



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:38 PM GMT

PDB ID : 1GLN  
Title : ARCHITECTURES OF CLASS-DEFINING AND SPECIFIC DOMAINS OF GLUTAMYL-TRNA SYNTHETASE  
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Deposited on : 1994-07-20  
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](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

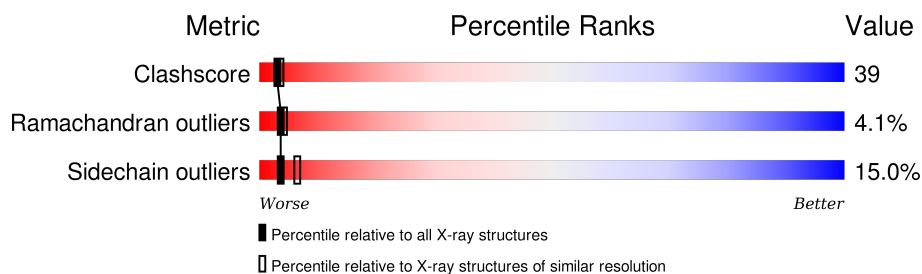
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	468	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3973 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 GLUTAMYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3813	2443	674	688	8			

- Molecule 2 is water.

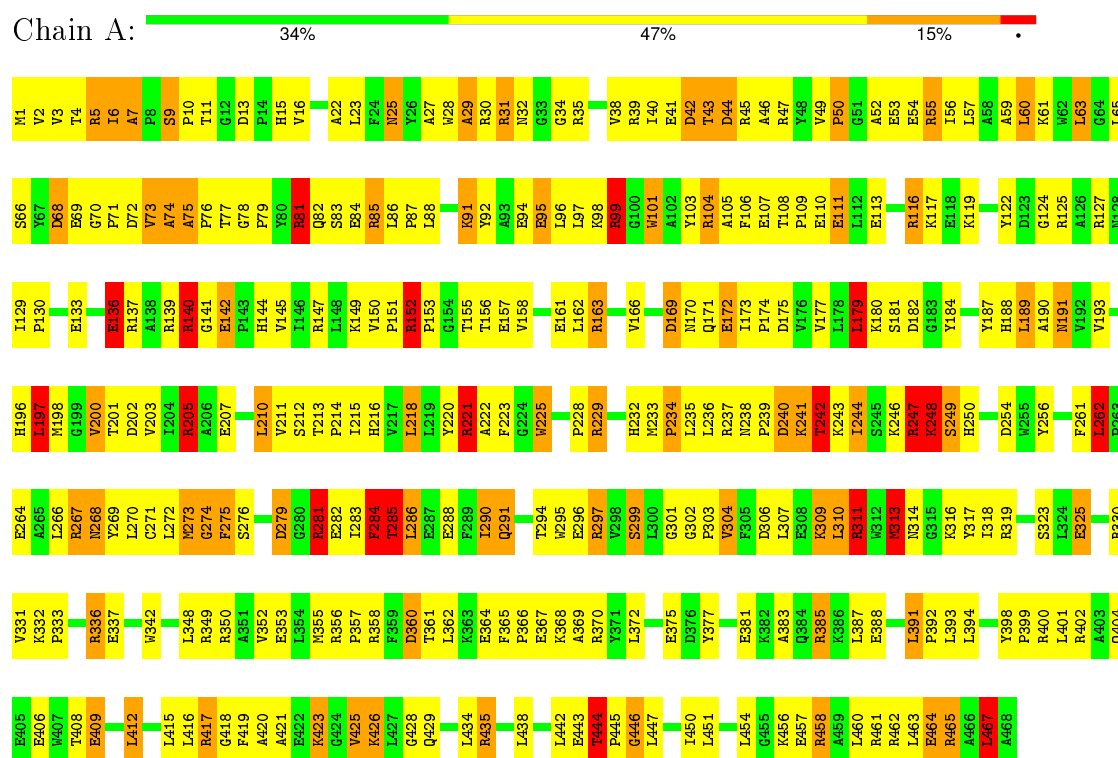
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	160	Total	O	0	0
			160	160		

### 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: GLUTAMYL-TRNA SYNTHETASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.75Å 110.09Å 67.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3973	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	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	0.99	0/3908	1.99	115/5292 (2.2%)

There are no bond length outliers.

