



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 PM UTC

PDB ID : 6HL7 / pdb_00006hl7
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 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

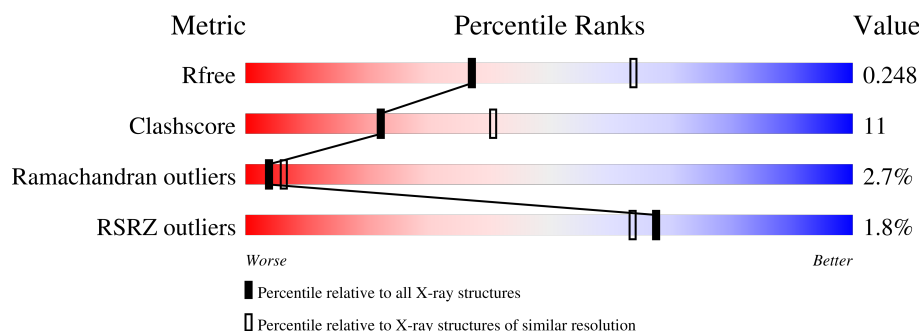
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	348	69% 25% • •
1	B	348	71% 19% • 9%
1	C	348	68% 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:

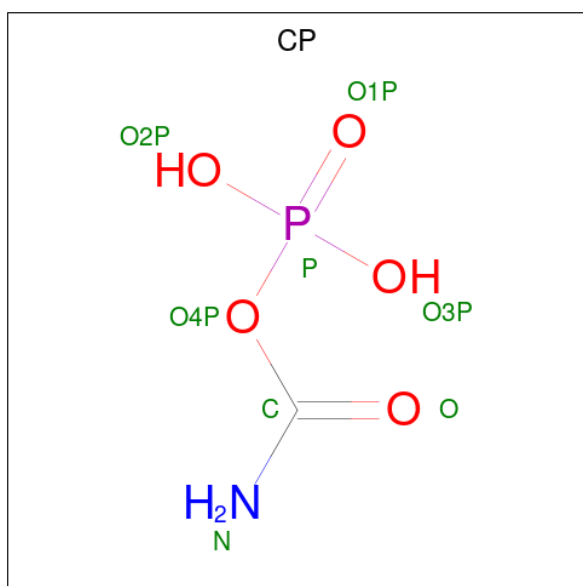
Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ALA	ARG	engineered mutation	UNP O15804
A	138	ALA	LYS	engineered mutation	UNP O15804
A	376	ALA	-	expression tag	UNP O15804
A	377	TRP	-	expression tag	UNP O15804
A	378	SER	-	expression tag	UNP O15804
A	379	HIS	-	expression tag	UNP O15804
A	380	PRO	-	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 (CCD ID: CP) (formula: $\text{CH}_4\text{NO}_5\text{P}$).



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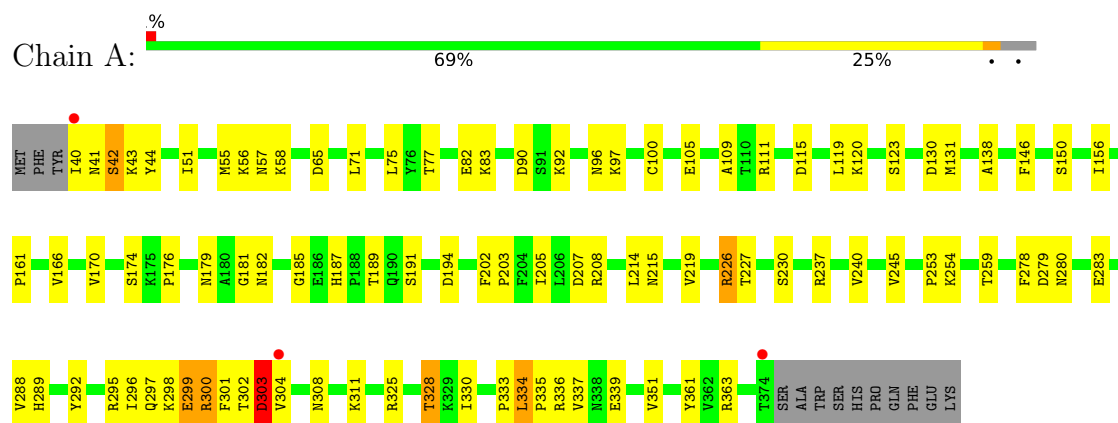
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	13	Total	O	0	0
			13	13		

