



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:10 PM UTC

PDB ID : 6ECK / pdb_00006eck
Title : Pyruvate Kinase Isoform L-type with phosphorylated Ser113 (pS113) in complex with FBP
Authors : Padyana, A.; Tong, S.
Deposited on : 2018-08-08
Resolution : 2.36 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

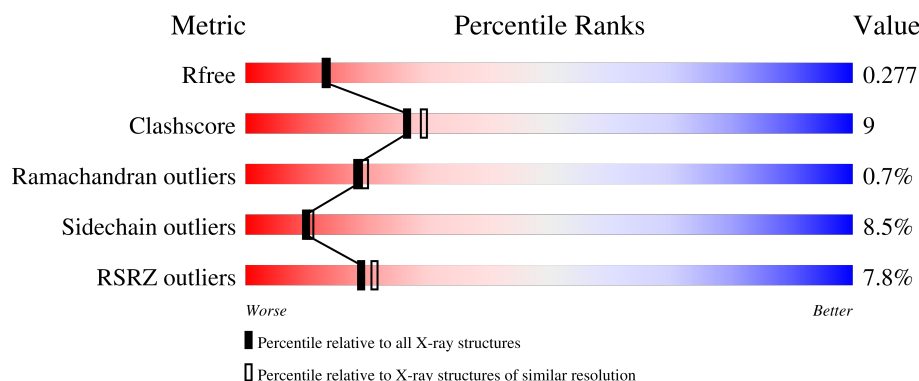
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	5% 77% 17% • •
1	B	550	10% 72% 21% • •

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	GOL	B	602	-	X	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8633 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.

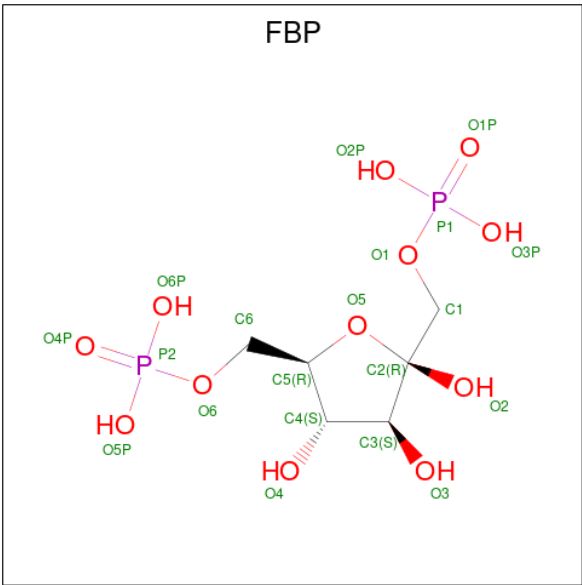
- Molecule 1 is a protein called Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	P	S	0	2	0
			4054	2547	725	762	1	19			
1	B	532	Total	C	N	O	P	S	0	3	0
			4085	2563	734	768	1	19			

There are 14 discrepancies between the modelled and reference sequences:

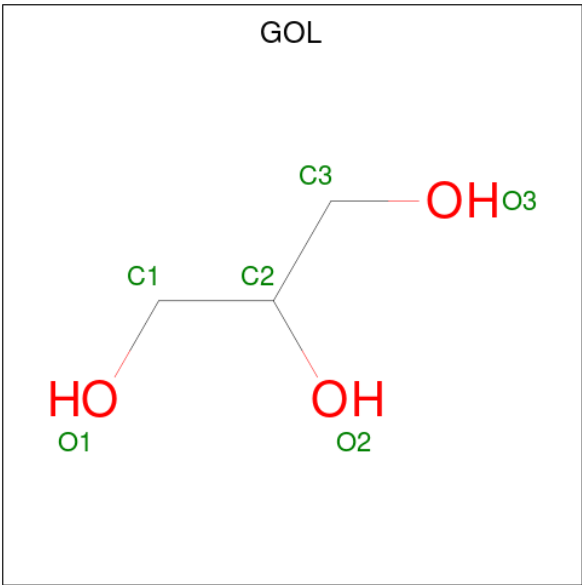
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P12928
A	544	HIS	-	expression tag	UNP P12928
A	546	HIS	-	expression tag	UNP P12928
A	547	HIS	-	expression tag	UNP P12928
A	548	HIS	-	expression tag	UNP P12928
A	549	HIS	-	expression tag	UNP P12928
A	550	HIS	-	expression tag	UNP P12928
B	0	HIS	-	expression tag	UNP P12928
B	544	HIS	-	expression tag	UNP P12928
B	545	HIS	-	expression tag	UNP P12928
B	546	HIS	-	expression tag	UNP P12928
B	547	HIS	-	expression tag	UNP P12928
B	548	HIS	-	expression tag	UNP P12928
B	549	HIS	-	expression tag	UNP P12928

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: C₆H₁₄O₁₂P₂).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



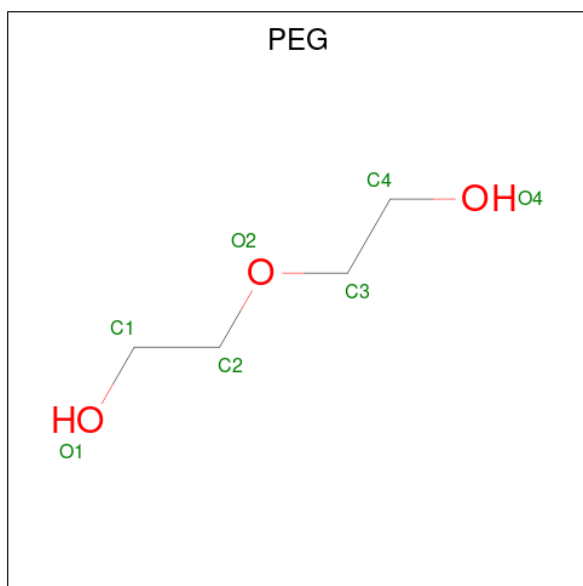
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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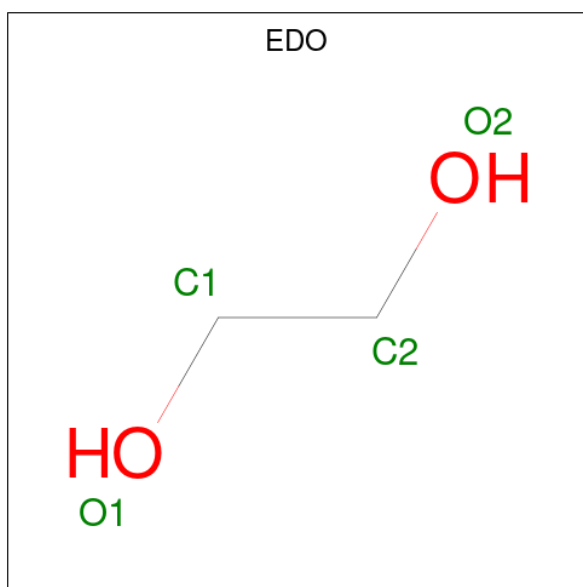
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



