



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 04:17 AM UTC

PDB ID : 5ILN / pdb_00005iln
Title : Crystal structure of Aspartate Transcarbamoylase from Plasmodium falciparum (PfATC) with bound citrate
Authors : Lunev, S.; Bosch, S.S.; Batista, F.D.A.; Wrenger, C.; Groves, M.R.
Deposited on : 2016-03-04
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

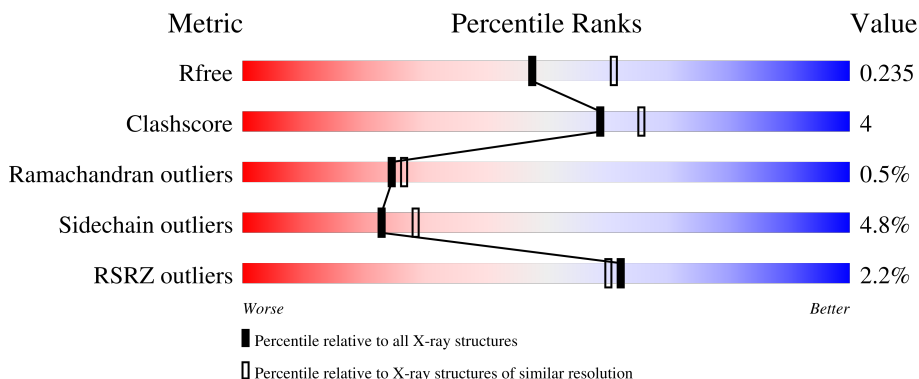
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	385	
1	B	385	
1	C	385	

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
4	FLC	C	401	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8418 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 Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2681	1715	440	517	9			
1	B	335	Total	C	N	O	S	0	0	0
			2727	1743	448	528	8			
1	C	343	Total	C	N	O	S	0	0	0
			2792	1784	457	542	9			

There are 30 discrepancies between the modelled and reference sequences:

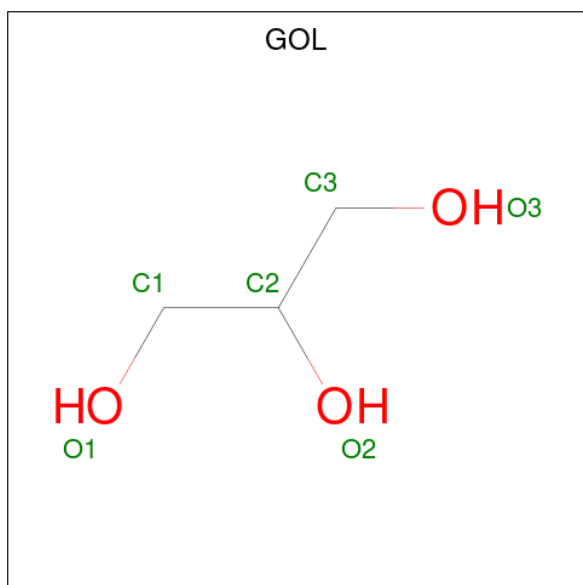
Chain	Residue	Modelled	Actual	Comment	Reference
A	376	SER	-	expression tag	UNP Q8IDP8
A	377	ALA	-	expression tag	UNP Q8IDP8
A	378	TRP	-	expression tag	UNP Q8IDP8
A	379	SER	-	expression tag	UNP Q8IDP8
A	380	HIS	-	expression tag	UNP Q8IDP8
A	381	PRO	-	expression tag	UNP Q8IDP8
A	382	GLN	-	expression tag	UNP Q8IDP8
A	383	PHE	-	expression tag	UNP Q8IDP8
A	384	GLU	-	expression tag	UNP Q8IDP8
A	385	LYS	-	expression tag	UNP Q8IDP8
B	376	SER	-	expression tag	UNP Q8IDP8
B	377	ALA	-	expression tag	UNP Q8IDP8
B	378	TRP	-	expression tag	UNP Q8IDP8
B	379	SER	-	expression tag	UNP Q8IDP8
B	380	HIS	-	expression tag	UNP Q8IDP8
B	381	PRO	-	expression tag	UNP Q8IDP8
B	382	GLN	-	expression tag	UNP Q8IDP8
B	383	PHE	-	expression tag	UNP Q8IDP8
B	384	GLU	-	expression tag	UNP Q8IDP8
B	385	LYS	-	expression tag	UNP Q8IDP8
C	376	SER	-	expression tag	UNP Q8IDP8
C	377	ALA	-	expression tag	UNP Q8IDP8
C	378	TRP	-	expression tag	UNP Q8IDP8