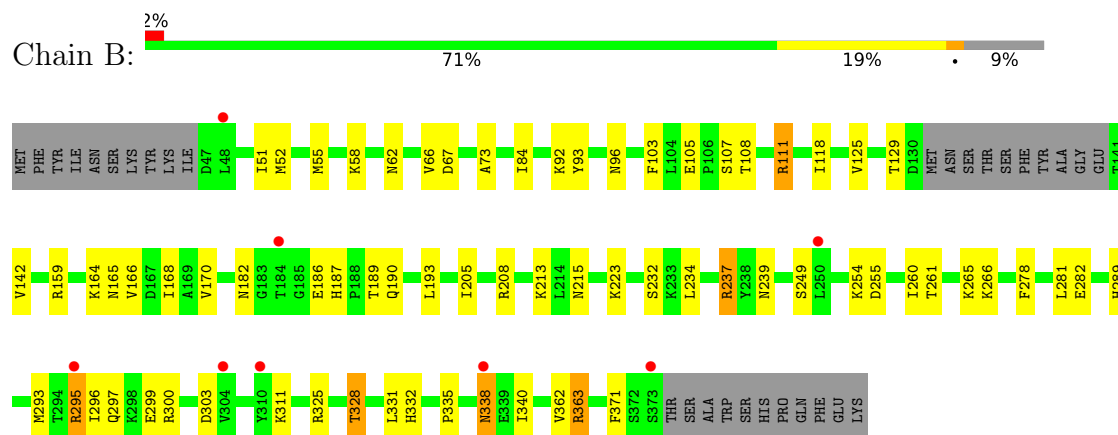
3 Residue-property plots [i](#)

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.

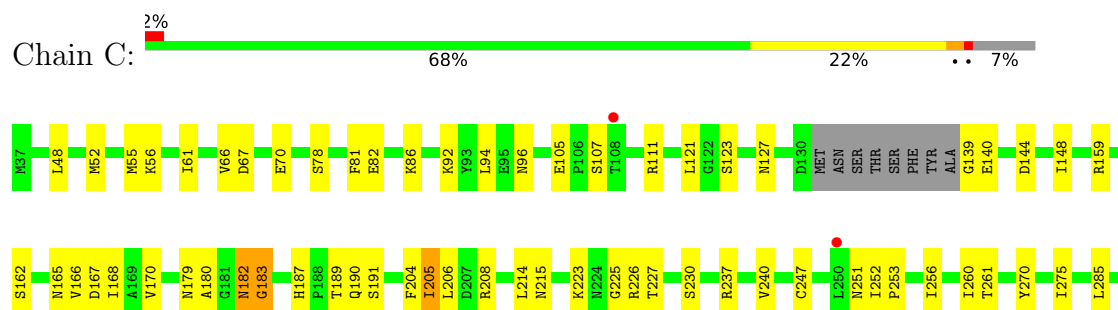
• Molecule 1: Aspartate transcarbamoylase

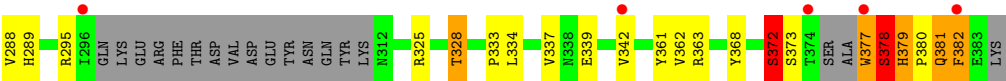


• Molecule 1: Aspartate transcarbamoylase



• Molecule 1: Aspartate transcarbamoylase





4 Data and refinement statistics

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 57.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (57.61-2.50) 94.8 (57.61-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.204 , 0.258 (Not available) , 0.248	Depositor DCC
R_{free} test set	2399 reflections (5.14%)	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 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

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: 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	1.13	0/2757	1.66	23/3726 (0.6%)
1	B	1.16	0/2602	1.66	19/3516 (0.5%)
1	C	1.14	0/2652	1.60	14/3582 (0.4%)
All	All	1.15	0/8011	1.64	56/10824 (0.5%)

