



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

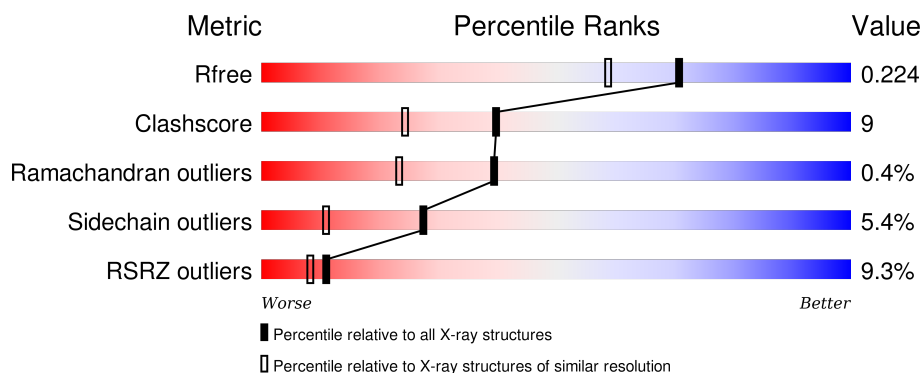
# 1 Overall quality at a glance

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  $\geq 3$ , 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			

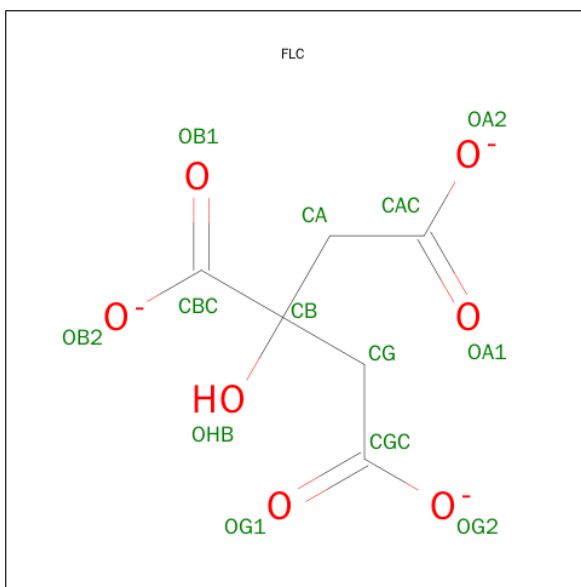
There are 4 discrepancies between the modelled and reference sequences:

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).

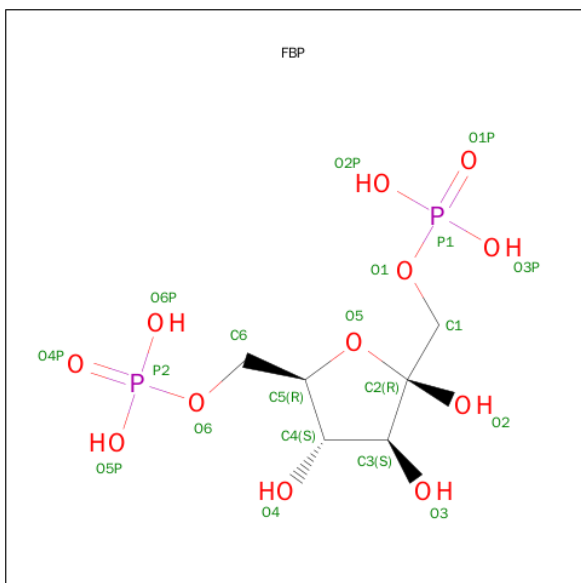
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



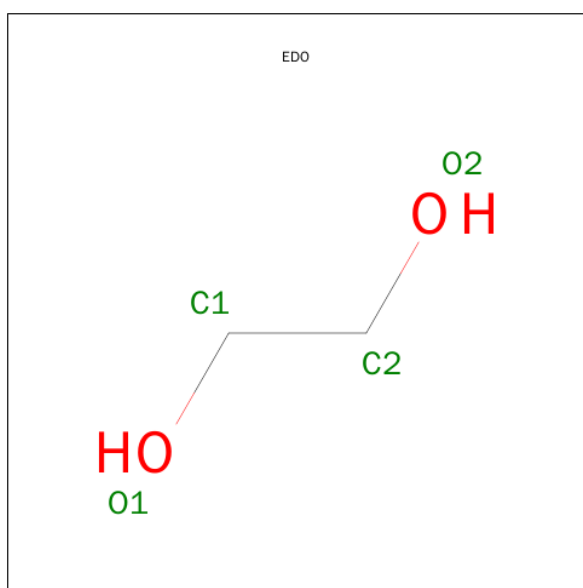
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

- 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:  $C_2H_6O_2$ ).



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	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

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

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

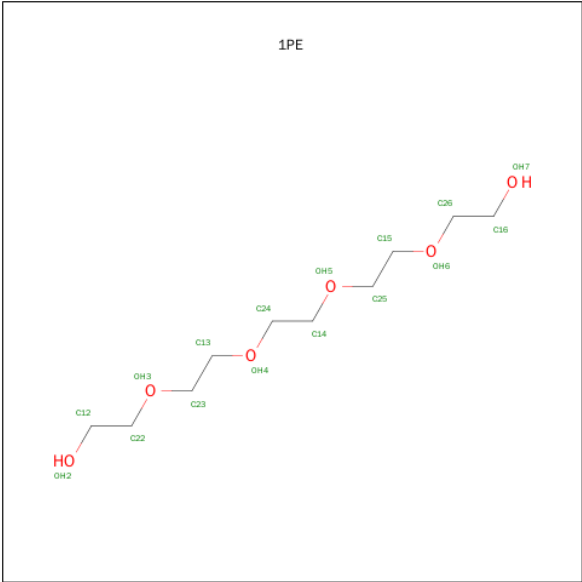


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		

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

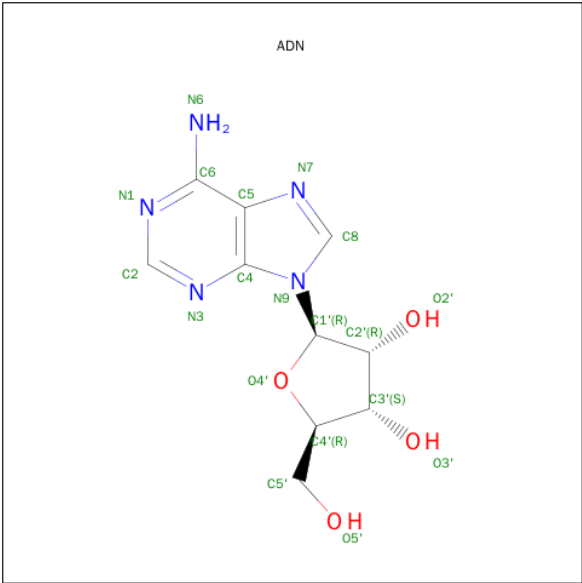
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		
7	A	1	Total	Na	0	0
			1	1		
7	D	1	Total	Na	0	0
			1	1		
7	C	1	Total	Na	0	0
			1	1		

- 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	0	0
			10	6	4		
8	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is ADENOSINE (three-letter code: ADN) (formula: C<sub>10</sub>H<sub>13</sub>N<sub>5</sub>O<sub>4</sub>).



