



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:16 am BST

PDB ID : 6AT1  
Title : STRUCTURAL CONSEQUENCES OF EFFECTOR BINDING TO THE T STATE OF ASPARTATE CARBAMOYLTRANSFERASE. CRYSTAL STRUCTURES OF THE UNLIGATED AND ATP-, AND CTP-COMPLEXED ENZYMES AT 2.6-ANGSTROMS RESOLUTION  
Authors : Stevens, R.C.; Gouaux, J.E.; Lipscomb, W.N.  
Deposited on : 1990-04-26  
Resolution : 2.60 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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

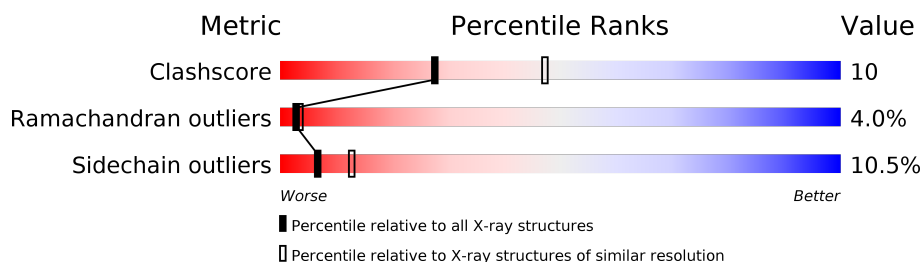
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	
1	C	310	
2	B	153	
2	D	153	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7108 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 (T STATE), CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLN	GLU	CONFLICT	UNP P0A786
A	147	GLN	GLU	CONFLICT	UNP P0A786
A	149	GLU	GLN	CONFLICT	UNP P0A786
A	196	GLU	GLN	CONFLICT	UNP P0A786
C	60	GLN	GLU	CONFLICT	UNP P0A786
C	147	GLN	GLU	CONFLICT	UNP P0A786
C	149	GLU	GLN	CONFLICT	UNP P0A786
C	196	GLU	GLN	CONFLICT	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	GLY	GLN	CONFLICT	UNP P0A7F3
D	8	GLY	GLN	CONFLICT	UNP P0A7F3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

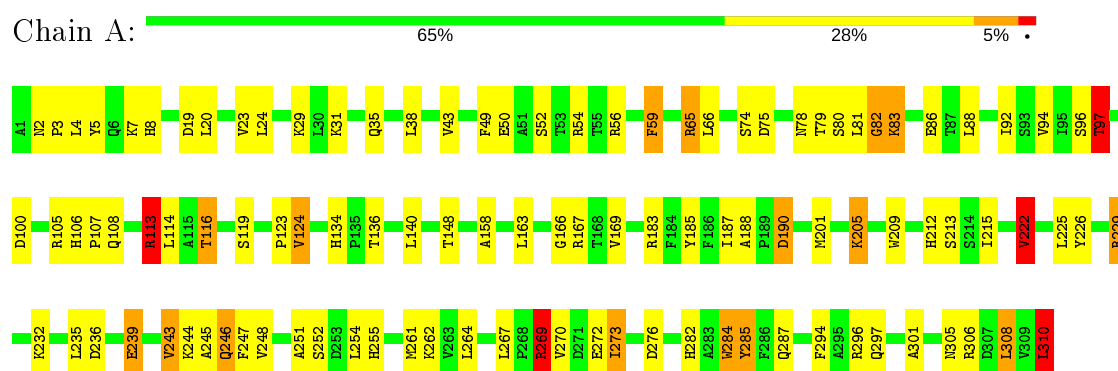
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