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 (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	PHE	CA-C-N	8.73	132.69	120.29
1	B	278	PHE	C-N-CA	8.73	132.69	120.29
1	B	338	ASN	CB-CA-C	7.71	123.52	111.95
1	C	204	PHE	CA-C-O	-7.36	110.58	119.49
1	C	382	PHE	N-CA-C	-7.07	104.65	113.20
1	A	130	ASP	CA-CB-CG	6.92	119.52	112.60
1	B	108	THR	CB-CA-C	6.82	121.68	110.90
1	C	67	ASP	CA-CB-CG	6.75	119.35	112.60
1	B	295	ARG	CB-CG-CD	6.74	126.79	111.30
1	A	205	ILE	N-CA-CB	6.58	121.91	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	377	TRP	CA-C-N	6.50	133.95	121.54
1	C	377	TRP	C-N-CA	6.50	133.95	121.54
1	C	372	SER	CA-C-N	6.45	133.86	121.54
1	C	372	SER	C-N-CA	6.45	133.86	121.54
1	B	111	ARG	CB-CA-C	6.28	121.22	110.79
1	B	295	ARG	CG-CD-NE	6.21	125.67	112.00
1	A	77	THR	CA-CB-OG1	-6.16	100.36	109.60
1	C	339	GLU	CB-CA-C	-6.15	100.22	110.68
1	A	278	PHE	CA-C-N	6.09	129.05	120.28
1	A	278	PHE	C-N-CA	6.09	129.05	120.28
1	C	205	ILE	N-CA-CB	6.01	119.97	110.54
1	A	339	GLU	CB-CA-C	-5.89	101.38	110.81
1	B	363	ARG	CB-CA-C	5.89	121.98	110.67
1	B	328	THR	N-CA-CB	5.86	118.67	109.83
1	B	363	ARG	N-CA-C	-5.83	105.05	111.82
1	A	298	LYS	CA-C-N	5.82	132.65	121.54
1	A	298	LYS	C-N-CA	5.82	132.65	121.54
1	A	174	SER	N-CA-C	-5.80	106.25	113.38
1	A	259	THR	CA-CB-OG1	-5.80	100.90	109.60
1	C	70	GLU	N-CA-C	-5.79	105.05	111.36
1	B	67	ASP	CA-CB-CG	5.68	118.28	112.60
1	C	328	THR	N-CA-CB	5.68	118.39	110.04
1	B	129	THR	CB-CA-C	5.61	118.81	110.62
1	C	379	HIS	CA-CB-CG	5.59	119.39	113.80
1	A	41	ASN	CA-C-N	5.56	132.16	121.54
1	A	41	ASN	C-N-CA	5.56	132.16	121.54
1	A	194	ASP	CA-C-N	5.50	127.64	120.28
1	A	194	ASP	C-N-CA	5.50	127.64	120.28
1	A	253	PRO	CA-C-N	5.41	128.93	120.82
1	A	253	PRO	C-N-CA	5.41	128.93	120.82
1	A	328	THR	N-CA-CB	5.34	117.90	110.04
1	A	226	ARG	N-CA-C	-5.31	105.60	111.71
1	B	335	PRO	N-CA-C	5.27	125.81	112.10
1	A	303	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	90	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	205	ILE	CA-C-O	-5.19	115.02	120.57
1	B	332	HIS	CB-CA-C	5.16	116.36	109.65
1	A	83	LYS	CA-C-N	5.16	127.01	120.72
1	A	83	LYS	C-N-CA	5.16	127.01	120.72
1	B	295	ARG	N-CA-CB	5.14	117.11	109.19
1	B	237	ARG	CB-CG-CD	5.14	123.12	111.30
1	C	382	PHE	CA-CB-CG	5.13	118.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	PHE	CA-C-O	-5.08	113.32	118.90
1	C	167	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	338	ASN	CA-C-N	5.03	131.38	121.58
1	B	338	ASN	C-N-CA	5.03	131.38	121.58

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	45	0
1	C	2604	0	2609	67	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	167	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 11.