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

- Molecule 10 is water.

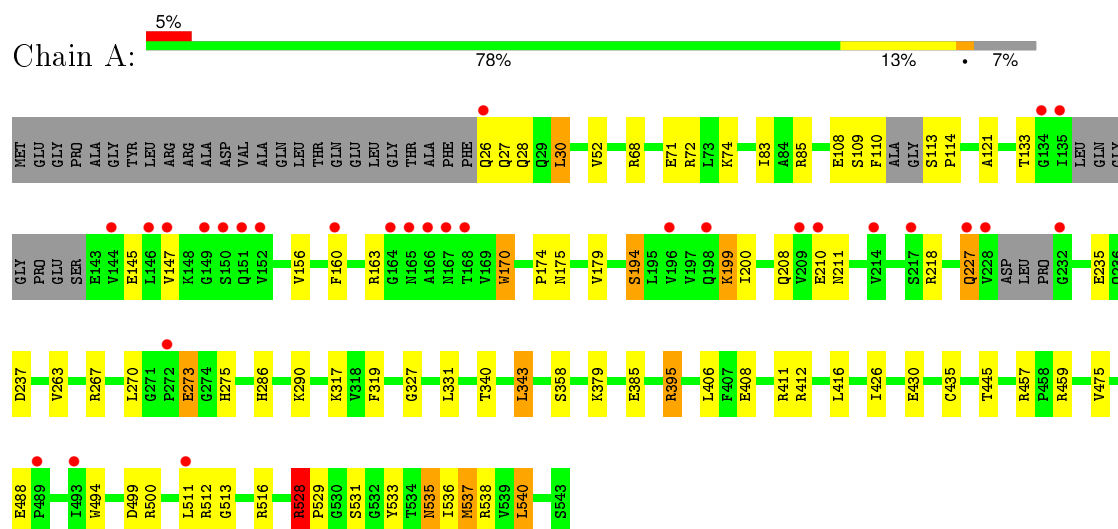


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	361	Total 361	O 361	0	0
10	B	324	Total 324	O 324	0	0
10	C	333	Total 333	O 333	0	0
10	D	306	Total 306	O 306	0	0

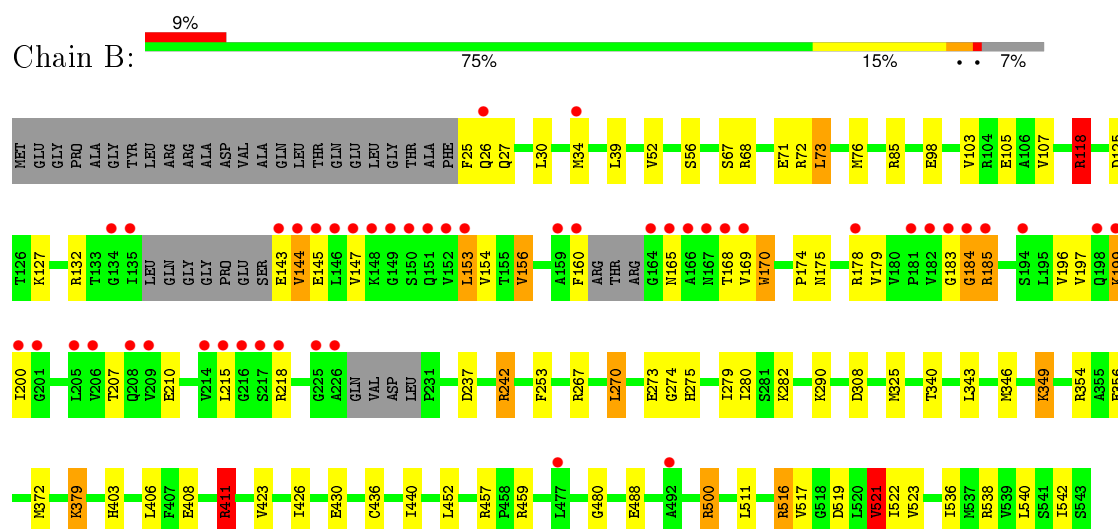
### 3 Residue-property plots [i](#)

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.

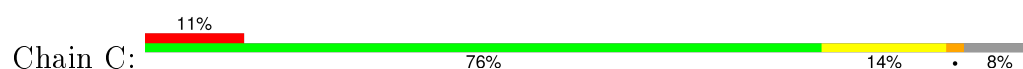
#### • Molecule 1: Pyruvate kinase isozymes L

