



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 06:40 AM EDT

PDB ID : 1GHD  
Title : Crystal structure of the glutaryl-7-aminocephalosporanic acid acylase by mad phasing  
Authors : Ding, Y.; Jiang, W.; Mao, X.; He, H.; Zhang, S.; Tang, H.; Bartlam, M.; Ye, S.; Jiang, F.; Liu, Y.; Zhao, G.; Rao, Z.  
Deposited on : unknown  
Resolution : 2.40 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

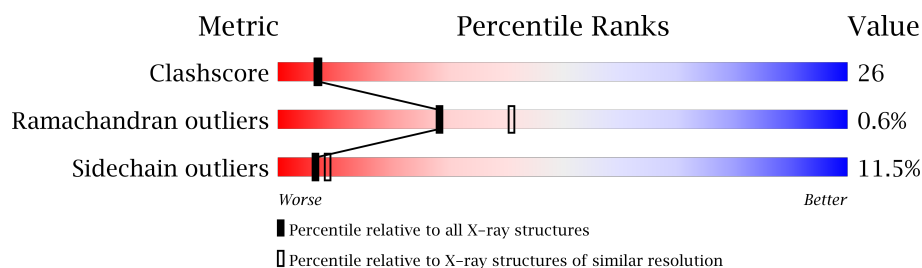
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)

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	171	 62% 23% 11%
2	B	522	 59% 31% 8%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5504 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 GLUTARYL-7-AMINOCEPHALOSPORANIC ACID ACYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	Se	0	0	0
			1201	764	212	224	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	MSE	MET	MODIFIED RESIDUE	UNP O86089

- Molecule 2 is a protein called GLUTARYL-7-AMINOCEPHALOSPORANIC ACID ACYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	520	Total	C	N	O	Se	0	0	0
			4105	2595	724	775	11			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	64	MSE	MET	MODIFIED RESIDUE	UNP O86089
B	73	MSE	MET	MODIFIED RESIDUE	UNP O86089
B	149	MSE	MET	MODIFIED RESIDUE	UNP O86089
B	156	MSE	MET	MODIFIED RESIDUE	UNP O86089
B	172	MSE	MET	MODIFIED RESIDUE	UNP O86089
B	282	MSE	MET	MODIFIED RESIDUE	UNP O86089
B	294	MSE	MET	MODIFIED RESIDUE	UNP O86089
B	304	MSE	MET	MODIFIED RESIDUE	UNP O86089
B	416	MSE	MET	MODIFIED RESIDUE	UNP O86089
B	460	MSE	MET	MODIFIED RESIDUE	UNP O86089
B	473	MSE	MET	MODIFIED RESIDUE	UNP O86089

- Molecule 3 is water.

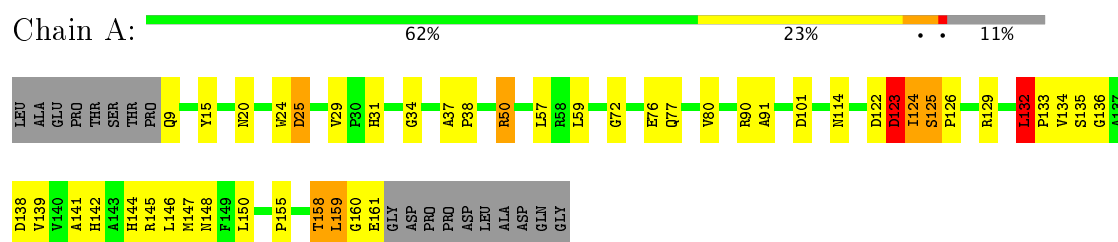
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	151	Total 151	O 151	0	0

