



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:33 PM GMT

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

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

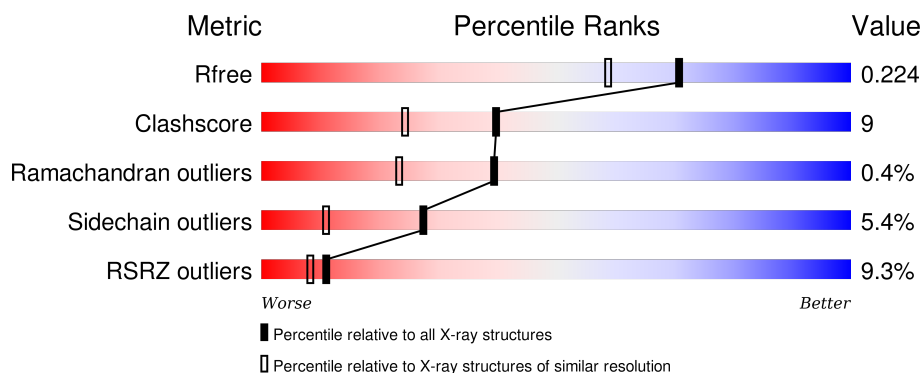
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	543	<div> <div>5%</div> <div>78% 13% • 7%</div> </div>
1	B	543	<div> <div>9%</div> <div>75% 15% • • 7%</div> </div>
1	C	543	<div> <div>11%</div> <div>76% 14% • 8%</div> </div>
1	D	543	<div> <div>10%</div> <div>76% 13% • • 7%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	B	602	-	-	X	-
6	PEG	A	606	-	-	X	-
7	NA	B	607	-	-	-	X
8	1PE	C	606	-	-	X	X
9	ADN	D	604[A]	-	-	-	X
9	ADN	D	604[B]	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17146 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate kinase isozymes L.

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

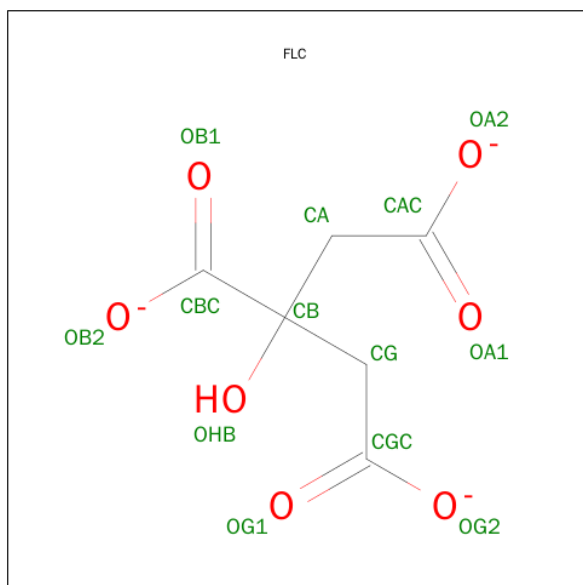
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ASP	SER	ENGINEERED MUTATION	UNP P30613
B	12	ASP	SER	ENGINEERED MUTATION	UNP P30613
C	12	ASP	SER	ENGINEERED MUTATION	UNP P30613
D	12	ASP	SER	ENGINEERED MUTATION	UNP P30613

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

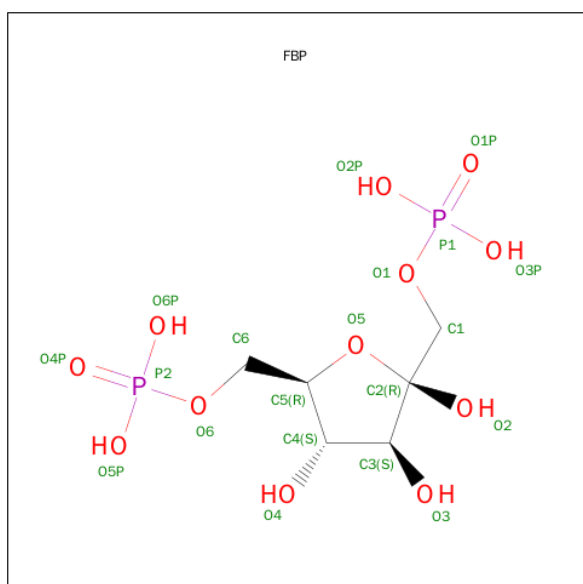
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