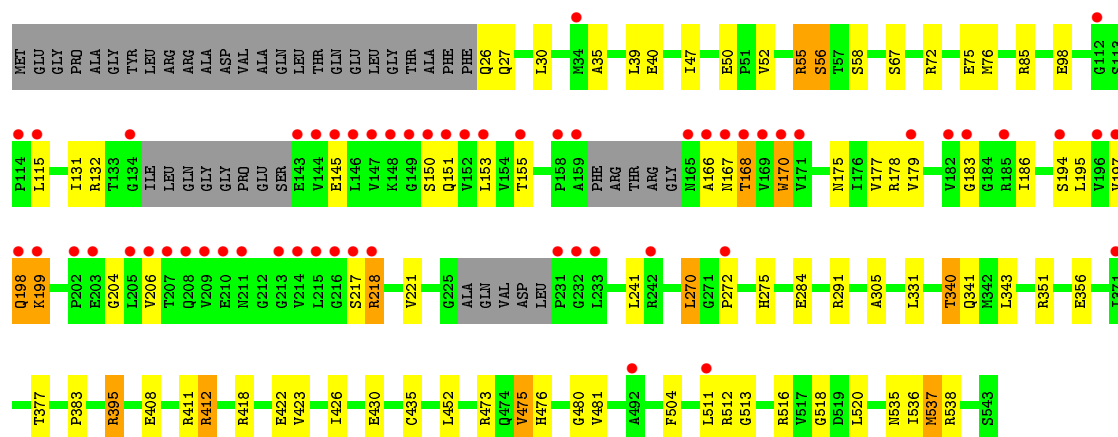


#### • Molecule 1: Pyruvate kinase isozymes L

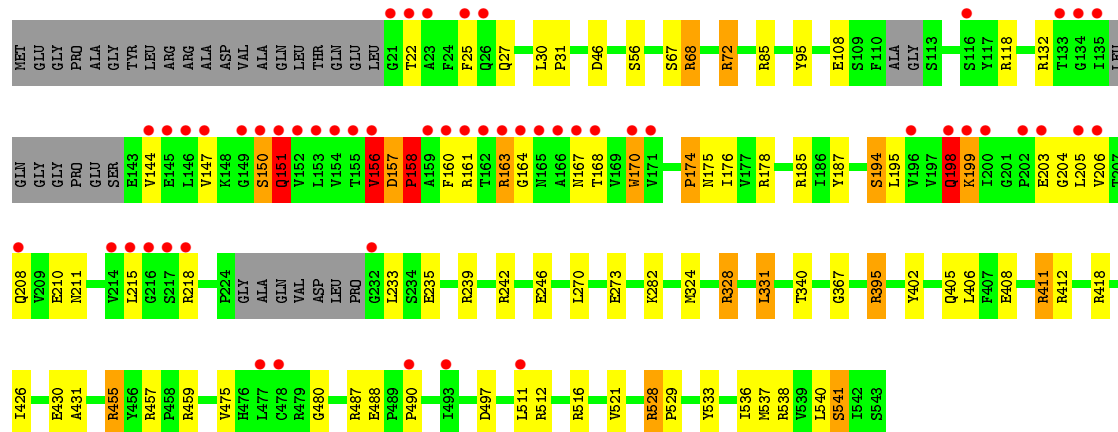
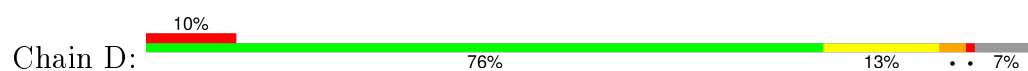


#### • Molecule 1: Pyruvate kinase isozymes L





### • 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.3	EDS
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

All (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
1	A	358	SER	CB-OG	-8.01	1.31	1.42
1	D	204	GLY	C-N	7.85	1.52	1.34
1	D	158	PRO	N-CA	7.38	1.59	1.47
1	D	156	VAL	CA-C	6.86	1.70	1.52
1	D	167	ASN	C-O	6.51	1.35	1.23
1	C	167	ASN	CG-ND2	6.29	1.48	1.32
1	A	494	TRP	CD2-CE2	6.14	1.48	1.41
1	B	105	GLU	CD-OE2	-5.97	1.19	1.25
1	D	204	GLY	C-O	5.91	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	170	TRP	CD2-CE2	5.51	1.48	1.41
1	B	71	GLU	CD-OE1	5.49	1.31	1.25
1	C	150	SER	CB-OG	5.46	1.49	1.42
1	A	170	TRP	CD2-CE2	5.40	1.47	1.41
1	D	367	GLY	N-CA	5.32	1.54	1.46
1	B	170	TRP	CD2-CE2	5.28	1.47	1.41
1	A	147	VAL	CB-CG1	5.22	1.63	1.52
1	C	56	SER	CB-OG	-5.21	1.35	1.42
1	C	170	TRP	CD2-CE2	5.17	1.47	1.41
1	B	273	GLU	CD-OE2	5.16	1.31	1.25
1	D	198	GLN	CG-CD	5.02	1.62	1.51
1	A	319	PHE	CG-CD2	5.01	1.46	1.38

All (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
1	D	395	ARG	NE-CZ-NH1	12.85	126.73	120.30
1	D	328	ARG	NE-CZ-NH1	12.23	126.42	120.30
1	A	395	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	D	537	MET	CG-SD-CE	-11.85	81.23	100.20
1	A	85	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	A	528	ARG	NE-CZ-NH2	-11.34	114.63	120.30
1	D	328	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	D	68	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	A	237	ASP	CB-CG-OD1	9.32	126.69	118.30
1	D	85	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	C	537	MET	CG-SD-CE	-9.06	85.71	100.20
1	B	349	LYS	CD-CE-NZ	-8.65	91.81	111.70
1	B	354	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	343	LEU	CB-CG-CD1	8.49	125.44	111.00
1	B	237	ASP	CB-CG-OD1	8.08	125.58	118.30
1	D	158	PRO	N-CA-CB	-7.92	93.79	103.30
1	A	263	VAL	CG1-CB-CG2	7.83	123.44	110.90
1	D	331	LEU	CB-CG-CD1	-7.74	97.85	111.00
1	D	132	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	C	475	VAL	CG1-CB-CG2	7.67	123.16	110.90
1	D	198	GLN	CG-CD-OE1	7.54	136.67	121.60
1	A	459	ARG	NE-CZ-NH2	-7.50	116.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	D	132	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	178	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	118[A]	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	118[B]	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	85	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	73	LEU	CB-CG-CD2	6.90	122.74	111.00
1	C	85	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	237	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	A	72	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	475	VAL	CG1-CB-CG2	6.64	121.53	110.90
1	A	72	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	D	72	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	540	LEU	CB-CG-CD2	-6.32	100.26	111.00
1	B	127	LYS	CD-CE-NZ	-6.24	97.35	111.70
1	B	325	MET	CA-CB-CG	-6.23	102.71	113.30
1	D	46	ASP	CB-CG-OD1	6.07	123.77	118.30
1	C	291	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	C	55	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	B	411	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	C	55	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	D	72	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	521	VAL	CG1-CB-CG2	5.76	120.12	110.90
1	D	151	GLN	C-N-CA	-5.67	107.53	121.70
1	D	487	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	308	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	537[A]	MET	CG-SD-CE	-5.60	91.24	100.20
1	A	537[B]	MET	CG-SD-CE	-5.60	91.24	100.20
1	B	85	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	85	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	153	LEU	CA-CB-CG	5.58	128.12	115.30
1	D	475	VAL	CG1-CB-CG2	5.57	119.82	110.90
1	B	411	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	290	LYS	CD-CE-NZ	-5.50	99.05	111.70
1	D	174	PRO	O-C-N	5.49	131.49	122.70
1	B	379	LYS	CD-CE-NZ	5.46	124.27	111.70
1	D	151	GLN	CA-CB-CG	-5.44	101.44	113.40
1	A	385	GLU	OE1-CD-OE2	-5.43	116.79	123.30
1	D	459	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	459	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	452	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	C	75	GLU	OE1-CD-OE2	-5.16	117.10	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	459	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	473	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	D	233	LEU	CA-CB-CG	5.12	127.06	115.30
1	C	512	ARG	NE-CZ-NH1	-5.04	117.78	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