### 3 Residue-property plots

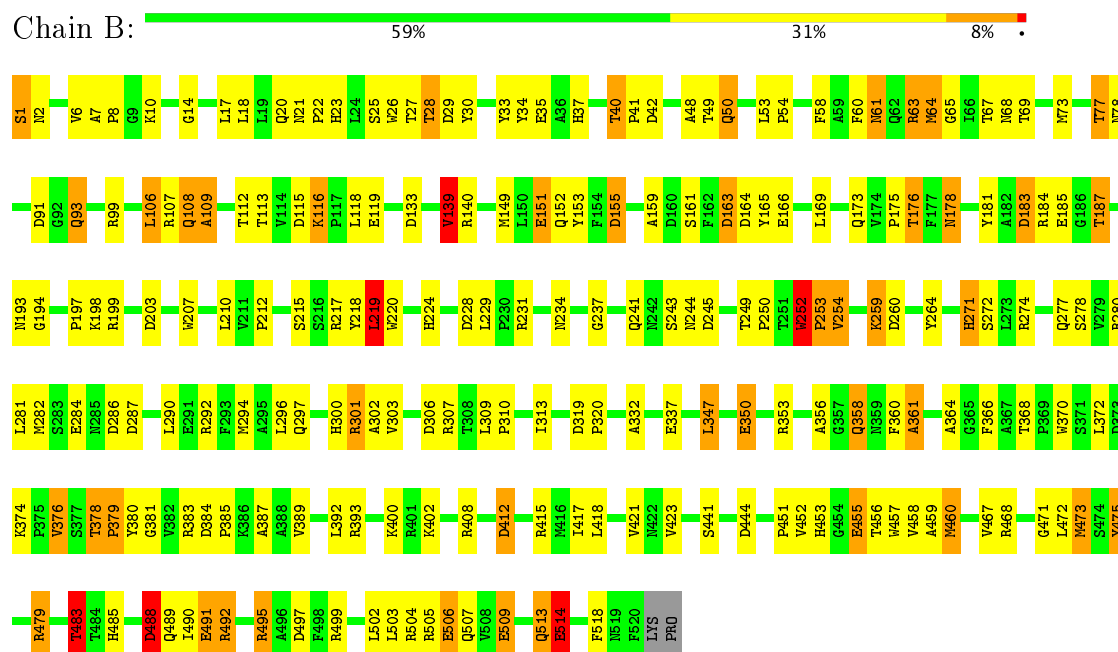
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: GLUTARYL-7-AMINOCEPHALOSPORANIC ACID ACYLASE



#### • Molecule 2: GLUTARYL-7-AMINOCEPHALOSPORANIC ACID ACYLASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.48 Å 73.48 Å 382.02 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	97.8 (30.00-2.40)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.218 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5504	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.92	3/1239 (0.2%)	1.09	8/1694 (0.5%)
2	B	0.96	11/4208 (0.3%)	1.12	31/5727 (0.5%)
All	All	0.95	14/5447 (0.3%)	1.11	39/7421 (0.5%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	514	GLU	CG-CD	15.97	1.75	1.51
2	B	514	GLU	CB-CG	15.20	1.81	1.52
1	A	123	ASP	CB-CG	11.22	1.75	1.51
2	B	509	GLU	CG-CD	10.54	1.67	1.51
2	B	509	GLU	CB-CG	10.52	1.72	1.52
2	B	514	GLU	CD-OE2	-8.53	1.16	1.25
2	B	151	GLU	CD-OE2	7.95	1.34	1.25
1	A	123	ASP	CA-CB	6.71	1.68	1.53
2	B	514	GLU	CA-CB	6.63	1.68	1.53
2	B	514	GLU	CD-OE1	-6.47	1.18	1.25
2	B	488	ASP	CB-CG	-6.07	1.39	1.51
2	B	203	ASP	CG-OD2	5.62	1.38	1.25
2	B	203	ASP	CA-CB	5.18	1.65	1.53
1	A	123	ASP	CA-C	5.15	1.66	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	514	GLU	OE1-CD-OE2	-21.37	97.66	123.30
1	A	123	ASP	CB-CG-OD2	16.25	132.92	118.30
1	A	123	ASP	OD1-CG-OD2	-12.78	99.02	123.30
2	B	155	ASP	CB-CG-OD2	10.67	127.90	118.30
2	B	203	ASP	CB-CG-OD1	-9.14	110.08	118.30
1	A	123	ASP	CB-CG-OD1	8.64	126.08	118.30
2	B	495	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	A	50	ARG	NE-CZ-NH1	-7.54	116.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	488	ASP	CB-CG-OD1	-7.48	111.56	118.30
2	B	378	THR	C-N-CD	7.42	143.99	128.40
2	B	163	ASP	CB-CG-OD1	7.24	124.82	118.30
2	B	514	GLU	CG-CD-OE1	7.22	132.75	118.30
2	B	183	ASP	CB-CA-C	-7.08	96.25	110.40
2	B	253	PRO	N-CA-C	-7.00	93.91	112.10
2	B	164	ASP	CB-CG-OD2	6.70	124.33	118.30
2	B	203	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	132	LEU	N-CA-C	6.44	128.39	111.00
2	B	361	ALA	N-CA-C	-6.39	93.76	111.00
2	B	509	GLU	OE1-CD-OE2	-6.19	115.87	123.30
2	B	260	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	124	ILE	CB-CA-C	-6.17	99.26	111.60
2	B	252	TRP	C-N-CD	5.76	140.49	128.40
2	B	155	ASP	CB-CG-OD1	-5.64	113.22	118.30
2	B	513	GLN	N-CA-C	-5.63	95.80	111.00
2	B	139	VAL	CB-CA-C	-5.57	100.81	111.40
2	B	178	ASN	N-CA-C	-5.57	95.95	111.00
2	B	219	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	125	SER	N-CA-C	5.51	125.88	111.00
2	B	483	THR	CB-CA-C	-5.49	96.77	111.60
2	B	379	PRO	N-CA-C	-5.39	98.08	112.10
2	B	503	LEU	CA-CB-CG	5.30	127.50	115.30
2	B	378	THR	N-CA-C	5.22	125.09	111.00
1	A	132	LEU	C-N-CD	5.20	139.32	128.40
2	B	378	THR	C-N-CA	-5.18	100.26	122.00
2	B	252	TRP	C-N-CA	-5.16	100.33	122.00
2	B	175	PRO	N-CA-C	5.08	125.31	112.10
2	B	514	GLU	CG-CD-OE2	5.08	128.45	118.30
2	B	1	SER	N-CA-C	5.03	124.59	111.00
2	B	364	ALA	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	1201	0	1118	49	0
2	B	4105	0	3936	229	0
3	A	47	0	0	2	0
3	B	151	0	0	8	0
All	All	5504	0	5054	265	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 26.

