Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:48 pm BST

PDB ID	:	6HL7
Title	:	Crystal structure of truncated aspartate transcarbamoylase from Plasmodium falciparum with mutated active site (R109A/K138A) and N-carbamoyl-L-phosphate bound
Authors	:	Bosch, S.S.; Lunev, S.; Wrenger, C.; Groves, M.R.
Deposited on	:	2018-09-10
Resolution	:	2.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

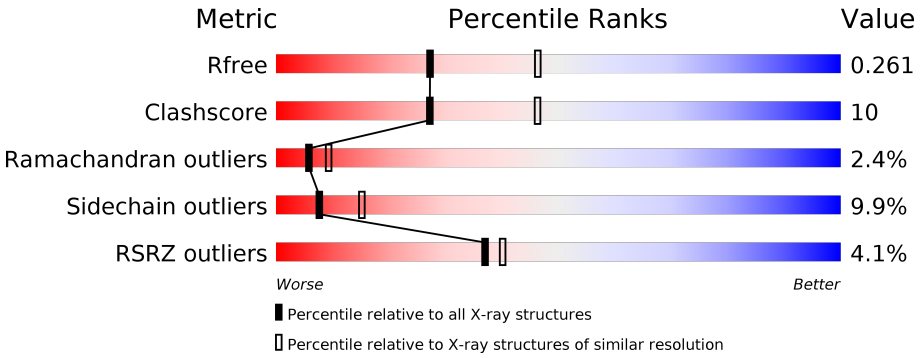
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	348	% 68% 23% 5%
1	B	348	6% 66% 23% 9%
1	C	348	5% 66% 22% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7928 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 transcarbamoylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2708	1729	443	528	8			
1	B	317	Total	C	N	O	S	0	0	0
			2558	1632	421	498	7			
1	C	322	Total	C	N	O	S	0	0	0
			2604	1670	425	501	8			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ALA	ARG	engineered mutation	UNP O15804
A	138	ALA	LYS	engineered mutation	UNP O15804
A	376	ALA	-	expression tag	UNP O15804
A	377	TRP	-	expression tag	UNP O15804
A	378	SER	-	expression tag	UNP O15804
A	379	HIS	-	expression tag	UNP O15804
A	380	PRO	-	expression tag	UNP O15804
A	381	GLN	-	expression tag	UNP O15804
A	382	PHE	-	expression tag	UNP O15804
A	383	GLU	-	expression tag	UNP O15804
A	384	LYS	-	expression tag	UNP O15804
B	109	ALA	ARG	engineered mutation	UNP O15804
B	138	ALA	LYS	engineered mutation	UNP O15804
B	376	ALA	-	expression tag	UNP O15804
B	377	TRP	-	expression tag	UNP O15804
B	378	SER	-	expression tag	UNP O15804
B	379	HIS	-	expression tag	UNP O15804
B	380	PRO	-	expression tag	UNP O15804
B	381	GLN	-	expression tag	UNP O15804
B	382	PHE	-	expression tag	UNP O15804
B	383	GLU	-	expression tag	UNP O15804
B	384	LYS	-	expression tag	UNP O15804
C	109	ALA	ARG	engineered mutation	UNP O15804

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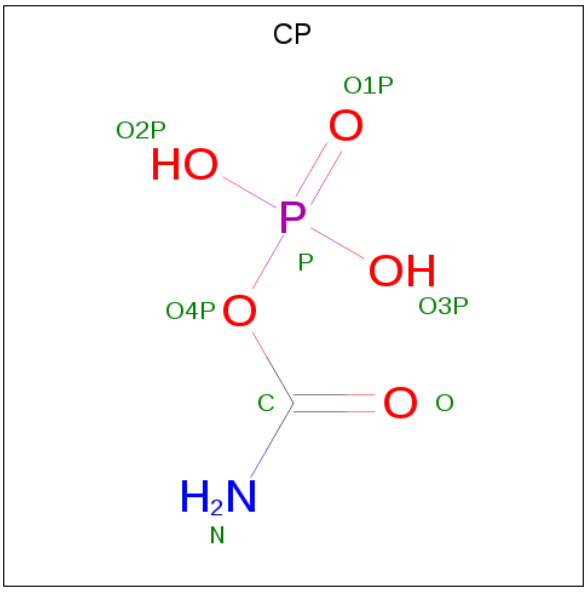
Chain	Residue	Modelled	Actual	Comment	Reference
C	138	ALA	LYS	engineered mutation	UNP O15804
C	376	ALA	-	expression tag	UNP O15804
C	377	TRP	-	expression tag	UNP O15804
C	378	SER	-	expression tag	UNP O15804
C	379	HIS	-	expression tag	UNP O15804
C	380	PRO	-	expression tag	UNP O15804
C	381	GLN	-	expression tag	UNP O15804
C	382	PHE	-	expression tag	UNP O15804
C	383	GLU	-	expression tag	UNP O15804
C	384	LYS	-	expression tag	UNP O15804