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

All (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
8:C:605:1PE:H241	8:C:605:1PE:H221	1.34	1.05
1:B:516:ARG:NH1	1:B:516:ARG:HG3	1.61	1.02
1:B:185:ARG:HH11	1:B:185:ARG:HG2	1.22	1.02
1:B:516:ARG:CG	1:B:516:ARG:HH11	1.74	0.99
1:B:185:ARG:CG	1:B:185:ARG:HH11	1.77	0.98
1:D:163:ARG:HG3	1:D:163:ARG:O	1.62	0.97
1:B:516:ARG:HG3	1:B:516:ARG:HH11	0.81	0.96
1:C:56:SER:O	8:C:606:1PE:H132	1.67	0.93
1:D:160:PHE:HD2	1:D:163:ARG:HG2	1.35	0.90
1:D:242[B]:ARG:HG2	1:D:242[B]:ARG:HH11	1.35	0.89
1:C:408:GLU:HG3	10:C:704:HOH:O	1.72	0.89
1:A:267[B]:ARG:HD2	10:A:800:HOH:O	1.74	0.88
1:D:455:ARG:NH1	1:D:455:ARG:HG3	1.88	0.88
1:A:430:GLU:OE2	1:B:430[B]:GLU:OE1	1.93	0.87
1:A:411:ARG:HH12	6:A:606:PEG:H41	1.41	0.85
1:A:528:ARG:HD2	1:A:533:TYR:CD1	2.13	0.83
1:A:327:GLY:O	1:A:331[B]:LEU:HD13	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HD2	1:B:196:VAL:HG22	1.61	0.82
8:C:605:1PE:H241	8:C:605:1PE:C22	2.10	0.81
1:D:418:ARG:NH1	10:D:954:HOH:O	2.11	0.81
1:C:538:ARG:HG2	1:D:536:ILE:HG12	1.61	0.81
1:D:147:VAL:O	1:D:150:SER:HB2	1.79	0.80
1:C:58:SER:H	8:C:606:1PE:H131	1.41	0.80
1:A:488[B]:GLU:OE1	1:A:500:ARG:NH2	2.14	0.80
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.65	0.79
1:A:227:GLN:HB2	10:A:883:HOH:O	1.82	0.78
1:C:72:ARG:NH1	10:C:998:HOH:O	1.88	0.78
1:A:331[A]:LEU:HD22	10:A:979:HOH:O	1.83	0.77
1:D:108:GLU:HG2	10:D:858:HOH:O	1.83	0.77
1:C:218:ARG:NH1	1:C:218:ARG:HB3	1.99	0.77
1:C:411:ARG:HG3	1:C:426:ILE:HD11	1.66	0.77
1:B:185:ARG:NH1	1:B:185:ARG:HG2	1.89	0.76
1:D:68:ARG:NH2	1:D:95:TYR:O	2.18	0.75
1:D:118[A]:ARG:HG2	10:D:747:HOH:O	1.86	0.75
10:C:832:HOH:O	1:D:411:ARG:HD2	1.84	0.75
6:A:606:PEG:H12	10:B:748:HOH:O	1.87	0.75
1:A:411:ARG:NH1	6:A:606:PEG:H41	2.00	0.75
1:C:58:SER:OG	8:C:606:1PE:H221	1.87	0.75
8:C:606:1PE:H121	10:C:734:HOH:O	1.86	0.74
1:C:430[A]:GLU:OE2	1:D:411:ARG:HD3	1.88	0.74
1:B:175:ASN:OD1	1:B:178:ARG:HD3	1.88	0.74
1:D:528:ARG:HD2	1:D:533:TYR:CD1	2.23	0.74
1:D:418:ARG:HG2	1:D:418:ARG:HH11	1.53	0.73
1:B:178:ARG:HB3	1:B:178:ARG:NH1	2.03	0.73
1:A:199:LYS:HG3	1:A:200:ILE:H	1.54	0.72
1:C:476:HIS:CE1	8:C:606:1PE:H122	2.25	0.72
1:A:74:LYS:HE3	1:A:109:SER:OG	1.89	0.71
1:C:56:SER:O	8:C:606:1PE:C23	2.38	0.71
1:B:185:ARG:HH11	1:B:185:ARG:CB	2.03	0.71
1:B:67:SER:HB2	1:B:76[B]:MET:SD	2.31	0.71
1:C:218:ARG:HH11	1:C:218:ARG:HB3	1.55	0.70
1:A:512:ARG:HD3	10:A:887:HOH:O	1.91	0.70
1:A:538:ARG:HG2	1:B:536:ILE:HG12	1.73	0.70
1:B:521:VAL:HB	1:B:542[A]:ILE:HD11	1.72	0.70
1:B:183:GLY:HA2	1:B:197:VAL:O	1.92	0.69
1:D:411:ARG:HG3	1:D:426:ILE:HD11	1.73	0.69
1:B:523:VAL:HG21	1:B:540[A]:LEU:HD12	1.73	0.69
1:A:331[B]:LEU:HD11	1:C:39:LEU:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ARG:CG	1:D:163:ARG:O	2.40	0.68
1:D:194:SER:HB2	1:D:211:ASN:HB2	1.74	0.68
1:A:411:ARG:HH22	6:A:606:PEG:H41	1.59	0.68
1:D:160:PHE:CD2	1:D:163:ARG:HG2	2.25	0.68
1:D:242[B]:ARG:CG	1:D:242[B]:ARG:HH11	2.04	0.68
9:D:604[B]:ADN:H2'	9:D:604[B]:ADN:O5'	1.94	0.68
1:D:198:GLN:HE22	1:D:208:GLN:HB3	1.58	0.68
1:C:56:SER:O	8:C:606:1PE:H231	1.94	0.67
1:A:331[A]:LEU:HD21	10:A:981:HOH:O	1.94	0.67
1:C:56:SER:O	8:C:606:1PE:C13	2.41	0.67
1:C:27:GLN:HE21	1:C:50:GLU:H	1.42	0.67
1:B:197:VAL:HG22	1:B:207:THR:HG22	1.77	0.67
1:C:177:VAL:HG21	1:C:204:GLY:HA2	1.76	0.67
1:B:519:ASP:O	1:B:542[A]:ILE:HD13	1.94	0.66
1:A:74:LYS:CE	1:A:109:SER:OG	2.43	0.66
1:C:198:GLN:HG3	10:C:907:HOH:O	1.95	0.66
1:A:199:LYS:HG3	1:A:200:ILE:N	2.10	0.66
1:B:156:VAL:CG2	1:B:174:PRO:HA	2.20	0.66
1:A:108:GLU:HG2	10:A:783:HOH:O	1.96	0.66
1:A:327:GLY:O	1:A:331[B]:LEU:CD1	2.44	0.65
1:C:67:SER:HB2	1:C:76[B]:MET:SD	2.37	0.65
1:C:411:ARG:HH21	1:C:412:ARG:HH11	1.45	0.65
1:A:499[B]:ASP:OD1	10:A:1039:HOH:O	2.15	0.65
1:B:185:ARG:CG	1:B:185:ARG:NH1	2.47	0.63
1:D:156:VAL:CG2	1:D:176:ILE:HG22	2.28	0.63
1:D:175:ASN:OD1	1:D:178:ARG:HD3	1.98	0.63
1:B:488:GLU:HG3	1:B:500:ARG:HH21	1.63	0.63
1:B:27:GLN:OE1	1:B:52:VAL:HG21	2.00	0.62
1:D:516:ARG:HH11	1:D:516:ARG:HG3	1.64	0.62
1:D:541:SER:HB3	10:D:874:HOH:O	1.99	0.62
1:A:411:ARG:NH2	6:A:606:PEG:H41	2.14	0.62