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	CD-NE-CZ	28.46	163.44	123.60
1	A	319	ARG	NE-CZ-NH2	-15.41	112.60	120.30
1	A	140	ARG	NE-CZ-NH1	13.59	127.09	120.30
1	A	55	ARG	CD-NE-CZ	12.54	141.16	123.60
1	A	319	ARG	NE-CZ-NH1	12.48	126.54	120.30
1	A	465	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	A	55	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	A	465	ARG	NE-CZ-NH2	-11.38	114.61	120.30
1	A	225	TRP	CA-CB-CG	11.29	135.16	113.70
1	A	283	ILE	C-N-CA	11.18	149.66	121.70
1	A	336	ARG	NE-CZ-NH2	-11.05	114.77	120.30
1	A	400	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	A	311	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	336	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	55	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	A	385	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	221	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	267	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	A	284	PHE	N-CA-CB	9.21	127.18	110.60
1	A	104	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	104	ARG	CD-NE-CZ	9.02	136.23	123.60
1	A	6	ILE	N-CA-CB	8.63	130.64	110.80
1	A	116	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	A	349	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	325	GLU	OE1-CD-OE2	-8.56	113.03	123.30
1	A	262	LEU	CA-CB-CG	8.09	133.90	115.30
1	A	99	ARG	NE-CZ-NH2	-7.84	116.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	GLU	CA-CB-CG	7.76	130.48	113.40
1	A	370	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	A	5	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	152	ARG	NE-CZ-NH1	-7.44	116.58	120.30
1	A	7	ALA	CB-CA-C	7.43	121.24	110.10
1	A	467	LEU	CA-CB-CG	7.37	132.24	115.30
1	A	44	ASP	CB-CG-OD2	7.31	124.88	118.30
1	A	247	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	152	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	A	229	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	175	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	A	205	ARG	CB-CG-CD	7.13	130.14	111.60
1	A	281	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	225	TRP	CB-CA-C	7.03	124.46	110.40
1	A	99	ARG	CA-CB-CG	6.91	128.60	113.40
1	A	177	VAL	CB-CA-C	6.85	124.41	111.40
1	A	400	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	319	ARG	CD-NE-CZ	6.70	132.98	123.60
1	A	152	ARG	NH1-CZ-NH2	6.69	126.76	119.40