- Molecule 2 is PHOSPHORIC ACID MONO(FORMAMIDE)ESTER (three-letter code: CP) (formula: CH_4NO_5P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			8	1	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	12	Total	O	0	0
			12	12		

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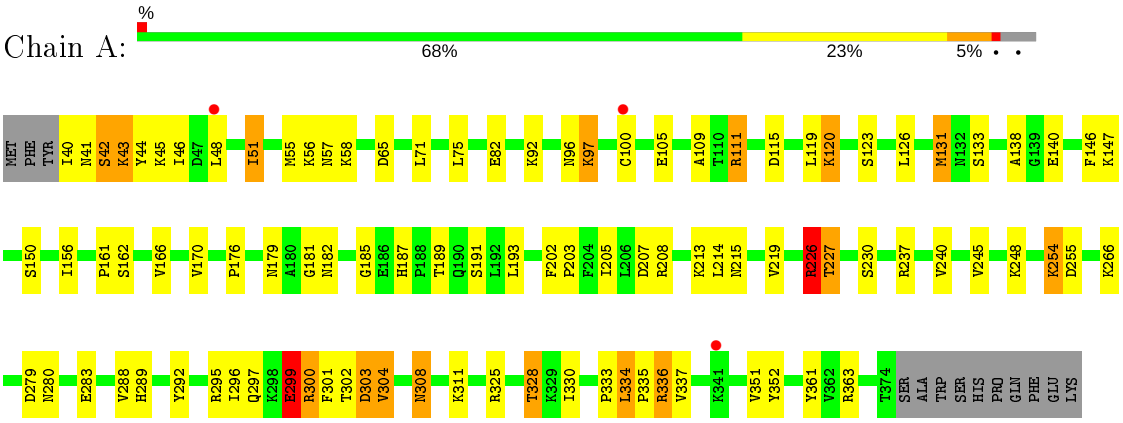
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	13	Total O 13 13	0	0

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 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.

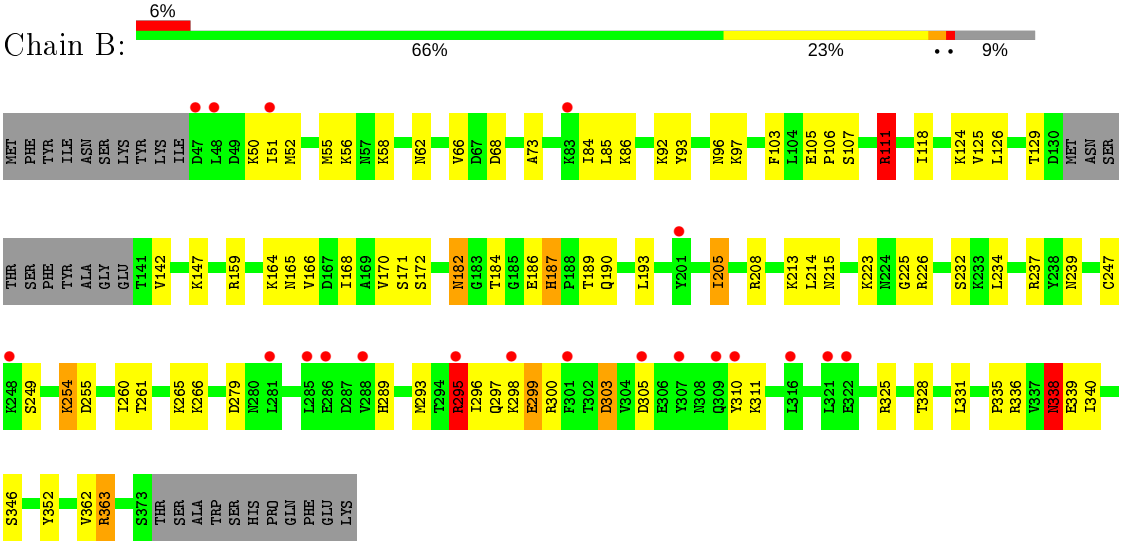
- Molecule 1: Aspartate transcarbamoylase