1:A:194:SER:HB3	1:A:211:ASN:HB2	1.80	0.61
1:A:331[B]:LEU:CD1	1:C:39:LEU:HD11	2.31	0.61
1:B:178:ARG:HB3	1:B:178:ARG:HH11	1.64	0.61
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.82	0.61
1:D:273:GLU:HG2	10:D:721:HOH:O	1.99	0.61
1:D:418:ARG:HG2	1:D:418:ARG:NH1	2.15	0.61
1:A:156:VAL:HG11	1:A:174:PRO:HA	1.84	0.60
1:C:58:SER:CA	8:C:606:1PE:H131	2.32	0.58
1:D:27:GLN:HG2	10:D:957:HOH:O	2.02	0.58
1:D:528:ARG:HD2	1:D:533:TYR:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:ARG:CG	1:D:455:ARG:NH1	2.57	0.58
1:C:518:GLY:O	1:D:418:ARG:NH2	2.37	0.58
1:C:58:SER:OG	8:C:606:1PE:C13	2.52	0.57
1:A:411:ARG:HG3	1:A:426:ILE:HD11	1.85	0.57
1:A:267[B]:ARG:HD2	10:A:869:HOH:O	2.03	0.57
1:D:455:ARG:HH11	1:D:455:ARG:CG	1.93	0.57
1:B:267[B]:ARG:HD2	1:B:279:ILE:HD12	1.87	0.57
1:C:26:GLN:HG2	10:C:805:HOH:O	2.04	0.56
1:D:282:LYS:HE3	3:D:602:FLC:OA2	2.05	0.56
1:D:160:PHE:HD2	1:D:163:ARG:CG	2.13	0.56
1:C:183:GLY:HA2	1:C:197:VAL:O	2.04	0.56
1:A:331[B]:LEU:HD11	1:C:39:LEU:CD1	2.36	0.56
1:C:27:GLN:NE2	1:C:50:GLU:H	2.04	0.56
1:D:156:VAL:CG1	1:D:174:PRO:HA	2.36	0.56
1:C:56:SER:HB2	1:C:480:GLY:CA	2.35	0.56
1:D:198:GLN:HE22	1:D:208:GLN:CB	2.19	0.56
8:C:606:1PE:C23	10:C:734:HOH:O	2.23	0.55
1:A:528:ARG:HD3	1:A:529:PRO:O	2.06	0.55
1:D:324:MET:SD	1:D:328:ARG:HD3	2.46	0.55
1:B:156:VAL:HG21	1:B:174:PRO:CA	2.23	0.55
1:B:67:SER:HA	1:B:72:ARG:HG2	1.86	0.55
1:B:56:SER:HB2	1:B:480:GLY:CA	2.36	0.55
1:C:177:VAL:CG2	1:C:204:GLY:HA2	2.36	0.55
1:D:194:SER:HB3	1:D:210:GLU:HB3	1.89	0.55
1:A:331[A]:LEU:CD2	10:A:981:HOH:O	2.54	0.54
1:D:156:VAL:HG21	1:D:176:ILE:HG22	1.89	0.54
1:A:445:THR:HB	1:A:531[B]:SER:OG	2.07	0.54
1:B:517:VAL:HG23	10:B:922:HOH:O	2.06	0.54
1:C:58:SER:N	8:C:606:1PE:C13	2.57	0.54
1:D:56:SER:HB2	1:D:480:GLY:HA2	1.89	0.54
1:B:516:ARG:CG	1:B:516:ARG:NH1	2.43	0.54
1:D:175:ASN:HB2	10:D:999:HOH:O	2.07	0.53
1:C:536:ILE:HG12	1:D:538[A]:ARG:HG2	1.89	0.53
1:A:411:ARG:CZ	6:A:606:PEG:H41	2.37	0.53
1:A:536:ILE:HG12	1:B:538:ARG:HG2	1.91	0.53
1:A:411:ARG:HH22	6:A:606:PEG:C4	2.21	0.53
1:C:343:LEU:HD23	1:C:356:GLU:HB3	1.91	0.53
1:C:55:ARG:HB2	1:C:395:ARG:HG3	1.91	0.52
1:D:156:VAL:HG11	1:D:174:PRO:HA	1.91	0.52
1:D:157:ASP:O	1:D:158:PRO:C	2.48	0.52
1:B:343:LEU:HD23	1:B:356:GLU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118[A]:ARG:HG2	10:B:702:HOH:O	2.10	0.52
1:A:267[B]:ARG:CD	10:A:869:HOH:O	2.57	0.52
1:B:196:VAL:HG23	1:B:210:GLU:HB2	1.92	0.52
1:A:513:GLY:HA2	1:A:516:ARG:HH21	1.74	0.52
1:A:535:ASN:OD1	1:A:536:ILE:HG13	2.09	0.52
1:B:160:PHE:HB2	1:B:170:TRP:CD1	2.45	0.52
1:B:523:VAL:HG21	1:B:540[A]:LEU:CD1	2.38	0.51
1:C:52:VAL:HG22	10:C:886:HOH:O	2.08	0.51
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.75	0.51
1:A:416:LEU:HD13	1:B:436:CYS:SG	2.51	0.51
1:C:411:ARG:HD2	1:D:430[A]:GLU:OE2	2.10	0.51
9:D:604[B]:ADN:H1'	10:D:756:HOH:O	2.11	0.51
1:D:490:PRO:HA	1:D:497:ASP:OD1	2.10	0.51
1:C:67:SER:HA	1:C:72:ARG:HG2	1.93	0.50
1:B:372:MET:CE	3:B:602:FLC:OA2	2.60	0.50
1:B:267[B]:ARG:HD2	1:B:279:ILE:CD1	2.41	0.50
1:A:163:ARG:NH1	1:A:163:ARG:HG2	2.27	0.49
1:A:331[B]:LEU:HD11	1:C:39:LEU:CG	2.41	0.49
1:B:178:ARG:CB	1:B:178:ARG:HH11	2.25	0.49
1:D:170:TRP:HZ3	1:D:218:ARG:HH22	1.60	0.49
1:B:372:MET:HE1	3:B:602:FLC:OA2	2.13	0.49
1:D:170:TRP:HZ3	1:D:218:ARG:NH2	2.10	0.49
1:D:235:GLU:HG2	1:D:239:ARG:NH1	2.28	0.49
1:C:58:SER:OG	8:C:606:1PE:H131	2.12	0.48
1:B:68:ARG:NH2	1:B:98:GLU:HB2	2.28	0.48
1:C:153:LEU:HB3	1:C:168:THR:HG23	1.94	0.48
1:C:58:SER:H	8:C:606:1PE:C13	2.19	0.48
1:B:98:GLU:HG3	10:B:859:HOH:O	2.14	0.48
9:D:604[B]:ADN:O5'	9:D:604[B]:ADN:C2'	2.62	0.47
1:D:235:GLU:HG2	1:D:239:ARG:HH12	1.79	0.47
1:C:155:THR:O	1:C:170:TRP:HA	2.15	0.47
1:B:132:ARG:HD2	1:B:218:ARG:HH21	1.79	0.47
1:D:402:TYR:CD2	1:D:405[A]:GLN:HB3	2.49	0.47
1:B:185:ARG:NH1	1:B:185:ARG:CB	2.74	0.47
1:D:147:VAL:O	1:D:150:SER:CB	2.57	0.47
1:A:435:CYS:HB3	1:B:423:VAL:CG2	2.45	0.47
1:A:194:SER:OG	1:A:210:GLU:OE1	2.32	0.47
1:B:488:GLU:HG3	1:B:500:ARG:NH2	2.30	0.47
1:C:199:LYS:HA	1:C:199:LYS:HZ3	1.80	0.47
1:C:435:CYS:HB2	1:C:520:LEU:HD12	1.96	0.47
