



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 01:23 AM EDT

PDB ID : 4GX1 / pdb\_00004gx1  
Title : Crystal structure of the GsuK bound to ADP  
Authors : Kong, C.; Zeng, W.; Ye, S.; Chen, L.; Sauer, D.B.; Lam, Y.; Derebe, M.G.; Jiang, Y.  
Deposited on : 2012-09-03  
Resolution : 2.80 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

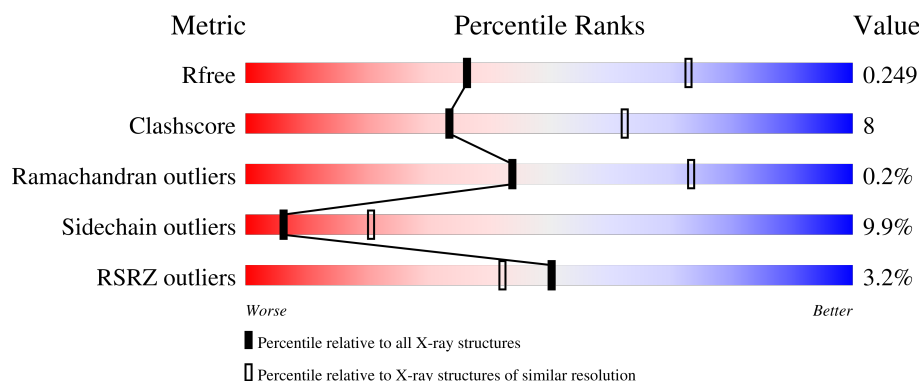
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	565	<div> <div>5%</div> <div>53% 12% 33%</div> </div>
1	B	565	<div> <div>5%</div> <div>72% 21%</div> </div>
1	C	565	<div> <div>3%</div> <div>75% 20%</div> </div>
1	D	565	<div> <div>5%</div> <div>52% 13% 33%</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
7	PO4	C	610	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14702 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 TrkA domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	0	0
			2931	1885	507	528	11			
1	B	547	Total	C	N	O	S	0	0	0
			4197	2687	725	770	15			
1	C	546	Total	C	N	O	S	0	0	0
			4188	2682	723	768	15			
1	D	376	Total	C	N	O	S	0	0	0
			2928	1883	507	527	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	expression tag	UNP Q74FS9
A	5	GLN	-	expression tag	UNP Q74FS9
A	6	ARG	-	expression tag	UNP Q74FS9
A	7	GLY	-	expression tag	UNP Q74FS9
A	8	SER	-	expression tag	UNP Q74FS9
A	52	ALA	GLU	engineered mutation	UNP Q74FS9
A	77	GLU	GLN	engineered mutation	UNP Q74FS9
A	97	ASP	LEU	engineered mutation	UNP Q74FS9
A	565	LEU	-	expression tag	UNP Q74FS9
A	566	VAL	-	expression tag	UNP Q74FS9
A	567	PRO	-	expression tag	UNP Q74FS9
A	568	ARG	-	expression tag	UNP Q74FS9
B	4	MET	-	expression tag	UNP Q74FS9
B	5	GLN	-	expression tag	UNP Q74FS9
B	6	ARG	-	expression tag	UNP Q74FS9
B	7	GLY	-	expression tag	UNP Q74FS9
B	8	SER	-	expression tag	UNP Q74FS9
B	52	ALA	GLU	engineered mutation	UNP Q74FS9
B	77	GLU	GLN	engineered mutation	UNP Q74FS9
B	97	ASP	LEU	engineered mutation	UNP Q74FS9
B	565	LEU	-	expression tag	UNP Q74FS9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	566	VAL	-	expression tag	UNP Q74FS9
B	567	PRO	-	expression tag	UNP Q74FS9
B	568	ARG	-	expression tag	UNP Q74FS9
C	4	MET	-	expression tag	UNP Q74FS9
C	5	GLN	-	expression tag	UNP Q74FS9
C	6	ARG	-	expression tag	UNP Q74FS9
C	7	GLY	-	expression tag	UNP Q74FS9
C	8	SER	-	expression tag	UNP Q74FS9
C	52	ALA	GLU	engineered mutation	UNP Q74FS9
C	77	GLU	GLN	engineered mutation	UNP Q74FS9
C	97	ASP	LEU	engineered mutation	UNP Q74FS9
C	565	LEU	-	expression tag	UNP Q74FS9
C	566	VAL	-	expression tag	UNP Q74FS9
C	567	PRO	-	expression tag	UNP Q74FS9
C	568	ARG	-	expression tag	UNP Q74FS9
D	4	MET	-	expression tag	UNP Q74FS9
D	5	GLN	-	expression tag	UNP Q74FS9
D	6	ARG	-	expression tag	UNP Q74FS9
D	7	GLY	-	expression tag	UNP Q74FS9
D	8	SER	-	expression tag	UNP Q74FS9
D	52	ALA	GLU	engineered mutation	UNP Q74FS9
D	77	GLU	GLN	engineered mutation	UNP Q74FS9
D	97	ASP	LEU	engineered mutation	UNP Q74FS9
D	565	LEU	-	expression tag	UNP Q74FS9
D	566	VAL	-	expression tag	UNP Q74FS9
D	567	PRO	-	expression tag	UNP Q74FS9
D	568	ARG	-	expression tag	UNP Q74FS9

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total K 3 3	0	0
2	B	3	Total K 3 3	0	0
2	C	3	Total K 3 3	0	0
2	D	2	Total K 2 2	0	0

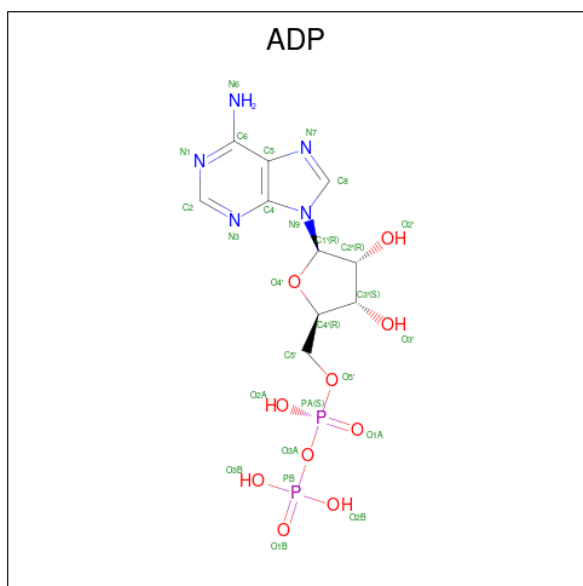
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



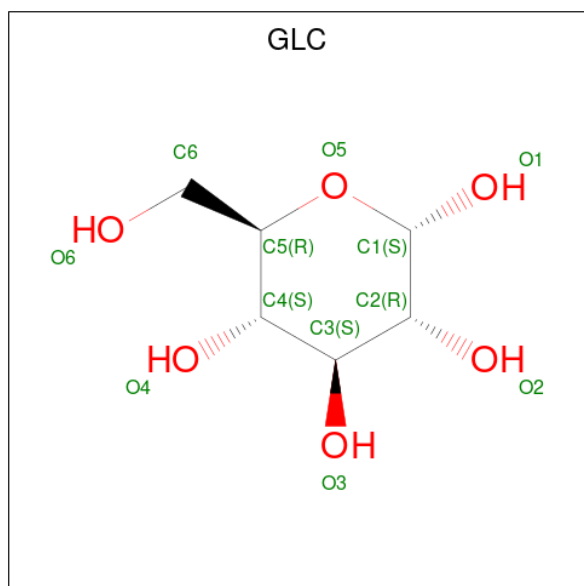
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	C	1	Total 27	C 10	N 5	O 10	P 2	0	0

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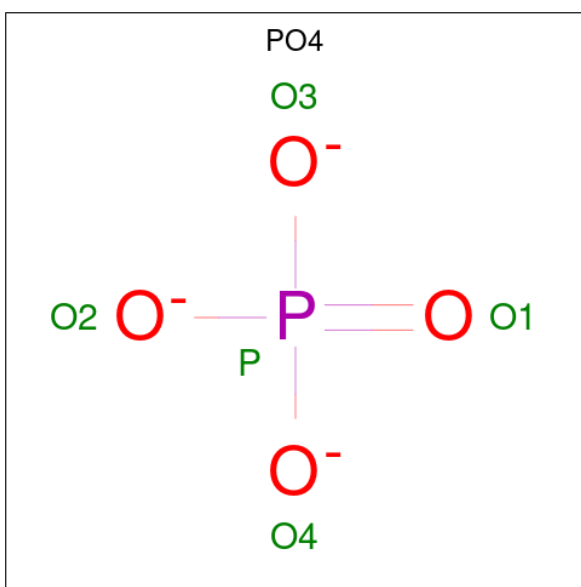
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			12	6	6		
6	C	1	Total	C	O	0	0
			12	6	6		
6	C	1	Total	C	O	0	0
			12	6	6		
6	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is water.