Chain A:



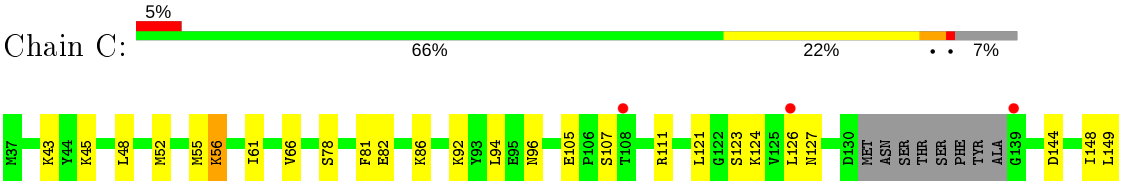
- Molecule 1: Aspartate transcarbamoylase

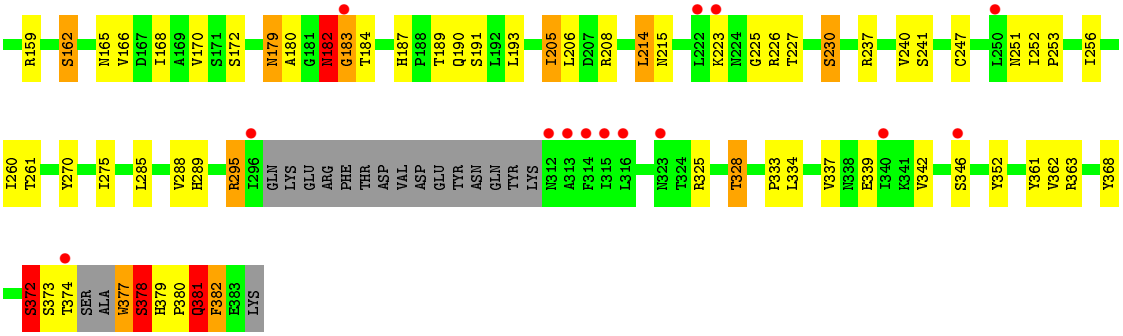
Chain B:



- Molecule 1: Aspartate transcarbamoylase

Chain C:




R159 S162 N165 V166 D167 I168 A169 V170 S171 S172 N179 A180 G181 N182 G183 T184 H187 P188 T189 Q190 S191 L192 L193 I205 L206 D207 R208 L214 N215 L222 K223 N224 G225 R226 T227 S230 R237 V240 S241 C247 L250 N251 I252 P253 I256
I260 T261 Y270 I275 L285 V288 H289 R295 I296 GLN LYS GLU ARG PHE THR ASP VAL ASP GLU TYR ASN GLN TYR LYS N312 A313 P314 I315 L316 N323 T324 R325 T328 P333 L334 V337 N338 E339 I340 K341 V342 S346 Y352 Y361 V362 R363 Y368
S372 S373 T374 SER ALA W377 S378 H379 P380 Q381 F382 E383 LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.00Å 89.72Å 121.64Å 90.00° 122.17° 90.00°	Depositor
Resolution (Å)	57.61 – 2.50 57.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (57.61-2.50) 98.0 (57.55-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.204 , 0.258 0.210 , 0.261	Depositor DCC
R_{free} test set	2399 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7928	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CP

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	0.78	0/2757	1.03	1/3726 (0.0%)
1	B	0.78	0/2602	1.04	6/3516 (0.2%)
1	C	0.78	0/2652	1.01	1/3582 (0.0%)
All	All	0.78	0/8011	1.03	8/10824 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	4
All	All	0	7

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	ARG	CG-CD-NE	6.61	125.67	111.80
1	B	338	ASN	CB-CA-C	6.56	123.52	110.40
1	A	226	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	B	295	ARG	CB-CG-CD	5.84	126.79	111.60
1	B	363	ARG	CB-CA-C	5.79	121.98	110.40
1	B	111	ARG	CB-CA-C	5.41	121.22	110.40
1	B	335	PRO	N-CA-C	5.27	125.81	112.10
1	C	339	GLU	CB-CA-C	-5.09	100.22	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	ASP	Peptide
1	B	107	SER	Peptide
1	B	338	ASN	Peptide
1	C	180	ALA	Peptide
1	C	247	CYS	Peptide
1	C	378	SER	Peptide
1	C	381	GLN	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	2708	0	2712	62	0
1	B	2558	0	2565	42	0
1	C	2604	0	2609	63	0
2	A	8	0	2	1	0
2	C	8	0	2	0	0
3	A	17	0	0	1	0
3	B	12	0	0	1	0
3	C	13	0	0	0	0
All	All	7928	0	7890	160	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 10.

