



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:21 PM GMT

PDB ID : 1ACM  
Title : ARGININE 54 IN THE ACTIVE SITE OF ESCHERICHIA COLI ASPARTATE TRANSCARBAMOYLASE IS CRITICAL FOR CATALYSIS: A SITE-SPECIFIC MUTAGENESIS, NMR AND X-RAY CRYSTALLOGRAPHY STUDY  
Authors : Stevens, R.C.; Kantrowitz, E.R.; Lipscomb, W.N.  
Deposited on : 1992-07-08  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

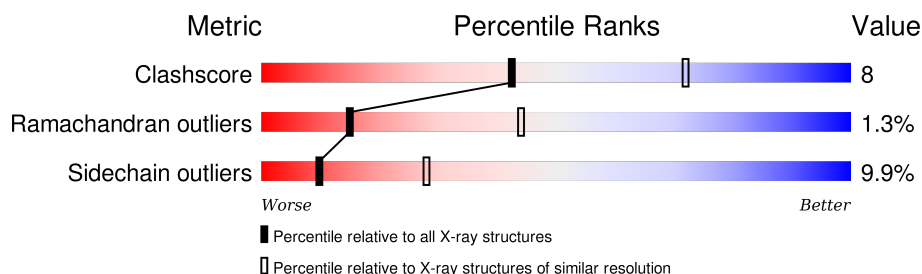
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	 75% 21% • •
1	C	310	 79% 17% •
2	B	153	 51% 33% 10% • 5%
2	D	153	 52% 35% 7% • 5%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7143 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, CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2409	1524	420	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2409	1524	420	456	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ALA	ARG	CONFLICT	UNP P0A786
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	54	ALA	ARG	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

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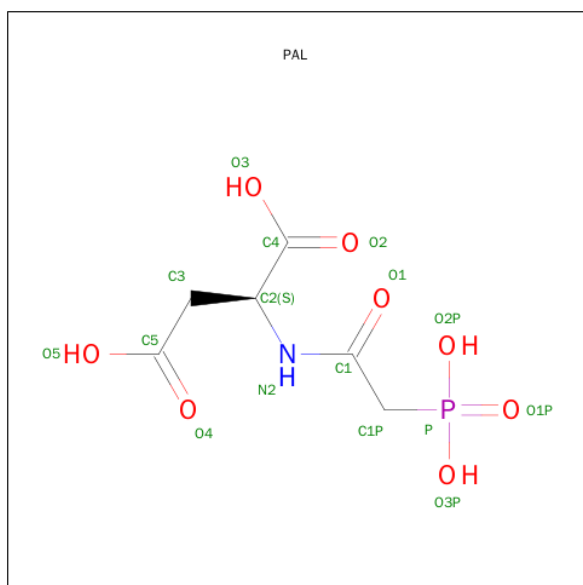
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Chain	Residue	Modelled	Actual	Comment	Reference
D	8	GLY	GLN	CONFLICT	UNP P0A7F3

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

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

- Molecule 4 is N-(PHOSPHONACETYL)-L-ASPARTIC ACID (three-letter code: PAL) (formula: C<sub>6</sub>H<sub>10</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 16 6 1 8 1	0	0
4	C	1	Total C N O P 16 6 1 8 1	0	0

- Molecule 5 is water.

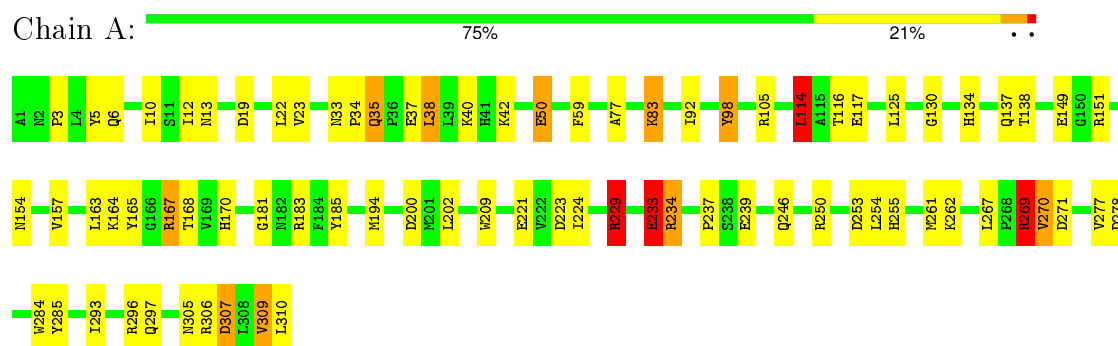
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0
5	C	7	Total O 7 7	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

#### • Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.20 Å 122.20 Å 156.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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, PAL

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	0.82	0/2455	1.55	28/3332 (0.8%)
1	C	0.86	0/2455	1.53	36/3332 (1.1%)
2	B	0.71	0/1155	1.53	16/1561 (1.0%)
2	D	0.75	0/1155	1.52	13/1561 (0.8%)
All	All	0.81	0/7220	1.54	93/9786 (1.0%)

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	3
1	C	0	3
2	B	0	2
2	D	0	3
All	All	0	11

There are no bond length outliers.

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ARG	NE-CZ-NH1	16.61	128.61	120.30
1	A	229	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	167	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	C	234	ARG	NE-CZ-NH2	-10.59	115.01	120.30
1	A	233	GLU	CA-CB-CG	9.92	135.22	113.40
1	C	306	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	C	284	TRP	CD1-CG-CD2	8.84	113.37	106.30
2	B	96	ARG	NE-CZ-NH2	-8.66	115.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	102	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	C	209	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	A	209	TRP	CD1-CG-CD2	8.33	112.96	106.30
1	A	167	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	A	114	LEU	CA-CB-CG	8.14	134.02	115.30
2	D	41	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	C	209	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	A	234	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	C	234	ARG	CG-CD-NE	-7.38	96.29	111.80
1	A	6	GLN	CA-CB-CG	-7.36	97.20	113.40
1	A	209	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	C	284	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	98	TYR	CB-CG-CD2	-7.28	116.63	121.00
1	C	303	VAL	CG1-CB-CG2	-7.26	99.28	110.90
1	C	114	LEU	CA-CB-CG	7.09	131.61	115.30
1	C	234	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	185	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	C	165	TYR	CB-CG-CD1	-6.91	116.86	121.00
1	C	113	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	C	229	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	183	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	284	TRP	CD1-CG-CD2	6.67	111.63	106.30
2	D	102	ARG	NE-CZ-NH1	6.67	123.63	120.30
2	B	55	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	284	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	A	296	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	C	309	VAL	CA-C-N	-6.42	103.07	117.20
2	D	128	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	B	130	ARG	NE-CZ-NH1	6.31	123.45	120.30
2	D	14	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	234	ARG	CG-CD-NE	-6.10	98.99	111.80
1	A	200	ASP	CB-CA-C	-6.03	98.34	110.40
2	B	152	ALA	N-CA-C	5.96	127.11	111.00