1:C:151:GLN:HE22	1:C:206:VAL:HG12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:O	1:B:107:VAL:HG23	2.15	0.47
1:A:275[A]:HIS:CD2	10:A:800:HOH:O	2.68	0.46
1:D:198:GLN:N	1:D:206:VAL:O	2.26	0.46
1:C:377:THR:HA	1:C:383:PRO:HB3	1.97	0.46
6:A:606:PEG:H11	1:B:403:HIS:HB2	1.97	0.46
1:D:185:ARG:HH21	1:D:210:GLU:CD	2.18	0.46
1:C:58:SER:CB	8:C:606:1PE:H131	2.46	0.46
1:D:25:PHE:O	1:D:31:PRO:HD3	2.15	0.46
1:C:284:GLU:HG2	1:C:305:ALA:HB3	1.97	0.46
1:D:406:LEU:HD21	1:D:457:ARG:HG3	1.97	0.46
1:B:406:LEU:HD21	1:B:457:ARG:HG3	1.98	0.46
1:B:516:ARG:NH1	10:B:946:HOH:O	2.47	0.46
1:C:175:ASN:HB2	10:C:836:HOH:O	2.15	0.46
1:A:199:LYS:HE2	1:A:200:ILE:H	1.80	0.46
1:B:267[B]:ARG:NH2	1:B:274:GLY:O	2.48	0.46
1:D:488:GLU:H	1:D:488:GLU:HG2	1.62	0.46
1:A:113:SER:HA	1:A:114:PRO:HD3	1.77	0.45
1:B:408:GLU:HA	1:B:411:ARG:HH21	1.81	0.45
1:D:56:SER:HB2	1:D:480:GLY:CA	2.46	0.45
1:C:199:LYS:HA	1:C:199:LYS:NZ	2.32	0.45
1:B:39:LEU:HD21	1:D:331:LEU:CD1	2.47	0.45
1:B:282:LYS:HE3	3:B:602:FLC:OA1	2.17	0.45
1:C:131:ILE:HB	1:C:221:VAL:HB	1.98	0.45
1:D:118[A]:ARG:HH12	1:D:512:ARG:HD3	1.81	0.45
1:A:199:LYS:CG	1:A:200:ILE:H	2.28	0.45
1:D:412:ARG:HB2	10:D:995:HOH:O	2.15	0.45
1:A:286:HIS:CE1	1:A:290:LYS:HG3	2.51	0.45
1:D:408:GLU:HA	1:D:411:ARG:HH21	1.81	0.45
1:B:267[A]:ARG:NH1	10:B:942:HOH:O	2.42	0.45
1:C:186:ILE:O	1:C:194:SER:HA	2.17	0.45
1:C:481:VAL:O	8:C:606:1PE:H121	2.17	0.44
1:A:537[A]:MET:HE3	1:A:537[A]:MET:HB2	1.78	0.44
1:A:28:GLN:HG2	1:A:30:LEU:HD22	2.00	0.44
1:A:411:ARG:HH12	6:A:606:PEG:C4	2.20	0.44
1:D:194:SER:O	1:D:195:LEU:HD23	2.17	0.44
1:D:516:ARG:NH1	1:D:516:ARG:HG3	2.30	0.44
1:B:199:LYS:HG3	1:B:200:ILE:N	2.31	0.44
1:B:125:ASP:OD2	3:B:602:FLC:OA1	2.35	0.44
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.99	0.44
1:C:272:PRO:HA	1:C:275[B]:HIS:CD2	2.53	0.44
1:A:435:CYS:HB3	1:B:423:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:SER:HA	1:D:72:ARG:HG2	1.99	0.43
1:B:144:VAL:HG21	1:B:165:ASN:HA	2.00	0.43
8:C:605:1PE:H242	8:C:605:1PE:H231	1.71	0.43
1:C:535:ASN:OD1	1:C:536:ILE:HG13	2.17	0.43
1:A:133:THR:HA	1:A:170:TRP:O	2.17	0.43
1:C:513:GLY:HA2	10:C:821:HOH:O	2.18	0.43
1:C:241:LEU:HD22	1:C:270[A]:LEU:HD11	2.00	0.43
1:A:110:PHE:HB2	10:A:867:HOH:O	2.18	0.43
1:D:161:ARG:HA	1:D:170:TRP:CD2	2.54	0.43
1:D:161:ARG:HA	1:D:170:TRP:CG	2.53	0.43
1:A:406:LEU:HD21	1:A:457:ARG:HG3	2.00	0.43
1:A:83:ILE:HG12	1:A:121:ALA:HB3	2.01	0.43
1:C:199:LYS:HA	1:C:199:LYS:CE	2.49	0.43
1:A:331[B]:LEU:HD11	1:C:39:LEU:HG	1.99	0.43
1:A:160:PHE:HA	1:A:163:ARG:HD2	2.01	0.42
1:C:35:ALA:HB1	1:C:40[A]:GLU:HB3	2.01	0.42
1:A:71[A]:GLU:HG3	10:A:773:HOH:O	2.18	0.42
1:B:267[B]:ARG:NH2	1:B:275:HIS:HA	2.34	0.42
1:D:242[A]:ARG:NH2	1:D:270:LEU:O	2.52	0.42
1:D:516:ARG:CG	1:D:516:ARG:NH1	2.80	0.42
1:D:218:ARG:HD2	10:D:925:HOH:O	2.17	0.42
1:B:242:ARG:NH2	1:B:270:LEU:O	2.52	0.42
1:B:440:ILE:HA	1:B:522:ILE:O	2.20	0.42
1:C:67:SER:CB	1:C:76[B]:MET:SD	3.08	0.42
1:A:317:LYS:HD3	1:C:47:ILE:O	2.20	0.41
1:B:346:MET:HA	1:B:349:LYS:O	2.21	0.41
1:C:408:GLU:OE1	1:D:408:GLU:OE2	2.38	0.41
1:C:331:LEU:HD23	1:C:331:LEU:HA	1.83	0.41
1:D:185:ARG:CD	1:D:187:TYR:CE1	3.03	0.41
1:D:528:ARG:HD3	1:D:529:PRO:O	2.21	0.41
1:D:242[B]:ARG:CG	1:D:242[B]:ARG:NH1	2.71	0.41
1:C:408:GLU:O	1:C:412:ARG:HB2	2.21	0.41
1:A:408[B]:GLU:OE1	1:A:412:ARG:HD3	2.20	0.41
1:C:422[A]:GLU:HG2	1:C:452:LEU:HD13	2.01	0.41
1:C:340:THR:HG22	1:C:341:GLN:HG3	2.01	0.41
1:A:528:ARG:CD	1:A:529:PRO:O	2.67	0.41
1:D:118[B]:ARG:NE	10:D:973:HOH:O	2.09	0.41
1:C:418:ARG:HD2	10:C:803:HOH:O	2.21	0.41
1:A:163:ARG:CG	1:A:163:ARG:HH11	2.33	0.40
1:B:253:PHE:HD1	1:B:280:ILE:HB	1.87	0.40
1:C:351:ARG:HB2	5:C:601:EDO:H21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:HD2	1:B:218:ARG:NH2	2.35	0.40
1:A:273:GLU:H	1:A:273:GLU:HG2	1.54	0.40
1:B:183:GLY:O	1:B:197:VAL:HB	2.21	0.40
1:D:198:GLN:HB3	1:D:199:LYS:H	1.63	0.40
6:B:605:PEG:H41	6:B:605:PEG:H21	1.89	0.40
1:C:115:LEU:HD23	1:C:504:PHE:CE1	2.57	0.40
1:C:423:VAL:HG12	1:D:431:ALA:HB1	2.03	0.40
1:C:132:ARG:HD2	1:C:218:ARG:HH12	1.86	0.40
1:B:183:GLY:O	1:B:184:GLY:O	2.39	0.40