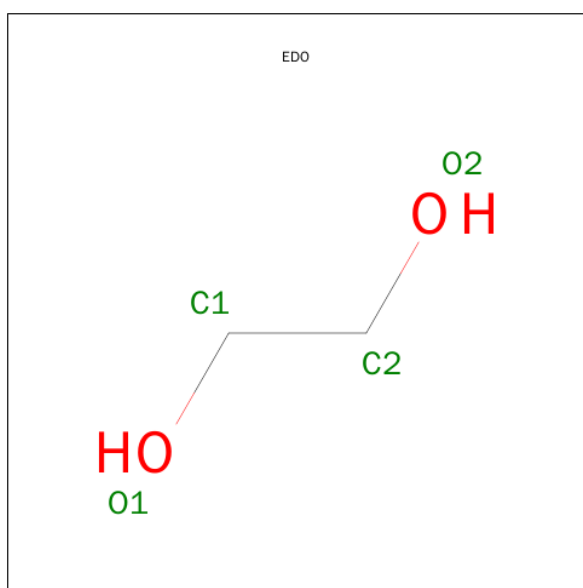
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is SUGAR (BETA-FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

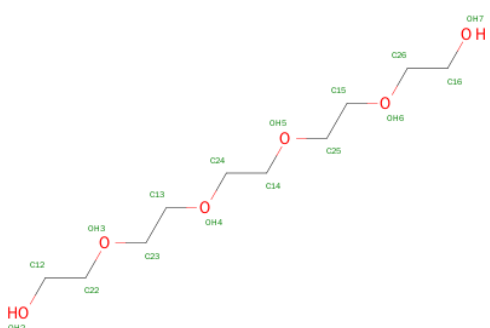


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

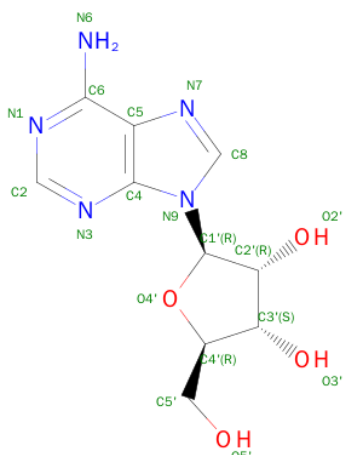
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		
7	A	1	Total	Na	0	0
			1	1		
7	D	1	Total	Na	0	0
			1	1		
7	C	1	Total	Na	0	0
			1	1		

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



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

- Molecule 9 is ADENOSINE (three-letter code: ADN) (formula: $\text{C}_{10}\text{H}_{13}\text{N}_5\text{O}_4$).