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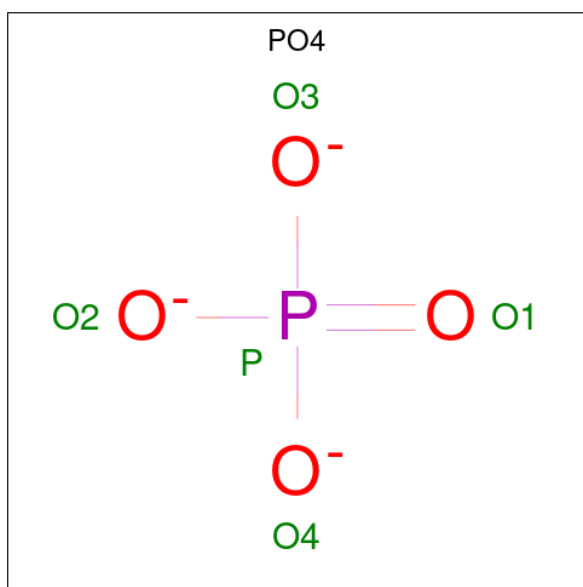
Chain	Residue	Modelled	Actual	Comment	Reference
C	379	SER	-	expression tag	UNP Q8IDP8
C	380	HIS	-	expression tag	UNP Q8IDP8
C	381	PRO	-	expression tag	UNP Q8IDP8
C	382	GLN	-	expression tag	UNP Q8IDP8
C	383	PHE	-	expression tag	UNP Q8IDP8
C	384	GLU	-	expression tag	UNP Q8IDP8
C	385	LYS	-	expression tag	UNP Q8IDP8

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



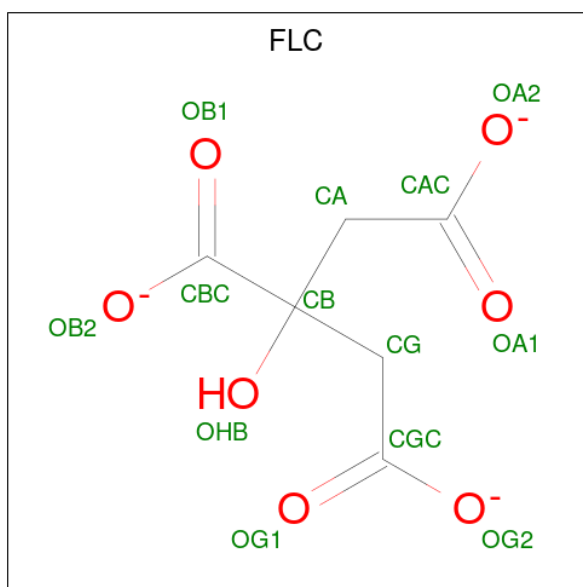
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



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

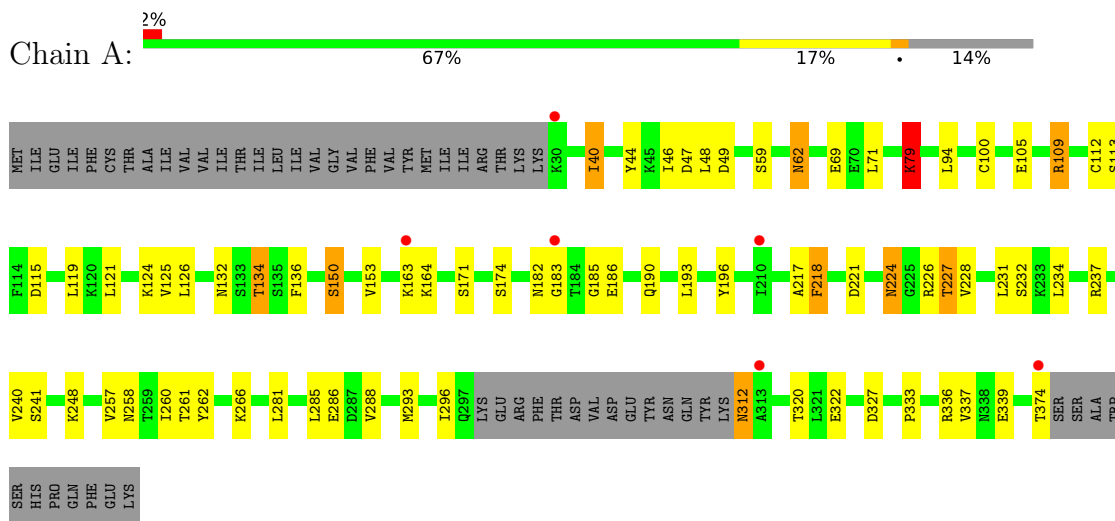
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	42	Total 42	O 42	0	0
5	B	54	Total 54	O 54	0	0
5	C	70	Total 70	O 70	0	0