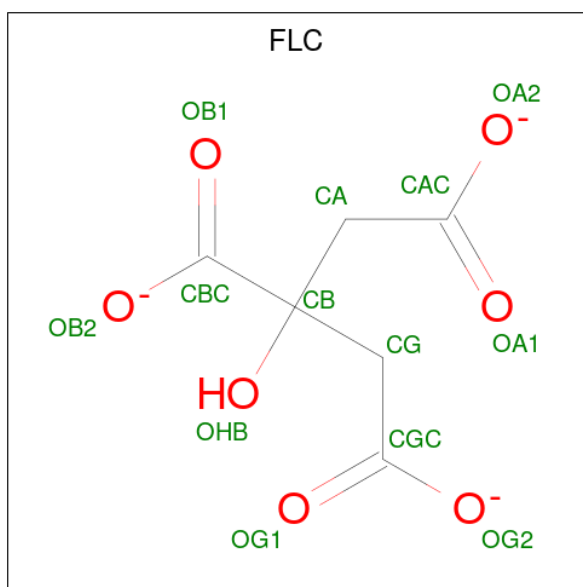
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



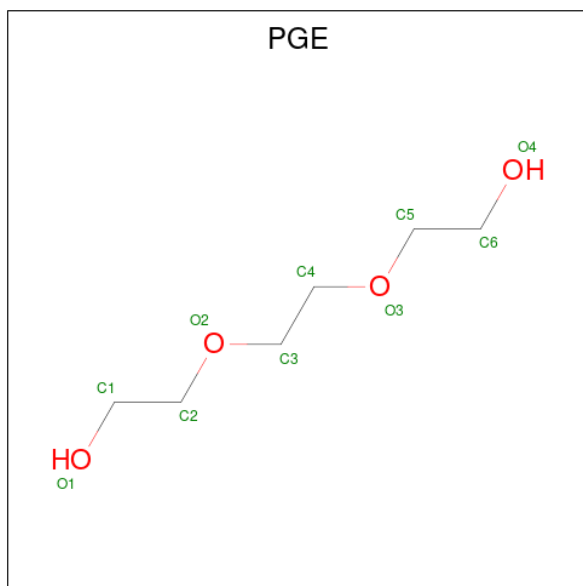
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7^-$).



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

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	229	Total	O	0	0
			229	229		
8	B	158	Total	O	0	0
			158	158		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.77Å 111.84Å 127.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.36 48.59 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.59-2.36) 97.6 (48.59-2.36)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.203 , 0.275 0.209 , 0.277	Depositor DCC
R_{free} test set	2815 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.3	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	0.95	EDS
Total number of atoms	8633	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: PGE, FLC, GOL, SEP, PEG, EDO, 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	1.00	4/4109 (0.1%)	1.12	4/5560 (0.1%)
1	B	0.95	0/4140	1.16	3/5604 (0.1%)
All	All	0.98	4/8249 (0.0%)	1.14	7/11164 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	PHE	N-CA	-6.63	1.38	1.46
1	A	179	VAL	N-CA	5.79	1.51	1.46
1	A	353	THR	C-O	-5.57	1.16	1.23
1	A	451	GLN	C-O	-5.09	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	293	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	530	GLY	CA-C-N	5.47	128.48	120.71
1	A	530	GLY	C-N-CA	5.47	128.48	120.71
1	B	377	THR	CA-CB-OG1	5.10	117.25	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	496	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ARG	Sidechain
1	A	412	ARG	Sidechain
1	A	528	ARG	Sidechain
1	B	339	ALA	Peptide
1	B	467	ARG	Sidechain

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	4054	0	4123	69	0
1	B	4085	0	4149	90	0
2	A	20	0	10	2	0
2	B	20	0	10	0	0
3	A	12	0	16	1	0
3	B	6	0	8	12	0
4	A	7	0	10	3	0
4	B	7	0	10	3	0
5	A	12	0	18	1	0
6	B	13	0	5	2	0
7	B	10	0	14	0	0
8	A	229	0	0	7	0
8	B	158	0	0	3	0
All	All	8633	0	8373	155	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 9.