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

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/543 (95%)	504 (98%)	11 (2%)	2 (0%)	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

All (7) Ramachandran outliers are listed below:



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

### 5.3.2 Protein sidechains ⓘ

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

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	GLN
1	A	30	LEU
1	A	52	VAL
1	A	68	ARG
1	A	145	GLU
1	A	175	ASN
1	A	179	VAL
1	A	194	SER
1	A	199	LYS
1	A	208	GLN
1	A	218	ARG
1	A	227	GLN
1	A	235	GLU
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	273	GLU
1	A	343	LEU
1	A	379	LYS
1	A	395	ARG
1	A	511	LEU
1	A	528	ARG
1	A	540	LEU
1	B	25	PHE
1	B	26	GLN
1	B	30	LEU
1	B	34	MET
1	B	73	LEU
1	B	118[A]	ARG
1	B	118[B]	ARG
1	B	143	GLU
1	B	144	VAL
1	B	145	GLU
1	B	147	VAL
1	B	153	LEU
1	B	154	VAL
1	B	156	VAL
1	B	168	THR
1	B	169	VAL
1	B	179	VAL
1	B	185	ARG
1	B	199	LYS
1	B	215	LEU
1	B	242	ARG
1	B	270	LEU
1	B	379	LYS
1	B	411	ARG
1	B	500	ARG
1	B	511	LEU
1	B	516	ARG
1	B	521	VAL
1	C	30	LEU
1	C	145	GLU
1	C	168	THR
1	C	179	VAL
1	C	195	LEU
1	C	198	GLN
1	C	199	LYS

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Mol	Chain	Res	Type
1	C	217	SER
1	C	218	ARG
1	C	270[A]	LEU
1	C	270[B]	LEU
1	C	395	ARG
1	C	412	ARG
1	C	475	VAL
1	C	511	LEU
1	C	516	ARG
1	C	537	MET
1	D	22	THR
1	D	30	LEU
1	D	144	VAL
1	D	150	SER
1	D	151	GLN
1	D	156	VAL
1	D	158	PRO
1	D	163	ARG
1	D	168	THR
1	D	194	SER
1	D	198	GLN
1	D	199	LYS
1	D	205	LEU
1	D	215	LEU
1	D	395	ARG
1	D	411	ARG
1	D	455	ARG
1	D	511	LEU
1	D	521	VAL
1	D	528	ARG
1	D	540	LEU
1	D	541	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	167	ASN
1	C	26	GLN
1	C	27	GLN
1	C	151	GLN
1	D	151	GLN
1	D	198	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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
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

All (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
8	C	605	1PE	OH3-C22	2.21	1.51	1.42
4	D	603	FBP	O2-C2	2.26	1.44	1.41
4	D	603	FBP	O4-C4	2.35	1.48	1.43
9	D	604[A]	ADN	C2-N3	2.41	1.36	1.32
8	C	605	1PE	C23-C13	2.41	1.61	1.48
4	A	603	FBP	O4-C4	2.57	1.49	1.43
3	C	603	FLC	CG-CB	2.72	1.58	1.54
3	A	602	FLC	CG-CB	2.96	1.59	1.54
8	C	605	1PE	OH3-C23	3.01	1.54	1.42
4	D	603	FBP	O5-C2	3.04	1.48	1.43
3	D	602	FLC	OHB-CB	3.09	1.48	1.43
8	C	605	1PE	OH4-C24	3.16	1.55	1.42
9	D	604[B]	ADN	C5-C4	3.18	1.47	1.40
9	D	604[A]	ADN	C5-C4	3.20	1.47	1.40
8	C	606	1PE	OH4-C13	3.47	1.60	1.42
3	C	603	FLC	OHB-CB	3.52	1.48	1.43
8	C	606	1PE	OH3-C23	4.97	1.63	1.42

All (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
9	D	604[B]	ADN	C4-C5-N7	-3.86	105.92	109.48
8	C	606	1PE	C23-OH3-C22	-3.71	97.37	113.31
4	D	603	FBP	O1-P1-O1P	-3.54	98.13	107.14
9	D	604[A]	ADN	C4-C5-N7	-3.47	106.28	109.48
9	D	604[B]	ADN	C2'-C3'-C4'	-2.98	96.48	102.61
4	D	603	FBP	O6-P2-O4P	-2.48	100.82	107.14
4	A	603	FBP	O6-P2-O4P	-2.38	101.07	107.14
9	D	604[A]	ADN	C1'-N9-C4	-2.31	123.46	126.94
6	A	606	PEG	O2-C2-C1	-2.25	100.08	110.43
3	D	602	FLC	CB-CG-CGC	-2.20	111.44	114.96
6	A	606	PEG	O2-C3-C4	-2.10	100.76	110.43
4	D	603	FBP	O5P-P2-O6	-2.02	100.75	106.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	FLC	CG-CB-CA	2.01	114.62	109.81
9	D	604[A]	ADN	C2-N1-C6	2.02	122.37	118.77
3	D	602	FLC	CG-CB-CA	2.04	114.69	109.81
8	C	605	1PE	OH4-C24-C14	2.46	121.77	110.43
4	D	603	FBP	O3P-P1-O1P	2.64	119.08	110.58
9	D	604[B]	ADN	O2'-C2'-C3'	2.69	120.59	111.83
4	D	603	FBP	O6P-P2-O5P	2.75	117.84	107.38
4	C	604	FBP	O3P-P1-O1P	2.75	119.43	110.58
8	C	605	1PE	OH3-C22-C12	2.87	123.67	110.43
4	B	603	FBP	O3P-P1-O1P	2.91	119.96	110.58
4	A	603	FBP	O3P-P1-O1P	3.01	120.27	110.58
4	D	603	FBP	O2-C2-O5	3.07	115.70	109.37
9	D	604[A]	ADN	O2'-C2'-C3'	3.24	122.37	111.83
4	B	603	FBP	O6P-P2-O5P	3.29	119.92	107.38
3	A	602	FLC	CG-CB-CA	3.90	119.14	109.81
4	A	603	FBP	O6P-P2-O5P	4.58	124.81	107.38
8	C	606	1PE	OH4-C13-C23	5.01	142.93	112.03
8	C	606	1PE	OH3-C23-C13	6.24	139.17	110.43

