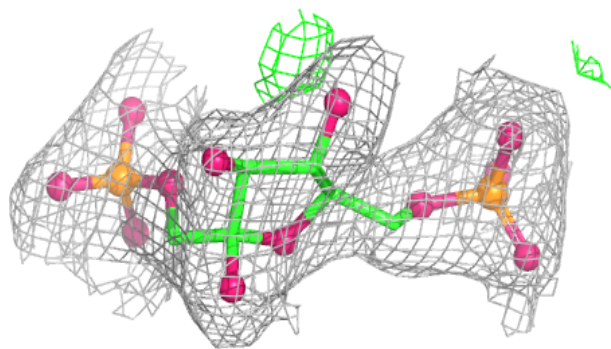
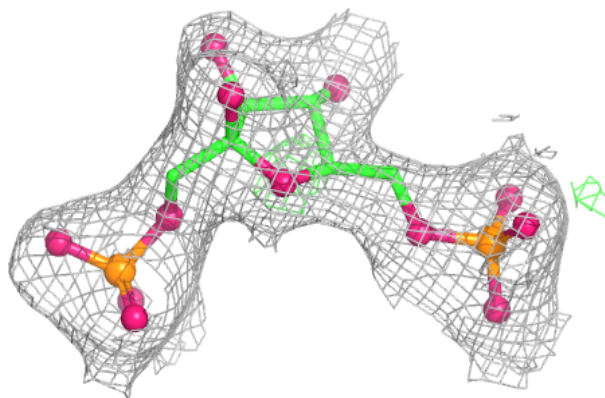
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FBP	A	600	20/20	0.98	0.04	35,40,48,48	0
4	FBP	B	600	20/20	0.99	0.04	33,38,45,45	0

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.

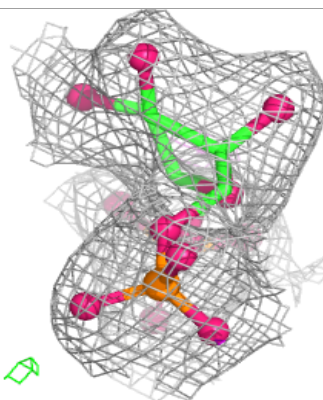
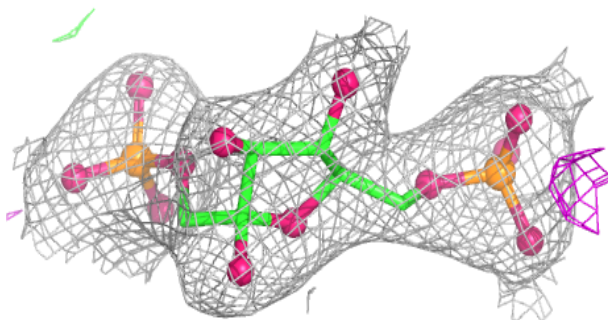
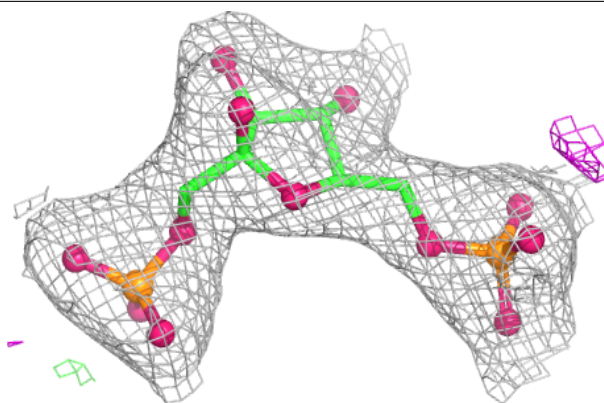
Electron density around FBP C 600:

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

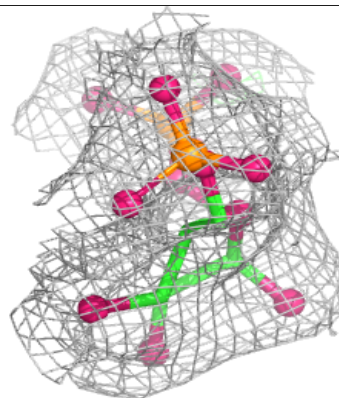
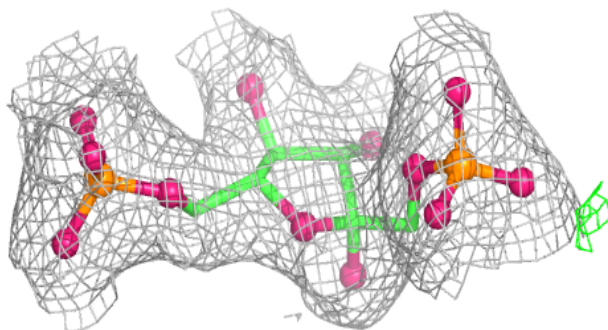
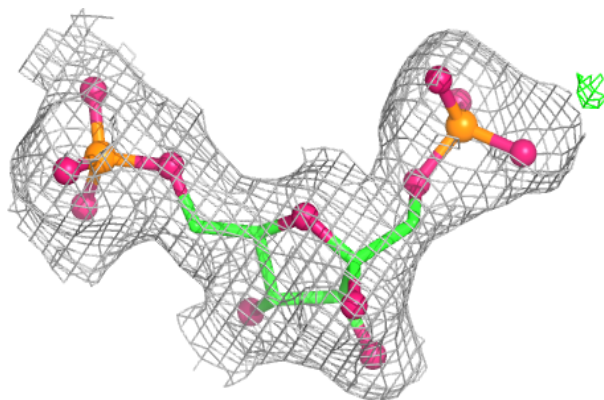


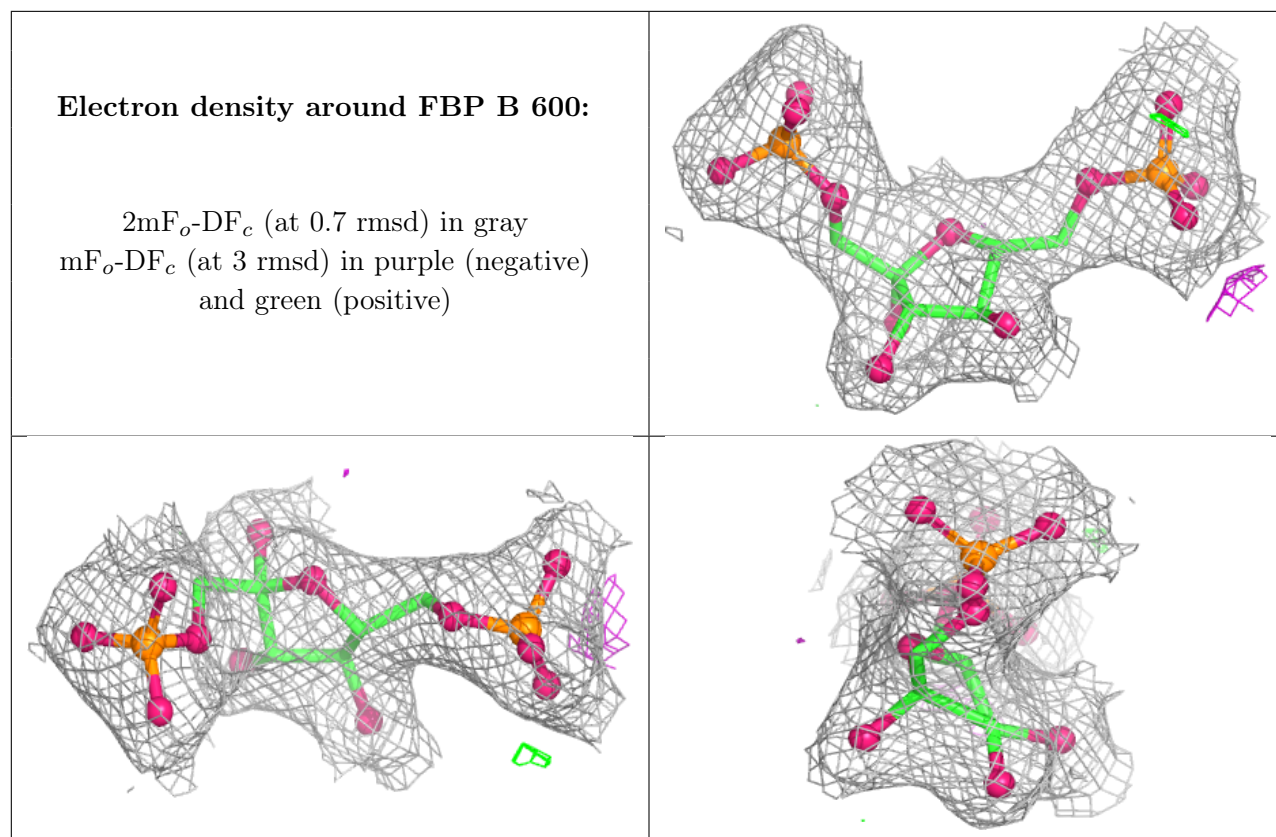
Electron density around FBP D 600:

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

**Electron density around FBP A 600:**

$2mF_o-DF_c$ (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.