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

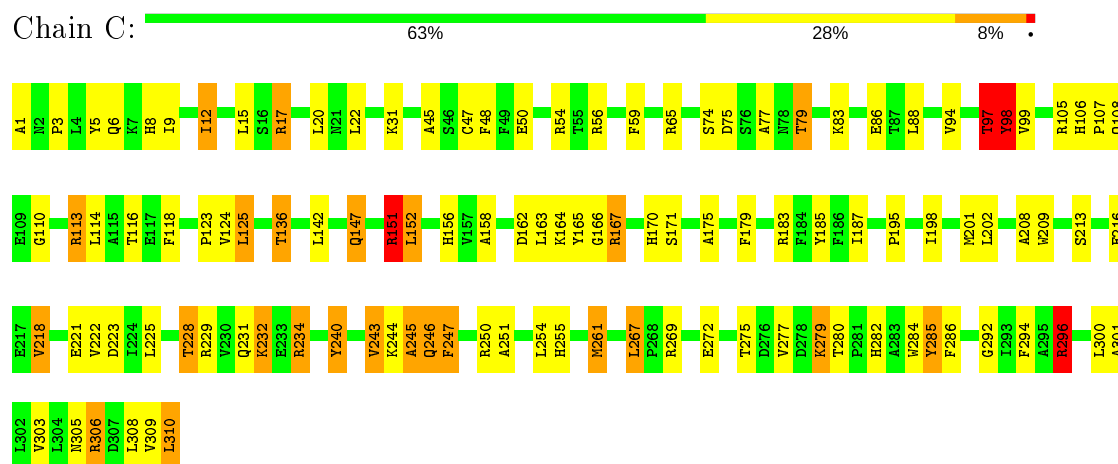
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

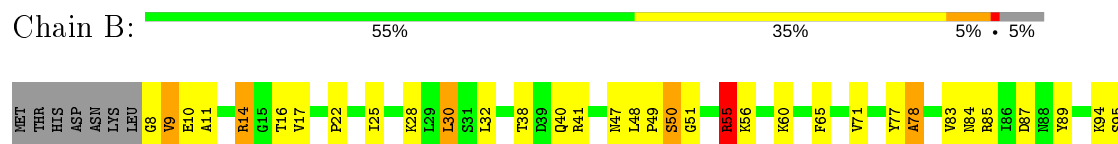
#### • Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE (T STATE), CATALYTIC CHAIN



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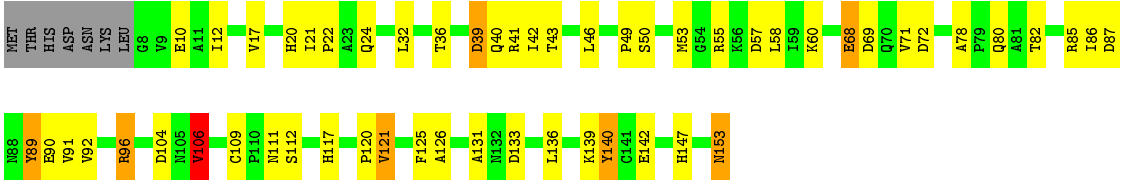


#### • Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.00 Å   122.00 Å   142.00 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7108	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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	0.87	0/2461	1.61	25/3339 (0.7%)
1	C	0.88	0/2461	1.69	43/3339 (1.3%)
2	B	0.81	0/1155	1.55	13/1561 (0.8%)
2	D	0.77	0/1155	1.52	10/1561 (0.6%)
All	All	0.85	0/7232	1.61	91/9800 (0.9%)

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	2
1	C	0	7
2	B	0	2
2	D	0	1
All	All	0	12