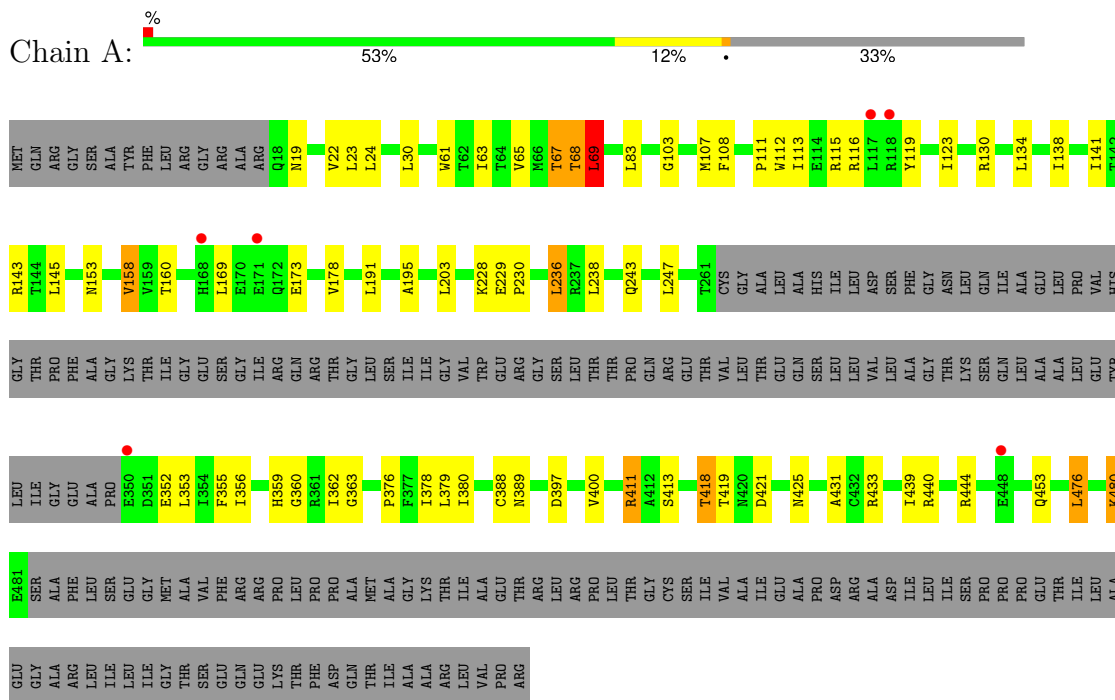
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	49	Total	O	0	0
			49	49		
8	B	91	Total	O	0	0
			91	91		
8	C	83	Total	O	0	0
			83	83		
8	D	50	Total	O	0	0
			50	50		



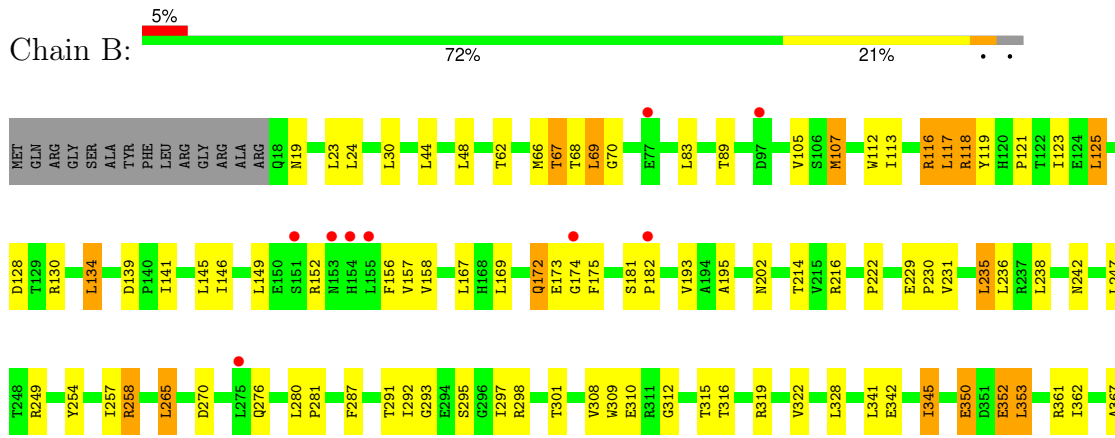
### 3 Residue-property plots

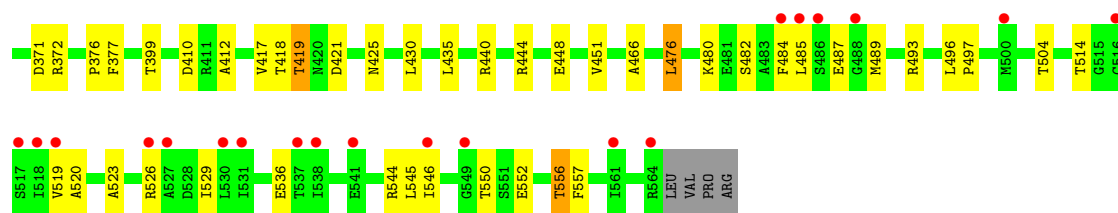
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: TrkA domain protein

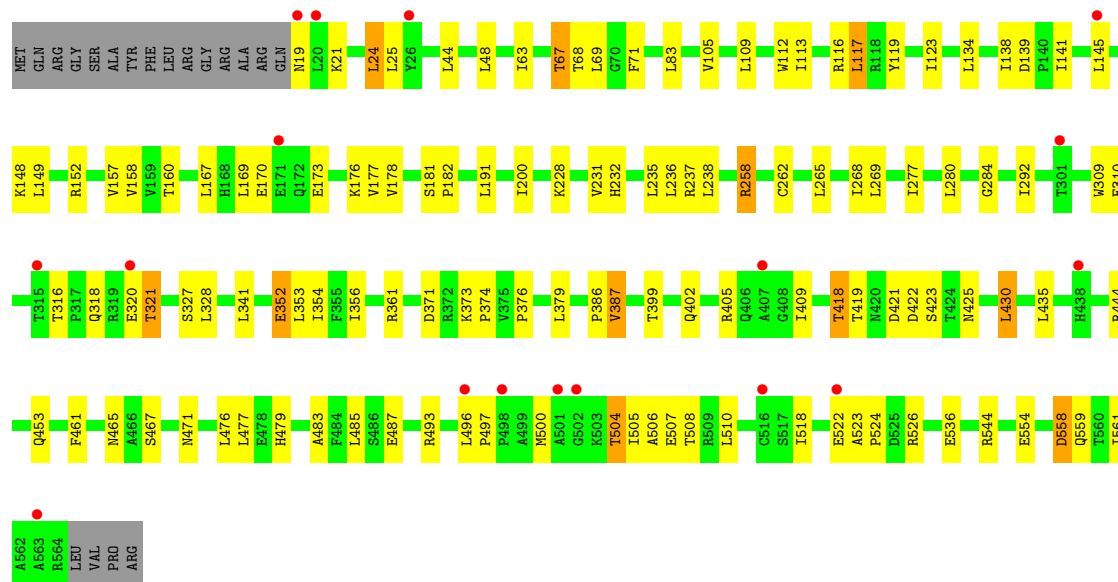
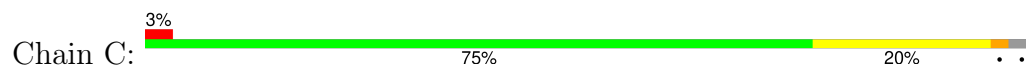