2	D	14	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	271	ASP	CB-CG-OD1	5.95	123.66	118.30
1	A	233	GLU	CB-CA-C	-5.95	98.50	110.40
2	D	55	ARG	CA-CB-CG	5.90	126.38	113.40
2	D	128	ARG	CA-CB-CG	5.86	126.29	113.40
2	B	140	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	C	157	VAL	CG1-CB-CG2	-5.77	101.67	110.90
1	C	56	ARG	CG-CD-NE	-5.71	99.82	111.80
1	C	309	VAL	O-C-N	5.68	131.79	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	C	209	TRP	CG-CD1-NE1	-5.65	104.45	110.10
2	B	128	ARG	CA-CB-CG	5.63	125.79	113.40
1	C	42	LYS	CA-CB-CG	-5.58	101.12	113.40
1	C	194	MET	CG-SD-CE	-5.56	91.30	100.20
2	D	74	LEU	CA-CB-CG	5.53	128.01	115.30
2	D	33	PHE	CB-CG-CD2	-5.51	116.94	120.80
1	C	240	TYR	CB-CG-CD2	-5.50	117.70	121.00
2	B	139	LYS	CA-CB-CG	5.50	125.50	113.40
2	D	105	ASN	N-CA-C	5.48	125.79	111.00
1	A	234	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	C	284	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	A	117	GLU	CA-CB-CG	-5.42	101.47	113.40
1	C	124	VAL	CG1-CB-CG2	-5.41	102.25	110.90
1	C	261	MET	CA-CB-CG	5.40	122.48	113.30
1	C	65	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	309	VAL	CA-C-N	-5.35	105.44	117.20
2	B	131	ALA	N-CA-CB	5.33	117.56	110.10
1	C	151	ARG	CA-CB-CG	5.33	125.11	113.40
1	A	209	TRP	CG-CD1-NE1	-5.32	104.78	110.10
2	D	130	ARG	CA-CB-CG	5.31	125.07	113.40
2	B	69	ASP	N-CA-CB	-5.28	101.10	110.60
1	A	42	LYS	CA-CB-CG	-5.27	101.80	113.40
1	C	100	ASP	CB-CG-OD1	5.27	123.04	118.30
1	C	56	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	209	TRP	CG-CD2-CE3	5.26	138.63	133.90
2	B	90	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	C	98	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	C	17	ARG	CA-CB-CG	5.23	124.90	113.40
1	A	50	GLU	OE1-CD-OE2	-5.21	117.05	123.30
1	A	37	GLU	CA-CB-CG	5.20	124.85	113.40
2	D	50	SER	N-CA-C	-5.16	97.07	111.00
1	C	209	TRP	CB-CG-CD1	-5.13	120.33	127.00
2	B	99	LEU	CA-CB-CG	5.13	127.10	115.30
2	B	131	ALA	CB-CA-C	-5.11	102.43	110.10
2	B	102	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	153	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	138	THR	N-CA-CB	-5.07	100.67	110.30
2	B	77	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	A	221	GLU	CA-CB-CG	5.05	124.52	113.40
1	C	151	ARG	N-CA-CB	-5.03	101.55	110.60
2	B	87	ASP	N-CA-C	-5.02	97.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	94	LYS	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	TYR	Sidechain
1	A	269	ARG	Sidechain
1	A	98	TYR	Sidechain
2	B	77	TYR	Sidechain
2	B	99	LEU	Peptide
1	C	165	TYR	Sidechain
1	C	234	ARG	Sidechain
1	C	240	TYR	Sidechain
2	D	125	PHE	Sidechain
2	D	140	TYR	Sidechain
2	D	77	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	2409	0	2414	26	0
1	C	2409	0	2414	19	0
2	B	1138	0	1154	38	0
2	D	1138	0	1154	39	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	6	0	0
4	C	16	0	6	0	0