All (160) 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:280:ASN:HD21	1:A:283:GLU:HG3	1.32	0.95
1:C:368:TYR:O	1:C:372:SER:OG	1.86	0.93
1:C:377:TRP:CD1	1:C:378:SER:N	2.38	0.91
1:C:377:TRP:HD1	1:C:378:SER:N	1.68	0.91
1:C:377:TRP:HD1	1:C:378:SER:CA	1.85	0.88
1:C:48:LEU:HD23	1:C:381:GLN:HB3	1.55	0.87
1:C:191:SER:OG	1:C:230:SER:HB3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:TRP:CD1	1:C:378:SER:CA	2.64	0.80
1:A:92:LYS:NZ	1:C:96:ASN:OD1	2.13	0.78
1:A:215:ASN:H	1:A:289:HIS:HD2	1.29	0.78
1:A:208:ARG:NH1	1:A:237:ARG:O	2.17	0.77
1:A:42:SER:HB2	1:A:43:LYS:HE3	1.67	0.75
1:B:295:ARG:HD3	1:B:295:ARG:H	1.52	0.74
1:A:308:ASN:C	1:A:308:ASN:HD22	1.90	0.74
1:C:208:ARG:NH1	1:C:237:ARG:O	2.21	0.74
1:C:377:TRP:HD1	1:C:378:SER:CB	2.02	0.73
1:B:208:ARG:NH1	1:B:237:ARG:O	2.21	0.72
1:A:325:ARG:O	1:A:328:THR:HG23	1.91	0.69
1:A:131:MET:CE	1:A:131:MET:HA	2.22	0.69
1:C:377:TRP:CD1	1:C:378:SER:CB	2.76	0.69
1:B:296:ILE:HG21	1:B:311:LYS:HA	1.77	0.66
1:A:214:LEU:O	1:A:240:VAL:HA	1.94	0.66
1:A:146:PHE:O	1:A:150:SER:HB3	1.96	0.66
1:B:62:ASN:HD22	1:B:186:GLU:HG3	1.60	0.66
1:B:189:THR:OG1	1:B:363:ARG:NH2	2.29	0.66
1:C:325:ARG:HB2	1:C:328:THR:HG22	1.79	0.65
1:A:227:THR:HG23	1:A:292:TYR:OH	1.96	0.65
1:A:215:ASN:H	1:A:289:HIS:CD2	2.11	0.65
1:B:297:GLN:OE1	1:B:300:ARG:NH1	2.30	0.64
1:C:377:TRP:CD1	1:C:378:SER:HB2	2.33	0.64
1:B:182:ASN:C	1:B:182:ASN:HD22	2.01	0.64
1:A:191:SER:OG	1:A:230:SER:HB3	1.98	0.63
1:A:166:VAL:HG21	1:A:182:ASN:HB3	1.80	0.63
1:A:187:HIS:HB2	1:A:226:ARG:HG3	1.78	0.63
1:C:379:HIS:HB3	1:C:381:GLN:HG3	1.80	0.63
1:A:96:ASN:OD1	1:B:92:LYS:HE3	1.99	0.63
1:B:66:VAL:O	1:B:237:ARG:NH2	2.31	0.63
1:B:187:HIS:HB3	3:B:412:HOH:O	2.00	0.61
1:C:48:LEU:CD2	1:C:381:GLN:HB3	2.30	0.61
1:A:187:HIS:HB2	1:A:226:ARG:CG	2.30	0.61
1:C:325:ARG:O	1:C:328:THR:HG23	2.01	0.61
1:A:227:THR:HG21	1:A:333:PRO:HG3	1.84	0.60
1:B:295:ARG:N	1:B:295:ARG:HD3	2.16	0.60
1:A:189:THR:OG1	1:A:363:ARG:NH2	2.35	0.59
1:A:166:VAL:O	1:A:170:VAL:HG23	2.03	0.59
1:B:293:MET:HG3	1:B:340:ILE:HD11	1.85	0.59
1:C:377:TRP:C	1:C:377:TRP:CD1	2.75	0.58
1:A:131:MET:HA	1:A:131:MET:HE2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ASN:H	1:B:289:HIS:HD2	1.51	0.58
1:A:334:LEU:HD13	1:C:148:ILE:HD11	1.87	0.57
1:A:295:ARG:HD3	1:A:335:PRO:HG2	1.86	0.56
1:A:308:ASN:ND2	1:A:308:ASN:C	2.59	0.55
1:C:165:ASN:HA	1:C:168:ILE:HD12	1.88	0.55