#### • Molecule 1: TrkA domain protein

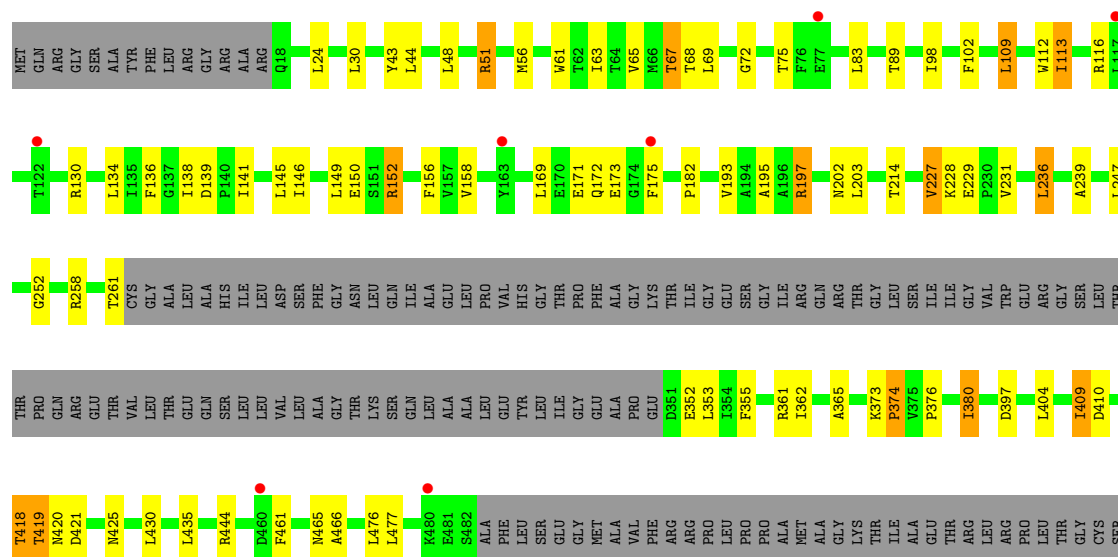




• Molecule 1: TrkA domain protein



• Molecule 1: TrkA domain protein



ILE	VAL	ALA	ILE	GLU	ALA	PRO	ASP	ARG	ALA	ASP	ILE	LEU	ILE	SER	PRO	PRO	PRO	GLU	THR	ILE	LEU	ALA	GLU	GLY	ALA	ARG	LEU	ILE	ILE	ILE	GLY	THR	SER	GLU	GLN	GLU	LYS	THR	PHE	ASP	GLN	THR	ILE	ALA	ALA	ARG	LEU	VAL	PRO	ARG
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	234.32Å 111.44Å 164.74Å 90.00° 134.93° 90.00°	Depositor
Resolution (Å)	41.47 – 2.80 41.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (41.47-2.80) 96.8 (41.47-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.212 , 0.255 0.207 , 0.249	Depositor DCC
$R_{free}$ test set	3624 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.7	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.089 for -h-2*k,h+1 0.015 for -h,-k,h+1 0.023 for -h-2*k,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3762e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 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: PO4, ZN, GLC, ADP, K, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.45	0/2991	0.82	5/4072 (0.1%)
1	B	0.41	0/4280	0.80	5/5829 (0.1%)
1	C	0.39	0/4271	0.81	1/5817 (0.0%)
1	D	0.39	0/2988	0.79	1/4068 (0.0%)
All	All	0.41	0/14530	0.81	12/19786 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	ILE	N-CA-C	8.10	118.14	110.53
1	A	400	VAL	N-CA-C	7.44	117.97	110.23
1	A	69	LEU	N-CA-C	-6.75	103.61	110.97
1	B	69	LEU	N-CA-C	-6.61	103.69	111.03
1	D	173	GLU	N-CA-C	6.04	118.04	108.79
1	A	173	GLU	N-CA-C	5.86	119.06	108.69
1	B	174	GLY	N-CA-C	-5.46	106.21	115.34
1	C	354	ILE	N-CA-C	5.30	115.21	107.37
1	A	229	GLU	CA-C-N	5.24	126.39	119.84
1	A	229	GLU	C-N-CA	5.24	126.39	119.84
1	B	229	GLU	CA-C-N	5.07	126.18	119.84
1	B	229	GLU	C-N-CA	5.07	126.18	119.84

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2931	0	2961	46	0
1	B	4197	0	4267	76	0
1	C	4188	0	4259	65	0
1	D	2928	0	2960	49	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	27	0	12	6	0
5	B	27	0	12	2	0
5	C	27	0	12	1	0
5	D	27	0	12	5	0
6	B	12	0	11	0	0
6	C	24	0	22	0	0
6	D	12	0	11	0	0
7	B	5	0	0	0	0
7	C	5	0	0	2	0
8	A	49	0	0	1	0
8	B	91	0	0	1	0
8	C	83	0	0	4	0
8	D	50	0	0	0	0
All	All	14702	0	14539	221	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 8.