5	A	8	0	0	0	0
5	C	7	0	0	0	0
All	All	7143	0	7148	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (118) 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)
2:B:22:PRO:HB2	2:B:25:ILE:HD12	1.60	0.84
2:D:102:ARG:NH2	2:D:124:SER:HB3	1.94	0.83
2:D:99:LEU:HD11	2:D:134:ILE:HD12	1.64	0.78
2:D:102:ARG:HH21	2:D:124:SER:HB3	1.47	0.78
2:D:22:PRO:HB2	2:D:25:ILE:HD12	1.70	0.72
1:A:270:VAL:HG23	1:A:271:ASP:H	1.56	0.69
2:D:76:LEU:HD22	2:D:103:ILE:HD13	1.76	0.67
1:A:154:ASN:HA	1:A:181:GLY:O	1.95	0.67
2:D:74:LEU:HD23	2:D:97:PRO:HG2	1.76	0.66
1:A:35:GLN:HG2	1:A:38:LEU:HG	1.77	0.65
2:D:128:ARG:HD2	2:D:130:ARG:HB2	1.79	0.65
2:B:71:VAL:HG13	2:B:83:VAL:HG21	1.80	0.63
1:C:1:ALA:HA	1:C:306:ARG:HG2	1.81	0.61
2:B:12:ILE:HG13	2:B:62:GLU:HG3	1.82	0.61
1:A:130:GLY:O	1:A:167:ARG:HD3	2.00	0.60
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.82	0.60
1:A:157:VAL:HG12	1:A:224:ILE:HB	1.82	0.60
1:A:10:ILE:HD11	1:A:116:THR:HG21	1.84	0.60
2:B:42:ILE:HG12	2:B:61:ILE:HG23	1.83	0.59
2:B:25:ILE:HA	2:B:28:LYS:HD3	1.86	0.56
2:D:49:PRO:HA	2:D:54:GLY:O	2.07	0.55
2:B:46:LEU:HD12	2:D:44:ILE:HD11	1.89	0.55
2:B:84:ASN:HD21	2:B:91:VAL:HG22	1.72	0.55
2:D:12:ILE:HG23	2:D:41:ARG:NH2	2.22	0.54
1:C:63:MET:SD	1:C:70:VAL:HG22	2.47	0.54
2:B:17:VAL:HG13	2:B:84:ASN:HB3	1.91	0.53
2:B:124:SER:HB3	2:B:139:LYS:HG2	1.91	0.53
1:A:254:LEU:HD11	1:A:277:VAL:HG13	1.90	0.53
1:C:254:LEU:HD11	1:C:277:VAL:HG13	1.90	0.53
1:A:77:ALA:O	1:A:83:LYS:HD3	2.08	0.52
1:A:10:ILE:HD11	1:A:116:THR:CG2	2.38	0.52
1:C:232:LYS:HE3	1:C:243:VAL:O	2.09	0.52
2:B:14:ARG:HG2	2:B:88:ASN:H	1.74	0.52
2:D:128:ARG:HG3	2:D:135:ALA:HB3	1.92	0.52
2:D:43:THR:HB	2:D:60:LYS:HB2	1.92	0.51
2:B:62:GLU:HG2	2:B:63:ASN:HD22	1.77	0.50
2:B:82:THR:HG23	2:B:96:ARG:NH1	2.27	0.50
1:C:130:GLY:HA2	1:C:234:ARG:HH21	1.76	0.50
1:C:35:GLN:HB3	1:C:38:LEU:HG	1.93	0.49
2:D:50:SER:HB2	2:D:52:GLU:OE2	2.13	0.49
2:B:111:ASN:O	2:B:117:HIS:HE1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:O	1:A:170:HIS:HE1	1.95	0.49
2:B:22:PRO:O	2:B:25:ILE:HB	2.13	0.48
2:D:13:LYS:HG2	2:D:89:TYR:CE1	2.48	0.48
1:A:223:ASP:O	1:A:261:MET:HA	2.14	0.48
2:D:126:ALA:O	2:D:136:LEU:HA	2.14	0.48
2:B:62:GLU:HG2	2:B:63:ASN:ND2	2.28	0.48
1:C:308:LEU:HG	1:C:310:LEU:HD12	1.96	0.48
2:B:14:ARG:HA	2:B:86:ILE:O	2.14	0.48
2:D:16:THR:OG1	2:D:65:PHE:HA	2.14	0.48
2:B:75:ALA:HB2	2:B:97:PRO:HB2	1.96	0.48
2:D:106:VAL:HG23	2:D:107:LEU:HG	1.96	0.47
2:D:72:ASP:HB3	2:D:100:PRO:HD3	1.97	0.47
2:B:44:ILE:HB	2:D:44:ILE:HD13	1.97	0.47
2:D:12:ILE:HG23	2:D:41:ARG:HH22	1.80	0.47
1:A:3:PRO:HD2	1:A:22:LEU:HD21	1.97	0.46
1:C:76:SER:HA	1:C:79:THR:HG23	1.97	0.46
2:B:84:ASN:ND2	2:B:86:ILE:HG23	2.30	0.46
2:D:10:GLU:HB2	2:D:43:THR:HG21	1.98	0.46
1:C:164:LYS:NZ	1:C:239:GLU:OE2	2.48	0.46
2:B:84:ASN:OD1	2:B:94:LYS:HD3	2.16	0.46
2:B:10:GLU:HG2	2:B:43:THR:HG21	1.98	0.46