All (265) 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:514:GLU:CB	2:B:514:GLU:CG	1.81	1.54
2:B:514:GLU:CD	2:B:514:GLU:CG	1.75	1.54
1:A:123:ASP:CB	1:A:123:ASP:CG	1.75	1.50
2:B:485:HIS:HE1	2:B:514:GLU:OE1	1.30	1.13
2:B:63:ARG:NH2	2:B:64:MSE:HE3	1.69	1.06
2:B:353:ARG:HD3	2:B:358:GLN:HE22	1.28	0.98
2:B:63:ARG:HH22	2:B:64:MSE:HE3	1.24	0.94
2:B:77:THR:HG21	2:B:220:TRP:HE1	1.34	0.93
2:B:485:HIS:CE1	2:B:514:GLU:OE1	2.22	0.92
2:B:244:ASN:HD22	2:B:274:ARG:HH22	0.93	0.92
2:B:20:GLN:HG2	2:B:67:THR:OG1	1.69	0.91
2:B:491:GLU:OE2	2:B:495:ARG:NH1	2.03	0.90
2:B:241:GLN:HG3	2:B:278:SER:OG	1.72	0.89
2:B:152:GLN:HE22	2:B:173:GLN:H	1.20	0.88
2:B:73:MSE:HB3	2:B:176:THR:HG22	1.56	0.87
2:B:152:GLN:NE2	2:B:173:GLN:H	1.73	0.85
2:B:77:THR:CG2	2:B:220:TRP:HE1	1.89	0.85
1:A:37:ALA:HB3	1:A:38:PRO:HD3	1.59	0.84
2:B:483:THR:HB	2:B:485:HIS:H	1.43	0.83
1:A:155:PRO:O	1:A:159:LEU:HB2	1.79	0.83
2:B:64:MSE:CE	2:B:159:ALA:HB3	2.09	0.83
2:B:64:MSE:HE1	2:B:159:ALA:HB3	1.61	0.83
1:A:158:THR:HB	2:B:78:ASN:OD1	1.79	0.82
2:B:244:ASN:ND2	2:B:274:ARG:HH22	1.77	0.80
2:B:307:ARG:NH1	2:B:379:PRO:HD2	1.96	0.80
1:A:144:HIS:HD2	1:A:148:ASN:HD22	1.27	0.78
2:B:307:ARG:HH12	2:B:379:PRO:HD2	1.45	0.78
2:B:50:GLN:HG2	2:B:53:LEU:HD12	1.65	0.78
2:B:479:ARG:HD3	3:B:537:HOH:O	1.82	0.77
2:B:50:GLN:HG2	2:B:53:LEU:CD1	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:PHE:HD2	2:B:67:THR:HG23	1.50	0.76
2:B:423:VAL:HG11	2:B:491:GLU:HB2	1.68	0.75
2:B:374:LYS:HB2	2:B:378:THR:HG23	1.69	0.75
2:B:21:ASN:ND2	2:B:297:GLN:HE21	1.85	0.74
1:A:114:ASN:HD21	1:A:134:VAL:H	1.34	0.74
2:B:229:LEU:O	2:B:231:ARG:HG3	1.88	0.74
2:B:183:ASP:HB3	2:B:185:GLU:H	1.52	0.73
2:B:106:LEU:HD12	2:B:116:LYS:HE3	1.71	0.73
1:A:147:MSE:SE	2:B:149:MSE:HE3	2.39	0.73
2:B:73:MSE:HE3	2:B:73:MSE:HA	1.70	0.73
2:B:374:LYS:HB2	2:B:378:THR:CG2	2.18	0.72
2:B:252:TRP:O	2:B:254:VAL:N	2.21	0.72
2:B:292:ARG:HG2	2:B:292:ARG:HH11	1.55	0.71
2:B:149:MSE:HE2	2:B:153:TYR:CE1	2.26	0.71
2:B:313:ILE:HD13	2:B:332:ALA:HB2	1.74	0.70
2:B:259:LYS:HE3	2:B:259:LYS:H	1.54	0.70
2:B:33:TYR:HB3	2:B:473:MSE:HE1	1.74	0.69
2:B:1:SER:HB2	2:B:23:HIS:CG	2.27	0.69
2:B:58:PHE:CD2	2:B:67:THR:HG23	2.27	0.69
2:B:64:MSE:HE2	2:B:181:TYR:HE1	1.58	0.69
1:A:144:HIS:HD2	1:A:148:ASN:ND2	1.91	0.69
2:B:33:TYR:CB	2:B:473:MSE:HE1	2.23	0.68
2:B:384:ASP:OD1	2:B:387:ALA:HB2	1.93	0.68