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

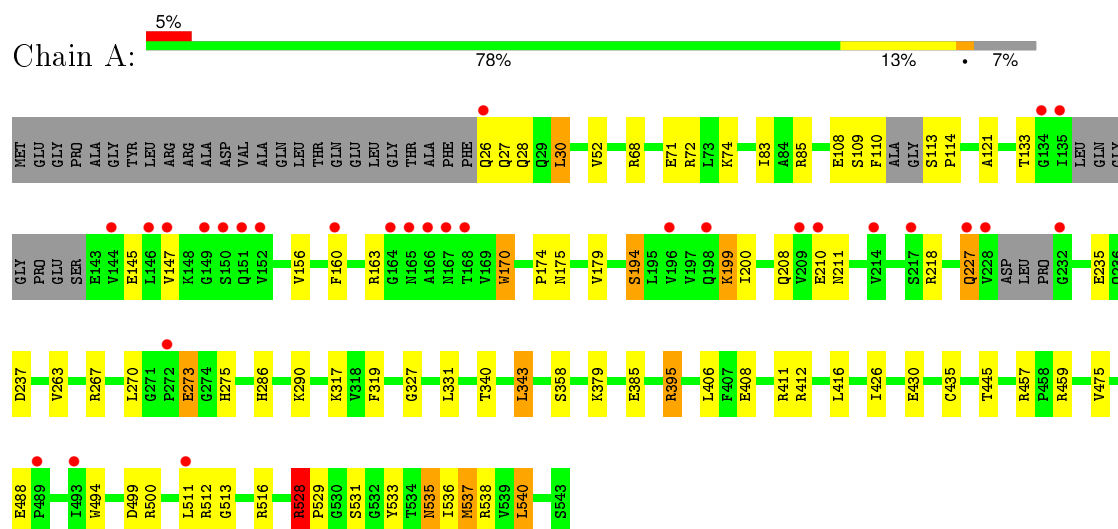
- Molecule 10 is water.

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

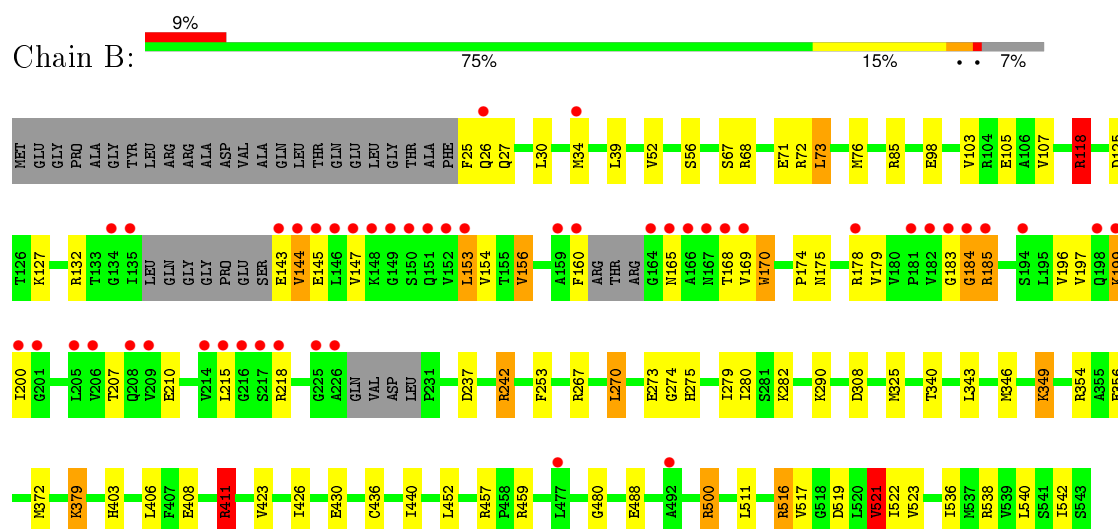
3 Residue-property plots [i](#)

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

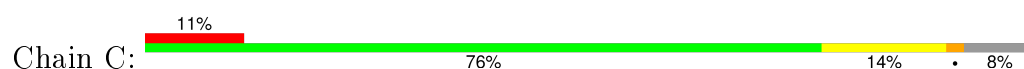
• Molecule 1: Pyruvate kinase isozymes L