3 Residue-property plots [i](#)

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

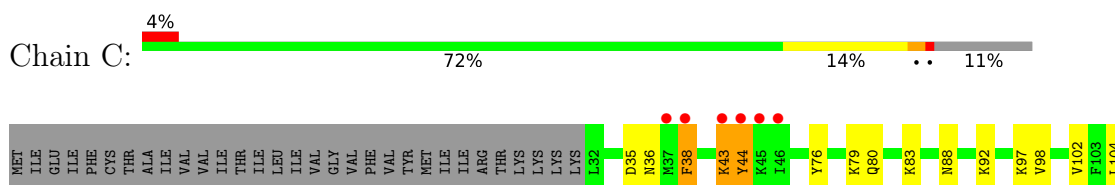
- Molecule 1: Aspartate carbamoyltransferase

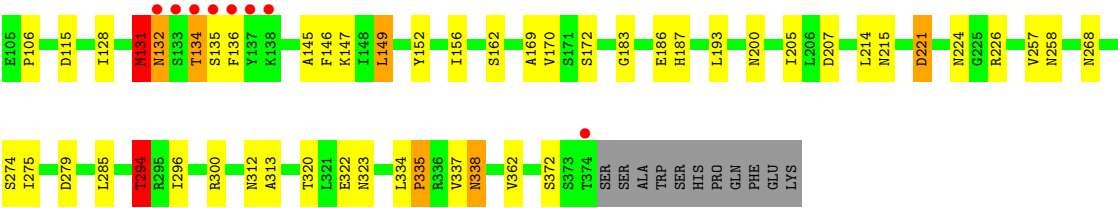


- Molecule 1: Aspartate carbamoyltransferase



- Molecule 1: Aspartate carbamoyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.45Å 107.29Å 87.32Å 90.00° 117.46° 90.00°	Depositor
Resolution (Å)	45.10 – 2.21 45.10 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.10-2.21) 97.6 (45.10-2.21)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.180 , 0.234 0.186 , 0.235	Depositor DCC
R_{free} test set	3470 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h-l,k,h 0.011 for l,k,-h-l 0.021 for h,-k,-h-l 0.023 for -h-l,-k,l 0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8418	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, FLC, CSO

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	1.49	16/2712 (0.6%)	1.42	18/3656 (0.5%)
1	B	1.51	17/2759 (0.6%)	1.34	11/3720 (0.3%)
1	C	1.56	21/2827 (0.7%)	1.35	14/3814 (0.4%)
All	All	1.52	54/8298 (0.7%)	1.37	43/11190 (0.4%)