All (221) 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:419:THR:HG22	1:A:421:ASP:H	1.36	0.90
1:C:112:TRP:HE1	1:C:116:ARG:HH11	1.24	0.84
1:C:419:THR:HG22	1:C:421:ASP:H	1.43	0.83
1:C:493:ARG:HD2	1:C:544:ARG:HD3	1.63	0.80
1:C:419:THR:HB	1:C:425:ASN:HD21	1.45	0.80
1:D:130:ARG:HG3	1:D:195:ALA:HB1	1.65	0.77
1:C:69:LEU:HD23	1:D:68:THR:HA	1.68	0.75
1:B:419:THR:HG22	1:B:421:ASP:H	1.52	0.73
1:C:523:ALA:HB3	1:C:526:ARG:HG3	1.70	0.73
1:C:169:LEU:HB3	1:C:177:VAL:HG21	1.71	0.72
1:B:139:ASP:OD2	1:B:202:ASN:ND2	2.24	0.71
1:B:361:ARG:NH1	8:B:728:HOH:O	2.22	0.70
1:A:359:HIS:ND1	8:A:737:HOH:O	2.24	0.70
1:A:119:TYR:HB2	1:B:118:ARG:HH12	1.59	0.68
1:C:419:THR:HB	1:C:425:ASN:ND2	2.08	0.67
1:D:419:THR:HG22	1:D:421:ASP:H	1.60	0.66
1:A:444:ARG:NH1	5:A:606:ADP:O1B	2.29	0.66
1:D:138:ILE:HG21	1:D:169:LEU:HD11	1.78	0.66
1:D:397:ASP:OD1	5:D:604:ADP:N6	2.29	0.65
1:B:172:GLN:O	1:B:172:GLN:NE2	2.30	0.65
1:D:229:GLU:OE1	1:D:361:ARG:NE	2.30	0.64
1:B:265:LEU:HD21	1:B:341:LEU:HD23	1.80	0.64
1:B:298:ARG:NH2	1:B:523:ALA:O	2.31	0.64
1:D:112:TRP:HD1	1:D:116:ARG:HH11	1.46	0.63
1:B:520:ALA:HB1	1:B:529:ILE:HD11	1.81	0.63
1:B:523:ALA:HB3	1:B:526:ARG:HB2	1.81	0.62
1:B:222:PRO:HB2	1:B:480:LYS:HE3	1.82	0.62
1:D:444:ARG:NH2	5:D:604:ADP:O2B	2.32	0.62
1:A:138:ILE:HG21	1:A:169:LEU:HD11	1.81	0.62
1:B:419:THR:HB	1:B:425:ASN:OD1	2.00	0.61
1:D:51:ARG:NH2	1:D:75:THR:O	2.30	0.61
1:C:19:ASN:N	8:C:710:HOH:O	2.32	0.60
1:C:430:LEU:HD11	1:D:239:ALA:HB2	1.83	0.60
1:C:402:GLN:OE1	1:C:405:ARG:NE	2.29	0.60
1:D:362:ILE:N	5:D:604:ADP:O1B	2.33	0.60
1:A:69:LEU:CD2	1:B:70:GLY:HA3	2.32	0.60
1:A:419:THR:HG23	5:A:606:ADP:C8	2.37	0.59
1:B:67:THR:O	1:B:68:THR:OG1	2.20	0.59
1:A:419:THR:HB	1:A:425:ASN:OD1	2.03	0.59
1:D:139:ASP:OD2	1:D:202:ASN:ND2	2.34	0.59
1:D:197:ARG:NH1	1:D:477:LEU:O	2.36	0.58
1:D:404:LEU:HB3	1:D:409:ILE:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:LEU:HD22	1:B:497:PRO:HD2	1.85	0.58
1:A:69:LEU:HD22	1:B:70:GLY:HA3	1.85	0.58
1:B:496:LEU:HD23	1:B:545:LEU:HD11	1.85	0.58
1:D:67:THR:O	1:D:68:THR:OG1	2.19	0.58
1:C:262:CYS:HA	1:C:284:GLY:HA3	1.84	0.58
1:C:361:ARG:N	5:C:607:ADP:O3B	2.29	0.58
1:A:19:ASN:HB3	1:A:107:MET:HE3	1.86	0.58
1:B:287:PHE:HD2	1:B:295:SER:HB2	1.67	0.58
1:A:433:ARG:NH1	1:A:439:ILE:O	2.30	0.58
1:A:355:PHE:CE2	1:A:380:ILE:HD11	2.39	0.57
7:C:610:PO4:O1	8:C:748:HOH:O	2.17	0.57
1:D:444:ARG:HE	1:D:465:ASN:HD21	1.52	0.57
1:C:352:GLU:O	1:C:376:PRO:HG2	2.04	0.57
1:C:505:ILE:HD13	1:C:518:ILE:HG21	1.85	0.57
1:A:108:PHE:HA	1:A:111:PRO:HD2	1.85	0.57
1:C:67:THR:O	1:C:68:THR:OG1	2.17	0.57
1:C:418:THR:HG22	1:C:444:ARG:HH11	1.70	0.56
1:A:355:PHE:HE2	1:A:380:ILE:HD11	1.70	0.56
1:C:113:ILE:HG23	1:C:117:LEU:HD23	1.87	0.56
1:B:362:ILE:H	5:B:606:ADP:PB	2.29	0.56
1:C:119:TYR:CE2	1:C:170:GLU:HG3	2.41	0.56
1:C:504:THR:HG22	1:C:507:GLU:H	1.71	0.56
1:D:252:GLY:HA3	1:D:365:ALA:HB3	1.88	0.55
1:C:232:HIS:HA	1:C:235:LEU:HD12	1.87	0.55
1:B:44:LEU:HB3	1:B:48:LEU:HD12	1.88	0.55
1:B:297:ILE:O	1:B:301:THR:OG1	2.23	0.54
1:B:520:ALA:HB3	1:B:546:ILE:HB	1.88	0.54
1:D:63:ILE:O	1:D:67:THR:HB	2.08	0.54
1:B:62:THR:HG22	1:B:66:MET:HE2	1.90	0.54
1:B:418:THR:HG23	1:B:444:ARG:HD3	1.90	0.54
1:A:411:ARG:H	1:A:411:ARG:HD3	1.73	0.53
1:C:228:LYS:HE3	8:C:730:HOH:O	2.08	0.53
1:D:146:ILE:HG21	1:D:175:PHE:HD2	1.74	0.53
1:C:21:LYS:HA	1:C:24:LEU:HD23	1.91	0.53
1:C:258:ARG:HG2	1:C:461:PHE:CD1	2.44	0.53
1:C:500:MET:HG3	1:C:508:THR:HG21	1.90	0.52
1:D:112:TRP:CD1	1:D:116:ARG:HH11	2.25	0.52
1:A:103:GLY:O	1:A:107:MET:HB3	2.10	0.52
1:C:265:LEU:HD23	1:C:280:LEU:HB2	1.91	0.52
1:B:169:LEU:HB3	1:B:175:PHE:HE1	1.75	0.52
1:D:355:PHE:HE2	1:D:380:ILE:HD11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:SER:HA	1:B:485:LEU:HB2	1.92	0.51
1:A:418:THR:HG22	1:A:444:ARG:HD2	1.93	0.51
1:A:130:ARG:HG2	1:A:195:ALA:HB1	1.93	0.51
1:B:489:MET:HG2	1:B:550:THR:HA	1.92	0.51
1:B:352:GLU:O	1:B:376:PRO:HG2	2.11	0.50
1:B:493:ARG:HD3	1:B:544:ARG:HD2	1.94	0.50
1:C:112:TRP:HZ3	1:D:113:ILE:HD13	1.77	0.50
1:A:141:ILE:HD13	1:A:247:LEU:HD13	1.92	0.50
1:B:146:ILE:HG21	1:B:175:PHE:CD2	2.47	0.50
1:B:112:TRP:CE2	1:B:116:ARG:HD2	2.47	0.50
1:D:352:GLU:O	1:D:376:PRO:HG2	2.12	0.50
1:C:200:ILE:HD11	1:C:477:LEU:HD11	1.94	0.50
1:C:496:LEU:HD22	1:C:497:PRO:HD2	1.94	0.50
1:A:360:GLY:HA3	5:A:606:ADP:O5'	2.12	0.49
1:B:216:ARG:NH1	1:B:242:ASN:OD1	2.45	0.49
1:B:113:ILE:HG23	1:B:117:LEU:HD23	1.94	0.49
1:C:71:PHE:O	1:D:72:GLY:HA3	2.11	0.49
1:B:444:ARG:NH2	5:B:606:ADP:O2B	2.46	0.49
1:C:178:VAL:HG11	1:C:191:LEU:HD21	1.92	0.49
1:A:67:THR:HG21	1:B:89:THR:CG2	2.42	0.48
1:C:310:GLU:OE1	1:C:327:SER:OG	2.21	0.48
1:D:149:LEU:HD12	1:D:156:PHE:HZ	1.77	0.48
1:C:405:ARG:HA	1:C:409:ILE:HG22	1.96	0.48
1:A:67:THR:O	1:A:68:THR:OG1	2.29	0.48
1:C:309:TRP:NE1	7:C:610:PO4:O2	2.45	0.48
1:C:67:THR:HG21	1:D:89:THR:CG2	2.44	0.47
1:D:419:THR:HB	1:D:425:ASN:OD1	2.14	0.47
1:D:112:TRP:CE3	1:D:113:ILE:HG13	2.49	0.47
1:A:61:TRP:O	1:A:65:VAL:HG23	2.15	0.47
1:A:397:ASP:OD2	5:A:606:ADP:N6	2.48	0.47
1:B:149:LEU:HB2	1:B:156:PHE:CE1	2.50	0.47
1:C:112:TRP:NE1	1:C:116:ARG:HH11	2.04	0.47
1:A:362:ILE:HB	5:A:606:ADP:O1B	2.15	0.47
1:A:63:ILE:O	1:A:67:THR:HB	2.15	0.47
1:B:149:LEU:HA	1:B:152:ARG:HG2	1.97	0.47
1:C:318:GLN:HB2	1:C:321:THR:HG22	1.97	0.47
1:A:431:ALA:HB2	1:B:235:LEU:HD21	1.97	0.46
1:D:44:LEU:O	1:D:48:LEU:HB2	2.15	0.46
1:D:203:LEU:O	1:D:228:LYS:NZ	2.48	0.46
1:D:146:ILE:HG21	1:D:175:PHE:CD2	2.51	0.46
1:A:203:LEU:O	1:A:228:LYS:NZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ASN:HB3	1:B:107:MET:SD	2.56	0.46
1:D:418:THR:HG22	1:D:444:ARG:HD2	1.97	0.46
1:C:112:TRP:HE1	1:C:116:ARG:NH1	2.04	0.46
1:A:425:ASN:ND2	1:A:444:ARG:O	2.43	0.45
1:A:363:GLY:N	5:A:606:ADP:O3B	2.35	0.45
1:B:265:LEU:HD23	1:B:342:GLU:HG3	1.99	0.45
1:D:227:VAL:HG23	1:D:236:LEU:HD22	1.98	0.45
1:A:158:VAL:HG21	1:A:169:LEU:HD13	1.98	0.45
1:A:388:CYS:SG	1:A:389:ASN:N	2.89	0.45
1:D:362:ILE:H	5:D:604:ADP:PB	2.40	0.45
1:B:552:GLU:O	1:B:556:THR:OG1	2.22	0.45
1:D:258:ARG:HG2	1:D:461:PHE:CD1	2.52	0.44
1:C:504:THR:HG22	1:C:507:GLU:N	2.32	0.44
1:B:125:LEU:HD21	1:B:157:VAL:HG21	1.98	0.44
1:C:237:ARG:NH2	8:C:745:HOH:O	2.49	0.44
1:C:157:VAL:HG22	1:C:176:LYS:HB3	1.99	0.44
1:C:522:GLU:HG3	1:C:544:ARG:HB3	1.98	0.44
1:A:178:VAL:HG11	1:A:191:LEU:HD21	2.00	0.44
1:C:63:ILE:O	1:C:67:THR:HB	2.18	0.44
1:B:112:TRP:CZ2	1:B:116:ARG:HD2	2.52	0.44
1:C:67:THR:HG21	1:D:89:THR:HG21	1.99	0.44
1:C:113:ILE:O	1:C:117:LEU:N	2.48	0.44
1:C:422:ASP:HA	1:C:425:ASN:HB2	2.00	0.44
1:D:112:TRP:CD1	1:D:116:ARG:HD2	2.53	0.44
1:B:141:ILE:HD13	1:B:466:ALA:HA	1.99	0.43
1:C:268:ILE:HB	1:C:277:ILE:HG22	2.00	0.43
1:B:117:LEU:HD13	1:B:117:LEU:HA	1.81	0.43
1:B:247:LEU:HD23	1:B:247:LEU:HA	1.86	0.43
1:C:44:LEU:O	1:C:48:LEU:HB2	2.17	0.43
1:C:69:LEU:HD11	1:C:71:PHE:CZ	2.54	0.43
1:C:504:THR:HG23	1:C:506:ALA:H	1.84	0.43
1:A:431:ALA:HA	1:B:235:LEU:HD11	2.01	0.43
1:B:67:THR:C	1:B:68:THR:HG1	2.23	0.43
1:B:418:THR:HG22	1:B:444:ARG:HH11	1.84	0.43
1:B:293:GLY:HA3	1:B:319:ARG:HG3	1.99	0.43
1:C:269:LEU:HB3	1:C:277:ILE:HB	2.00	0.43
1:C:496:LEU:HA	1:C:497:PRO:HD2	1.89	0.43
1:D:109:LEU:HD12	1:D:109:LEU:HA	1.90	0.43
1:B:476:LEU:O	1:B:480:LYS:HG2	2.19	0.43
1:C:444:ARG:HE	1:C:465:ASN:HD21	1.67	0.43
1:D:420:ASN:HB3	5:D:604:ADP:O2A	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ILE:HB	1:C:379:LEU:HD23	2.00	0.43
1:A:359:HIS:CD2	1:A:379:LEU:HD13	2.53	0.42
1:A:67:THR:HG21	1:B:89:THR:HG21	2.01	0.42
1:B:134:LEU:HD23	1:B:193:VAL:HG12	2.01	0.42
1:C:105:VAL:HG13	1:C:109:LEU:HD23	2.01	0.42
1:C:479:HIS:O	1:C:483:ALA:N	2.51	0.42
1:D:61:TRP:O	1:D:65:VAL:HG23	2.19	0.42
1:B:119:TYR:CZ	1:B:121:PRO:HA	2.55	0.42
1:B:448:GLU:HA	1:B:451:VAL:HG23	2.01	0.42
1:B:514:THR:HG21	1:B:557:PHE:HD1	1.84	0.42
1:D:136:PHE:CD1	1:D:182:PRO:HB3	2.54	0.42
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.85	0.42
1:B:309:TRP:CZ2	1:B:312:GLY:HA2	2.54	0.42
1:A:453:GLN:HE21	1:B:214:THR:HA	1.85	0.42
1:B:291:THR:HG22	1:B:322:VAL:HG22	2.01	0.42
1:B:493:ARG:HG3	1:B:546:ILE:HG12	2.02	0.42
1:C:386:PRO:HG2	1:C:387:VAL:HG13	2.02	0.42
1:A:476:LEU:O	1:A:480:LYS:HB2	2.20	0.42
1:D:98:ILE:O	1:D:102:PHE:HB3	2.20	0.42
1:B:350:GLU:H	1:B:350:GLU:HG2	1.58	0.42
1:B:173:GLU:C	1:B:175:PHE:H	2.28	0.41
1:B:270:ASP:OD1	1:B:276:GLN:NE2	2.43	0.41
1:C:558:ASP:OD1	1:C:558:ASP:N	2.52	0.41
1:B:130:ARG:HD2	1:B:195:ALA:HB1	2.02	0.41
1:C:112:TRP:CZ3	1:D:113:ILE:HD13	2.54	0.41
1:B:128:ASP:O	1:B:130:ARG:HG2	2.20	0.41
1:B:149:LEU:HB2	1:B:156:PHE:HE1	1.85	0.41
1:D:43:TYR:HD2	1:D:44:LEU:HD23	1.85	0.41
1:D:247:LEU:HD23	1:D:247:LEU:HA	1.85	0.41
1:C:318:GLN:H	1:C:321:THR:CG2	2.32	0.41
1:D:373:LYS:HA	1:D:374:PRO:HD2	1.90	0.41
1:A:355:PHE:CE1	1:A:378:ILE:HD12	2.54	0.41
1:A:356:ILE:HB	1:A:379:LEU:HD23	2.03	0.41
1:B:216:ARG:HD3	1:B:216:ARG:HA	1.90	0.41
1:C:67:THR:C	1:C:68:THR:HG1	2.23	0.41
1:A:352:GLU:O	1:A:376:PRO:HG2	2.20	0.41
1:B:230:PRO:HB3	1:B:249:ARG:HH11	1.86	0.41
1:B:292:ILE:HD11	1:B:308:VAL:HG21	2.03	0.41
1:B:280:LEU:HA	1:B:281:PRO:HD2	1.95	0.41
1:A:107:MET:HE2	1:A:108:PHE:CD2	2.56	0.41
1:A:476:LEU:HD12	1:A:476:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:TYR:HD1	1:B:257:ILE:HD11	1.86	0.41
1:C:181:SER:HA	1:C:182:PRO:HD3	1.89	0.41
1:D:141:ILE:HD13	1:D:466:ALA:HA	2.03	0.41
1:B:258:ARG:O	1:B:440:ARG:HD3	2.21	0.41
1:C:453:GLN:HE21	1:D:214:THR:HA	1.86	0.41
1:A:112:TRP:O	1:A:116:ARG:HB2	2.21	0.40
1:C:138:ILE:HG21	1:C:169:LEU:HD11	2.03	0.40
1:A:352:GLU:HG3	1:A:413:SER:OG	2.21	0.40
1:B:181:SER:HA	1:B:182:PRO:HD3	1.92	0.40
1:B:353:LEU:HB3	1:B:412:ALA:HA	2.04	0.40
1:B:484:PHE:HA	1:B:487:GLU:HB3	2.04	0.40
1:C:419:THR:HG22	1:C:421:ASP:N	2.23	0.40
1:B:67:THR:C	1:B:68:THR:OG1	2.63	0.40
1:B:367:ALA:HB1	1:B:377:PHE:CE1	2.57	0.40
1:D:152:ARG:HD2	1:D:152:ARG:H	1.84	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/565 (66%)	356 (96%)	15 (4%)	1 (0%)	37	67
1	B	545/565 (96%)	527 (97%)	18 (3%)	0	100	100
1	C	544/565 (96%)	522 (96%)	20 (4%)	2 (0%)	30	61
1	D	372/565 (66%)	357 (96%)	14 (4%)	1 (0%)	37	67
All	All	1833/2260 (81%)	1762 (96%)	67 (4%)	4 (0%)	44	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	524	PRO
1	C	374	PRO
1	D	374	PRO
1	A	230	PRO