2:D:71:VAL:O	2:D:74:LEU:HB3	2.16	0.45
2:B:102:ARG:HA	2:B:125:PHE:O	2.16	0.45
2:B:106:VAL:HG12	2:B:107:LEU:HD23	1.98	0.45
1:C:163:LEU:HG	1:C:188:ALA:HB2	1.98	0.45
2:D:76:LEU:HD22	2:D:103:ILE:CD1	2.45	0.45
1:A:151:ARG:NH1	1:A:154:ASN:O	2.49	0.45
2:D:133:ASP:HB2	2:D:147:HIS:CE1	2.51	0.45
1:C:229:ARG:NH2	1:C:233:GLU:OE1	2.49	0.45
1:A:50:GLU:CD	1:A:234:ARG:HH22	2.20	0.45
2:D:12:ILE:HG21	2:D:62:GLU:HA	1.99	0.45
2:B:147:HIS:O	2:B:151:LEU:HG	2.16	0.45
1:A:293:ILE:O	1:A:297:GLN:HB2	2.17	0.45
2:D:128:ARG:NH1	2:D:130:ARG:HG3	2.33	0.44
2:B:12:ILE:HD11	2:B:62:GLU:HA	1.98	0.44
1:C:279:LYS:HD2	1:C:279:LYS:N	2.32	0.44
2:D:9:VAL:O	2:D:60:LYS:NZ	2.50	0.44
2:B:96:ARG:HB2	2:B:96:ARG:NH1	2.32	0.44
2:D:23:ALA:HB2	2:D:55:ARG:HB3	1.98	0.44
2:D:114:CYS:SG	2:D:116:SER:HB3	2.58	0.44
2:B:9:VAL:O	2:B:60:LYS:NZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:LEU:HB2	2:D:42:ILE:HB	2.00	0.44
1:A:19:ASP:O	1:A:23:VAL:HG23	2.17	0.44
1:C:223:ASP:O	1:C:261:MET:HA	2.18	0.44
2:B:82:THR:HG23	2:B:96:ARG:HH12	1.82	0.43
1:A:269:ARG:NH2	1:A:278:ASP:OD1	2.52	0.43
1:C:91:THR:O	1:C:95:ILE:HG12	2.18	0.43
2:B:134:ILE:O	2:B:147:HIS:HB3	2.19	0.43
2:D:109:CYS:HA	2:D:110:PRO:HD3	1.83	0.43
2:B:34:LYS:NZ	2:B:37:GLU:OE1	2.52	0.43
1:A:270:VAL:HG23	1:A:271:ASP:N	2.29	0.42
2:B:66:LEU:HD12	2:B:71:VAL:HG22	2.01	0.42
2:D:147:HIS:O	2:D:151:LEU:HG	2.19	0.42
1:A:229:ARG:HH22	1:A:233:GLU:CD	2.22	0.42
2:B:16:THR:HG1	2:B:65:PHE:HA	1.85	0.42
1:A:5:TYR:CE2	1:A:306:ARG:HD3	2.55	0.42
2:D:48:LEU:HD11	2:D:58:LEU:HD22	2.02	0.42
2:B:82:THR:OG1	2:B:96:ARG:NH2	2.53	0.42
1:C:275:THR:O	1:C:279:LYS:HE3	2.20	0.42
2:D:42:ILE:HG12	2:D:61:ILE:HG23	2.01	0.42
1:C:37:GLU:OE2	1:C:40:LYS:NZ	2.53	0.41
1:A:12:ILE:HA	1:A:12:ILE:HD13	1.81	0.41
1:C:23:VAL:HG11	1:C:139:LEU:HD13	2.02	0.41
2:B:21:ILE:HD12	2:B:58:LEU:HA	2.02	0.41
2:B:68:GLU:O	2:B:71:VAL:HB	2.19	0.41
1:A:33:ASN:HA	1:A:34:PRO:HD3	1.66	0.41
2:D:50:SER:O	2:D:54:GLY:N	2.54	0.41
1:A:50:GLU:HB3	1:A:105:ARG:HG2	2.03	0.41
2:D:58:LEU:HD21	2:D:60:LYS:NZ	2.35	0.41
1:C:137:GLN:O	1:C:140:LEU:HG	2.21	0.41
1:A:164:LYS:NZ	1:A:239:GLU:OE2	2.52	0.41
2:B:13:LYS:HE2	2:B:88:ASN:OD1	2.22	0.40
1:C:7:LYS:HD3	1:C:7:LYS:HA	1.94	0.40
2:D:23:ALA:CB	2:D:55:ARG:HD3	2.52	0.40
1:A:114:LEU:HD21	2:B:119:GLU:HG3	2.04	0.40
2:D:104:ASP:HA	2:D:124:SER:HA	2.04	0.40
2:D:129:LYS:HD2	2:D:129:LYS:H	1.87	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%)	298 (97%)	7 (2%)	3 (1%)	19	52
1	C	308/310 (99%)	300 (97%)	7 (2%)	1 (0%)	46	79
2	B	144/153 (94%)	122 (85%)	16 (11%)	6 (4%)	3	11
2	D	144/153 (94%)	130 (90%)	12 (8%)	2 (1%)	14	42
All	All	904/926 (98%)	850 (94%)	42 (5%)	12 (1%)	15	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	VAL
2	B	10	GLU
2	B	152	ALA
2	B	131	ALA
2	D	131	ALA
2	D	54	GLY
1	A	307	ASP
2	B	88	ASN
2	B	54	GLY
1	A	309	VAL
1	A	270	VAL
1	C	270	VAL