All (155) 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:188:ILE:HD12	1:A:193:ILE:HD11	1.54	0.89
1:B:58:SER:OG	3:B:602:GOL:H12	1.83	0.79
1:B:303:MET:CE	1:B:372:MET:HE1	2.14	0.78
1:B:55:ARG:HD3	1:B:391:HIS:ND1	2.00	0.77
1:B:303:MET:HE2	1:B:372:MET:HE1	1.72	0.72
1:A:136:LEU:HB2	8:A:860:HOH:O	1.90	0.71
1:B:58:SER:CB	3:B:602:GOL:H12	2.21	0.70
1:A:421:THR:HG22	1:A:452:LEU:HD12	1.74	0.69
1:B:137:GLN:HE22	1:B:144:VAL:CG2	2.08	0.67
1:A:303:MET:CE	1:A:372:MET:HE1	2.24	0.67
1:B:538[B]:ARG:HH11	1:B:540:LEU:HD11	1.60	0.67
1:A:178:ARG:NE	8:A:701:HOH:O	2.26	0.66
1:A:412:ARG:NH2	1:B:408:GLU:OE1	2.30	0.65
1:A:303:MET:HE2	1:A:372:MET:HE1	1.77	0.65
1:B:528:ARG:HD2	1:B:529:PRO:O	1.98	0.64
1:A:60:ILE:HG21	1:A:372:MET:HE2	1.80	0.62
1:A:257:VAL:HG21	1:A:281:SER:HB3	1.79	0.62
1:A:319:PHE:CE2	1:A:320:LEU:HD13	2.35	0.62
1:B:81:MET:CE	1:B:84:ALA:HB2	2.30	0.61
1:A:232:GLY:C	1:A:233:LEU:HD12	2.26	0.61
1:A:54:ALA:HA	5:A:606:EDO:O1	2.00	0.61
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.83	0.60
1:B:16:LEU:O	1:B:18:GLN:N	2.35	0.60
1:B:114:PRO:HB3	1:B:487:ARG:HH11	1.67	0.60
1:A:188:ILE:CD1	1:A:193:ILE:HD11	2.28	0.59
1:B:58:SER:CA	3:B:602:GOL:H31	2.33	0.59
1:B:56:SER:O	3:B:602:GOL:H2	2.02	0.59
1:A:536:ILE:HG12	1:B:538[A]:ARG:HG2	1.84	0.58
1:B:382:PHE:HB3	1:B:385:GLU:HG2	1.86	0.57
1:B:156:VAL:HG13	1:B:174:HIS:CD2	2.39	0.57
1:A:132:ARG:HA	1:A:219:LYS:O	2.05	0.57
1:B:141:GLU:HB3	8:B:706:HOH:O	2.04	0.57
1:B:58:SER:HA	3:B:602:GOL:H31	1.87	0.56
3:B:602:GOL:H32	8:B:740:HOH:O	2.06	0.56
1:B:419:ASP:OD1	1:B:419:ASP:C	2.50	0.55
1:A:189:ASP:O	1:A:190:ASP:C	2.49	0.55
1:A:330:ASN:HD21	1:A:367:GLY:HA3	1.72	0.55
1:A:85:ARG:HH22	3:A:603:GOL:H32	1.73	0.54
1:A:118:ARG:NE	8:A:704:HOH:O	2.32	0.54
1:A:457:ARG:HH11	1:A:479:ARG:NE	2.05	0.53
1:A:538[A]:ARG:HG2	1:B:536:ILE:HG12	1.90	0.53
1:B:85:ARG:NE	1:B:125:ASP:OD2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:HIS:HB2	8:A:925:HOH:O	2.08	0.53
1:B:150:SER:OG	1:B:151:GLN:N	2.42	0.53
1:A:538[B]:ARG:HG2	1:B:536:ILE:HG12	1.90	0.52
1:A:70:VAL:HG12	8:A:845:HOH:O	2.09	0.52
1:A:187:TYR:O	1:A:221:VAL:HA	2.09	0.52
1:A:457:ARG:NH1	1:A:479:ARG:NE	2.58	0.52
1:B:129:PRO:HG2	1:B:258:ARG:NH2	2.25	0.52
1:A:408:GLU:OE1	1:B:411:ARG:NH2	2.42	0.52
1:A:188:ILE:HB	1:A:193:ILE:CG1	2.39	0.51
1:B:241:LEU:O	1:B:244:GLY:N	2.42	0.51
1:B:341:GLN:HG2	1:B:344:GLU:HG2	1.93	0.51
1:B:344:GLU:HA	1:B:344:GLU:OE1	2.11	0.51
1:B:538[B]:ARG:NH1	1:B:540:LEU:HD11	2.25	0.51
1:B:309:LEU:O	1:B:313:ILE:HG12	2.11	0.51
1:A:457:ARG:NH1	1:A:479:ARG:CB	2.74	0.50
1:B:343:LEU:HD23	1:B:356:GLU:HB3	1.93	0.50
1:B:528:ARG:HD3	1:B:529:PRO:HD2	1.93	0.50
1:A:540:LEU:CD2	4:A:604:PEG:H41	2.41	0.50
1:B:179:VAL:HG12	1:B:226:THR:CG2	2.41	0.50
1:B:267:ARG:NH2	1:B:300:ASP:OD2	2.45	0.50
1:B:56:SER:O	3:B:602:GOL:C2	2.61	0.49
1:B:58:SER:N	3:B:602:GOL:H11	2.27	0.49
1:A:195:LEU:CD2	1:A:209:VAL:HG22	2.42	0.49
1:A:188:ILE:HB	1:A:193:ILE:HG13	1.95	0.49
1:B:335:PRO:HB3	1:B:477:LEU:O	2.12	0.49
1:A:17:THR:HG22	1:A:25:PHE:CD2	2.47	0.49
1:B:254:ALA:O	1:B:257:VAL:HG23	2.14	0.48
1:A:178:ARG:NH1	8:A:711:HOH:O	2.45	0.48
1:A:136:LEU:HA	1:A:164:GLY:HA3	1.94	0.48
1:A:501:ARG:NH2	2:A:601:FBP:O2P	2.47	0.48
6:B:603:FLC:OA1	6:B:603:FLC:OHB	2.30	0.48
1:A:523:VAL:HG21	1:A:540:LEU:HD12	1.94	0.48
1:B:523:VAL:HG21	1:B:540:LEU:HD12	1.95	0.48
1:A:501:ARG:HH22	2:A:601:FBP:P1	2.35	0.48
1:B:83:ILE:HG12	1:B:121:ALA:HB3	1.95	0.48