1	A	31	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	42	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	A	73	VAL	N-CA-CB	-6.38	97.46	111.50
1	A	99	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	136	GLU	CG-CD-OE2	6.31	130.92	118.30
1	A	400	ARG	CD-NE-CZ	6.29	132.41	123.60
1	A	95	GLU	CA-CB-CG	6.25	127.14	113.40
1	A	197	LEU	CB-CA-C	6.25	122.07	110.20
1	A	85	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	A	458	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	A	311	ARG	CD-NE-CZ	6.15	132.21	123.60
1	A	28	TRP	CB-CA-C	6.12	122.65	110.40
1	A	297	ARG	CD-NE-CZ	-6.12	115.03	123.60
1	A	74	ALA	N-CA-CB	6.04	118.56	110.10
1	A	385	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	254	ASP	CA-CB-CG	5.99	126.58	113.40
1	A	444	THR	CA-CB-CG2	5.97	120.77	112.40
1	A	267	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	349	ARG	CD-NE-CZ	5.90	131.86	123.60
1	A	279	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	A	306	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	A	16	VAL	CA-CB-CG1	5.89	119.73	110.90
1	A	169	ASP	CB-CG-OD1	5.87	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	6	ILE	N-CA-C	-5.85	95.22	111.00
1	A	457	GLU	CG-CD-OE1	5.84	129.99	118.30
1	A	172	GLU	CG-CD-OE1	-5.81	106.68	118.30
1	A	325	GLU	CG-CD-OE2	5.80	129.91	118.30
1	A	116	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	330	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	285	THR	C-N-CA	5.73	136.03	121.70
1	A	281	ARG	CD-NE-CZ	-5.72	115.59	123.60
1	A	172	GLU	OE1-CD-OE2	5.70	130.14	123.30
1	A	95	GLU	CG-CD-OE1	5.68	129.66	118.30
1	A	248	LYS	CA-CB-CG	5.68	125.90	113.40
1	A	205	ARG	CD-NE-CZ	5.66	131.52	123.60
1	A	250	HIS	N-CA-CB	5.61	120.70	110.60
1	A	273	MET	CG-SD-CE	5.59	109.14	100.20
1	A	284	PHE	CB-CA-C	-5.49	99.43	110.40
1	A	254	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	211	VAL	CG1-CB-CG2	5.46	119.64	110.90
1	A	360	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	50	PRO	N-CA-C	5.44	126.25	112.10
1	A	147	ARG	CD-NE-CZ	-5.41	116.03	123.60
1	A	25	ASN	O-C-N	5.40	131.34	122.70
1	A	264	GLU	CG-CD-OE2	-5.34	107.62	118.30
1	A	435	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	264	GLU	CG-CD-OE1	5.28	128.86	118.30
1	A	81	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	205	ARG	CA-CB-CG	5.22	124.89	113.40
1	A	104	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
1	A	313	MET	CG-SD-CE	5.21	108.53	100.20