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	NE-CZ-NH2	14.40	127.50	120.30
1	A	269	ARG	NE-CZ-NH2	12.95	126.77	120.30
1	C	113	ARG	NE-CZ-NH1	-11.59	114.50	120.30
1	A	56	ARG	NE-CZ-NH2	11.03	125.82	120.30
1	A	56	ARG	NE-CZ-NH1	-10.05	115.28	120.30
1	C	56	ARG	NE-CZ-NH1	-9.85	115.38	120.30
1	C	285	TYR	CB-CG-CD2	-9.03	115.58	121.00
1	A	65	ARG	NE-CZ-NH1	-8.51	116.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	105	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	C	209	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	A	43	VAL	CG1-CB-CG2	-7.97	98.14	110.90
2	D	89	TYR	N-CA-C	7.95	132.45	111.00
1	C	284	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	C	284	TRP	CG-CD2-CE3	7.79	140.91	133.90
2	B	128	ARG	NE-CZ-NH1	-7.78	116.41	120.30
1	A	284	TRP	CE2-CD2-CG	-7.74	101.11	107.30
1	A	209	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	C	250	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	A	284	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	C	113	ARG	NE-CZ-NH2	7.57	124.08	120.30
1	C	269	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	A	113	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	167	ARG	CA-CB-CG	7.34	129.56	113.40
1	C	296	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	A	100	ASP	CB-CG-OD1	7.31	124.88	118.30
1	C	209	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	269	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	C	125	LEU	CA-CB-CG	7.24	131.96	115.30
1	C	284	TRP	CE2-CD2-CG	-7.24	101.51	107.30
2	B	128	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	C	17	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	A	209	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	C	136	THR	N-CA-CB	-7.07	96.88	110.30
1	C	98	TYR	CB-CG-CD1	-7.05	116.77	121.00
1	C	284	TRP	CB-CG-CD1	-6.92	118.00	127.00
1	C	97	THR	N-CA-CB	-6.78	97.43	110.30
1	C	79	THR	N-CA-C	-6.70	92.92	111.00
1	C	105	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	C	167	ARG	NE-CZ-NH2	6.57	123.59	120.30
1	C	56	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	A	97	THR	N-CA-CB	-6.41	98.12	110.30
1	A	229	ARG	CA-CB-CG	6.40	127.48	113.40
2	B	85	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	C	98	TYR	CB-CA-C	-6.37	97.67	110.40
2	D	46	LEU	CB-CG-CD1	-6.36	100.19	111.00
2	B	32	LEU	CA-CB-CG	6.32	129.84	115.30
2	D	106	VAL	N-CA-CB	-6.32	97.59	111.50
2	B	41	ARG	NE-CZ-NH2	6.30	123.45	120.30
2	D	55	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	C	306	ARG	NE-CZ-NH2	6.15	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	46	LEU	CA-CB-CG	6.13	129.40	115.30
2	B	30	LEU	CA-CB-CG	5.97	129.03	115.30
2	D	55	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	C	65	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	C	261	MET	CG-SD-CE	-5.82	90.88	100.20
2	B	55	ARG	CA-CB-CG	5.80	126.16	113.40
2	D	96	ARG	NE-CZ-NH2	5.71	123.16	120.30
2	D	85	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	C	296	ARG	CA-CB-CG	5.62	125.76	113.40
1	A	190	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	54	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	C	310	LEU	N-CA-C	-5.39	96.44	111.00
1	C	309	VAL	CA-C-N	-5.37	105.40	117.20
1	C	234	ARG	NE-CZ-NH2	5.32	122.96	120.30
2	B	77	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	A	43	VAL	N-CA-C	-5.31	96.67	111.00
2	B	11	ALA	N-CA-C	5.27	125.23	111.00
1	C	303	VAL	CG1-CB-CG2	-5.19	102.60	110.90
1	C	223	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	5	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	C	151	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	17	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	218	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	C	218	VAL	N-CA-CB	-5.14	100.20	111.50
1	A	269	ARG	N-CA-C	-5.13	97.14	111.00
1	A	310	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	140	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	269	ARG	N-CA-C	-5.13	97.16	111.00
2	B	147	HIS	CA-CB-CG	5.09	122.26	113.60
1	C	209	TRP	CG-CD1-NE1	-5.08	105.02	110.10
2	B	134	ILE	N-CA-C	-5.08	97.28	111.00
2	D	153	ASN	N-CA-C	5.08	124.72	111.00
1	A	243	VAL	CA-CB-CG1	-5.08	103.29	110.90
2	D	86	ILE	N-CA-C	-5.08	97.29	111.00
1	C	300	LEU	CB-CG-CD2	-5.07	102.39	111.00
1	C	284	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	A	222	VAL	N-CA-CB	-5.06	100.37	111.50
1	A	273	ILE	N-CA-C	-5.05	97.37	111.00
1	C	218	VAL	CG1-CB-CG2	5.03	118.95	110.90
2	B	106	VAL	N-CA-CB	-5.01	100.47	111.50
2	B	105	ASN	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	TYR	Sidechain
1	A	285	TYR	Sidechain
2	B	78	ALA	Peptide
2	B	89	TYR	Sidechain
1	C	118	PHE	Sidechain
1	C	185	TYR	Sidechain
1	C	240	TYR	Sidechain
1	C	247	PHE	Sidechain
1	C	286	PHE	Sidechain
1	C	294	PHE	Sidechain
1	C	98	TYR	Sidechain
2	D	140	TYR	Sidechain