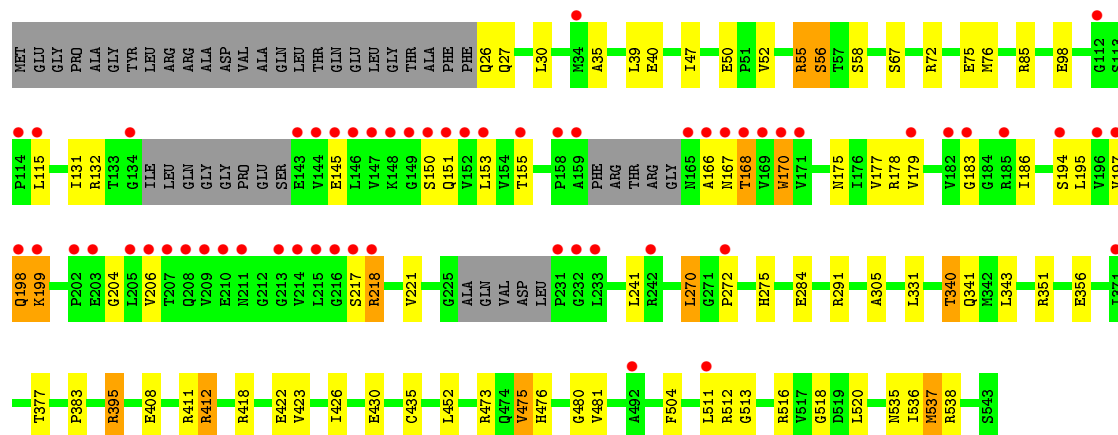


• Molecule 1: Pyruvate kinase isozymes L

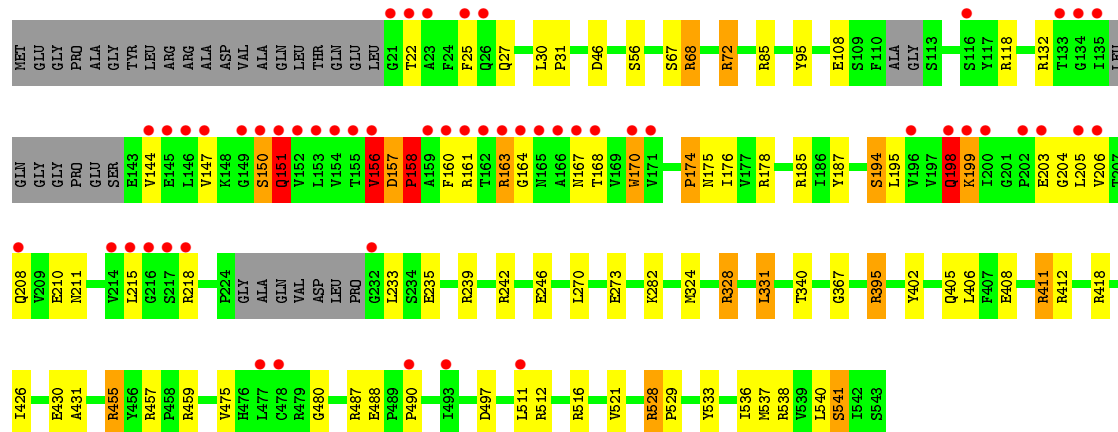
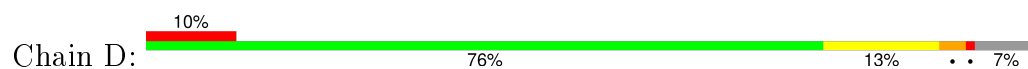


• Molecule 1: Pyruvate kinase isozymes L





• Molecule 1: Pyruvate kinase isozymes L



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.14Å 205.08Å 83.91Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	37.53 – 1.80 37.53 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (37.53-1.80) 97.5 (37.53-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.187 , 0.226 0.186 , 0.224	Depositor DCC
R_{free} test set	11896 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.3	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 236781 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17146	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, NA, MN, EDO, 1PE, ADN, FLC, PEG

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	1.13	5/4061 (0.1%)	1.17	19/5494 (0.3%)
1	B	1.05	4/3976 (0.1%)	1.09	18/5380 (0.3%)
1	C	1.06	4/3924 (0.1%)	1.04	11/5313 (0.2%)
1	D	1.23	13/4018 (0.3%)	1.19	24/5436 (0.4%)
All	All	1.12	26/15979 (0.2%)	1.12	72/21623 (0.3%)