### 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	314/463 (68%)	288 (92%)	26 (8%)	9	28
1	B	448/463 (97%)	403 (90%)	45 (10%)	6	20
1	C	447/463 (96%)	398 (89%)	49 (11%)	5	17
1	D	314/463 (68%)	283 (90%)	31 (10%)	6	21
All	All	1523/1852 (82%)	1372 (90%)	151 (10%)	6	21

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	23	LEU
1	A	24	LEU
1	A	30	LEU
1	A	67	THR
1	A	68	THR
1	A	69	LEU
1	A	83	LEU
1	A	113	ILE
1	A	115	ARG
1	A	123	ILE
1	A	134	LEU
1	A	143	ARG
1	A	145	LEU
1	A	153	ASN
1	A	158	VAL
1	A	160	THR
1	A	236	LEU

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Mol	Chain	Res	Type
1	A	238	LEU
1	A	243	GLN
1	A	353	LEU
1	A	411	ARG
1	A	418	THR
1	A	440	ARG
1	A	476	LEU
1	A	480	LYS
1	B	23	LEU
1	B	24	LEU
1	B	30	LEU
1	B	67	THR
1	B	69	LEU
1	B	83	LEU
1	B	105	VAL
1	B	107	MET
1	B	116	ARG
1	B	117	LEU
1	B	118	ARG
1	B	123	ILE
1	B	125	LEU
1	B	134	LEU
1	B	145	LEU
1	B	158	VAL
1	B	167	LEU
1	B	172	GLN
1	B	231	VAL
1	B	235	LEU
1	B	236	LEU
1	B	238	LEU
1	B	258	ARG
1	B	265	LEU
1	B	310	GLU
1	B	315	THR
1	B	316	THR
1	B	328	LEU
1	B	345	ILE
1	B	350	GLU
1	B	352	GLU
1	B	353	LEU
1	B	371	ASP
1	B	372	ARG

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Mol	Chain	Res	Type
1	B	399	THR
1	B	410	ASP
1	B	417	VAL
1	B	419	THR
1	B	430	LEU
1	B	435	LEU
1	B	476	LEU
1	B	504	THR
1	B	519	VAL
1	B	536	GLU
1	B	556	THR
1	C	24	LEU
1	C	25	LEU
1	C	67	THR
1	C	83	LEU
1	C	117	LEU
1	C	123	ILE
1	C	134	LEU
1	C	139	ASP
1	C	141	ILE
1	C	145	LEU
1	C	148	LYS
1	C	149	LEU
1	C	152	ARG
1	C	158	VAL
1	C	160	THR
1	C	167	LEU
1	C	173	GLU
1	C	231	VAL
1	C	236	LEU
1	C	238	LEU
1	C	258	ARG
1	C	292	ILE
1	C	316	THR
1	C	320	GLU
1	C	321	THR
1	C	328	LEU
1	C	341	LEU
1	C	352	GLU
1	C	353	LEU
1	C	371	ASP
1	C	373	LYS

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Mol	Chain	Res	Type
1	C	387	VAL
1	C	399	THR
1	C	418	THR
1	C	423	SER
1	C	430	LEU
1	C	435	LEU
1	C	467	SER
1	C	471	ASN
1	C	476	LEU
1	C	485	LEU
1	C	487	GLU
1	C	504	THR
1	C	510	LEU
1	C	536	GLU
1	C	554	GLU
1	C	558	ASP
1	C	559	GLN
1	C	561	ILE
1	D	24	LEU
1	D	30	LEU
1	D	51	ARG
1	D	56	MET
1	D	67	THR
1	D	69	LEU
1	D	83	LEU
1	D	109	LEU
1	D	113	ILE
1	D	134	LEU
1	D	145	LEU
1	D	150	GLU
1	D	152	ARG
1	D	158	VAL
1	D	171	GLU
1	D	172	GLN
1	D	193	VAL
1	D	197	ARG
1	D	227	VAL
1	D	231	VAL
1	D	236	LEU
1	D	261	THR
1	D	353	LEU
1	D	380	ILE

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Mol	Chain	Res	Type
1	D	409	ILE
1	D	410	ASP
1	D	418	THR
1	D	419	THR
1	D	430	LEU
1	D	435	LEU
1	D	476	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	168	HIS
1	B	172	GLN
1	B	267	HIS
1	C	47	HIS
1	C	425	ASN
1	C	453	GLN
1	C	465	ASN
1	D	465	ASN
1	D	479	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 19 are monoatomic - leaving 10 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
5	ADP	D	604	-	24,29,29	1.65	6 (25%)	29,45,45	1.94	6 (20%)
7	PO4	C	610	-	4,4,4	0.96	0	6,6,6	0.37	0
5	ADP	A	606	-	24,29,29	1.56	6 (25%)	29,45,45	2.02	4 (13%)
5	ADP	C	607	-	24,29,29	1.58	6 (25%)	29,45,45	1.86	4 (13%)
6	GLC	C	608	-	12,12,12	1.70	2 (16%)	17,17,17	1.17	1 (5%)
6	GLC	D	605	-	12,12,12	1.69	2 (16%)	17,17,17	1.15	2 (11%)
6	GLC	B	607	-	12,12,12	1.74	2 (16%)	17,17,17	1.20	0
5	ADP	B	606	-	24,29,29	1.70	6 (25%)	29,45,45	1.91	5 (17%)
6	GLC	C	609	-	12,12,12	1.71	2 (16%)	17,17,17	1.15	1 (5%)
7	PO4	B	608	-	4,4,4	0.99	0	6,6,6	0.47	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
5	ADP	D	604	-	-	3/12/32/32	0/3/3/3
5	ADP	A	606	-	-	10/12/32/32	0/3/3/3
5	ADP	C	607	-	-	2/12/32/32	0/3/3/3
6	GLC	C	608	-	-	2/2/22/22	0/1/1/1
6	GLC	D	605	-	-	0/2/22/22	0/1/1/1
6	GLC	B	607	-	-	2/2/22/22	0/1/1/1
5	ADP	B	606	-	-	3/12/32/32	0/3/3/3
6	GLC	C	609	-	-	2/2/22/22	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	607	GLC	C4-C3	-3.88	1.42	1.52
6	C	609	GLC	C4-C3	-3.87	1.42	1.52
6	D	605	GLC	C4-C3	-3.82	1.42	1.52
6	C	608	GLC	C4-C3	-3.79	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	604	ADP	PA-O3A	-3.75	1.55	1.59
5	B	606	ADP	PA-O3A	-3.66	1.55	1.59
5	A	606	ADP	C2'-C3'	-3.64	1.43	1.53
5	B	606	ADP	C2'-C3'	-3.60	1.43	1.53
5	C	607	ADP	C2'-C3'	-3.57	1.43	1.53
5	D	604	ADP	C2'-C3'	-3.52	1.43	1.53
6	C	608	GLC	C3-C2	-3.36	1.43	1.52
6	B	607	GLC	C3-C2	-3.33	1.43	1.52
6	C	609	GLC	C3-C2	-3.24	1.43	1.52
6	D	605	GLC	C3-C2	-3.17	1.44	1.52
5	A	606	ADP	O4'-C1'	2.85	1.44	1.40
5	B	606	ADP	O4'-C1'	2.78	1.44	1.40
5	C	607	ADP	O4'-C4'	-2.77	1.38	1.45
5	D	604	ADP	O4'-C4'	-2.74	1.38	1.45
5	C	607	ADP	PA-O3A	-2.63	1.56	1.59
5	B	606	ADP	O4'-C4'	-2.52	1.39	1.45
5	A	606	ADP	C6-N6	2.49	1.43	1.34
5	B	606	ADP	C6-N6	2.47	1.42	1.34
5	C	607	ADP	C6-N6	2.45	1.42	1.34
5	D	604	ADP	C6-N6	2.44	1.42	1.34
5	A	606	ADP	O4'-C4'	-2.38	1.39	1.45
5	D	604	ADP	C1'-N9	-2.33	1.44	1.49
5	D	604	ADP	O4'-C1'	2.20	1.43	1.40
5	B	606	ADP	C1'-N9	-2.17	1.44	1.49
5	A	606	ADP	C1'-N9	-2.14	1.44	1.49
5	A	606	ADP	PA-O3A	-2.13	1.57	1.59
5	C	607	ADP	O4'-C1'	2.13	1.43	1.40
5	C	607	ADP	C1'-N9	-2.12	1.44	1.49