## 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	2415	0	2422	50	0
1	C	2415	0	2422	48	0
2	B	1138	0	1154	28	0
2	D	1138	0	1154	18	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
All	All	7108	0	7152	142	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 (142) 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:136:THR:HB	1:A:296:ARG:NH2	1.95	0.80
1:C:251:ALA:HA	1:C:254:LEU:HD12	1.67	0.74
1:A:50:GLU:HB2	1:A:107:PRO:HD3	1.67	0.73
2:B:14:ARG:HG3	2:B:87:ASP:HA	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:LEU:O	2:B:55:ARG:HA	1.90	0.71
2:B:130:ARG:NH1	2:B:131:ALA:HB2	2.07	0.69
1:C:243:VAL:HG11	1:C:247:PHE:HE2	1.57	0.69
2:B:17:VAL:HG22	2:B:60:LYS:HG2	1.74	0.69
1:A:8:HIS:HD2	1:A:124:VAL:H	1.42	0.68
1:C:94:VAL:O	1:C:97:THR:HB	1.95	0.67
1:C:50:GLU:HB2	1:C:107:PRO:HD3	1.76	0.67
2:B:8:GLY:N	2:B:50:SER:HG	1.94	0.66
1:C:292:GLY:O	1:C:296:ARG:HB2	1.95	0.66
1:C:183:ARG:HG2	1:C:208:ALA:HB3	1.79	0.63
1:A:183:ARG:HH21	1:A:185:TYR:HE2	1.48	0.62
2:B:14:ARG:HG2	2:B:65:PHE:HZ	1.64	0.62
1:C:163:LEU:O	1:C:170:HIS:HE1	1.82	0.61
1:C:277:VAL:O	1:C:280:THR:HB	2.01	0.61
2:D:133:ASP:HB2	2:D:147:HIS:CE1	2.35	0.60
2:B:38:THR:HG22	2:B:40:GLN:H	1.67	0.60
2:B:110:PRO:HD2	2:B:145:PHE:CE1	2.38	0.59
2:B:71:VAL:HG22	2:B:83:VAL:HG11	1.85	0.59
1:C:245:ALA:O	1:C:246:GLN:HB2	2.03	0.58
1:A:114:LEU:HD12	2:B:121:VAL:HG11	1.86	0.58
1:C:106:HIS:HD2	1:C:108:GLN:H	1.49	0.58
2:D:133:ASP:HB2	2:D:147:HIS:HE1	1.68	0.58
1:A:158:ALA:HB2	1:A:222:VAL:HG21	1.86	0.58
2:D:96:ARG:HB2	2:D:96:ARG:NH2	2.19	0.57
1:A:243:VAL:HG23	1:A:246:GLN:OE1	2.04	0.57
2:D:96:ARG:HB2	2:D:96:ARG:HH21	1.70	0.56
1:C:142:LEU:HD11	1:C:175:ALA:HB1	1.88	0.56
1:A:8:HIS:CD2	1:A:124:VAL:H	2.25	0.55
1:A:4:LEU:HD23	1:A:7:LYS:HD2	1.89	0.55
1:A:82:GLY:HA2	1:A:86:GLU:HB2	1.90	0.54
1:A:187:ILE:HG12	1:A:212:HIS:HB2	1.90	0.54
2:D:20:HIS:CE1	2:D:53:MET:SD	3.01	0.53
1:A:166:GLY:O	1:A:169:VAL:HG22	2.09	0.53
2:D:126:ALA:O	2:D:136:LEU:HA	2.08	0.52
2:B:129:LYS:HE3	2:B:133:ASP:HB3	1.92	0.52
1:A:35:GLN:HE22	1:A:310:LEU:HB3	1.74	0.52
1:A:148:THR:HG21	1:A:262:LYS:HG3	1.90	0.52
2:D:68:GLU:O	2:D:71:VAL:HB	2.10	0.52
1:A:8:HIS:CD2	1:A:123:PRO:HA	2.46	0.51
1:C:8:HIS:HD2	1:C:124:VAL:H	1.58	0.51
1:C:151:ARG:HG3	1:C:151:ARG:HH21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:ALA:HA	1:C:306:ARG:HD2	1.94	0.50
1:A:269:ARG:HA	1:A:272:GLU:OE2	2.11	0.50
1:A:78:ASN:ND2	1:A:83:LYS:HB2	2.27	0.49
1:A:49:PHE:O	1:A:75:ASP:HB2	2.12	0.49
1:C:136:THR:HG23	1:C:296:ARG:NH2	2.26	0.49
2:B:109:CYS:HA	2:B:125:PHE:HZ	1.78	0.49
1:C:301:ALA:O	1:C:305:ASN:HB2	2.12	0.49
1:A:261:MET:O	1:A:282:HIS:HD2	1.96	0.49
2:B:83:VAL:HB	2:B:95:SER:HB2	1.95	0.49
1:C:88:LEU:HD23	1:C:114:LEU:HD22	1.95	0.48
2:B:25:ILE:HD13	2:B:28:LYS:HD2	1.96	0.48
1:A:31:LYS:HG3	1:A:294:PHE:CE2	2.49	0.48
2:B:99:LEU:HD12	2:B:100:PRO:HD2	1.96	0.48
1:C:113:ARG:HH21	1:C:113:ARG:HG2	1.79	0.48
2:B:25:ILE:O	2:B:28:LYS:HB3	2.14	0.48
1:A:20:LEU:O	1:A:24:LEU:HD13	2.13	0.47
1:C:229:ARG:HA	1:C:272:GLU:OE2	2.15	0.47
1:C:31:LYS:NZ	1:C:147:GLN:OE1	2.47	0.47
1:C:3:PRO:HD2	1:C:22:LEU:HD21	1.95	0.47
1:A:66:LEU:HG	1:A:297:GLN:HE21	1.79	0.47
2:D:87:ASP:CG	2:D:92:VAL:HG11	2.35	0.47
1:A:29:LYS:HD2	1:A:310:LEU:HD13	1.97	0.46
1:A:50:GLU:HB3	1:A:105:ARG:HG2	1.97	0.46
1:C:48:PHE:O	1:C:74:SER:HA	2.14	0.46
1:A:236:ASP:H	1:A:239:GLU:HG2	1.79	0.46
1:A:301:ALA:O	1:A:305:ASN:HB2	2.16	0.46