1	A	179	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	16	VAL	CB-CA-C	5.19	121.26	111.40
1	A	133	GLU	CG-CD-OE1	-5.18	107.93	118.30
1	A	271	CYS	N-CA-CB	5.18	119.92	110.60
1	A	63	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	205	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	68	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	417	ARG	CD-NE-CZ	-5.09	116.47	123.60
1	A	240	ASP	C-N-CA	5.08	134.40	121.70
1	A	409	GLU	CG-CD-OE1	-5.07	108.16	118.30
1	A	161	GLU	CG-CD-OE1	5.07	128.44	118.30
1	A	147	ARG	O-C-N	5.03	130.75	122.70
1	A	353	GLU	OE1-CD-OE2	5.03	129.33	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	THR	N-CA-CB	5.03	119.85	110.30
1	A	461	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	240	ASP	CB-CG-OD1	5.00	122.80	118.30
1	A	269	TYR	CB-CG-CD2	-5.00	118.00	121.00

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	3813	0	3821	295	0
2	A	160	0	0	16	0
All	All	3973	0	3821	295	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 39.

All (295) 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:127:ARG:HH21	1:A:149:LYS:HG3	1.24	1.02
1:A:77:THR:HG21	1:A:198:MET:HA	1.40	1.01
1:A:75:ALA:HB1	1:A:76:PRO:HD2	1.47	0.96
1:A:262:LEU:H	1:A:314:ASN:HD21	1.15	0.94
1:A:268:ASN:HA	1:A:285:THR:HG23	1.55	0.89
1:A:284:PHE:HD2	1:A:288:GLU:HB2	1.40	0.86
1:A:136:GLU:HG3	1:A:137:ARG:N	1.90	0.85
1:A:75:ALA:HB1	1:A:76:PRO:CD	2.06	0.85
1:A:127:ARG:HH21	1:A:149:LYS:CG	1.90	0.84
1:A:444:THR:HG23	1:A:445:PRO:HD2	1.59	0.84
1:A:152:ARG:HG3	1:A:171:GLN:HE22	1.41	0.83
1:A:279:ASP:OD1	1:A:281:ARG:HB2	1.80	0.82
1:A:4:THR:HB	1:A:25:ASN:HD22	1.44	0.81
1:A:311:ARG:NH2	1:A:364:GLU:OE2	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:NH2	1:A:149:LYS:HG3	1.95	0.81
1:A:262:LEU:H	1:A:314:ASN:ND2	1.81	0.79
1:A:332:LYS:HD3	1:A:342:TRP:CZ2	2.18	0.78
1:A:385:ARG:O	1:A:388:GLU:HG2	1.85	0.76
1:A:291:GLN:HG2	2:A:804:HOH:O	1.85	0.76
1:A:237:ARG:CZ	1:A:302:GLY:HA3	2.17	0.74
1:A:267:ARG:HG2	1:A:285:THR:HG21	1.69	0.74
1:A:74:ALA:O	1:A:75:ALA:HB2	1.86	0.73
1:A:213:THR:N	1:A:214:PRO:HD2	2.03	0.73
1:A:272:LEU:HD21	1:A:282:GLU:HB3	1.68	0.73
1:A:435:ARG:HD2	1:A:444:THR:HB	1.69	0.72
1:A:152:ARG:HH12	1:A:171:GLN:HA	1.53	0.72
1:A:77:THR:HG21	1:A:198:MET:CA	2.19	0.72
1:A:267:ARG:HE	1:A:285:THR:HB	1.55	0.72
1:A:404:GLN:NE2	1:A:415:LEU:HD12	2.05	0.72
1:A:268:ASN:CA	1:A:285:THR:HG23	2.22	0.70
1:A:234:PRO:O	1:A:235:LEU:HB3	1.91	0.70
1:A:55:ARG:HD2	2:A:555:HOH:O	1.93	0.69