1:B:92:SER:O	1:B:95:TYR:HB3	2.14	0.48
1:B:81:MET:HE2	1:B:84:ALA:HB2	1.95	0.47
1:B:108:GLU:HA	1:B:108:GLU:OE1	2.14	0.47
1:B:56:SER:O	3:B:602:GOL:H11	2.15	0.46
1:B:187:TYR:HB3	1:B:191:GLY:HA2	1.97	0.46
1:B:154:VAL:HA	1:B:169:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLN:HG2	1:B:344:GLU:CG	2.45	0.46
1:A:156:VAL:HG12	1:A:156:VAL:O	2.16	0.45
1:A:538[B]:ARG:CG	1:B:536:ILE:HG12	2.46	0.45
1:B:285:ASN:HB2	1:B:312:GLU:CD	2.42	0.45
1:A:487:ARG:HH11	1:A:487:ARG:HG2	1.81	0.45
1:B:58:SER:N	3:B:602:GOL:C1	2.80	0.45
1:A:233:LEU:HD12	1:A:233:LEU:N	2.31	0.45
1:A:538[B]:ARG:HH21	4:A:604:PEG:H41	1.81	0.45
1:A:13:VAL:O	1:A:17:THR:HG23	2.16	0.45
1:B:153:LEU:HD13	1:B:155:THR:HG23	1.97	0.45
1:B:480:GLY:HA3	4:B:604:PEG:H42	1.98	0.45
1:B:81:MET:HE1	1:B:84:ALA:HB2	1.99	0.45
1:B:256:PHE:N	1:B:284:GLU:OE1	2.42	0.45
1:A:303:MET:HE2	1:A:372:MET:CE	2.47	0.45
1:B:28:GLN:O	1:B:459[A]:ARG:NH1	2.50	0.45
1:A:233:LEU:HD13	1:A:265:ALA:HB1	1.99	0.44
1:A:303:MET:HE1	1:A:372:MET:HE1	1.98	0.44
1:B:249:VAL:O	1:B:277:ILE:HD13	2.16	0.44
1:B:38:PHE:O	1:B:41:HIS:HB3	2.17	0.44
1:B:144:VAL:CG1	1:B:166:ALA:HB2	2.47	0.44
1:B:173:TYR:CE1	1:B:229:ASP:HB3	2.52	0.44
1:B:484:LEU:HD13	1:B:508:SER:CB	2.47	0.44
1:B:30:LEU:N	1:B:31:PRO:CD	2.81	0.44
1:B:126:THR:HG22	1:B:255:SER:HB2	2.00	0.44
1:B:468:SER:HB3	1:B:471:ALA:HB3	1.99	0.44
1:B:58:SER:OG	3:B:602:GOL:C3	2.65	0.44
1:A:346:MET:HA	1:A:349:LYS:O	2.18	0.43
1:A:160:PHE:HD2	1:A:168:THR:HG21	1.84	0.43
1:B:243:PHE:C	1:B:243:PHE:CD1	2.96	0.43
1:B:230:LEU:O	1:B:258:ARG:NH1	2.49	0.43
1:B:85:ARG:NH2	1:B:125:ASP:OD2	2.50	0.43
1:A:459:ARG:NH2	8:A:721:HOH:O	2.51	0.43
1:B:16:LEU:HD12	1:B:16:LEU:C	2.44	0.43
1:B:60:ILE:HG21	1:B:372:MET:HE2	2.01	0.43
1:A:324:MET:SD	1:A:328:ARG:HD2	2.59	0.42
1:A:135:VAL:O	1:A:136:LEU:C	2.62	0.42
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.87	0.42
1:A:30:LEU:O	1:A:34:MET:HG2	2.18	0.42
1:A:155:THR:HG1	1:A:157:ASP:H	1.67	0.42
1:A:284:GLU:HG2	1:A:305:ALA:HB3	2.00	0.42
1:A:540:LEU:HD22	4:A:604:PEG:H41	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASP:HB3	8:B:727:HOH:O	2.19	0.42
1:B:457:ARG:HA	4:B:604:PEG:H32	2.00	0.42
1:B:56:SER:HB2	1:B:480:GLY:CA	2.48	0.42
1:A:260:ALA:O	1:A:263:VAL:N	2.47	0.42
1:B:56:SER:CB	1:B:480:GLY:HA2	2.50	0.42
1:A:193:ILE:C	1:A:193:ILE:HD12	2.44	0.42
1:A:335:PRO:HB3	1:A:477:LEU:O	2.20	0.41
1:B:479:ARG:HA	3:B:602:GOL:O1	2.20	0.41
1:B:153:LEU:CD1	1:B:155:THR:HG23	2.49	0.41
1:B:303:MET:HE1	1:B:372:MET:HE1	1.97	0.41
1:A:189:ASP:O	1:A:192:LEU:HB2	2.21	0.41
1:A:408:GLU:OE2	1:B:408:GLU:HG3	2.20	0.41
1:B:73:LEU:HD13	1:B:103:ILE:HA	2.02	0.41
1:B:342:MET:HE2	1:B:360:VAL:HG22	2.03	0.41
1:A:243:PHE:CE2	1:A:247:HIS:NE2	2.89	0.41
1:A:382:PHE:N	1:A:383:PRO:CD	2.84	0.41
1:B:124:LEU:C	1:B:124:LEU:HD23	2.46	0.41
1:A:136:LEU:HD23	1:A:164:GLY:HA3	2.02	0.41
1:A:156:VAL:O	1:A:156:VAL:CG1	2.68	0.41
1:B:148:LYS:H	1:B:148:LYS:HG3	1.75	0.41
1:B:435:CYS:HB2	1:B:520:LEU:HD12	2.03	0.40
1:B:341:GLN:HA	1:B:344:GLU:HG2	2.03	0.40
1:B:479:ARG:CG	4:B:604:PEG:H31	2.51	0.40
1:A:535:ASN:OD1	1:A:536:ILE:HG13	2.21	0.40
1:B:55:ARG:NH2	1:B:82:ASN:OD1	2.54	0.40
1:B:286:HIS:NE2	1:B:290:LYS:HE2	2.36	0.40
6:B:603:FLC:OHB	6:B:603:FLC:OG1	2.35	0.40
1:B:85:ARG:HH21	1:B:125:ASP:CG	2.30	0.40
1:A:124:LEU:C	1:A:124:LEU:HD23	2.46	0.40
1:A:250:ASP:C	1:A:251:ILE:HG13	2.47	0.40
1:B:156:VAL:CG1	1:B:174:HIS:NE2	2.84	0.40