2:D:32:LEU:HD22	2:D:106:VAL:HG13	1.98	0.46
1:A:5:TYR:CD2	1:A:306:ARG:HA	2.51	0.46
1:C:280:THR:HG22	1:C:282:HIS:H	1.79	0.46
2:D:22:PRO:HD2	2:D:78:ALA:HB1	1.97	0.46
1:C:12:ILE:HD13	1:C:15:LEU:HD12	1.98	0.46
1:A:80:SER:O	1:A:82:GLY:N	2.49	0.46
2:D:111:ASN:O	2:D:117:HIS:CE1	2.69	0.46
1:C:12:ILE:HD13	1:C:12:ILE:HA	1.77	0.45
1:C:158:ALA:HB3	1:C:225:LEU:HD12	1.98	0.45
2:B:22:PRO:HG2	2:B:25:ILE:HG13	1.98	0.45
1:A:269:ARG:HG3	1:A:273:ILE:HB	1.98	0.45
1:A:246:GLN:HB3	1:A:248:VAL:HG13	1.99	0.45
1:A:94:VAL:O	1:A:97:THR:HB	2.17	0.45
2:B:14:ARG:HG2	2:B:65:PHE:CZ	2.50	0.44
1:C:301:ALA:HB1	1:C:308:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HG	1:A:188:ALA:HB2	1.99	0.44
1:A:201:MET:HG2	1:A:205:LYS:NZ	2.32	0.44
2:B:47:ASN:ND2	2:D:39:ASP:HA	2.33	0.44
1:C:261:MET:O	1:C:282:HIS:HD2	2.00	0.44
2:B:127:VAL:HA	2:B:136:LEU:HD23	1.99	0.44
1:A:136:THR:HB	1:A:296:ARG:HH22	1.79	0.44
1:C:45:ALA:HB2	1:C:99:VAL:HG11	1.99	0.44
1:A:96:SER:OG	1:A:119:SER:HA	2.18	0.43
1:A:183:ARG:NH2	1:A:185:TYR:HE2	2.15	0.43
2:B:111:ASN:HB2	2:B:145:PHE:HZ	1.83	0.43
1:C:54:ARG:HH11	1:C:267:LEU:HD13	1.83	0.43
2:D:109:CYS:HA	2:D:125:PHE:HZ	1.83	0.43
1:A:106:HIS:HD2	1:A:108:GLN:H	1.66	0.43
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.33	0.43
2:D:42:ILE:HA	2:D:60:LYS:O	2.17	0.43
1:C:152:LEU:HD23	1:C:179:PHE:CZ	2.53	0.43
1:C:301:ALA:CB	1:C:308:LEU:HD11	2.48	0.43
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.99	0.43
1:C:162:ASP:O	1:C:228:THR:HG21	2.18	0.43
1:A:308:LEU:HB3	1:A:310:LEU:HD11	2.01	0.43
1:C:232:LYS:HA	1:C:240:TYR:CE2	2.54	0.43
1:C:187:ILE:HG22	1:C:247:PHE:CE1	2.54	0.42
1:C:45:ALA:HB1	1:C:47:CYS:SG	2.59	0.42
1:A:38:LEU:HG	1:A:305:ASN:ND2	2.34	0.42
2:B:84:ASN:OD1	2:B:94:LYS:HE2	2.20	0.42
2:D:17:VAL:HG13	2:D:58:LEU:HD21	2.00	0.42
1:C:151:ARG:HH21	1:C:151:ARG:CG	2.32	0.42
1:C:198:ILE:HD13	1:C:198:ILE:HA	1.94	0.42
2:B:111:ASN:O	2:B:117:HIS:CE1	2.73	0.42
1:A:59:PHE:CZ	1:A:136:THR:HG21	2.54	0.42
2:B:51:GLY:HA3	2:B:56:LYS:HD3	2.02	0.42
1:C:20:LEU:HA	1:C:20:LEU:HD23	1.82	0.42
1:C:8:HIS:HD2	1:C:124:VAL:N	2.17	0.42
1:A:187:ILE:HD13	1:A:215:ILE:HA	2.01	0.42
1:A:235:LEU:HG	1:A:239:GLU:CG	2.50	0.42
1:C:201:MET:C	1:C:201:MET:SD	2.98	0.42
1:C:218:VAL:O	1:C:222:VAL:HG23	2.20	0.42
1:A:19:ASP:O	1:A:23:VAL:HG23	2.20	0.41
1:A:251:ALA:O	1:A:254:LEU:HB2	2.20	0.41
1:C:8:HIS:CD2	1:C:123:PRO:HA	2.55	0.41
1:C:164:LYS:HA	1:C:195:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ARG:O	1:A:116:THR:HB	2.20	0.41
1:C:110:GLY:O	1:C:113:ARG:HB3	2.20	0.41
2:B:138:CYS:O	2:B:142:GLU:HA	2.20	0.41
1:C:202:LEU:HA	1:C:202:LEU:HD23	1.89	0.41
1:A:52:SER:HB2	1:A:105:ARG:NH2	2.36	0.41
1:A:88:LEU:O	1:A:92:ILE:HG12	2.21	0.41
2:B:109:CYS:HA	2:B:110:PRO:HD3	1.89	0.41
2:B:105:ASN:HA	2:B:123:SER:OG	2.20	0.41
1:C:279:LYS:H	1:C:279:LYS:HG2	1.66	0.41
2:B:14:ARG:HB3	2:B:14:ARG:NH2	2.36	0.41
1:A:2:ASN:ND2	1:A:305:ASN:O	2.53	0.40
2:D:139:LYS:HD3	2:D:140:TYR:CZ	2.57	0.40
2:D:121:VAL:HG22	2:D:140:TYR:OH	2.21	0.40
1:A:4:LEU:O	1:A:7:LYS:HB2	2.22	0.40
1:C:164:LYS:HD3	1:C:165:TYR:CZ	2.56	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	308/310 (99%)	286 (93%)	13 (4%)	9 (3%)	4	7
1	C	308/310 (99%)	278 (90%)	19 (6%)	11 (4%)	3	4
2	B	144/153 (94%)	125 (87%)	11 (8%)	8 (6%)	2	2
2	D	144/153 (94%)	122 (85%)	14 (10%)	8 (6%)	2	2
All	All	904/926 (98%)	811 (90%)	57 (6%)	36 (4%)	3	3