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	C	0	1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	LEU	CA-C	7.91	1.62	1.52
1	C	275	ILE	C-O	-7.61	1.15	1.24
1	A	71	LEU	N-CA	-7.33	1.37	1.46
1	A	237	ARG	C-O	6.86	1.33	1.24
1	C	221	ASP	CA-C	-6.78	1.45	1.53
1	C	294	THR	CB-CG2	-6.58	1.30	1.52
1	C	97	LYS	CA-C	-6.54	1.44	1.52
1	C	98	VAL	N-CA	-6.46	1.38	1.46
1	C	200	ASN	N-CA	-6.34	1.38	1.46
1	C	205	ILE	C-O	-6.17	1.16	1.24
1	C	296	ILE	C-O	-6.12	1.17	1.23
1	B	333	PRO	C-O	-6.03	1.16	1.24
1	A	115	ASP	N-CA	6.02	1.54	1.46
1	B	71	LEU	CA-C	-5.94	1.45	1.52
1	A	327	ASP	CA-C	5.93	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	CYS	C-O	-5.89	1.16	1.24
1	C	134	THR	N-CA	5.88	1.53	1.46
1	B	209	ASN	N-CA	-5.80	1.39	1.46
1	C	268	ASN	CA-C	-5.77	1.45	1.53
1	C	312	ASN	C-O	-5.75	1.16	1.24
1	C	296	ILE	N-CA	-5.70	1.40	1.46
1	B	258	ASN	N-CA	-5.69	1.39	1.46
1	B	296	ILE	C-O	-5.64	1.18	1.24
1	B	161	PRO	C-O	-5.60	1.17	1.24
1	B	285	LEU	CA-C	-5.59	1.44	1.52
1	C	274	SER	CA-C	5.59	1.60	1.52
1	B	72	LEU	C-O	-5.54	1.17	1.24
1	B	154	ASP	CA-CB	-5.47	1.44	1.53
1	B	56	LYS	CA-C	5.46	1.59	1.52
1	A	59	SER	CA-C	-5.44	1.46	1.52
1	C	215	ASN	C-O	5.43	1.30	1.24
1	C	279	ASP	CA-C	-5.42	1.46	1.52
1	A	171	SER	C-O	-5.40	1.17	1.24
1	C	258	ASN	CA-C	-5.40	1.45	1.52
1	A	258	ASN	CA-C	-5.39	1.45	1.52
1	A	79	LYS	CA-C	-5.39	1.45	1.52
1	B	188	PRO	C-O	-5.38	1.18	1.24
1	B	125	VAL	C-O	-5.38	1.18	1.24
1	A	47	ASP	CA-C	5.36	1.59	1.53
1	A	62	ASN	N-CA	5.35	1.52	1.45
1	C	152	TYR	N-CA	5.33	1.53	1.46
1	B	51	ILE	C-O	-5.33	1.18	1.24
1	C	102	VAL	C-O	-5.26	1.18	1.24
1	C	224	ASN	CA-C	-5.24	1.45	1.52
1	B	191	SER	CA-C	-5.19	1.45	1.52
1	A	183	GLY	N-CA	5.15	1.52	1.45
1	A	44	TYR	N-CA	5.15	1.52	1.45
1	B	56	LYS	C-O	-5.14	1.17	1.24
1	C	169	ALA	N-CA	-5.14	1.40	1.46
1	C	104	LEU	C-O	-5.12	1.17	1.24
1	B	84	ILE	C-O	-5.11	1.18	1.24
1	B	171	SER	C-O	-5.11	1.17	1.24
1	A	218	PHE	CA-CB	-5.08	1.46	1.53
1	A	293	MET	CA-C	5.01	1.59	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	TYR	N-CA-C	-9.92	95.84	110.52
1	A	44	TYR	CA-C-N	-8.69	111.15	122.79
1	A	44	TYR	C-N-CA	-8.69	111.15	122.79
1	A	150	SER	CB-CA-C	-7.09	98.62	110.68
1	A	224	ASN	N-CA-C	7.01	121.07	112.23
1	A	109	ARG	N-CA-C	6.94	119.69	111.71
1	C	131	MET	CG-SD-CE	-6.78	85.98	100.90
1	A	79	LYS	CB-CA-C	-6.67	99.71	110.79
1	A	231	LEU	N-CA-C	-6.53	104.24	111.36
1	B	279	ASP	CB-CA-C	-6.49	97.88	109.24
1	A	132	ASN	N-CA-C	6.49	120.45	112.54
1	C	285	LEU	N-CA-C	6.26	120.77	113.20
1	B	57	ASN	N-CA-C	6.14	120.73	113.23
1	C	186	GLU	CA-C-N	5.99	127.55	122.28
1	C	186	GLU	C-N-CA	5.99	127.55	122.28
1	A	105	GLU	N-CA-C	-5.84	102.75	110.40
1	B	85	LEU	N-CA-C	5.78	117.58	111.28
1	A	125	VAL	N-CA-C	5.75	116.56	108.17
1	A	183	GLY	N-CA-C	5.70	121.73	114.66
1	C	170	VAL	CB-CA-C	-5.69	104.45	112.14
1	C	38	PHE	N-CA-C	5.64	117.23	111.14
1	B	362	VAL	N-CA-C	5.55	116.32	110.72
1	C	172	SER	N-CA-C	5.51	118.05	111.71
1	A	40	ILE	CB-CA-C	5.42	119.69	112.22
1	A	266	LYS	N-CA-C	5.40	118.67	111.75
1	C	200	ASN	N-CA-C	5.40	120.28	111.37
1	C	294	THR	N-CA-CB	-5.38	102.34	111.69
1	B	164	LYS	N-CA-C	5.37	116.94	111.14
1	C	323	ASN	N-CA-C	5.31	118.88	112.93
1	C	323	ASN	CB-CA-C	-5.28	101.67	110.81
1	C	313	ALA	N-CA-C	5.25	116.69	111.07
1	B	140	GLU	N-CA-C	5.22	117.80	110.23
1	B	308	ASN	N-CA-C	5.20	117.85	111.82
1	A	257	VAL	CB-CA-C	-5.16	105.28	112.04
1	B	264	LEU	CA-C-N	5.15	127.18	120.28
1	B	264	LEU	C-N-CA	5.15	127.18	120.28
1	B	278	PHE	CA-C-N	5.14	131.29	122.09
1	B	278	PHE	C-N-CA	5.14	131.29	122.09
1	C	79	LYS	CB-CA-C	-5.13	102.82	110.88
1	A	339	GLU	N-CA-C	5.09	118.95	112.34
1	A	153	VAL	N-CA-C	5.08	116.02	108.65
1	C	300	ARG	N-CA-CB	-5.08	103.19	110.65
1	A	227	THR	CB-CA-C	5.05	119.18	110.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	131	MET	Peptide