There are no symmetry-related clashes.

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	525/550 (96%)	500 (95%)	23 (4%)	2 (0%)	30	34
1	B	532/550 (97%)	490 (92%)	37 (7%)	5 (1%)	14	14
All	All	1057/1100 (96%)	990 (94%)	60 (6%)	7 (1%)	18	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	THR
1	B	340	THR
1	A	129	PRO
1	A	340	THR
1	B	234	SER
1	B	129	PRO
1	B	80	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	433/446 (97%)	404 (93%)	29 (7%)	15	17
1	B	435/446 (98%)	391 (90%)	44 (10%)	7	6
All	All	868/892 (97%)	795 (92%)	73 (8%)	10	11

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	45	LEU
1	A	52	VAL
1	A	73	LEU
1	A	109	SER
1	A	112	THR

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Mol	Chain	Res	Type
1	A	132	ARG
1	A	141	GLU
1	A	147	VAL
1	A	150	SER
1	A	155	THR
1	A	162	THR
1	A	163	ARG
1	A	167	LYS
1	A	192	LEU
1	A	197	VAL
1	A	199	LYS
1	A	230	LEU
1	A	238	LEU
1	A	296	LEU
1	A	313	ILE
1	A	320	LEU
1	A	357	THR
1	A	358	SER
1	A	416	LEU
1	A	479	ARG
1	A	500	ARG
1	A	501	ARG
1	A	550	HIS
1	B	15	GLN
1	B	16	LEU
1	B	18	GLN
1	B	19	GLU
1	B	26	GLN
1	B	68	ARG
1	B	75	GLU
1	B	78	LYS
1	B	98	GLU
1	B	99	SER
1	B	126	THR
1	B	135	VAL
1	B	145	GLU
1	B	146	ILE
1	B	148	LYS
1	B	151	GLN
1	B	153	LEU
1	B	155	THR
1	B	157	ASP

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Mol	Chain	Res	Type
1	B	162	THR
1	B	192	LEU
1	B	207	THR
1	B	208	GLU
1	B	210	GLU
1	B	214	ILE
1	B	215	LEU
1	B	221	VAL
1	B	223	LEU
1	B	230	LEU
1	B	234	SER
1	B	256	PHE
1	B	277	ILE
1	B	278	LYS
1	B	312	GLU
1	B	331	LEU
1	B	344	GLU
1	B	358	SER
1	B	385	GLU
1	B	389	MET
1	B	411	ARG
1	B	475	VAL
1	B	488	GLU
1	B	491	GLU
1	B	528	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	50	GLN
1	A	96	HIS
1	A	198	GLN
1	A	211	HIS
1	A	330	ASN
1	A	470	GLN
1	B	15	GLN
1	B	18	GLN
1	B	26	GLN
1	B	87	ASN
1	B	96	HIS
1	B	137	GLN

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Mol	Chain	Res	Type
1	B	151	GLN
1	B	236	GLN
1	B	247	HIS
1	B	535	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SEP	A	113	1	8,9,10	0.70	0	7,12,14	2.05	2 (28%)
1	SEP	B	113	1	8,9,10	0.68	0	7,12,14	1.21	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
1	SEP	A	113	1	-	5/6/8/10	-
1	SEP	B	113	1	-	1/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	SEP	O3P-P-O2P	3.39	120.52	107.80
1	A	113	SEP	O2P-P-OG	-3.38	97.86	106.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	113	SEP	N-CA-CB-OG
1	A	113	SEP	C-CA-CB-OG
1	A	113	SEP	CB-OG-P-O2P
1	A	113	SEP	CB-OG-P-O3P
1	B	113	SEP	CB-OG-P-O1P
1	A	113	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	602	-	5,5,5	1.13	0	5,5,5	1.26	1 (20%)
5	EDO	A	605	-	3,3,3	0.43	0	2,2,2	0.34	0
3	GOL	A	603	-	5,5,5	0.64	0	5,5,5	0.40	0
2	FBP	B	601	-	18,20,20	1.05	1 (5%)	21,32,32	1.79	7 (33%)
4	PEG	A	604	-	6,6,6	1.00	0	5,5,5	1.17	0
5	EDO	A	606	-	3,3,3	0.67	0	2,2,2	0.26	0
7	PGE	B	605	-	9,9,9	0.66	0	8,8,8	0.67	0
2	FBP	A	601	-	18,20,20	1.08	2 (11%)	21,32,32	1.85	7 (33%)
3	GOL	B	602	-	5,5,5	1.36	1 (20%)	5,5,5	2.18	3 (60%)
6	FLC	B	603	-	12,12,12	1.43	1 (8%)	17,17,17	1.64	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	607	-	3,3,3	0.57	0	2,2,2	0.28	0
4	PEG	B	604	-	6,6,6	0.61	0	5,5,5	0.84	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
3	GOL	A	602	-	-	4/4/4/4	-
5	EDO	A	605	-	-	0/1/1/1	-
3	GOL	A	603	-	-	2/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
4	PEG	A	604	-	-	1/4/4/4	-
5	EDO	A	606	-	-	0/1/1/1	-
7	PGE	B	605	-	-	5/7/7/7	-
2	FBP	A	601	-	-	1/13/32/32	0/1/1/1
3	GOL	B	602	-	-	3/4/4/4	-
6	FLC	B	603	-	-	9/16/16/16	-
5	EDO	A	607	-	-	1/1/1/1	-
4	PEG	B	604	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	603	FLC	CB-CBC	2.83	1.56	1.53
2	A	601	FBP	C4-C5	-2.41	1.46	1.53
2	A	601	FBP	P1-O2P	-2.37	1.46	1.54
2	B	601	FBP	O5-C5	2.25	1.48	1.43
3	B	602	GOL	O2-C2	2.20	1.49	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	603	FLC	OB2-CBC-CB	5.19	123.10	113.14
2	B	601	FBP	O6P-P2-O5P	4.06	123.01	107.80
2	A	601	FBP	O3P-P1-O1	-3.41	97.77	106.67
2	A	601	FBP	O5-C5-C6	3.19	117.00	109.50
3	B	602	GOL	O1-C1-C2	3.12	124.43	110.38
2	A	601	FBP	O6P-P2-O4P	3.09	122.88	110.83
2	B	601	FBP	O3P-P1-O2P	2.96	118.92	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FBP	O3P-P1-O1P	2.80	121.76	110.83
2	B	601	FBP	O1-P1-O1P	2.80	114.00	106.44
2	B	601	FBP	O6-C6-C5	2.62	117.92	108.99
3	B	602	GOL	O2-C2-C3	2.59	119.89	109.18
6	B	603	FLC	OB2-CBC-OB1	-2.58	115.61	123.86
2	B	601	FBP	O6P-P2-O6	-2.50	100.14	106.67
2	A	601	FBP	O6-P2-O4P	-2.42	99.90	106.44
2	A	601	FBP	O1-P1-O1P	-2.23	100.42	106.44
2	B	601	FBP	O3P-P1-O1	-2.15	101.08	106.67
6	B	603	FLC	CA-CB-CBC	2.11	114.70	110.03
3	A	602	GOL	O2-C2-C3	2.11	117.91	109.18
3	B	602	GOL	O3-C3-C2	2.11	119.86	110.38
2	A	601	FBP	O6P-P2-O6	-2.01	101.42	106.67
2	B	601	FBP	O5-C5-C6	2.01	114.22	109.50