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	190	ASP
1	A	246	GLN
2	B	105	ASN
2	B	129	LYS
1	C	244	LYS
1	C	245	ALA
1	C	246	GLN
2	D	68	GLU
2	D	89	TYR
1	A	82	GLY
1	A	245	ALA
2	B	9	VAL
2	B	14	ARG
2	B	49	PRO
1	C	77	ALA
1	C	86	GLU
2	D	49	PRO
2	D	91	VAL
1	A	83	LYS
1	A	232	LYS
2	B	50	SER
1	C	75	ASP
1	C	275	THR
2	D	131	ALA
2	D	142	GLU
2	B	131	ALA
1	C	166	GLY
2	B	78	ALA
1	C	232	LYS
2	D	50	SER
1	A	244	LYS
1	C	243	VAL
1	C	267	LEU
2	D	120	PRO
1	A	267	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	261/261 (100%)	235 (90%)	26 (10%)	7	14
1	C	261/261 (100%)	233 (89%)	28 (11%)	6	12
2	B	129/136 (95%)	119 (92%)	10 (8%)	12	25
2	D	129/136 (95%)	111 (86%)	18 (14%)	3	6
All	All	780/794 (98%)	698 (90%)	82 (10%)	7	13

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	59	PHE
1	A	65	ARG
1	A	74	SER
1	A	79	THR
1	A	97	THR
1	A	113	ARG
1	A	116	THR
1	A	124	VAL
1	A	134	HIS
1	A	205	LYS
1	A	213	SER
1	A	222	VAL
1	A	225	LEU
1	A	229	ARG
1	A	239	GLU
1	A	247	PHE
1	A	252	SER
1	A	255	HIS
1	A	264	LEU
1	A	269	ARG
1	A	270	VAL
1	A	276	ASP
1	A	285	TYR
1	A	308	LEU
1	A	310	LEU
2	B	9	VAL
2	B	10	GLU
2	B	16	THR
2	B	30	LEU
2	B	55	ARG