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	ADP	N3-C2-N1	-6.54	119.79	128.67
5	D	604	ADP	N3-C2-N1	-6.52	119.83	128.67
5	C	607	ADP	N3-C2-N1	-6.30	120.12	128.67
5	A	606	ADP	N3-C2-N1	-6.19	120.27	128.67
5	A	606	ADP	C4'-O4'-C1'	-5.02	105.33	109.92
5	C	607	ADP	C4'-O4'-C1'	-4.61	105.70	109.92
5	A	606	ADP	O4'-C1'-N9	4.51	114.73	108.75
5	B	606	ADP	O4'-C1'-N9	4.37	114.53	108.75
5	D	604	ADP	C4'-O4'-C1'	-4.06	106.21	109.92
5	D	604	ADP	O4'-C1'-N9	3.69	113.64	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	607	ADP	O4'-C1'-N9	3.37	113.22	108.75
5	A	606	ADP	O2B-PB-O3A	3.19	115.33	104.64
5	B	606	ADP	C4'-O4'-C1'	-3.02	107.16	109.92
5	B	606	ADP	O5'-C5'-C4'	2.96	119.06	108.99
5	D	604	ADP	O5'-C5'-C4'	2.76	118.40	108.99
5	C	607	ADP	O5'-C5'-C4'	2.72	118.24	108.99
5	D	604	ADP	C1'-N9-C4	-2.32	122.56	126.64
6	C	608	GLC	O6-C6-C5	2.32	119.22	111.33
5	B	606	ADP	C2'-C3'-C4'	2.19	106.84	102.61
6	C	609	GLC	O6-C6-C5	2.10	118.49	111.33
6	D	605	GLC	O5-C1-C2	2.05	113.91	110.30
5	D	604	ADP	O3B-PB-O3A	2.04	111.47	104.64
6	D	605	GLC	O6-C6-C5	2.01	118.17	111.33

There are no chirality outliers.

All (24) torsion outliers are listed below:

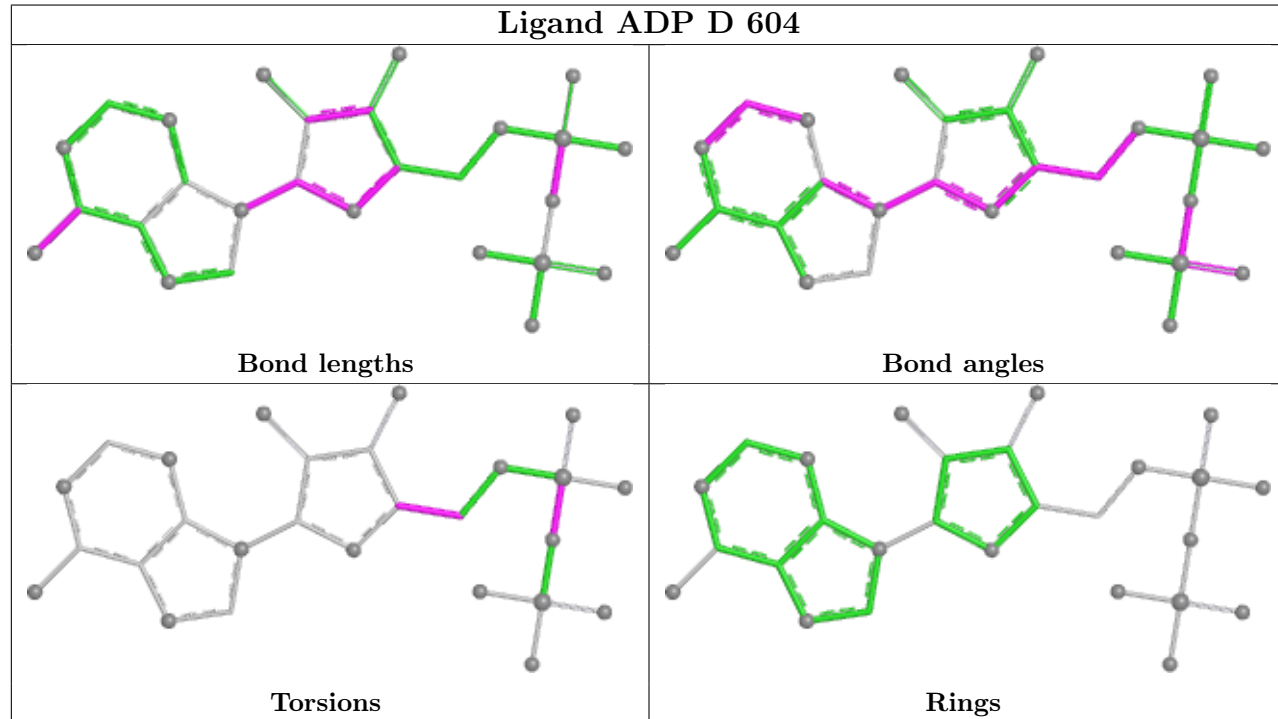
Mol	Chain	Res	Type	Atoms
5	A	606	ADP	PA-O3A-PB-O2B
5	A	606	ADP	C5'-O5'-PA-O1A
5	A	606	ADP	C5'-O5'-PA-O2A
5	A	606	ADP	C5'-O5'-PA-O3A
6	C	609	GLC	O5-C5-C6-O6
5	B	606	ADP	O4'-C4'-C5'-O5'
5	D	604	ADP	O4'-C4'-C5'-O5'
6	B	607	GLC	O5-C5-C6-O6
6	C	608	GLC	O5-C5-C6-O6
5	A	606	ADP	O4'-C4'-C5'-O5'
5	B	606	ADP	C3'-C4'-C5'-O5'
5	D	604	ADP	C3'-C4'-C5'-O5'
6	C	609	GLC	C4-C5-C6-O6
5	A	606	ADP	C3'-C4'-C5'-O5'
6	B	607	GLC	C4-C5-C6-O6
5	A	606	ADP	PB-O3A-PA-O5'
5	B	606	ADP	PB-O3A-PA-O5'
5	D	604	ADP	PB-O3A-PA-O5'
5	C	607	ADP	C5'-O5'-PA-O1A
6	C	608	GLC	C4-C5-C6-O6
5	A	606	ADP	PB-O3A-PA-O1A
5	C	607	ADP	O4'-C4'-C5'-O5'
5	A	606	ADP	PA-O3A-PB-O1B
5	A	606	ADP	PA-O3A-PB-O3B