1:C:285:LEU:O	1:C:288:VAL:HG22	2.06	0.55
1:B:96:ASN:ND2	1:C:92:LYS:HE3	2.21	0.55
1:B:62:ASN:ND2	1:B:186:GLU:HG3	2.22	0.55
1:B:223:LYS:HE3	1:B:249:SER:O	2.07	0.55
1:B:62:ASN:HD22	1:B:186:GLU:CG	2.19	0.55
1:C:189:THR:OG1	1:C:363:ARG:NH2	2.40	0.55
1:B:51:ILE:HG21	1:B:73:ALA:HB2	1.90	0.54
1:A:330:ILE:O	1:A:351:VAL:HG22	2.07	0.54
1:C:205:ILE:HD12	1:C:206:LEU:N	2.22	0.54
1:B:232:SER:HB3	1:B:260:ILE:HD11	1.89	0.53
1:A:296:ILE:HG23	1:A:296:ILE:O	2.08	0.53
1:A:280:ASN:ND2	1:A:283:GLU:H	2.05	0.53
1:A:57:ASN:HA	1:A:176:PRO:HG2	1.91	0.53
1:B:84:ILE:HD13	1:B:93:TYR:HE2	1.74	0.53
1:C:66:VAL:O	1:C:237:ARG:NH2	2.40	0.53
1:A:82:GLU:HG3	1:A:361:TYR:CE2	2.44	0.52
1:A:302:THR:O	1:A:303:ASP:HB3	2.10	0.52
1:C:205:ILE:HD12	1:C:206:LEU:H	1.73	0.52
1:A:325:ARG:HB2	1:A:328:THR:HG22	1.90	0.52
1:C:215:ASN:H	1:C:289:HIS:CD2	2.28	0.52
1:C:81:PHE:CZ	1:C:380:PRO:HG2	2.44	0.52
1:B:52:MET:O	1:B:55:MET:N	2.41	0.52
1:B:213:LYS:HD3	1:B:239:ASN:OD1	2.10	0.52
1:A:111:ARG:NH1	1:C:127:ASN:O	2.42	0.52
1:C:215:ASN:H	1:C:289:HIS:HD2	1.56	0.52
1:A:40:ILE:HA	1:A:44:TYR:O	2.11	0.51
1:B:325:ARG:HB2	1:B:328:THR:CG2	2.40	0.51
1:C:48:LEU:HD23	1:C:381:GLN:CB	2.35	0.51
1:A:51:ILE:O	1:A:55:MET:HG3	2.11	0.51
1:C:260:ILE:HG22	1:C:275:ILE:HD11	1.92	0.51
1:A:120:LYS:HA	1:A:120:LYS:HE3	1.91	0.51
1:A:55:MET:O	1:A:56:LYS:C	2.49	0.51
1:C:377:TRP:CD1	1:C:378:SER:C	2.85	0.50
1:A:302:THR:O	1:A:303:ASP:CB	2.58	0.50
1:B:325:ARG:HB2	1:B:328:THR:HG22	1.94	0.50
1:C:223:LYS:HA	1:C:253:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLU:HB3	1:A:161:PRO:HD3	1.94	0.49
1:C:48:LEU:O	1:C:52:MET:HG3	2.12	0.49
1:A:296:ILE:HG21	1:A:311:LYS:HB2	1.94	0.48
1:C:162:SER:OG	1:C:165:ASN:ND2	2.46	0.48
1:C:179:ASN:HD21	1:C:182:ASN:HB3	1.79	0.48
1:C:52:MET:CE	1:C:381:GLN:NE2	2.76	0.48
1:B:205:ILE:HD12	1:B:205:ILE:N	2.29	0.48
1:C:252:ILE:HD11	1:C:256:ILE:HG21	1.96	0.48
1:C:105:GLU:OE1	1:C:159:ARG:HD3	2.13	0.48
1:A:120:LYS:HA	1:A:120:LYS:CE	2.44	0.47
1:A:115:ASP:O	1:A:119:LEU:HG	2.13	0.47
1:C:78:SER:OG	1:C:362:VAL:HA	2.13	0.47
1:C:94:LEU:O	1:C:123:SER:OG	2.28	0.47
1:C:94:LEU:HB3	1:C:121:LEU:HB3	1.97	0.47
1:A:296:ILE:HG21	1:A:311:LYS:CB	2.43	0.47
1:B:164:LYS:O	1:B:168:ILE:HD12	2.15	0.47
1:A:254:LYS:HE3	1:A:254:LYS:HA	1.96	0.47
1:A:299:GLU:O	1:A:300:ARG:HG3	2.15	0.47
1:C:82:GLU:OE2	1:C:86:LYS:HE2	2.15	0.47
1:A:300:ARG:O	1:A:301:PHE:CD1	2.68	0.46
1:A:166:VAL:HG22	3:A:515:HOH:O	2.15	0.46