2:B:73:MSE:HB3	2:B:176:THR:CG2	2.23	0.67
2:B:108:GLN:O	2:B:109:ALA:CB	2.42	0.67
2:B:64:MSE:HE2	2:B:181:TYR:CE1	2.29	0.67
2:B:241:GLN:CG	2:B:278:SER:OG	2.42	0.67
2:B:244:ASN:HD22	2:B:274:ARG:NH2	1.79	0.67
2:B:181:TYR:OH	2:B:183:ASP:OD1	2.11	0.67
2:B:224:HIS:HE1	2:B:264:TYR:OH	1.78	0.66
1:A:132:LEU:O	1:A:134:VAL:N	2.28	0.65
2:B:21:ASN:HD21	2:B:297:GLN:HE21	1.45	0.65
1:A:132:LEU:HD12	1:A:132:LEU:O	1.97	0.65
1:A:122:ASP:C	1:A:124:ILE:H	1.99	0.65
2:B:20:GLN:HA	2:B:67:THR:HG21	1.78	0.65
2:B:301:ARG:HG3	2:B:302:ALA:N	2.12	0.65
1:A:146:LEU:HD21	2:B:50:GLN:HG3	1.79	0.64
2:B:301:ARG:HD3	2:B:306:ASP:OD2	1.98	0.64
2:B:106:LEU:HD12	2:B:116:LYS:CE	2.27	0.64
1:A:91:ALA:CB	1:A:141:ALA:HB2	2.28	0.64
2:B:1:SER:CB	2:B:244:ASN:HD21	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:LYS:HE3	2:B:259:LYS:N	2.14	0.63
1:A:142:HIS:HE1	3:B:567:HOH:O	1.81	0.63
2:B:40:THR:HG22	2:B:42:ASP:H	1.63	0.63
1:A:77:GLN:HA	1:A:77:GLN:NE2	2.15	0.62
1:A:20:ASN:HB3	2:B:518:PHE:CZ	2.35	0.62
2:B:455:GLU:HG3	2:B:458:VAL:HG21	1.81	0.61
2:B:108:GLN:HB2	2:B:112:THR:O	2.00	0.61
2:B:61:ASN:ND2	2:B:64:MSE:H	1.98	0.61
2:B:40:THR:HG23	2:B:41:PRO:HD2	1.80	0.61
2:B:252:TRP:O	2:B:253:PRO:C	2.35	0.61
2:B:1:SER:H3	2:B:22:PRO:HA	1.65	0.61
2:B:485:HIS:HD2	2:B:488:ASP:OD2	1.83	0.61
2:B:1:SER:HB2	2:B:23:HIS:ND1	2.16	0.60
2:B:271:HIS:HD2	3:B:526:HOH:O	1.84	0.60
2:B:197:PRO:HB3	2:B:220:TRP:CD2	2.37	0.60
2:B:224:HIS:HD2	2:B:228:ASP:OD2	1.85	0.59
2:B:224:HIS:CE1	2:B:264:TYR:OH	2.55	0.59
2:B:199:ARG:HD2	2:B:207:TRP:CE2	2.38	0.59
2:B:67:THR:CG2	3:B:664:HOH:O	2.50	0.59
2:B:152:GLN:HE22	2:B:173:GLN:N	1.96	0.59
2:B:513:GLN:O	2:B:514:GLU:O	2.21	0.59
2:B:378:THR:O	2:B:379:PRO:C	2.36	0.58
2:B:166:GLU:OE2	2:B:231:ARG:NH2	2.31	0.58
2:B:108:GLN:O	2:B:109:ALA:HB2	2.04	0.58
1:A:90:ARG:HH21	1:A:144:HIS:CE1	2.21	0.58
2:B:25:SER:CB	2:B:28:THR:HG23	2.33	0.58
2:B:67:THR:HG22	2:B:68:ASN:N	2.18	0.58
2:B:149:MSE:HE2	2:B:153:TYR:HE1	1.67	0.58
2:B:353:ARG:HD3	2:B:358:GLN:NE2	2.09	0.58
2:B:6:VAL:HG22	2:B:17:LEU:HB2	1.84	0.58
2:B:183:ASP:HB3	2:B:185:GLU:N	2.19	0.57
2:B:108:GLN:HA	2:B:108:GLN:NE2	2.19	0.57
2:B:26:TRP:CZ3	2:B:451:PRO:HG2	2.40	0.57
2:B:502:LEU:HD22	2:B:507:GLN:HB3	1.85	0.57
2:B:1:SER:HB2	2:B:23:HIS:HB2	1.88	0.56
2:B:378:THR:O	2:B:380:TYR:N	2.38	0.56
2:B:370:TRP:HD1	2:B:379:PRO:HD3	1.70	0.56