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	B	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3
6	B	603	FLC	CAC-CA-CB-CBC
6	B	603	FLC	CAC-CA-CB-CG
6	B	603	FLC	CAC-CA-CB-OHB
6	B	603	FLC	CA-CB-CBC-OB1
6	B	603	FLC	CA-CB-CBC-OB2
6	B	603	FLC	OHB-CB-CBC-OB1
6	B	603	FLC	OHB-CB-CBC-OB2
2	B	601	FBP	C4-C5-C6-O6
4	A	604	PEG	O1-C1-C2-O2
7	B	605	PGE	O3-C5-C6-O4
3	A	603	GOL	C1-C2-C3-O3
3	A	602	GOL	O2-C2-C3-O3
2	A	601	FBP	C4-C5-C6-O6
7	B	605	PGE	O1-C1-C2-O2
2	B	601	FBP	O5-C5-C6-O6
7	B	605	PGE	C1-C2-O2-C3
7	B	605	PGE	C4-C3-O2-C2
4	B	604	PEG	C4-C3-O2-C2

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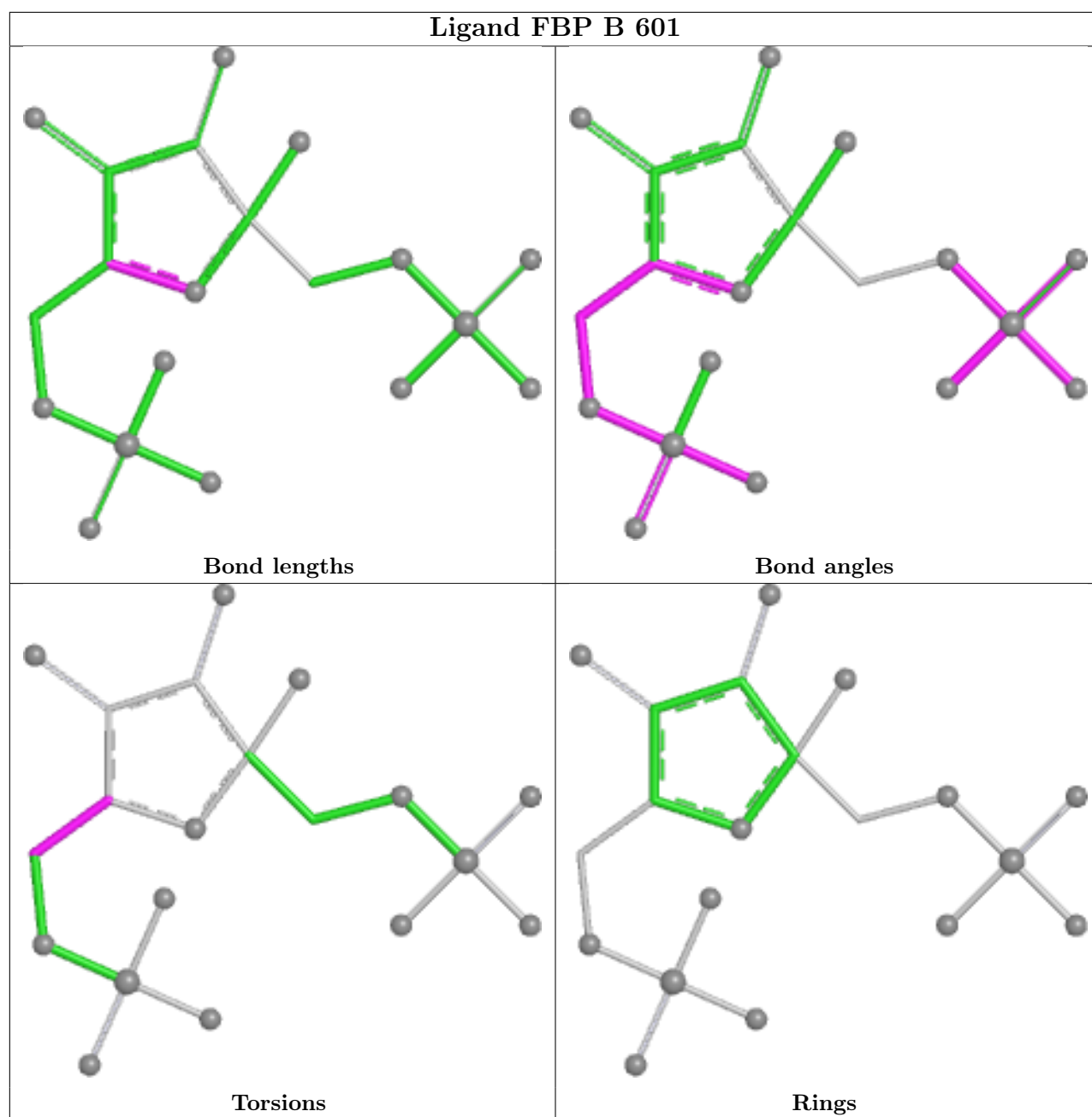
Mol	Chain	Res	Type	Atoms
7	B	605	PGE	C3-C4-O3-C5
3	A	603	GOL	O2-C2-C3-O3
6	B	603	FLC	CA-CB-CG-CGC
3	B	602	GOL	O1-C1-C2-O2
5	A	607	EDO	O1-C1-C2-O2
6	B	603	FLC	CG-CB-CBC-OB2