### 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	260/260 (100%)	232 (89%)	28 (11%)	8	23
1	C	260/260 (100%)	245 (94%)	15 (6%)	25	57
2	B	129/136 (95%)	112 (87%)	17 (13%)	5	14
2	D	129/136 (95%)	112 (87%)	17 (13%)	5	14
All	All	778/792 (98%)	701 (90%)	77 (10%)	10	28

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	35	GLN
1	A	38	LEU
1	A	40	LYS
1	A	59	PHE
1	A	83	LYS
1	A	92	ILE
1	A	114	LEU
1	A	125	LEU
1	A	134	HIS
1	A	149	GLU
1	A	183	ARG
1	A	194	MET
1	A	202	LEU
1	A	229	ARG
1	A	233	GLU
1	A	237	PRO
1	A	246	GLN
1	A	250	ARG
1	A	253	ASP
1	A	255	HIS
1	A	262	LYS
1	A	267	LEU
1	A	269	ARG
1	A	285	TYR
1	A	305	ASN
1	A	307	ASP
1	A	310	LEU
2	B	14	ARG
2	B	19	ASP
2	B	30	LEU
2	B	31	SER
2	B	52	GLU

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Mol	Chain	Res	Type
2	B	53	MET
2	B	60	LYS
2	B	69	ASP
2	B	80	GLN
2	B	82	THR
2	B	84	ASN
2	B	86	ILE
2	B	99	LEU
2	B	128	ARG
2	B	136	LEU
2	B	139	LYS
2	B	153	ASN
1	C	15	LEU
1	C	37	GLU
1	C	59	PHE
1	C	60	GLN
1	C	69	SER
1	C	121	ASN
1	C	151	ARG
1	C	183	ARG
1	C	194	MET
1	C	205	LYS
1	C	213	SER
1	C	256	ASN
1	C	271	ASP
1	C	279	LYS
1	C	285	TYR
2	D	16	THR
2	D	24	GLN
2	D	29	LEU
2	D	31	SER
2	D	32	LEU
2	D	36	THR
2	D	37	GLU
2	D	52	GLU
2	D	58	LEU
2	D	67	SER
2	D	74	LEU
2	D	98	SER
2	D	128	ARG
2	D	129	LYS
2	D	130	ARG

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Mol	Chain	Res	Type
2	D	151	LEU
2	D	153	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	154	ASN
1	A	170	HIS
1	A	246	GLN
1	A	256	ASN
1	A	305	ASN
2	B	63	ASN
2	B	70	GLN
2	B	84	ASN
2	B	117	HIS
2	B	153	ASN
1	C	60	GLN
1	C	256	ASN
1	C	291	ASN
2	D	20	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PAL	A	311	-	9,15,15	1.52	2 (22%)	12,21,21	1.05	1 (8%)
4	PAL	C	311	-	9,15,15	1.12	1 (11%)	12,21,21	0.95	1 (8%)

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
4	PAL	A	311	-	-	0/11/17/17	0/0/0/0
4	PAL	C	311	-	-	0/11/17/17	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	311	PAL	P-O1P	2.19	1.55	1.50
4	A	311	PAL	P-O1P	2.78	1.56	1.50
4	A	311	PAL	P-C1P	3.17	1.84	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	311	PAL	O3P-P-O1P	-2.19	106.80	112.40
4	C	311	PAL	P-C1P-C1	-2.07	109.36	114.41

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

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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.