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Mol	Chain	Res	Type
2	B	98	SER
2	B	101	GLU
2	B	122	SER
2	B	148	ASN
2	B	153	ASN
1	C	6	GLN
1	C	9	ILE
1	C	12	ILE
1	C	17	ARG
1	C	59	PHE
1	C	79	THR
1	C	83	LYS
1	C	97	THR
1	C	98	TYR
1	C	116	THR
1	C	125	LEU
1	C	147	GLN
1	C	151	ARG
1	C	152	LEU
1	C	156	HIS
1	C	167	ARG
1	C	171	SER
1	C	213	SER
1	C	216	GLU
1	C	221	GLU
1	C	228	THR
1	C	231	GLN
1	C	234	ARG
1	C	255	HIS
1	C	279	LYS
1	C	285	TYR
1	C	296	ARG
1	C	310	LEU
2	D	10	GLU
2	D	12	ILE
2	D	24	GLN
2	D	36	THR
2	D	39	ASP
2	D	40	GLN
2	D	41	ARG
2	D	43	THR
2	D	69	ASP

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Mol	Chain	Res	Type
2	D	72	ASP
2	D	80	GLN
2	D	82	THR
2	D	90	GLU
2	D	104	ASP
2	D	106	VAL
2	D	112	SER
2	D	121	VAL
2	D	153	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	HIS
1	A	21	ASN
1	A	78	ASN
1	A	106	HIS
1	A	170	HIS
1	A	287	GLN
1	A	297	GLN
1	A	305	ASN
1	C	8	HIS
1	C	60	GLN
1	C	106	HIS
1	C	134	HIS
1	C	170	HIS
1	C	282	HIS
1	C	291	ASN
2	D	24	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.