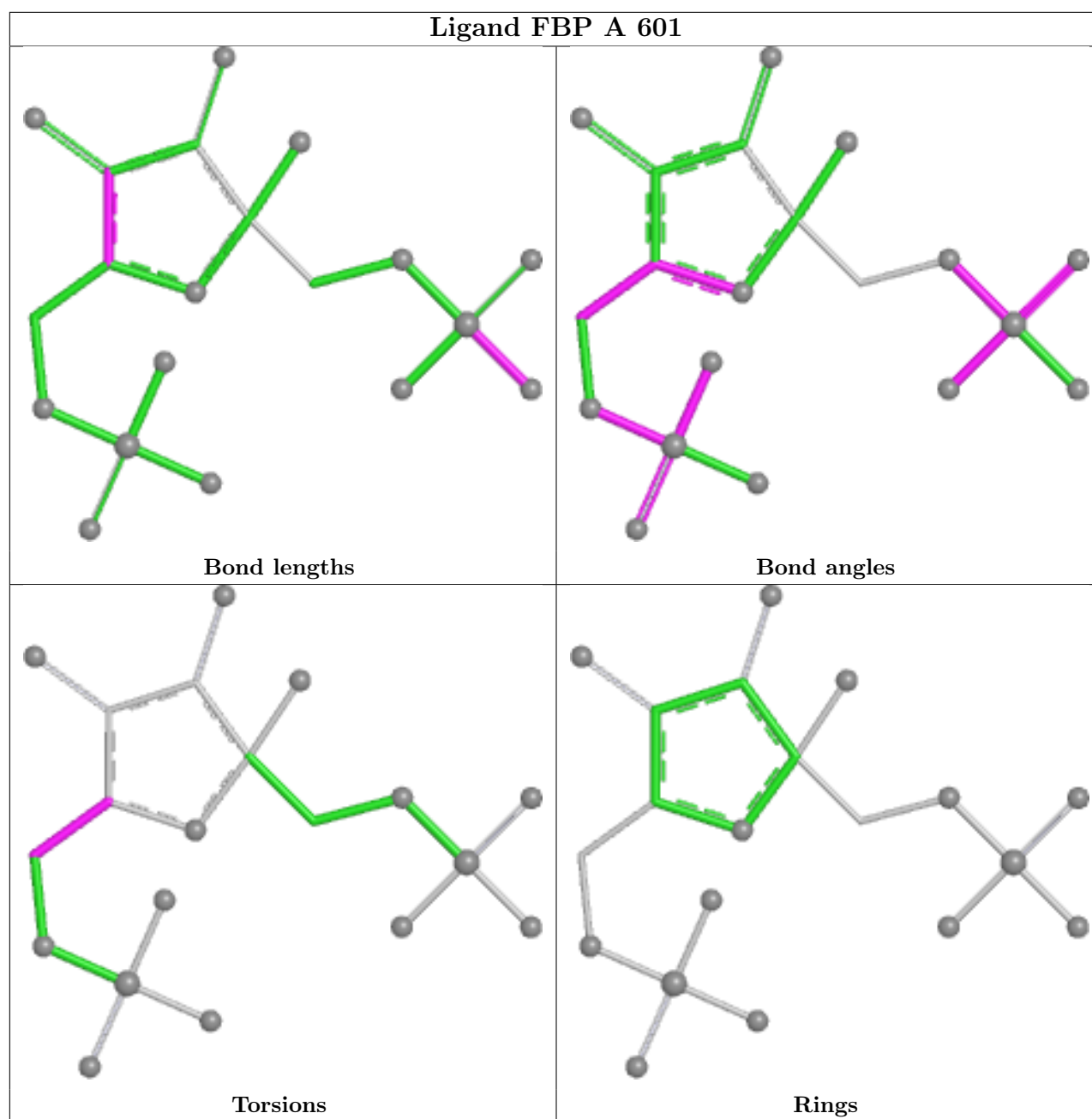
There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	GOL	1	0
4	A	604	PEG	3	0
5	A	606	EDO	1	0
2	A	601	FBP	2	0
3	B	602	GOL	12	0
6	B	603	FLC	2	0
4	B	604	PEG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	528/550 (96%)	0.28	26 (4%)	35 41	20, 48, 96, 135	2 (0%)
1	B	531/550 (96%)	0.69	57 (10%)	11 13	18, 56, 136, 206	3 (0%)
All	All	1059/1100 (96%)	0.48	83 (7%)	19 21	18, 53, 126, 206	5 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	ILE	5.4
1	B	545	HIS	4.7
1	A	13	VAL	4.6
1	A	136	LEU	4.4
1	B	215	LEU	4.2
1	B	216	GLY	4.2
1	A	193	ILE	4.0
1	B	16	LEU	3.9
1	B	169	VAL	3.8
1	B	154	VAL	3.8
1	B	134	GLY	3.7
1	A	52	VAL	3.7
1	A	550	HIS	3.6
1	B	52	VAL	3.4
1	B	20	LEU	3.4
1	B	14	ALA	3.3
1	B	135	VAL	3.2
1	B	166	ALA	3.2
1	B	136	LEU	3.2
1	B	173	TYR	3.2
1	B	228	VAL	3.1
1	B	25	PHE	3.1
1	B	191	GLY	3.1
1	B	171	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	156	VAL	3.0
1	A	135	VAL	3.0
1	B	221	VAL	3.0
1	B	200	ILE	3.0
1	A	232	GLY	3.0
1	A	189	ASP	2.9
1	B	17	THR	2.9
1	B	233	LEU	2.9
1	A	214	ILE	2.8
1	B	206	VAL	2.8
1	B	133	THR	2.8
1	B	152	VAL	2.7
1	B	140	PRO	2.7
1	B	115	LEU	2.7
1	B	193	ILE	2.6
1	B	153	LEU	2.6
1	A	160	PHE	2.6
1	B	232	GLY	2.6
1	B	147	VAL	2.5
1	A	34	MET	2.5
1	A	231	PRO	2.5
1	B	155	THR	2.5
1	A	233	LEU	2.5
1	B	202	PRO	2.5
1	A	25	PHE	2.4
1	B	103	ILE	2.4
1	A	124	LEU	2.4
1	A	217	SER	2.4
1	A	146	ILE	2.4
1	B	77	ILE	2.4
1	B	199	LYS	2.4
1	B	146	ILE	2.4
1	B	176	ILE	2.4
1	B	256	PHE	2.4
1	B	53	ALA	2.3
1	A	132	ARG	2.3
1	B	144	VAL	2.3
1	A	150	SER	2.3
1	B	182	VAL	2.3
1	B	139	GLY	2.2
1	A	209	VAL	2.2
1	B	138	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	170	TRP	2.2
1	B	89	SER	2.2
1	A	144	VAL	2.2
1	A	243	PHE	2.2
1	B	197	VAL	2.1
1	B	272	PRO	2.1
1	B	168	THR	2.1
1	B	177	THR	2.1
1	B	24	PHE	2.1
1	B	76	MET	2.1
1	A	149	GLY	2.1
1	B	160	PHE	2.1
1	A	151	GLN	2.0
1	A	238	LEU	2.0
1	B	93	HIS	2.0
1	A	20	LEU	2.0
1	B	239	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	B	113	10/11	0.77	0.10	81,88,111,130	0
1	SEP	A	113	10/11	0.93	0.07	57,69,84,84	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