1:C:183:GLY:HA2	1:C:226:ARG:NH1	2.31	0.46
1:C:252:ILE:HD12	1:C:253:PRO:HD2	1.97	0.46
1:C:382:PHE:N	1:C:382:PHE:CD1	2.83	0.46
1:B:166:VAL:O	1:B:170:VAL:HG23	2.16	0.46
1:A:179:ASN:ND2	1:A:181:GLY:H	2.14	0.46
1:A:304:VAL:O	1:A:308:ASN:N	2.46	0.46
1:C:107:SER:HB3	1:C:111:ARG:HB2	1.98	0.46
1:A:97:LYS:HB2	1:A:123:SER:OG	2.16	0.46
1:C:187:HIS:HB2	1:C:226:ARG:HG3	1.96	0.46
1:B:215:ASN:H	1:B:289:HIS:CD2	2.33	0.46
1:B:55:MET:O	1:B:58:LYS:HB2	2.16	0.45
1:C:377:TRP:C	1:C:377:TRP:HD1	2.15	0.45
1:B:51:ILE:HG21	1:B:73:ALA:CB	2.47	0.45
1:A:336:ARG:NH2	1:C:144:ASP:OD1	2.49	0.45
1:A:71:LEU:O	1:A:75:LEU:HG	2.17	0.45
1:A:44:TYR:OH	1:A:207:ASP:HA	2.17	0.45
1:B:105:GLU:OE1	1:B:159:ARG:NH2	2.50	0.44
1:C:61:ILE:HA	1:C:179:ASN:HB2	2.00	0.44
1:C:261:THR:HG23	1:C:270:TYR:CE1	2.52	0.44
1:B:261:THR:O	1:B:265:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:TYR:CZ	1:C:380:PRO:HD2	2.53	0.44
1:A:58:LYS:HE3	1:A:65:ASP:O	2.18	0.43
1:B:190:GLN:O	1:B:193:LEU:HG	2.18	0.43
1:A:219:VAL:HG22	1:A:245:VAL:HB	1.99	0.43
1:B:182:ASN:C	1:B:182:ASN:ND2	2.71	0.43
1:A:227:THR:CG2	1:A:292:TYR:OH	2.65	0.43
1:A:215:ASN:HB2	1:A:288:VAL:HA	2.01	0.43
1:C:260:ILE:CG2	1:C:275:ILE:HD11	2.49	0.43
1:A:334:LEU:HA	1:A:335:PRO:C	2.40	0.42
1:B:166:VAL:HG21	1:B:182:ASN:HB2	2.01	0.42
1:C:214:LEU:O	1:C:240:VAL:HA	2.19	0.42
1:C:55:MET:O	1:C:56:LYS:C	2.58	0.42
1:B:234:LEU:O	1:B:237:ARG:HB2	2.20	0.42
1:B:193:LEU:HA	1:B:362:VAL:HG21	2.02	0.42
1:C:377:TRP:NE1	1:C:378:SER:HB2	2.34	0.42
1:C:190:GLN:HG2	1:C:227:THR:HG22	2.01	0.42
1:C:82:GLU:HG3	1:C:361:TYR:CE2	2.54	0.42
1:C:166:VAL:O	1:C:170:VAL:HG23	2.20	0.42
1:A:109:ALA:HB3	2:A:401:CP:O1P	2.19	0.41
1:B:142:VAL:HG21	1:B:165:ASN:ND2	2.35	0.41
1:B:265:LYS:O	1:B:266:LYS:C	2.59	0.41
1:A:297:GLN:O	1:A:301:PHE:HD1	2.03	0.41
1:A:100:CYS:O	1:A:156:ILE:HA	2.21	0.41
1:A:202:PHE:N	1:A:203:PRO:HD3	2.36	0.41
1:B:118:ILE:HG21	1:B:125:VAL:HB	2.01	0.40
1:B:103:PHE:CE2	1:B:111:ARG:HB2	2.57	0.40
1:C:381:GLN:H	1:C:381:GLN:HG3	1.81	0.40
1:B:331:LEU:HD12	1:B:331:LEU:N	2.36	0.40
1:A:336:ARG:HH21	1:C:144:ASP:CG	2.24	0.40
1:C:333:PRO:O	1:C:334:LEU:HB2	2.21	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	333/348 (96%)	306 (92%)	19 (6%)	8 (2%)	6 9
1	B	313/348 (90%)	285 (91%)	23 (7%)	5 (2%)	9 17
1	C	314/348 (90%)	281 (90%)	23 (7%)	10 (3%)	4 5
All	All	960/1044 (92%)	872 (91%)	65 (7%)	23 (2%)	6 9