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	2681	0	2709	32	0
1	B	2727	0	2742	15	0
1	C	2792	0	2800	25	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	C	13	0	5	4	0
5	A	42	0	0	5	0
5	B	54	0	0	2	0
5	C	70	0	0	1	0
All	All	8418	0	8288	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (72) 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:B:112:CSO:SG	1:B:112:CSO:OD	1.96	1.23
4:C:401:FLC:OA1	5:C:501:HOH:O	1.80	1.00
1:C:187:HIS:HE1	4:C:401:FLC:OA2	1.69	0.75
1:C:38:PHE:CE2	1:C:76:TYR:CE1	2.80	0.69
1:C:106:PRO:CD	1:C:131:MET:HE1	2.23	0.69
1:A:182:ASN:O	1:A:226:ARG:NH2	2.27	0.67
1:A:185:GLY:HA2	1:A:226:ARG:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PRO:N	1:C:131:MET:HE1	2.12	0.65
1:A:134:THR:HG21	1:A:136:PHE:CD2	2.33	0.63
1:B:306:GLU:O	1:B:309:GLN:HB2	1.99	0.62
1:A:79:LYS:HE3	1:A:196:TYR:OH	1.99	0.62
4:C:401:FLC:OG1	4:C:401:FLC:CBC	2.50	0.59
1:B:187:HIS:HD2	5:B:506:HOH:O	1.85	0.59
1:C:187:HIS:CE1	4:C:401:FLC:OA2	2.54	0.59
1:A:218:PHE:CD1	1:A:228:VAL:HG13	2.38	0.59
1:C:334:LEU:HB3	1:C:335:PRO:HA	1.83	0.58
1:A:221:ASP:OD2	1:A:224:ASN:HB2	2.03	0.58
1:A:217:ALA:HB2	1:A:288:VAL:HG11	1.85	0.58
1:A:46:ILE:HD12	1:A:48:LEU:HD13	1.86	0.57
1:B:62:ASN:HA	1:B:186:GLU:CG	2.34	0.56
1:C:38:PHE:CZ	1:C:76:TYR:HE1	2.25	0.54
1:C:338:ASN:H	1:C:338:ASN:HD22	1.56	0.54
1:B:62:ASN:OD1	1:B:186:GLU:HG2	2.08	0.54
1:A:109:ARG:HD2	5:A:515:HOH:O	2.07	0.53
1:B:46:ILE:HD13	1:B:72:LEU:HD13	1.88	0.53
1:C:44:TYR:OH	1:C:207:ASP:OD1	2.26	0.53
1:C:106:PRO:HG3	1:C:131:MET:CE	2.40	0.52
1:A:232:SER:HB3	1:A:260:ILE:HD11	1.90	0.52
1:B:160:ASP:O	1:B:182:ASN:HA	2.09	0.52
1:C:221:ASP:H	1:C:294:THR:CG2	2.23	0.52
1:A:281:LEU:HD13	1:A:320:THR:HG21	1.92	0.51
1:C:183:GLY:O	1:C:226:ARG:HD3	2.11	0.51
1:C:36:ASN:OD1	1:C:80:GLN:NE2	2.42	0.51
1:A:62:ASN:OD1	1:A:186:GLU:HG3	2.11	0.51
1:B:62:ASN:HA	1:B:186:GLU:HG3	1.92	0.51
1:C:38:PHE:CZ	1:C:76:TYR:CE1	2.99	0.50