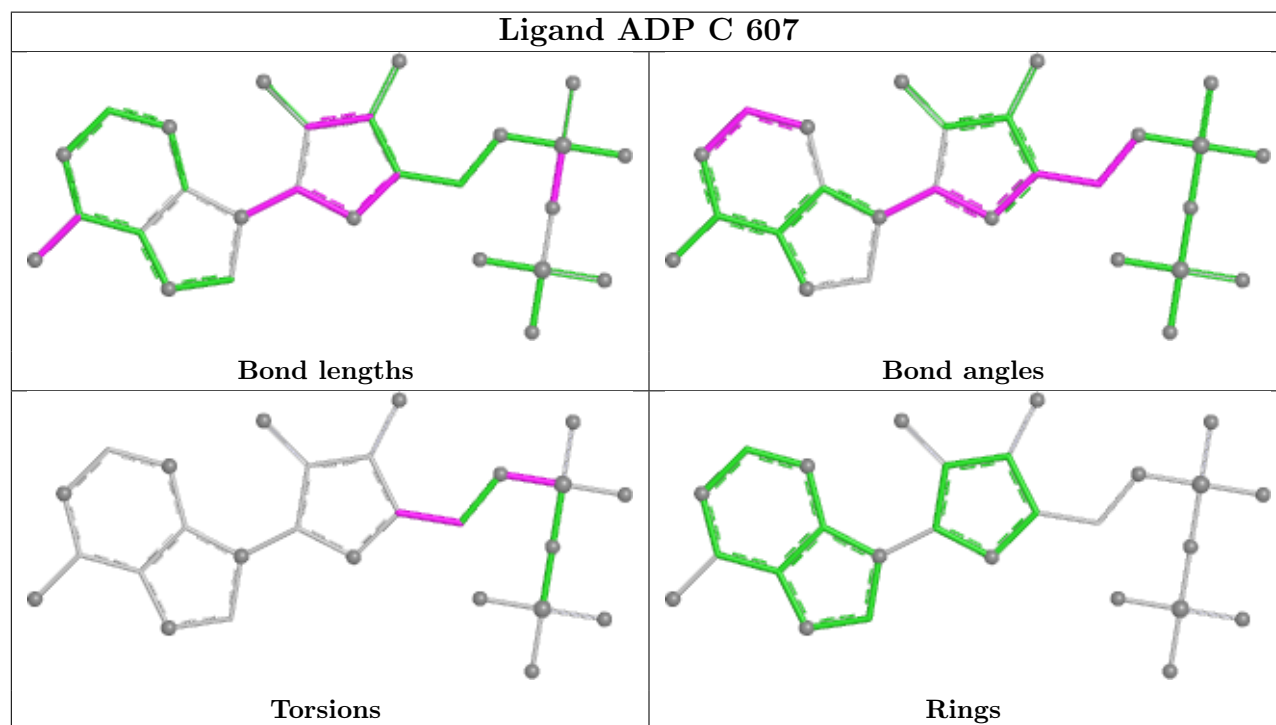
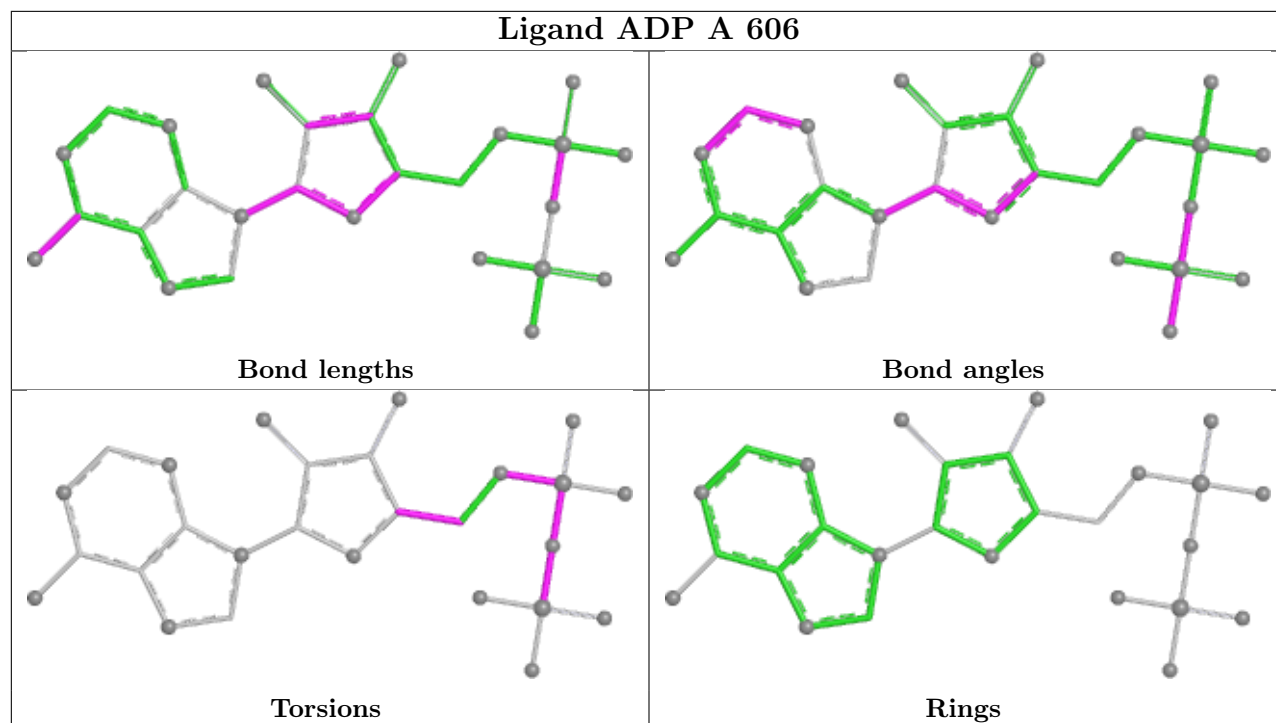
There are no ring outliers.

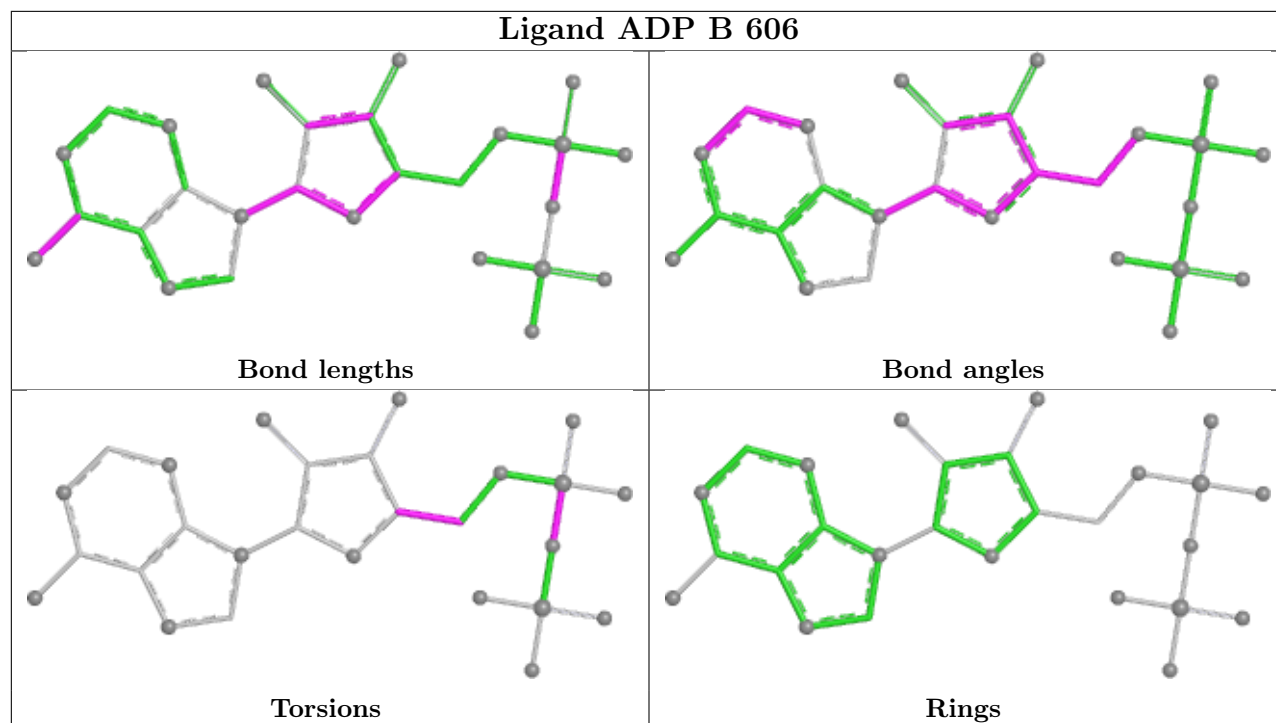
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	604	ADP	5	0
7	C	610	PO4	2	0
5	A	606	ADP	6	0
5	C	607	ADP	1	0
5	B	606	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	376/565 (66%)	-0.29	6 (1%) 70 63	45, 68, 135, 186	0
1	B	547/565 (96%)	0.08	29 (5%) 33 26	49, 81, 190, 249	0
1	C	546/565 (96%)	-0.03	17 (3%) 51 43	50, 79, 150, 217	0
1	D	376/565 (66%)	-0.24	7 (1%) 66 58	45, 70, 138, 197	0
All	All	1845/2260 (81%)	-0.09	59 (3%) 50 42	45, 75, 159, 249	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	517	SER	4.4
1	D	175	PHE	4.4
1	B	538	ILE	4.2
1	B	561	ILE	4.1
1	B	527	ALA	4.0
1	B	518	ILE	3.9
1	C	502	GLY	3.7
1	A	168	HIS	3.6
1	B	537	THR	3.6
1	B	564	ARG	3.6
1	B	516	CYS	3.6
1	B	519	VAL	3.4
1	C	438	HIS	3.2
1	A	448	GLU	3.2
1	C	501	ALA	3.1
1	C	498	PRO	3.0
1	C	26	TYR	3.0
1	C	320	GLU	3.0
1	A	171	GLU	2.9
1	B	153	ASN	2.9
1	D	117	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	350	GLU	2.7
1	C	19	ASN	2.7
1	C	563	ALA	2.7
1	B	531	ILE	2.6
1	B	530	LEU	2.6
1	B	485	LEU	2.6
1	B	97	ASP	2.4
1	B	174	GLY	2.4
1	C	145	LEU	2.4
1	B	154	HIS	2.4
1	D	163	TYR	2.3
1	C	407	ALA	2.3
1	C	315	THR	2.3
1	D	460	ASP	2.3
1	C	516	CYS	2.3
1	B	549	GLY	2.3
1	B	546	ILE	2.3
1	B	541	GLU	2.3
1	B	155	LEU	2.3
1	A	117	LEU	2.2
1	C	496	LEU	2.2
1	B	182	PRO	2.2
1	B	77	GLU	2.2
1	D	77	GLU	2.2
1	B	151	SER	2.2
1	D	122	THR	2.2
1	C	522	GLU	2.2
1	C	20	LEU	2.2
1	B	484	PHE	2.1
1	B	500	MET	2.1
1	A	118	ARG	2.1
1	B	488	GLY	2.1
1	B	486	SER	2.1
1	B	526	ARG	2.0
1	D	480	LYS	2.0
1	C	301	THR	2.0
1	C	171	GLU	2.0
1	B	275	LEU	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 [i](#)

There are no monosaccharides 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, 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.