1:A:152:ARG:HG3	1:A:171:GLN:NE2	2.08	0.68
1:A:92:TYR:HB3	1:A:223:PHE:CE1	2.29	0.68
1:A:57:LEU:O	1:A:61:LYS:HD2	1.92	0.68
1:A:202:ASP:OD2	1:A:229:ARG:NH1	2.27	0.68
1:A:77:THR:CG2	1:A:198:MET:HG2	2.24	0.67
1:A:11:THR:CG2	1:A:47:ARG:HB3	2.25	0.67
1:A:5:ARG:HG2	1:A:200:VAL:HG11	1.77	0.67
1:A:406:GLU:HG2	1:A:408:THR:HG23	1.76	0.67
1:A:205:ARG:HH22	1:A:216:HIS:CD2	2.13	0.67
1:A:221:ARG:HB3	1:A:221:ARG:HH11	1.60	0.67
1:A:247:ARG:O	1:A:248:LYS:HB2	1.95	0.67
1:A:137:ARG:HD2	1:A:142:GLU:OE2	1.95	0.66
1:A:307:LEU:O	1:A:311:ARG:HG3	1.96	0.66
1:A:294:THR:HG22	1:A:296:GLU:HB3	1.78	0.65
1:A:239:PRO:O	1:A:240:ASP:HB2	1.97	0.65
1:A:284:PHE:HA	2:A:631:HOH:O	1.96	0.65
1:A:332:LYS:HE3	1:A:348:LEU:CD2	2.27	0.64
1:A:15:HIS:HE1	1:A:244:ILE:HD12	1.62	0.64
1:A:10:PRO:HD3	1:A:40:ILE:HG23	1.79	0.64
1:A:79:PRO:HB2	1:A:85:ARG:HG2	1.80	0.63
1:A:11:THR:HG21	1:A:47:ARG:HB3	1.81	0.63
1:A:408:THR:O	1:A:412:LEU:HB2	1.98	0.63
1:A:332:LYS:HB2	1:A:333:PRO:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASN:HA	1:A:173:ILE:HD12	1.80	0.62
1:A:262:LEU:N	1:A:314:ASN:HD21	1.93	0.62
1:A:96:LEU:HD13	1:A:223:PHE:CZ	2.34	0.62
1:A:74:ALA:O	1:A:75:ALA:CB	2.47	0.62
1:A:29:ALA:O	1:A:32:ASN:N	2.27	0.62
1:A:5:ARG:CG	1:A:200:VAL:HG11	2.30	0.62
1:A:284:PHE:HD2	1:A:288:GLU:CB	2.13	0.61
1:A:169:ASP:O	1:A:172:GLU:HG3	2.01	0.61
1:A:365:PHE:HB3	1:A:366:PRO:HD3	1.82	0.61
1:A:235:LEU:HD11	1:A:243:LYS:HG2	1.83	0.61
1:A:77:THR:O	1:A:77:THR:HG22	2.01	0.60
1:A:119:LYS:NZ	1:A:125:ARG:HH22	1.99	0.60
1:A:221:ARG:CB	1:A:221:ARG:HH11	2.14	0.60
1:A:325:GLU:OE1	1:A:325:GLU:N	2.34	0.60
1:A:77:THR:HG21	1:A:198:MET:HG2	1.83	0.60
1:A:238:ASN:O	1:A:241:LYS:HA	2.01	0.60
1:A:205:ARG:HD3	1:A:232:HIS:CE1	2.38	0.59
1:A:438:LEU:HD11	1:A:451:LEU:HG	1.84	0.59
1:A:113:GLU:OE2	1:A:116:ARG:NH1	2.35	0.59
1:A:45:ARG:NH1	1:A:83:SER:HB2	2.17	0.59
1:A:40:ILE:HB	1:A:81:ARG:HG3	1.84	0.58
1:A:276:SER:O	1:A:297:ARG:NH1	2.36	0.58
1:A:205:ARG:HH11	1:A:232:HIS:HE1	1.51	0.57
1:A:3:VAL:HG13	1:A:35:ARG:HB2	1.87	0.57
1:A:275:PHE:HA	1:A:297:ARG:O	2.04	0.57
1:A:86:LEU:HB3	1:A:87:PRO:HD3	1.86	0.57
1:A:45:ARG:NE	2:A:528:HOH:O	2.36	0.57
1:A:267:ARG:HG2	1:A:285:THR:CG2	2.34	0.57
1:A:267:ARG:CG	1:A:285:THR:HG21	2.35	0.56
1:A:323:SER:HB2	2:A:511:HOH:O	2.04	0.56
1:A:52:ALA:O	1:A:56:ILE:HG13	2.05	0.56
1:A:444:THR:HG23	1:A:445:PRO:CD	2.34	0.56
1:A:456:LYS:HG2	1:A:460:LEU:HD12	1.87	0.56
1:A:122:TYR:CE2	1:A:124:GLY:HA2	2.41	0.55