1:A:31:HIS:HD2	2:B:37:HIS:ND1	2.04	0.56
2:B:108:GLN:CA	2:B:108:GLN:HE21	2.18	0.56
2:B:78:ASN:OD1	2:B:139:VAL:HG13	2.05	0.56
2:B:455:GLU:HG3	2:B:458:VAL:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:HIS:CE1	2:B:514:GLU:OE2	2.59	0.55
2:B:376:VAL:HG13	2:B:376:VAL:O	2.06	0.55
2:B:50:GLN:HG2	2:B:53:LEU:HD11	1.89	0.55
2:B:77:THR:CG2	2:B:220:TRP:NE1	2.66	0.55
1:A:90:ARG:HH21	1:A:144:HIS:HE1	1.54	0.54
2:B:505:ARG:HE	2:B:509:GLU:HG3	1.73	0.54
2:B:77:THR:HB	3:B:665:HOH:O	2.08	0.54
2:B:67:THR:HG22	2:B:68:ASN:H	1.73	0.54
1:A:20:ASN:HB3	2:B:518:PHE:CE1	2.44	0.53
2:B:347:LEU:O	2:B:347:LEU:HD22	2.08	0.53
1:A:25:ASP:OD2	1:A:31:HIS:HE1	1.92	0.53
2:B:67:THR:HG21	3:B:664:HOH:O	2.08	0.53
2:B:215:SER:C	2:B:217:ARG:H	2.11	0.53
2:B:374:LYS:CB	2:B:378:THR:HG23	2.38	0.53
2:B:183:ASP:OD2	2:B:187:THR:HG23	2.09	0.53
1:A:122:ASP:C	1:A:124:ILE:N	2.63	0.52
1:A:9:GLN:HG3	1:A:9:GLN:O	2.08	0.52
1:A:24:TRP:O	2:B:513:GLN:O	2.27	0.52
2:B:108:GLN:N	2:B:112:THR:O	2.42	0.52
2:B:2:ASN:ND2	2:B:274:ARG:HH11	2.08	0.52
2:B:77:THR:HG21	2:B:220:TRP:NE1	2.15	0.52
2:B:108:GLN:CA	2:B:108:GLN:NE2	2.72	0.51
2:B:133:ASP:C	2:B:133:ASP:OD1	2.49	0.51
2:B:356:ALA:O	2:B:361:ALA:O	2.27	0.51
2:B:8:PRO:HB3	2:B:14:GLY:O	2.09	0.51
2:B:249:THR:N	2:B:250:PRO:CD	2.73	0.51
2:B:40:THR:HG23	2:B:41:PRO:CD	2.40	0.51
2:B:99:ARG:HG2	2:B:99:ARG:HH11	1.74	0.51
2:B:99:ARG:HG2	2:B:99:ARG:NH1	2.25	0.51
2:B:441:SER:HB3	2:B:452:VAL:HG23	1.93	0.50
2:B:277:GLN:HG2	2:B:303:VAL:HG21	1.94	0.50
2:B:212:PRO:HG2	2:B:218:TYR:CE2	2.46	0.50
2:B:152:GLN:HE21	2:B:173:GLN:HB2	1.77	0.50
2:B:6:VAL:HG21	2:B:17:LEU:HD12	1.94	0.50
1:A:129:ARG:O	1:A:132:LEU:HB2	2.12	0.50
2:B:193:ASN:CG	2:B:194:GLY:N	2.66	0.49
2:B:198:LYS:HA	2:B:224:HIS:CE1	2.47	0.49
2:B:27:THR:O	2:B:28:THR:C	2.49	0.49
2:B:1:SER:HB2	2:B:23:HIS:CB	2.42	0.49
2:B:513:GLN:C	2:B:514:GLU:O	2.50	0.49
2:B:63:ARG:HH21	2:B:159:ALA:C	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ALA:HB1	1:A:141:ALA:HB2	1.94	0.49
2:B:444:ASP:C	2:B:444:ASP:OD2	2.51	0.49
2:B:408:ARG:NE	2:B:412:ASP:OD2	2.34	0.49
1:A:122:ASP:O	1:A:124:ILE:N	2.45	0.48
2:B:1:SER:HB3	2:B:244:ASN:HD21	1.76	0.48
2:B:252:TRP:HA	2:B:252:TRP:CE3	2.48	0.48
2:B:485:HIS:HE1	2:B:514:GLU:OE2	1.93	0.48
2:B:376:VAL:CG1	2:B:376:VAL:O	2.61	0.48
2:B:25:SER:OG	2:B:28:THR:HG23	2.13	0.48