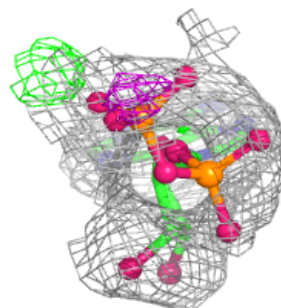
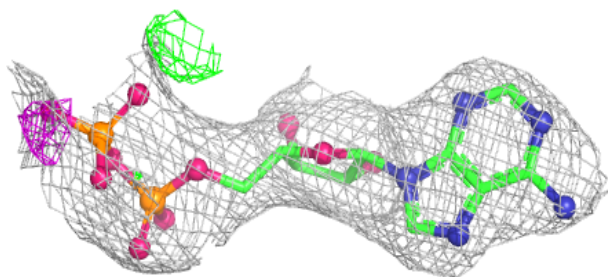
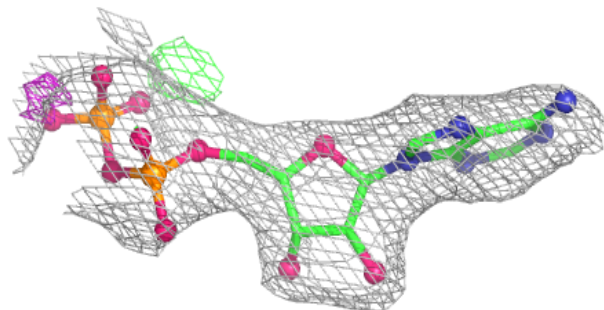
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	K	B	603	1/1	0.23	0.26	182,182,182,182	1
2	K	A	603	1/1	0.57	0.40	127,127,127,127	1
2	K	D	601	1/1	0.62	0.39	127,127,127,127	1
6	GLC	C	608	12/12	0.72	0.14	118,127,128,128	0
6	GLC	C	609	12/12	0.72	0.15	120,127,129,129	0
2	K	C	603	1/1	0.84	0.10	71,71,71,71	1
2	K	C	601	1/1	0.84	0.09	54,54,54,54	1
6	GLC	B	607	12/12	0.85	0.11	148,153,155,155	0
6	GLC	D	605	12/12	0.85	0.10	133,138,139,139	0
2	K	A	602	1/1	0.88	0.13	47,47,47,47	1
2	K	A	601	1/1	0.91	0.10	55,55,55,55	1
5	ADP	D	604	27/27	0.91	0.09	64,71,124,128	0
5	ADP	B	606	27/27	0.94	0.08	62,68,130,155	0
5	ADP	A	606	27/27	0.94	0.09	65,71,203,203	0
7	PO4	C	610	5/5	0.94	0.08	86,91,92,93	0
7	PO4	B	608	5/5	0.95	0.11	80,81,87,87	0
5	ADP	C	607	27/27	0.95	0.08	48,71,176,177	0
2	K	B	601	1/1	0.96	0.05	75,75,75,75	1
4	CA	B	605	1/1	0.96	0.07	64,64,64,64	0
2	K	D	602	1/1	0.97	0.30	121,121,121,121	1
4	CA	A	605	1/1	0.98	0.06	65,65,65,65	0
2	K	B	602	1/1	0.98	0.25	152,152,152,152	1
2	K	C	602	1/1	0.99	0.04	55,55,55,55	1
3	ZN	A	604	1/1	0.99	0.09	70,70,70,70	0
4	CA	C	605	1/1	0.99	0.07	62,62,62,62	0
4	CA	C	606	1/1	0.99	0.09	68,68,68,68	0
3	ZN	B	604	1/1	0.99	0.09	73,73,73,73	0
3	ZN	C	604	1/1	0.99	0.08	68,68,68,68	0
3	ZN	D	603	1/1	0.99	0.08	68,68,68,68	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.

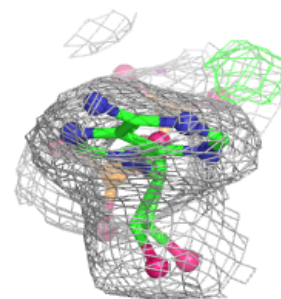
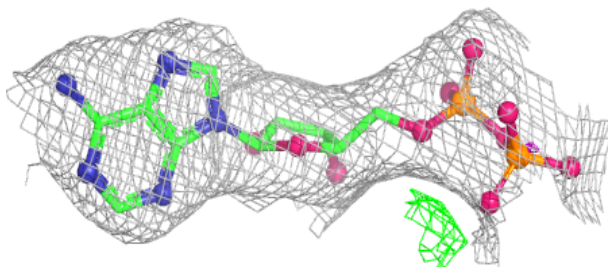
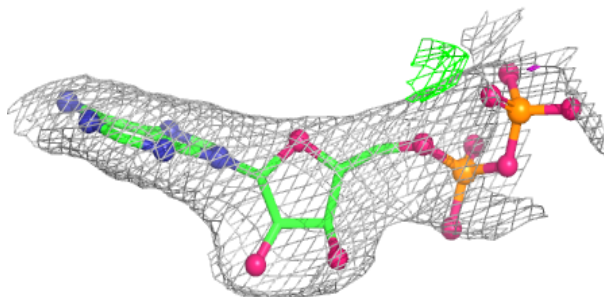
**Electron density around ADP D 604:**

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



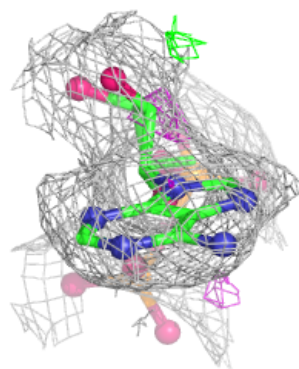
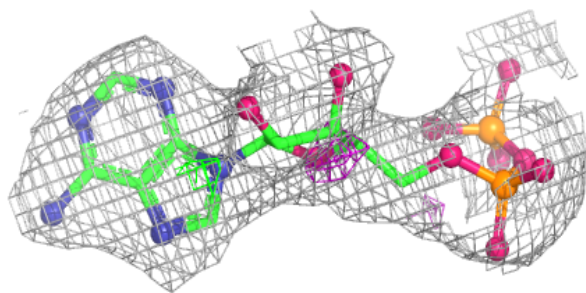
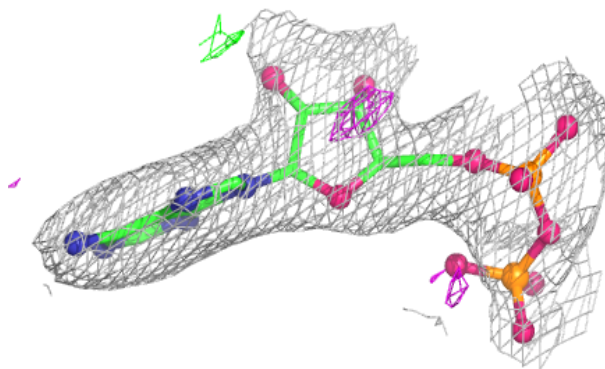
**Electron density around ADP B 606:**

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

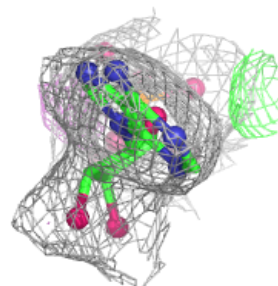
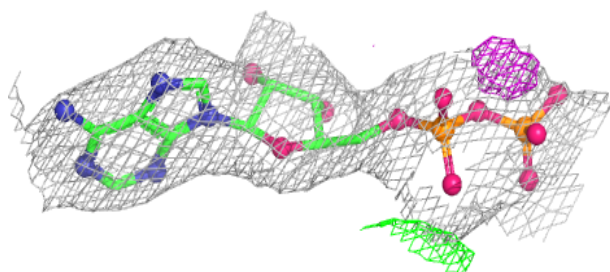
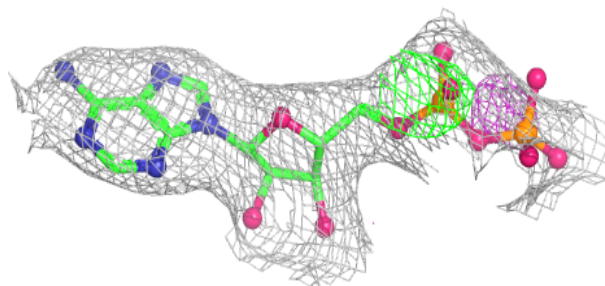


**Electron density around ADP A 606:**

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

**Electron density around ADP C 607:**

$2mF_o-DF_c$  (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.