1:A:23:LEU:HD13	1:A:65:LEU:HD21	1.87	0.55
1:A:276:SER:CB	1:A:297:ARG:HH12	2.18	0.55
1:A:91:LYS:NZ	1:A:91:LYS:CB	2.70	0.55
1:A:446:GLY:O	1:A:450:ILE:HG12	2.07	0.55
1:A:91:LYS:HZ3	1:A:91:LYS:HB2	1.72	0.55
1:A:106:PHE:CD2	1:A:144:HIS:HB3	2.42	0.54
1:A:276:SER:OG	1:A:297:ARG:NH1	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:PRO:O	1:A:446:GLY:C	2.45	0.54
1:A:242:THR:O	1:A:243:LYS:C	2.46	0.54
1:A:196:HIS:HD2	2:A:508:HOH:O	1.91	0.54
1:A:237:ARG:HD3	1:A:241:LYS:HB3	1.90	0.53
1:A:163:ARG:NH2	1:A:232:HIS:O	2.41	0.53
1:A:314:ASN:O	1:A:318:ILE:HG13	2.08	0.53
1:A:77:THR:HG22	1:A:198:MET:HG2	1.89	0.53
1:A:393:LEU:HD23	1:A:429:GLN:O	2.09	0.53
1:A:1:MET:O	1:A:3:VAL:HG23	2.09	0.53
1:A:95:GLU:HG2	1:A:99:ARG:HH21	1.74	0.53
1:A:103:TYR:CE2	1:A:127:ARG:HG2	2.44	0.53
1:A:290:ILE:O	1:A:290:ILE:HG13	2.09	0.53
1:A:82:GLN:OE1	1:A:190:ALA:HB1	2.09	0.52
1:A:86:LEU:HD21	1:A:184:TYR:CE1	2.44	0.52
1:A:398:TYR:N	1:A:399:PRO:HD2	2.23	0.52
1:A:75:ALA:CB	1:A:76:PRO:CD	2.78	0.52
1:A:72:ASP:OD1	1:A:73:VAL:N	2.42	0.52
1:A:332:LYS:HE3	1:A:348:LEU:HD21	1.90	0.52
1:A:40:ILE:HG22	1:A:42:ASP:HB3	1.91	0.52
1:A:267:ARG:NH2	2:A:607:HOH:O	2.42	0.52
1:A:332:LYS:HD3	1:A:342:TRP:CH2	2.45	0.52
1:A:267:ARG:HE	1:A:285:THR:CB	2.22	0.51
1:A:136:GLU:CD	1:A:140:ARG:HH11	2.13	0.51
1:A:237:ARG:HH11	1:A:241:LYS:CE	2.23	0.51
1:A:119:LYS:HZ1	1:A:125:ARG:HH22	1.57	0.51
1:A:179:LEU:HD23	1:A:189:LEU:HD12	1.93	0.51
1:A:282:GLU:OE2	1:A:309:LYS:NZ	2.43	0.51
1:A:97:LEU:O	1:A:99:ARG:N	2.43	0.51
1:A:27:ALA:CB	1:A:290:ILE:HG22	2.41	0.51
1:A:22:ALA:CB	1:A:60:LEU:HD21	2.41	0.51
1:A:188:HIS:CD2	1:A:216:HIS:HE1	2.29	0.51
1:A:398:TYR:O	1:A:402:ARG:HG3	2.11	0.50
1:A:124:GLY:O	1:A:127:ARG:HG3	2.11	0.50
1:A:188:HIS:CD2	1:A:216:HIS:CE1	2.98	0.50
1:A:136:GLU:CG	1:A:137:ARG:N	2.66	0.50
1:A:243:LYS:HZ3	1:A:244:ILE:HG13	1.76	0.50
1:A:237:ARG:HH11	1:A:241:LYS:NZ	2.10	0.50
1:A:136:GLU:OE2	1:A:140:ARG:HD2	2.12	0.50
1:A:361:THR:OG1	1:A:364:GLU:HG3	2.11	0.50
1:A:381:GLU:O	1:A:385:ARG:HG2	2.12	0.50
1:A:237:ARG:NH1	1:A:301:GLY:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ARG:NH2	1:A:302:GLY:HA3	2.26	0.49
1:A:92:TYR:O	1:A:96:LEU:HB2	2.11	0.49
1:A:94:GLU:CD	1:A:98:LYS:HZ2	2.15	0.49
1:A:237:ARG:NH1	1:A:241:LYS:NZ	2.61	0.49
1:A:246:LYS:NZ	1:A:247:ARG:HH12	2.10	0.49
1:A:464:GLU:O	1:A:465:ARG:C	2.49	0.49
1:A:213:THR:N	1:A:214:PRO:CD	2.72	0.49
1:A:332:LYS:O	1:A:336:ARG:HG2	2.12	0.49