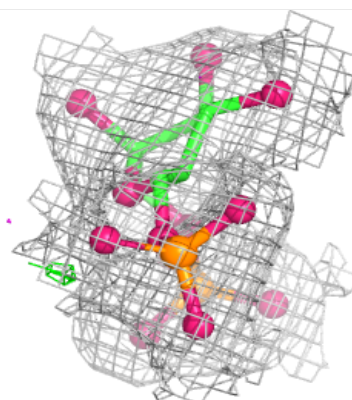
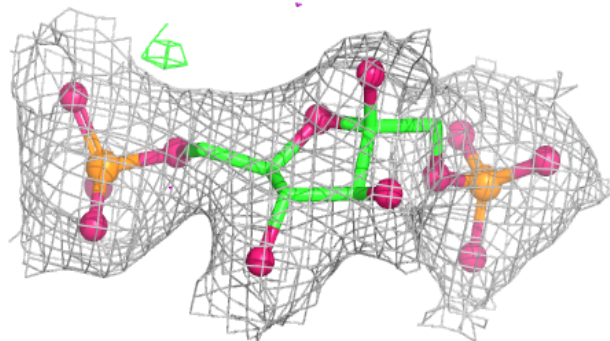
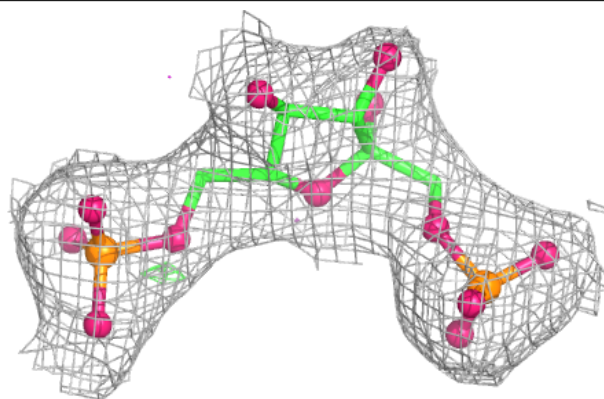
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

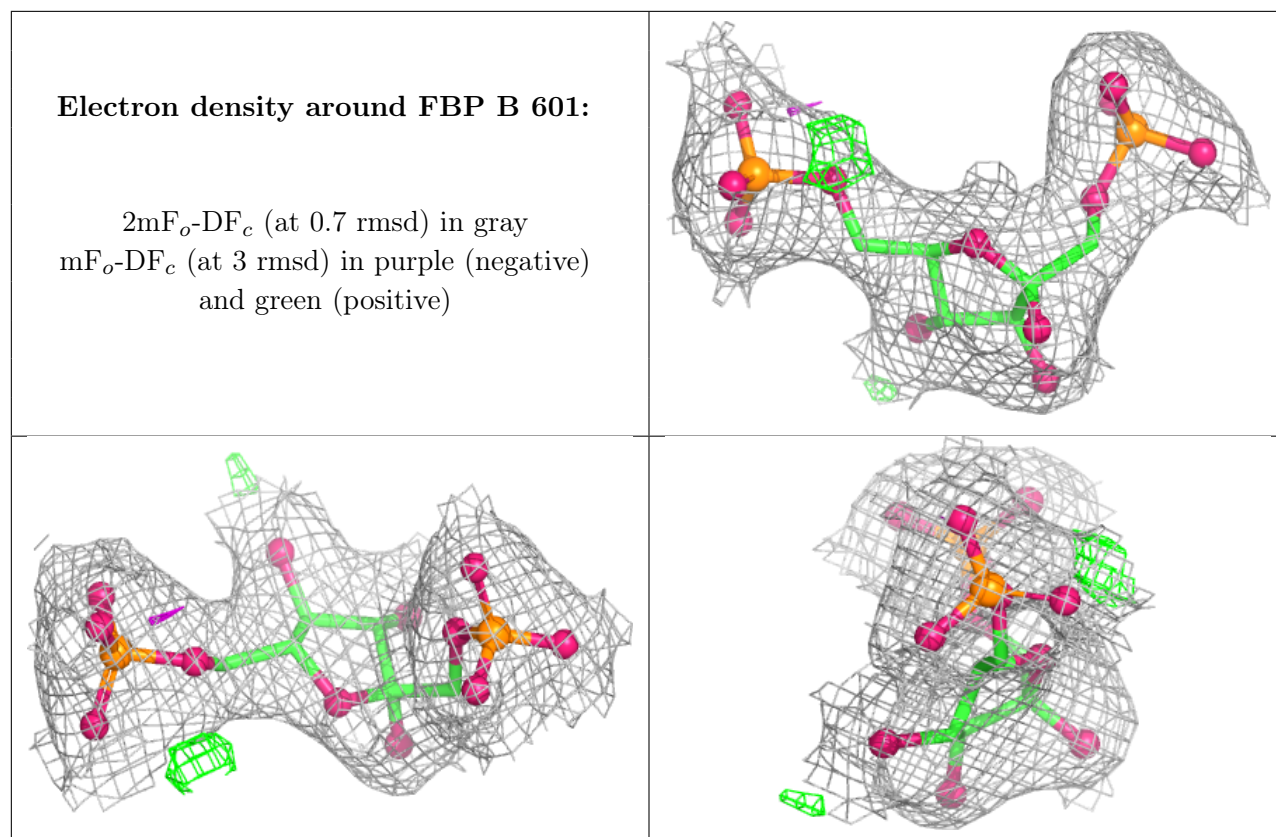
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	606	4/4	0.70	0.24	76,77,81,81	0
5	EDO	A	605	4/4	0.79	0.18	72,79,80,83	0
5	EDO	A	607	4/4	0.83	0.21	68,70,74,80	0
6	FLC	B	603	13/13	0.85	0.13	67,77,84,95	0
4	PEG	B	604	7/7	0.87	0.20	66,75,82,85	0
4	PEG	A	604	7/7	0.88	0.15	62,70,80,83	0
3	GOL	A	602	6/6	0.90	0.16	62,73,74,77	0
3	GOL	A	603	6/6	0.90	0.14	61,70,75,78	0
7	PGE	B	605	10/10	0.90	0.17	67,73,76,77	0
3	GOL	B	602	6/6	0.92	0.11	44,45,52,52	0
2	FBP	A	601	20/20	0.98	0.05	28,33,42,44	0
2	FBP	B	601	20/20	0.98	0.05	30,36,43,43	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 601:

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.