1:A:119:LEU:HD12	1:B:126:LEU:HD21	1.93	0.49
1:A:312:ASN:N	1:A:312:ASN:HD22	2.09	0.49
1:A:186:GLU:OE1	5:A:501:HOH:O	2.20	0.48
1:A:150:SER:HB3	1:A:174:SER:OG	2.13	0.48
1:C:132:ASN:HD22	1:C:132:ASN:N	2.12	0.47
1:C:38:PHE:CE2	1:C:76:TYR:CD1	3.02	0.47
1:A:190:GLN:NE2	5:A:504:HOH:O	2.48	0.47
1:C:145:ALA:O	1:C:149:LEU:HB2	2.15	0.47
1:A:281:LEU:HB3	1:A:285:LEU:HD22	1.96	0.47
1:C:43:LYS:N	1:C:43:LYS:HD3	2.30	0.47
1:B:158:TYR:CE1	1:B:160:ASP:HB2	2.50	0.46
1:C:35:ASP:OD1	1:C:83:LYS:NZ	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ILE:CD1	1:B:69:GLU:HB3	2.46	0.46
1:A:134:THR:CG2	1:A:136:PHE:H	2.29	0.45
1:A:109:ARG:O	1:A:113:SER:HB2	2.17	0.45
1:A:193:LEU:HD12	1:A:193:LEU:C	2.42	0.45
1:C:146:PHE:HE1	1:C:156:ILE:HG21	1.82	0.45
1:C:38:PHE:CE2	1:C:76:TYR:HE1	2.32	0.44
1:A:134:THR:HG22	1:A:136:PHE:H	1.82	0.44
1:B:193:LEU:C	1:B:193:LEU:HD12	2.43	0.44
1:A:46:ILE:CD1	1:A:48:LEU:HD13	2.47	0.43
1:A:79:LYS:NZ	5:A:506:HOH:O	2.50	0.43
1:B:221:ASP:OD2	5:B:501:HOH:O	2.21	0.43
1:C:128:ILE:HG21	1:C:136:PHE:CE1	2.52	0.43
1:B:58:LYS:NZ	1:B:65:ASP:O	2.38	0.43
1:C:106:PRO:CG	1:C:131:MET:HE1	2.47	0.43
1:A:261:THR:O	1:A:262:TYR:C	2.58	0.43
1:B:232:SER:HB3	1:B:260:ILE:HD11	2.01	0.43
1:A:240:VAL:HG12	1:A:241:SER:N	2.33	0.43
1:A:164:LYS:HA	5:A:530:HOH:O	2.19	0.42
1:A:227:THR:HG21	1:A:333:PRO:HG3	2.02	0.42
1:C:193:LEU:HA	1:C:362:VAL:HG21	2.02	0.41
1:A:94:LEU:HB3	1:A:121:LEU:HB3	2.02	0.41
1:A:126:LEU:HD22	1:C:115:ASP:HB3	2.02	0.41
1:A:134:THR:HG21	1:A:136:PHE:HD2	1.84	0.40
1:A:109:ARG:CZ	1:A:109:ARG:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	325/385 (84%)	306 (94%)	18 (6%)	1 (0%)	36 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	329/385 (86%)	318 (97%)	9 (3%)	2 (1%)	21	22
1	C	339/385 (88%)	319 (94%)	18 (5%)	2 (1%)	21	22
All	All	993/1155 (86%)	943 (95%)	45 (4%)	5 (0%)	24	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	VAL
1	C	88	ASN
1	C	337	VAL
1	B	337	VAL
1	B	334	LEU