2:B:10:LYS:NZ	2:B:282:MSE:O	2.46	0.48
2:B:40:THR:CG2	2:B:42:ASP:H	2.26	0.48
2:B:380:TYR:CG	2:B:381:GLY:N	2.81	0.48
2:B:294:MSE:HG2	2:B:460:MSE:HE3	1.95	0.48
1:A:132:LEU:O	1:A:133:PRO:C	2.43	0.48
1:A:101:ASP:OD1	1:A:101:ASP:N	2.47	0.47
2:B:1:SER:N	2:B:22:PRO:HA	2.29	0.47
2:B:61:ASN:HB2	3:B:543:HOH:O	2.13	0.47
2:B:93:GLN:N	2:B:93:GLN:OE1	2.47	0.47
2:B:149:MSE:HE2	2:B:153:TYR:CD1	2.49	0.47
1:A:76:GLU:O	1:A:80:VAL:HG23	2.14	0.47
2:B:64:MSE:CE	2:B:181:TYR:HE1	2.27	0.47
2:B:252:TRP:HA	2:B:252:TRP:HE3	1.80	0.47
2:B:64:MSE:HE1	2:B:165:TYR:HB2	1.97	0.47
1:A:132:LEU:HD13	1:A:132:LEU:HA	1.65	0.46
2:B:215:SER:C	2:B:217:ARG:N	2.68	0.46
2:B:29:ASP:OD2	2:B:30:TYR:N	2.48	0.46
2:B:106:LEU:O	2:B:113:THR:HA	2.15	0.46
2:B:99:ARG:NH1	2:B:119:GLU:OE1	2.48	0.46
2:B:73:MSE:CB	2:B:176:THR:HG22	2.36	0.46
2:B:151:GLU:OE2	2:B:155:ASP:OD2	2.33	0.46
2:B:237:GLY:HA3	2:B:253:PRO:HD2	1.96	0.46
2:B:504:ARG:NH1	2:B:506:GLU:OE2	2.48	0.46
1:A:139:VAL:HG13	2:B:54:PRO:HD3	1.97	0.46
2:B:20:GLN:NE2	2:B:457:TRP:HE1	2.14	0.46
2:B:513:GLN:O	2:B:514:GLU:HB2	2.16	0.46
2:B:456:THR:HG22	2:B:475:TYR:CE1	2.52	0.45
2:B:210:LEU:HD23	2:B:210:LEU:HA	1.81	0.45
2:B:491:GLU:CD	2:B:495:ARG:NH1	2.68	0.45
2:B:1:SER:CB	2:B:23:HIS:HB2	2.47	0.45
2:B:40:THR:HG21	3:B:530:HOH:O	2.17	0.45
2:B:69:THR:OG1	2:B:178:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:LEU:HD22	2:B:296:LEU:HD22	1.98	0.45
1:A:34:GLY:O	2:B:41:PRO:HD3	2.17	0.45
2:B:385:PRO:O	2:B:389:VAL:HG23	2.16	0.45
2:B:61:ASN:HD22	2:B:61:ASN:C	2.20	0.45
2:B:140:ARG:CZ	2:B:219:LEU:HD22	2.47	0.44
2:B:417:ILE:HA	2:B:421:VAL:O	2.16	0.44
2:B:457:TRP:CZ2	2:B:459:ALA:HB2	2.52	0.44
1:A:135:SER:O	1:A:136:GLY:C	2.55	0.44
2:B:152:GLN:NE2	2:B:173:GLN:N	2.53	0.44
2:B:63:ARG:HA	2:B:184:ARG:HD2	1.98	0.44
2:B:280:ARG:HD2	2:B:284:GLU:OE2	2.17	0.44
2:B:7:ALA:O	2:B:8:PRO:C	2.55	0.44
1:A:142:HIS:HD2	3:A:218:HOH:O	1.99	0.44
2:B:366:PHE:HA	2:B:381:GLY:O	2.18	0.44
2:B:489:GLN:OE1	2:B:499:ARG:NH1	2.49	0.44
2:B:107:ARG:HG2	2:B:107:ARG:HH11	1.82	0.44
1:A:15:TYR:CE1	2:B:505:ARG:HG2	2.53	0.44
2:B:1:SER:O	2:B:243:SER:HA	2.17	0.44
2:B:458:VAL:O	2:B:471:GLY:HA2	2.17	0.43
2:B:252:TRP:HB3	2:B:253:PRO:HD3	2.01	0.43
1:A:72:GLY:CA	2:B:107:ARG:HB3	2.48	0.43
2:B:294:MSE:SE	2:B:460:MSE:HE3	2.69	0.43
2:B:350:GLU:OE1	2:B:402:LYS:NZ	2.41	0.43
2:B:292:ARG:HG2	2:B:292:ARG:NH1	2.26	0.43