All (167) 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
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:308:ASN:HD22	1:A:308:ASN:C	1.90	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: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:C:52:MET:HE1	1:C:381:GLN:HE22	1.58	0.69
1:A:131:MET:HA	1:A:131:MET:CE	2.22	0.69
1:C:377:TRP:CD1	1:C:378:SER:CB	2.76	0.69
1:B:182:ASN:C	1:B:182:ASN:HD22	2.01	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:C:52:MET:HE1	1:C:381:GLN:NE2	2.12	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:C:377:TRP:CD1	1:C:377:TRP:C	2.75	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:B:295:ARG:N	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: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:C	1:A:308:ASN:ND2	2.59	0.56
1:A:55:MET:O	1:A:56:LYS:C	2.49	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:C:377:TRP:CD1	1:C:378:SER:C	2.85	0.55
1:B:62:ASN:HD22	1:B:186:GLU:CG	2.19	0.55
1:B:223:LYS:HE3	1:B:249:SER:O	2.07	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:57:ASN:HA	1:A:176:PRO:HG2	1.91	0.53
1:A:280:ASN:ND2	1:A:283:GLU:H	2.05	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:A:111:ARG:NH1	1:C:127:ASN:O	2.42	0.52
1:B:213:LYS:HD3	1:B:239:ASN:OD1	2.10	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:A:131:MET:HA	1:A:131:MET:HE2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:A:120:LYS:HA	1.91	0.51
1:C:377:TRP:HD1	1:C:377:TRP:C	2.15	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
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:N	1:B:205:ILE:HD12	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:B:182:ASN:C	1:B:182:ASN:ND2	2.71	0.47
1:A:334:LEU:HA	1:A:335:PRO:C	2.40	0.47
1:C:55:MET:O	1:C:56:LYS:C	2.58	0.47
1:C:78:SER:OG	1:C:362:VAL:HA	2.13	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:HA	1:A:254:LYS:HE3	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:B:265:LYS:O	1:B:266:LYS:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:336:ARG:HH21	1:C:144:ASP:CG	2.24	0.45
1:B:105:GLU:OE1	1:B:159:ARG:NH2	2.50	0.44
1:B:255:ASP:OD1	1:B:255:ASP:C	2.60	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
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:C:94:LEU:O	1:C:123:SER:OG	2.28	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:C:182:ASN:O	1:C:182:ASN:CG	2.60	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: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:B:193:LEU:HA	1:B:362:VAL:HG21	2.02	0.42
1:B:234:LEU:O	1:B:237:ARG:HB2	2.20	0.42
1:C:377:TRP:NE1	1:C:378:SER:HB2	2.34	0.42
1:C:82:GLU:HG3	1:C:361:TYR:CE2	2.54	0.42
1:C:190:GLN:HG2	1:C:227:THR:HG22	2.01	0.42
1:C:139:GLY:O	1:C:140:GLU:C	2.62	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:281:LEU:O	1:B:282:GLU:C	2.64	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:193:LEU:HD12	1:B:193:LEU:C	2.46	0.40
1:B:103:PHE:CE2	1:B:111:ARG:HB2	2.57	0.40
1:C:381:GLN:HG3	1:C:381:GLN:H	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:LEU:HD12	1:B:331:LEU:N	2.36	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%)	4	8
1	B	121/348 (35%)	110 (91%)	8 (7%)	3 (2%)	4	7
1	C	314/348 (90%)	281 (90%)	23 (7%)	10 (3%)	3	4
All	All	768/1044 (74%)	697 (91%)	50 (6%)	21 (3%)	4	6

All (21) 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	C	183	GLY
1	A	138	ALA
1	A	337	VAL
1	B	254	LYS
1	C	337	VAL
1	C	342	VAL

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Mol	Chain	Res	Type
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](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

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	C	401	-	6,7,7	4.06	4 (66%)	7,10,10	1.89	2 (28%)
2	CP	A	401	-	6,7,7	4.34	3 (50%)	7,10,10	1.77	3 (42%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	CP	C-N	8.03	1.48	1.33
2	C	401	CP	C-N	7.22	1.46	1.33
2	A	401	CP	P-O4P	5.89	1.70	1.59
2	C	401	CP	P-O4P	5.26	1.69	1.59
2	C	401	CP	P-O3P	3.73	1.68	1.54
2	A	401	CP	P-O3P	3.18	1.66	1.54
2	C	401	CP	P-O2P	-2.23	1.46	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	CP	O3P-P-O4P	4.01	116.99	105.32
2	A	401	CP	O2P-P-O4P	2.79	113.44	105.32
2	A	401	CP	O2P-P-O1P	-2.63	100.61	110.83
2	C	401	CP	O2P-P-O1P	-2.34	101.74	110.83
2	A	401	CP	O-C-N	-2.13	122.22	125.58

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/348 (96%)	0.02	3 (0%) 81 78	40, 62, 102, 130	0
1	B	317/348 (91%)	0.24	8 (2%) 58 54	44, 73, 117, 154	0
1	C	322/348 (92%)	0.08	7 (2%) 62 58	48, 67, 101, 123	0
All	All	974/1044 (93%)	0.11	18 (1%) 67 64	40, 67, 105, 154	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	TYR	4.4
1	C	382	PHE	3.5
1	A	374	THR	3.5
1	B	373	SER	3.3
1	A	40	ILE	3.2
1	B	304	VAL	2.9
1	B	48	LEU	2.8
1	B	338	ASN	2.8
1	B	295	ARG	2.7
1	B	184	THR	2.7
1	C	108	THR	2.4
1	A	304	VAL	2.3
1	C	296	ILE	2.3
1	C	374	THR	2.2
1	C	377	TRP	2.2
1	C	342	VAL	2.1
1	B	250	LEU	2.1
1	C	250	LEU	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 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($\text{\AA}^2$)	Q<0.9
2	CP	C	401	8/8	0.84	0.10	76,91,111,119	0
2	CP	A	401	8/8	0.86	0.11	80,93,107,111	0

6.5 Other polymers [i](#)

There are no such residues in this entry.