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLU
1	A	303	ASP
1	B	299	GLU
1	C	251	ASN
1	C	295	ARG
1	C	373	SER
1	C	378	SER
1	A	42	SER
1	A	300	ARG
1	B	225	GLY
1	B	310	TYR
1	C	183	GLY
1	A	138	ALA
1	A	337	VAL
1	B	254	LYS
1	C	337	VAL
1	C	342	VAL
1	B	303	ASP
1	C	182	ASN
1	C	225	GLY
1	C	372	SER
1	A	185	GLY
1	A	334	LEU

5.3.2 Protein sidechains (i)

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	313/325 (96%)	283 (90%)	30 (10%)	8 16
1	B	296/325 (91%)	262 (88%)	34 (12%)	5 11
1	C	301/325 (93%)	275 (91%)	26 (9%)	10 20
All	All	910/975 (93%)	820 (90%)	90 (10%)	8 15

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	43	LYS
1	A	45	LYS
1	A	46	ILE
1	A	48	LEU
1	A	51	ILE
1	A	97	LYS
1	A	111	ARG
1	A	120	LYS
1	A	126	LEU
1	A	131	MET
1	A	133	SER
1	A	140	GLU
1	A	147	LYS
1	A	162	SER
1	A	193	LEU
1	A	205	ILE
1	A	213	LYS
1	A	226	ARG
1	A	227	THR
1	A	248	LYS
1	A	254	LYS
1	A	255	ASP
1	A	266	LYS
1	A	299	GLU
1	A	304	VAL
1	A	308	ASN
1	A	328	THR
1	A	336	ARG
1	A	352	TYR
1	B	50	LYS
1	B	56	LYS

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Mol	Chain	Res	Type
1	B	68	ASP
1	B	85	LEU
1	B	86	LYS
1	B	97	LYS
1	B	106	PRO
1	B	111	ARG
1	B	124	LYS
1	B	126	LEU
1	B	129	THR
1	B	147	LYS
1	B	171	SER
1	B	172	SER
1	B	182	ASN
1	B	184	THR
1	B	187	HIS
1	B	205	ILE
1	B	214	LEU
1	B	226	ARG
1	B	247	CYS
1	B	254	LYS
1	B	255	ASP
1	B	279	ASP
1	B	295	ARG
1	B	298	LYS
1	B	299	GLU
1	B	303	ASP
1	B	305	ASP
1	B	336	ARG
1	B	338	ASN
1	B	339	GLU
1	B	346	SER
1	B	352	TYR
1	C	43	LYS
1	C	45	LYS
1	C	56	LYS
1	C	124	LYS
1	C	126	LEU
1	C	149	LEU
1	C	162	SER
1	C	172	SER
1	C	179	ASN
1	C	182	ASN