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	309/360 (86%)	295 (96%)	14 (4%)	24	31
1	B	313/360 (87%)	299 (96%)	14 (4%)	24	31
1	C	321/360 (89%)	304 (95%)	17 (5%)	20	24
All	All	943/1080 (87%)	898 (95%)	45 (5%)	23	28

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	A	49	ASP
1	A	69	GLU
1	A	79	LYS
1	A	124	LYS
1	A	134	THR
1	A	163	LYS
1	A	248	LYS
1	A	286	GLU

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Mol	Chain	Res	Type
1	A	296	ILE
1	A	312	ASN
1	A	322	GLU
1	A	336	ARG
1	A	374	THR
1	B	49	ASP
1	B	83	LYS
1	B	108	THR
1	B	124	LYS
1	B	149	LEU
1	B	200	ASN
1	B	241	SER
1	B	248	LYS
1	B	249	SER
1	B	254	LYS
1	B	271	SER
1	B	281	LEU
1	B	295	ARG
1	B	373	SER
1	C	43	LYS
1	C	44	TYR
1	C	92	LYS
1	C	132	ASN
1	C	134	THR
1	C	135	SER
1	C	147	LYS
1	C	149	LEU
1	C	162	SER
1	C	214	LEU
1	C	257	VAL
1	C	294	THR
1	C	320	THR
1	C	322	GLU
1	C	335	PRO
1	C	338	ASN
1	C	372	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
1	A	200	ASN

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Mol	Chain	Res	Type
1	A	215	ASN
1	A	267	ASN
1	A	318	ASN
1	B	87	ASN
1	B	96	ASN
1	B	127	ASN
1	B	187	HIS
1	B	243	ASN
1	B	338	ASN
1	B	358	ASN
1	C	36	ASN
1	C	80	GLN
1	C	87	ASN
1	C	132	ASN
1	C	187	HIS
1	C	200	ASN
1	C	251	ASN
1	C	308	ASN
1	C	312	ASN
1	C	338	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSO	B	247	1	3,6,7	1.71	0	1,6,8	1.06	0
1	CSO	C	112	1	3,6,7	0.78	0	1,6,8	0.55	0
1	CSO	C	247	1	3,6,7	0.59	0	1,6,8	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSO	B	112	1	3,6,7	1.47	1 (33%)	1,6,8	0.36	0
1	CSO	A	112	1	3,6,7	1.70	1 (33%)	1,6,8	1.62	0
1	CSO	A	247	1	3,6,7	0.78	0	1,6,8	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	B	247	1	-	0/1/5/7	-
1	CSO	C	112	1	-	0/1/5/7	-
1	CSO	C	247	1	-	0/1/5/7	-
1	CSO	B	112	1	-	0/1/5/7	-
1	CSO	A	112	1	-	0/1/5/7	-
1	CSO	A	247	1	-	1/1/5/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	112	CSO	CB-CA	2.42	1.59	1.53
1	A	112	CSO	O-C	2.11	1.28	1.20