1:A:135:SER:N	1:A:138:ASP:OD2	2.44	0.43
2:B:485:HIS:HE1	2:B:514:GLU:CD	2.10	0.43
1:A:144:HIS:CD2	1:A:148:ASN:ND2	2.79	0.43
2:B:140:ARG:HG2	2:B:220:TRP:CH2	2.54	0.43
2:B:313:ILE:HD13	2:B:332:ALA:CB	2.45	0.43
2:B:61:ASN:HD21	2:B:64:MSE:H	1.64	0.43
1:A:160:GLY:O	1:A:161:GLU:C	2.58	0.43
2:B:152:GLN:NE2	2:B:173:GLN:HB2	2.33	0.43
2:B:34:TYR:O	2:B:48:ALA:HA	2.19	0.43
1:A:114:ASN:HD21	1:A:134:VAL:HG22	1.84	0.42
1:A:114:ASN:ND2	1:A:134:VAL:HG22	2.34	0.42
2:B:301:ARG:HG2	2:B:303:VAL:HG23	2.00	0.42
2:B:492:ARG:HD3	2:B:497:ASP:HB3	2.02	0.42
2:B:374:LYS:HB2	2:B:378:THR:HG21	2.01	0.42
2:B:280:ARG:HD3	2:B:376:VAL:HG13	2.02	0.42
2:B:2:ASN:HD21	2:B:274:ARG:HH11	1.67	0.42
2:B:108:GLN:HA	2:B:108:GLN:HE21	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:ILE:O	2:B:418:LEU:HD23	2.19	0.42
1:A:145:ARG:HD3	3:A:218:HOH:O	2.19	0.42
1:A:72:GLY:HA2	2:B:107:ARG:HB3	2.02	0.42
2:B:187:THR:HA	2:B:234:ASN:OD1	2.19	0.42
2:B:380:TYR:CD2	2:B:381:GLY:N	2.88	0.42
2:B:393:ARG:HH11	2:B:393:ARG:HG3	1.85	0.42
1:A:125:SER:HA	1:A:126:PRO:HD3	1.90	0.42
2:B:64:MSE:HE3	2:B:159:ALA:HB3	1.94	0.42
2:B:252:TRP:O	2:B:252:TRP:CE3	2.73	0.42
2:B:309:LEU:N	2:B:310:PRO:CD	2.82	0.42
2:B:35:GLU:CD	2:B:499:ARG:HH22	2.23	0.41
1:A:90:ARG:NH2	1:A:144:HIS:HE1	2.17	0.41
2:B:492:ARG:CD	2:B:497:ASP:O	2.68	0.41
2:B:60:PHE:HA	2:B:65:GLY:HA2	2.01	0.41
2:B:107:ARG:HG2	2:B:107:ARG:NH1	2.36	0.41
2:B:485:HIS:CD2	2:B:488:ASP:OD2	2.70	0.41
2:B:300:HIS:HD2	2:B:337:GLU:OE1	2.04	0.41
2:B:360:PHE:C	2:B:361:ALA:O	2.57	0.41
2:B:472:LEU:HD23	2:B:499:ARG:HG3	2.02	0.41
2:B:489:GLN:O	2:B:492:ARG:HB2	2.21	0.41
2:B:245:ASP:N	2:B:245:ASP:OD2	2.52	0.41
1:A:132:LEU:O	1:A:132:LEU:CD1	2.69	0.41
2:B:2:ASN:HB2	2:B:21:ASN:HB3	2.02	0.41
2:B:319:ASP:HA	2:B:320:PRO:HD3	1.80	0.41
1:A:25:ASP:HB2	1:A:29:VAL:HB	2.03	0.40
2:B:370:TRP:HD1	2:B:379:PRO:CD	2.34	0.40
1:A:31:HIS:CD2	2:B:37:HIS:ND1	2.87	0.40
2:B:490:ILE:HA	2:B:490:ILE:HD12	1.77	0.40
2:B:199:ARG:HD2	2:B:207:TRP:CD2	2.56	0.40
2:B:63:ARG:NH2	2:B:161:SER:N	2.70	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	151/171 (88%)	139 (92%)	10 (7%)	2 (1%)	14	19
2	B	518/522 (99%)	477 (92%)	39 (8%)	2 (0%)	38	54
All	All	669/693 (96%)	616 (92%)	49 (7%)	4 (1%)	28	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
2	B	109	ALA
2	B	514	GLU
1	A	123	ASP