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Mol	Chain	Res	Type
1	C	184	THR
1	C	193	LEU
1	C	205	ILE
1	C	214	LEU
1	C	230	SER
1	C	241	SER
1	C	295	ARG
1	C	328	THR
1	C	346	SER
1	C	352	TYR
1	C	372	SER
1	C	374	THR
1	C	377	TRP
1	C	378	SER
1	C	381	GLN
1	C	382	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	165	ASN
1	A	179	ASN
1	A	243	ASN
1	A	267	ASN
1	A	280	ASN
1	A	289	HIS
1	A	308	ASN
1	A	323	ASN
1	A	338	ASN
1	B	62	ASN
1	B	96	ASN
1	B	179	ASN
1	B	182	ASN
1	B	211	ASN
1	B	243	ASN
1	B	289	HIS
1	B	323	ASN
1	B	338	ASN
1	C	62	ASN
1	C	165	ASN
1	C	179	ASN

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Mol	Chain	Res	Type
1	C	243	ASN
1	C	268	ASN
1	C	280	ASN
1	C	289	HIS
1	C	323	ASN
1	C	381	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

2 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	$\#\|Z\| > 2$
2	CP	A	401	-	6,7,7	4.59	3 (50%)	7,10,10	1.71	2 (28%)
2	CP	C	401	-	6,7,7	4.27	4 (66%)	7,10,10	1.81	2 (28%)

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	CP	A	401	-	-	1/3/5/5	-
2	CP	C	401	-	-	0/3/5/5	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CP	C-N	7.77	1.48	1.33
2	A	401	CP	P-O4P	7.30	1.70	1.59
2	C	401	CP	C-N	6.98	1.46	1.33
2	C	401	CP	P-O4P	6.55	1.69	1.59
2	C	401	CP	P-O3P	3.58	1.68	1.54
2	A	401	CP	P-O3P	3.05	1.66	1.54
2	C	401	CP	P-O2P	-2.16	1.46	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	CP	O3P-P-O4P	3.85	116.99	105.25
2	A	401	CP	O2P-P-O4P	2.69	113.44	105.25
2	A	401	CP	O2P-P-O1P	-2.57	100.61	110.68
2	C	401	CP	O2P-P-O1P	-2.28	101.74	110.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CP	C-O4P-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CP	1	0

5.7 Other polymers (i)

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^{th} 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	335/348 (96%)	0.30	3 (0%)	84	86	40, 62, 102, 130	0
1	B	317/348 (91%)	0.50	20 (6%)	20	21	44, 73, 117, 154	0
1	C	322/348 (92%)	0.38	17 (5%)	26	28	48, 67, 101, 123	0
All	All	974/1044 (93%)	0.39	40 (4%)	37	40	40, 67, 105, 154	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	TYR	6.4
1	C	315	ILE	5.2
1	C	314	PHE	4.6
1	B	47	ASP	4.4
1	C	346	SER	3.6
1	B	309	GLN	3.3
1	C	183	GLY	3.2
1	B	51	ILE	3.2
1	A	341	LYS	3.1
1	C	323	ASN	3.0
1	B	305	ASP	2.8
1	C	250	LEU	2.8
1	B	307	TYR	2.7
1	C	296	ILE	2.7
1	A	48	LEU	2.7
1	B	286	GLU	2.6
1	C	316	LEU	2.6
1	C	139	GLY	2.6
1	C	108	THR	2.5
1	C	223	LYS	2.5
1	C	312	ASN	2.5
1	B	83	LYS	2.4
1	B	298	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	301	PHE	2.4
1	B	281	LEU	2.4
1	B	248	LYS	2.3
1	C	340	ILE	2.3
1	B	48	LEU	2.2
1	B	322	GLU	2.2
1	B	295	ARG	2.2
1	B	316	LEU	2.2
1	C	374	THR	2.2
1	C	126	LEU	2.2
1	B	285	LEU	2.1
1	B	288	VAL	2.1
1	C	313	ALA	2.1
1	A	100	CYS	2.1
1	C	222	LEU	2.1
1	B	321	LEU	2.0
1	B	201	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	CP	C	401	8/8	0.90	0.22	76,91,111,119	0
2	CP	A	401	8/8	0.93	0.12	80,93,107,111	0

6.5 Other polymers (i)

There are no such residues in this entry.