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	247	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	112	CSO	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	B	402	-	4,4,4	0.86	0	6,6,6	1.00	0
2	GOL	B	401	-	5,5,5	0.77	0	5,5,5	0.90	0
4	FLC	C	401	-	12,12,12	1.81	4 (33%)	17,17,17	1.95	6 (35%)
3	PO4	C	404	-	4,4,4	1.29	0	6,6,6	0.97	0
2	GOL	A	401	-	5,5,5	0.94	0	5,5,5	1.04	0
2	GOL	C	402	-	5,5,5	0.35	0	5,5,5	0.81	0
3	PO4	A	402	-	4,4,4	1.13	0	6,6,6	0.85	0
2	GOL	C	403	-	5,5,5	0.57	0	5,5,5	0.45	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
2	GOL	B	401	-	-	3/4/4/4	-
4	FLC	C	401	-	-	5/16/16/16	-
2	GOL	A	401	-	-	2/4/4/4	-
2	GOL	C	402	-	-	1/4/4/4	-
2	GOL	C	403	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	FLC	CB-CBC	3.22	1.56	1.53
4	C	401	FLC	CG-CB	-2.59	1.50	1.54
4	C	401	FLC	OA1-CAC	2.43	1.30	1.22
4	C	401	FLC	OHB-CB	2.22	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	FLC	OG1-CGC-CG	-4.40	110.49	122.95
4	C	401	FLC	CB-CG-CGC	-3.31	104.87	113.92
4	C	401	FLC	OB2-CBC-CB	3.10	119.09	113.14
4	C	401	FLC	OG2-CGC-CG	2.77	123.13	114.35
4	C	401	FLC	OHB-CB-CA	2.35	114.74	109.38
4	C	401	FLC	OHB-CB-CG	-2.10	104.58	109.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	C1-C2-C3-O3
2	B	401	GOL	C1-C2-C3-O3
2	B	401	GOL	O2-C2-C3-O3
2	C	403	GOL	O1-C1-C2-O2
2	C	403	GOL	C1-C2-C3-O3
4	C	401	FLC	CAC-CA-CB-CBC
4	C	401	FLC	CAC-CA-CB-CG
4	C	401	FLC	CAC-CA-CB-OHB
2	A	401	GOL	O2-C2-C3-O3
2	C	403	GOL	O2-C2-C3-O3
2	C	403	GOL	O1-C1-C2-C3
2	C	402	GOL	O2-C2-C3-O3
4	C	401	FLC	OHB-CB-CBC-OB2
2	B	401	GOL	O1-C1-C2-O2
4	C	401	FLC	OHB-CB-CBC-OB1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	401	FLC	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	329/385 (85%)	0.06	6 (1%) 67 65	36, 51, 85, 117	0
1	B	333/385 (86%)	-0.15	2 (0%) 85 84	31, 47, 74, 92	0
1	C	341/385 (88%)	-0.22	14 (4%) 41 38	31, 44, 86, 114	0
All	All	1003/1155 (86%)	-0.11	22 (2%) 62 60	31, 47, 81, 117	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	LYS	4.6
1	A	374	THR	4.0
1	A	313	ALA	3.7
1	C	134	THR	3.4
1	C	37	MET	3.0
1	C	38	PHE	2.8
1	C	133	SER	2.7
1	A	30	LYS	2.7
1	A	163	LYS	2.7
1	C	45	LYS	2.7
1	C	137	TYR	2.6
1	C	135	SER	2.6
1	B	373	SER	2.5
1	C	46	ILE	2.5
1	C	374	THR	2.4
1	C	136	PHE	2.4
1	C	43	LYS	2.3
1	C	132	ASN	2.3
1	C	44	TYR	2.1
1	A	183	GLY	2.1
1	B	139	GLY	2.0
1	A	210	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSO	A	247	7/8	0.87	0.10	90,105,112,115	0
1	CSO	B	112	7/8	0.93	0.09	40,43,46,53	0
1	CSO	A	112	7/8	0.94	0.08	38,40,49,53	0
1	CSO	B	247	7/8	0.96	0.08	51,57,61,64	0
1	CSO	C	247	7/8	0.96	0.07	45,51,54,55	0
1	CSO	C	112	7/8	0.97	0.06	35,38,40,50	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	401	6/6	0.84	0.17	58,74,81,83	0
3	PO4	B	402	5/5	0.84	0.12	57,61,74,80	5
3	PO4	A	402	5/5	0.85	0.12	55,63,75,76	5
2	GOL	C	403	6/6	0.85	0.15	82,88,93,93	0
2	GOL	B	401	6/6	0.87	0.18	57,69,72,85	0
4	FLC	C	401	13/13	0.89	0.10	37,47,54,54	0
2	GOL	C	402	6/6	0.94	0.09	42,53,53,55	0
3	PO4	C	404	5/5	0.99	0.04	41,41,48,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.