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

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

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	203	GLU	CD-OE1	21.85	1.49	1.25
1	D	203	GLU	CD-OE2	13.51	1.40	1.25
1	D	198	GLN	CD-NE2	10.51	1.59	1.32
1	D	174	PRO	C-N	9.33	1.55	1.34
1	D	164	GLY	C-O	9.12	1.38	1.23

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ARG	NE-CZ-NH1	14.99	127.80	120.30
1	D	68	ARG	NE-CZ-NH2	-14.62	112.99	120.30
1	D	395	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	A	528	ARG	NE-CZ-NH1	12.97	126.78	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	395	ARG	NE-CZ-NH1	12.85	126.73	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	151	GLN	Mainchain
1	D	157	ASP	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3944	0	4061	64	1
1	B	3882	0	3990	72	0
1	C	3831	0	3928	76	0
1	D	3920	0	4026	77	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	4	0	0
3	B	13	0	4	4	0
3	C	13	0	4	0	0
3	D	13	0	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	8	0	12	0	0
5	B	8	0	12	0	0
5	C	8	0	12	1	0
5	D	12	0	18	0	0
6	A	7	0	10	9	0
6	B	7	0	10	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	C	17	0	22	22	0
9	D	38	0	26	3	0
10	A	361	0	0	13	1
10	B	324	0	0	6	0
10	C	333	0	0	12	0
10	D	306	0	0	11	0
All	All	17146	0	16183	280	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 280 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:606:1PE:H232	10:C:734:HOH:O	1.45	1.17
1:C:58:SER:N	8:C:606:1PE:H131	1.66	1.09
1:D:455:ARG:HH11	1:D:455:ARG:HG3	1.10	1.09
1:B:156:VAL:HG21	1:B:174:PRO:HA	1.34	1.08
1:C:476:HIS:ND1	8:C:606:1PE:H122	1.70	1.06

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:994:HOH:O	10:A:1017:HOH:O[1_455]	1.83	0.37
1:A:74:LYS:NZ	1:D:246:GLU:OE1[2_645]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/543 (95%)	504 (98%)	11 (2%)	2 (0%)	39	23
1	B	508/543 (94%)	491 (97%)	15 (3%)	2 (0%)	39	23
1	C	503/543 (93%)	492 (98%)	9 (2%)	2 (0%)	39	23
1	D	511/543 (94%)	494 (97%)	16 (3%)	1 (0%)	52	35
All	All	2039/2172 (94%)	1981 (97%)	51 (2%)	7 (0%)	39	29

5 of 7 Ramachandran outliers are listed below:

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

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	426/433 (98%)	404 (95%)	22 (5%)	29	12
1	B	415/433 (96%)	387 (93%)	28 (7%)	20	6
1	C	412/433 (95%)	395 (96%)	17 (4%)	37	19
1	D	420/433 (97%)	398 (95%)	22 (5%)	29	12
All	All	1673/1732 (97%)	1584 (95%)	89 (5%)	27	11