### 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	117/130 (90%)	109 (93%)	8 (7%)	18	29
2	B	429/420 (102%)	374 (87%)	55 (13%)	5	6
All	All	546/550 (99%)	483 (88%)	63 (12%)	6	9

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	50	ARG
1	A	57	LEU
1	A	59	LEU
1	A	132	LEU
1	A	150	LEU
1	A	158	THR
1	A	159	LEU
2	B	18	LEU

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Mol	Chain	Res	Type
2	B	28	THR
2	B	40	THR
2	B	49	THR
2	B	50	GLN
2	B	61	ASN
2	B	63	ARG
2	B	64	MSE
2	B	77	THR
2	B	91	ASP
2	B	93	GLN
2	B	106	LEU
2	B	108	GLN
2	B	115	ASP
2	B	116	LYS
2	B	118	LEU
2	B	139	VAL
2	B	163	ASP
2	B	169	LEU
2	B	176	THR
2	B	187	THR
2	B	219	LEU
2	B	252	TRP
2	B	254	VAL
2	B	259	LYS
2	B	271	HIS
2	B	272	SER
2	B	286	ASP
2	B	287	ASP
2	B	290	LEU
2	B	301	ARG
2	B	347	LEU
2	B	350	GLU
2	B	358	GLN
2	B	368	THR
2	B	372	LEU
2	B	376	VAL
2	B	383	ARG
2	B	392	LEU
2	B	400	LYS
2	B	412	ASP
2	B	415	ARG
2	B	453	HIS

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Mol	Chain	Res	Type
2	B	455	GLU
2	B	460	MSE
2	B	467	VAL
2	B	468	ARG
2	B	473	MSE
2	B	475	TYR
2	B	479	ARG
2	B	483	THR
2	B	488	ASP
2	B	491	GLU
2	B	492	ARG
2	B	506	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	55	ASN
1	A	77	GLN
1	A	98	GLN
1	A	114	ASN
1	A	130	GLN
1	A	142	HIS
1	A	144	HIS
1	A	148	ASN
2	B	2	ASN
2	B	20	GLN
2	B	21	ASN
2	B	61	ASN
2	B	84	GLN
2	B	108	GLN
2	B	152	GLN
2	B	189	ASN
2	B	224	HIS
2	B	244	ASN
2	B	271	HIS
2	B	300	HIS
2	B	358	GLN
2	B	485	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](#)

There are no ligands in this entry.

### 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.