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	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%)

All (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
1	A	144	VAL	6.1
1	D	151	GLN	6.0
1	B	146	LEU	5.8
1	D	149	GLY	5.8
1	D	205	LEU	5.5
1	D	215	LEU	5.4
1	B	182	VAL	5.3
1	C	182	VAL	5.2
1	B	147	VAL	5.1
1	B	215	LEU	5.0
1	B	152	VAL	5.0
1	D	22	THR	4.8
1	B	168	THR	4.7
1	B	183	GLY	4.6
1	C	152	VAL	4.6
1	C	214	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	149	GLY	4.6
1	D	23	ALA	4.6
1	D	160	PHE	4.6
1	D	164	GLY	4.6
1	C	146	LEU	4.5
1	B	151	GLN	4.5
1	D	167	ASN	4.5
1	B	214	VAL	4.4
1	D	171	VAL	4.4
1	C	215	LEU	4.3
1	D	163	ARG	4.3
1	C	199	LYS	4.3
1	C	167	ASN	4.3
1	B	160	PHE	4.2
1	D	168	THR	4.2
1	B	166	ALA	4.2
1	D	134	GLY	4.1
1	D	165	ASN	4.1
1	C	208	GLN	4.1
1	B	208	GLN	4.0
1	C	198	GLN	4.0
1	B	134	GLY	4.0
1	B	34	MET	3.9
1	A	166	ALA	3.9
1	D	152	VAL	3.9
1	D	490	PRO	3.9
1	B	181	PRO	3.9
1	C	155	THR	3.9
1	D	146	LEU	3.9
1	D	217	SER	3.9
1	D	208	GLN	3.8
1	B	209	VAL	3.8
1	D	21	GLY	3.8
1	B	135	ILE	3.8
1	C	183	GLY	3.8
1	C	209	VAL	3.7
1	C	151	GLN	3.7
1	B	26	GLN	3.7
1	C	150	SER	3.7
1	D	26	GLN	3.6
1	D	25	PHE	3.6
1	A	228	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	169	VAL	3.6
1	C	147	VAL	3.6
1	B	217	SER	3.6
1	B	225	GLY	3.6
1	D	200	ILE	3.6
1	D	153	LEU	3.5
1	A	149	GLY	3.5
1	C	206	VAL	3.5
1	A	146	LEU	3.5
1	A	167	ASN	3.5
1	B	165	ASN	3.4
1	D	150	SER	3.4
1	B	218	ARG	3.4
1	A	135	ILE	3.4
1	C	165	ASN	3.4
1	C	216	GLY	3.3
1	A	26	GLN	3.3
1	C	143	GLU	3.3
1	B	167	ASN	3.3
1	B	198	GLN	3.3
1	C	218	ARG	3.2
1	D	170	TRP	3.2
1	D	196	VAL	3.2
1	A	272	PRO	3.2
1	A	150	SER	3.1
1	C	231	PRO	3.1
1	D	198	GLN	3.1
1	B	216	GLY	3.1
1	A	151	GLN	3.1
1	C	492	ALA	3.1
1	C	158	PRO	3.1
1	C	203	GLU	3.0
1	C	166	ALA	3.0
1	B	206	VAL	3.0
1	B	143	GLU	3.0
1	D	218	ARG	3.0
1	B	200	ILE	3.0
1	B	205	LEU	3.0
1	D	203	GLU	3.0
1	C	34	MET	3.0
1	B	201	GLY	2.9
1	D	155[A]	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	153	LEU	2.9
1	C	170	TRP	2.9
1	A	164	GLY	2.9
1	C	196	VAL	2.8
1	C	145	GLU	2.8
1	D	154	VAL	2.8
1	D	161	ARG	2.8
1	B	184	GLY	2.8
1	B	185	ARG	2.8
1	A	196[A]	VAL	2.7
1	C	171	VAL	2.7
1	A	165	ASN	2.7
1	C	242	ARG	2.7
1	A	134	GLY	2.7
1	D	144	VAL	2.7
1	D	162	THR	2.7
1	A	227	GLN	2.7
1	B	159	ALA	2.6
1	A	198	GLN	2.6
1	B	226	ALA	2.6
1	B	150	SER	2.6
1	D	214	VAL	2.6
1	B	148	LYS	2.6
1	D	159	ALA	2.6
1	B	145	GLU	2.6
1	C	115	LEU	2.6
1	C	149	GLY	2.6
1	B	178	ARG	2.6
1	C	169	VAL	2.6
1	C	148	LYS	2.5
1	D	147	VAL	2.5
1	D	232	GLY	2.5
1	C	202	PRO	2.5
1	A	152	VAL	2.5
1	B	194	SER	2.5
1	D	477	LEU	2.5
1	A	147	VAL	2.5
1	D	166	ALA	2.5
1	D	493	ILE	2.4
1	B	153	LEU	2.4
1	A	493	ILE	2.4
1	C	134	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	216	GLY	2.4
1	A	511	LEU	2.4
1	D	199	LYS	2.4
1	B	164	GLY	2.4
1	C	511	LEU	2.3
1	C	233	LEU	2.3
1	A	214	VAL	2.3
1	C	114	PRO	2.3
1	B	492	ALA	2.3
1	C	185	ARG	2.3
1	D	145	GLU	2.3
1	A	217	SER	2.2
1	B	199	LYS	2.2
1	A	209	VAL	2.2
1	C	213	GLY	2.2
1	A	160	PHE	2.2
1	C	112	GLY	2.2
1	D	133	THR	2.2
1	C	159	ALA	2.2
1	C	207	THR	2.2
1	D	478	CYS	2.2
1	C	205	LEU	2.2
1	D	116[A]	SER	2.2
1	D	156	VAL	2.2
1	C	194	SER	2.1
1	A	489	PRO	2.1
1	C	179	VAL	2.1
1	D	206	VAL	2.1
1	C	211	ASN	2.1
1	D	202	PRO	2.1
1	D	511	LEU	2.1
1	A	232	GLY	2.1
1	A	210	GLU	2.0
1	B	477	LEU	2.0
1	C	197	VAL	2.0
1	C	210	GLU	2.0
1	C	232	GLY	2.0
1	A	168	THR	2.0
1	C	272	PRO	2.0
1	C	371	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
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 [i](#)

There are no such residues in this entry.