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	199	LYS
1	B	521	VAL
1	D	411	ARG
1	B	215	LEU
1	B	411	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	27	GLN
1	D	198	GLN
1	C	151	GLN
1	C	26	GLN
1	D	151	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FLC	A	602	2	3,12,12	2.10	1 (33%)	3,17,17	2.43	1 (33%)
4	FBP	A	603	-	18,20,20	1.10	1 (5%)	21,32,32	1.68	3 (14%)
5	EDO	A	604	-	3,3,3	0.74	0	2,2,2	0.94	0
5	EDO	A	605	-	3,3,3	0.74	0	2,2,2	0.59	0
6	PEG	A	606	-	6,6,6	0.67	0	5,5,5	1.51	2 (40%)
3	FLC	B	602	2	3,12,12	0.44	0	3,17,17	1.33	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FBP	B	603	-	18,20,20	1.08	1 (5%)	21,32,32	1.77	3 (14%)
5	EDO	B	604	-	3,3,3	0.77	0	2,2,2	0.84	0
6	PEG	B	605	-	6,6,6	0.92	0	5,5,5	0.52	0
5	EDO	B	606	-	3,3,3	1.52	0	2,2,2	0.64	0
5	EDO	C	601	-	3,3,3	0.88	0	2,2,2	1.08	0
3	FLC	C	603	2	3,12,12	2.57	2 (66%)	3,17,17	1.27	0
4	FBP	C	604	-	18,20,20	0.88	0	21,32,32	1.39	2 (9%)
8	1PE	C	605	-	9,9,15	2.12	5 (55%)	8,8,14	1.65	2 (25%)
8	1PE	C	606	-	6,6,15	2.64	2 (33%)	5,5,14	3.97	3 (60%)
5	EDO	C	607	-	3,3,3	0.80	0	2,2,2	0.33	0
3	FLC	D	602	2	3,12,12	2.13	1 (33%)	3,17,17	1.76	2 (66%)
4	FBP	D	603	-	18,20,20	1.50	4 (22%)	21,32,32	1.76	6 (28%)
9	ADN	D	604[A]	-	16,21,21	1.34	3 (18%)	16,31,31	2.40	5 (31%)
9	ADN	D	604[B]	-	16,21,21	1.20	2 (12%)	16,31,31	2.91	5 (31%)
5	EDO	D	605	-	3,3,3	0.97	0	2,2,2	0.75	0
5	EDO	D	606	-	3,3,3	0.78	0	2,2,2	1.19	0
5	EDO	D	607	-	3,3,3	1.09	0	2,2,2	0.27	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	FLC	A	602	2	-	0/6/16/16	0/0/0/0
4	FBP	A	603	-	-	0/13/32/32	0/1/1/1
5	EDO	A	604	-	-	0/1/1/1	0/0/0/0
5	EDO	A	605	-	-	0/1/1/1	0/0/0/0
6	PEG	A	606	-	-	0/4/4/4	0/0/0/0
3	FLC	B	602	2	-	0/6/16/16	0/0/0/0
4	FBP	B	603	-	-	0/13/32/32	0/1/1/1
5	EDO	B	604	-	-	0/1/1/1	0/0/0/0
6	PEG	B	605	-	-	0/4/4/4	0/0/0/0
5	EDO	B	606	-	-	0/1/1/1	0/0/0/0
5	EDO	C	601	-	-	0/1/1/1	0/0/0/0
3	FLC	C	603	2	-	0/6/16/16	0/0/0/0
4	FBP	C	604	-	-	0/13/32/32	0/1/1/1
8	1PE	C	605	-	-	0/7/7/13	0/0/0/0
8	1PE	C	606	-	-	0/4/4/13	0/0/0/0
5	EDO	C	607	-	-	0/1/1/1	0/0/0/0
3	FLC	D	602	2	-	0/6/16/16	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FBP	D	603	-	-	0/13/32/32	0/1/1/1
9	ADN	D	604[A]	-	-	0/2/22/22	0/3/3/3
9	ADN	D	604[B]	-	-	0/2/22/22	0/3/3/3
5	EDO	D	605	-	-	0/1/1/1	0/0/0/0
5	EDO	D	606	-	-	0/1/1/1	0/0/0/0
5	EDO	D	607	-	-	0/1/1/1	0/0/0/0

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	FBP	P1-O1	2.00	1.67	1.60
4	B	603	FBP	O2-C2	2.06	1.44	1.41
8	C	605	1PE	OH4-C13	2.07	1.50	1.42
9	D	604[B]	ADN	O4'-C1'	2.18	1.44	1.41
9	D	604[A]	ADN	O4'-C1'	2.20	1.44	1.41

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	604[B]	ADN	N3-C2-N1	-8.44	122.44	128.89
9	D	604[A]	ADN	N3-C2-N1	-6.90	123.61	128.89
9	D	604[B]	ADN	C2'-C1'-N9	-4.48	107.44	114.29
4	B	603	FBP	O1-P1-O1P	-4.26	96.30	107.14
4	C	604	FBP	O1-P1-O1P	-4.22	96.39	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 41 short contacts:

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

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	506/543 (93%)	0.08	29 (5%) 27 22	18, 32, 73, 103	0
1	B	505/543 (93%)	0.26	47 (9%) 11 8	20, 33, 96, 125	0
1	C	500/543 (92%)	0.37	58 (11%) 6 5	19, 35, 95, 120	1 (0%)
1	D	507/543 (93%)	0.34	53 (10%) 8 6	20, 34, 115, 197	0
All	All	2018/2172 (92%)	0.26	187 (9%) 11 8	18, 34, 96, 197	1 (0%)

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	135	ILE	8.5
1	B	144	VAL	6.6
1	C	144	VAL	6.5
1	C	217	SER	6.4
1	C	168	THR	6.2

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
9	ADN	D	604[B]	19/19	0.92	0.20	10.90	26,30,47,49	19
9	ADN	D	604[A]	19/19	0.92	0.20	10.83	26,30,41,43	19
7	NA	B	607	1/1	0.92	0.15	4.47	37,37,37,37	0
8	1PE	C	606	7/16	0.93	0.21	2.76	29,32,41,42	0
5	EDO	B	606	4/4	0.85	0.14	1.05	32,36,36,44	0
6	PEG	A	606	7/7	0.88	0.15	0.94	37,42,47,48	0
5	EDO	A	605	4/4	0.94	0.13	0.71	30,35,36,38	0
5	EDO	A	604	4/4	0.97	0.12	0.33	25,27,28,34	0
5	EDO	D	607	4/4	0.96	0.15	0.31	31,35,36,38	0
7	NA	C	608	1/1	0.95	0.09	0.14	41,41,41,41	0
5	EDO	D	606	4/4	0.95	0.11	-0.01	42,43,52,55	0
5	EDO	C	601	4/4	0.95	0.10	-0.17	35,35,37,38	0
4	FBP	B	603	20/20	0.98	0.07	-0.49	23,26,29,30	0
5	EDO	B	604	4/4	0.97	0.10	-0.86	27,32,34,37	0
5	EDO	D	605	4/4	0.95	0.11	-0.90	27,29,32,38	0
4	FBP	A	603	20/20	0.99	0.06	-0.95	22,25,28,28	0
4	FBP	C	604	20/20	0.98	0.07	-1.05	23,27,29,30	0
3	FLC	C	603	13/13	0.97	0.07	-1.15	24,31,41,47	0
4	FBP	D	603	20/20	0.98	0.06	-1.27	26,28,32,32	0
7	NA	A	607	1/1	0.96	0.07	-1.40	40,40,40,40	0
3	FLC	B	602	13/13	0.97	0.07	-1.68	26,30,42,44	0
3	FLC	D	602	13/13	0.95	0.07	-1.69	25,32,42,42	0
3	FLC	A	602	13/13	0.96	0.07	-1.73	21,27,36,39	0
7	NA	D	608	1/1	0.98	0.06	-1.91	38,38,38,38	0
5	EDO	C	607	4/4	0.84	0.14	-	44,52,55,56	0
6	PEG	B	605	7/7	0.87	0.26	-	42,50,59,60	0
2	MN	A	601	1/1	1.00	0.07	-	26,26,26,26	0
2	MN	B	601	1/1	1.00	0.05	-	27,27,27,27	0
2	MN	C	602	1/1	1.00	0.04	-	28,28,28,28	0
2	MN	D	601	1/1	1.00	0.07	-	28,28,28,28	0
8	1PE	C	605	10/16	0.83	0.16	-	41,46,48,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.