1:A:95:GLU:OE2	1:A:99:ARG:NH2	2.44	0.49
1:A:236:LEU:HD12	1:A:303:PRO:HG2	1.95	0.49
1:A:152:ARG:CG	1:A:171:GLN:HE22	2.21	0.49
1:A:92:TYR:HB3	1:A:223:PHE:CZ	2.47	0.49
1:A:267:ARG:NH1	2:A:556:HOH:O	2.43	0.48
1:A:243:LYS:NZ	1:A:244:ILE:HG13	2.28	0.48
1:A:152:ARG:NH1	1:A:152:ARG:HG3	2.28	0.48
1:A:276:SER:O	1:A:297:ARG:HD3	2.12	0.48
1:A:415:LEU:HD23	1:A:415:LEU:C	2.33	0.48
1:A:220:TYR:CZ	1:A:228:PRO:HD3	2.48	0.48
1:A:356:ARG:N	1:A:357:PRO:CD	2.76	0.48
1:A:152:ARG:NH1	1:A:170:ASN:O	2.46	0.48
1:A:96:LEU:HD13	1:A:223:PHE:CE1	2.48	0.48
1:A:205:ARG:HH11	1:A:232:HIS:CE1	2.32	0.48
1:A:7:ALA:HA	1:A:39:ARG:O	2.12	0.48
1:A:187:TYR:O	1:A:191:ASN:HB3	2.14	0.48
1:A:247:ARG:O	1:A:248:LYS:CB	2.61	0.48
1:A:191:ASN:ND2	2:A:538:HOH:O	2.45	0.48
1:A:137:ARG:CD	1:A:142:GLU:OE2	2.61	0.48
1:A:201:THR:HB	2:A:821:HOH:O	2.13	0.48
1:A:241:LYS:O	1:A:242:THR:HG23	2.13	0.47
1:A:248:LYS:O	1:A:249:SER:HB2	2.14	0.47
1:A:419:PHE:CE2	1:A:423:LYS:NZ	2.80	0.47
1:A:53:GLU:O	1:A:56:ILE:HB	2.14	0.47
1:A:88:LEU:O	1:A:92:TYR:HD2	1.96	0.47
1:A:401:LEU:HD12	1:A:463:LEU:CD1	2.44	0.47
1:A:381:GLU:OE2	1:A:385:ARG:NH2	2.48	0.47
1:A:43:THR:O	1:A:45:ARG:HG2	2.15	0.47
1:A:355:MET:HG3	1:A:369:ALA:HB2	1.95	0.47
1:A:63:LEU:O	1:A:267:ARG:HD3	2.15	0.47
1:A:163:ARG:NH1	1:A:207:GLU:OE2	2.48	0.47
1:A:157:GLU:HG3	2:A:560:HOH:O	2.15	0.47
1:A:458:ARG:NE	2:A:635:HOH:O	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:O	1:A:352:VAL:HG23	2.16	0.46
1:A:401:LEU:HD12	1:A:463:LEU:HD12	1.97	0.46
1:A:107:GLU:HB3	1:A:111:GLU:HB3	1.98	0.46
1:A:152:ARG:N	1:A:153:PRO:CD	2.78	0.46
1:A:391:LEU:CD2	1:A:394:LEU:HD12	2.46	0.46
1:A:72:ASP:OD1	1:A:73:VAL:HB	2.15	0.46
1:A:417:ARG:CB	1:A:417:ARG:NH1	2.78	0.46
1:A:59:ALA:O	1:A:63:LEU:HD12	2.15	0.46
1:A:79:PRO:HB2	1:A:85:ARG:CG	2.45	0.46
1:A:274:GLY:O	1:A:275:PHE:CB	2.63	0.46
1:A:166:VAL:HG23	2:A:502:HOH:O	2.15	0.46
1:A:210:LEU:HD12	1:A:210:LEU:O	2.16	0.46
1:A:98:LYS:O	1:A:99:ARG:HG3	2.16	0.46
1:A:356:ARG:CB	1:A:357:PRO:HD3	2.46	0.46
1:A:248:LYS:O	1:A:249:SER:CB	2.63	0.46
1:A:86:LEU:CB	1:A:87:PRO:HD3	2.46	0.45
1:A:418:GLY:O	1:A:421:ALA:HB3	2.16	0.45
1:A:158:VAL:HG21	1:A:214:PRO:HA	1.98	0.45
1:A:284:PHE:CD2	1:A:285:THR:O	2.69	0.45
1:A:71:PRO:C	1:A:73:VAL:H	2.20	0.45
1:A:239:PRO:HA	1:A:304:VAL:HG21	1.98	0.45
1:A:247:ARG:HH11	1:A:247:ARG:HG2	1.82	0.45
1:A:434:LEU:CD2	1:A:451:LEU:HD11	2.47	0.45
1:A:218:LEU:O	1:A:222:ALA:N	2.42	0.45
1:A:234:PRO:HG3	1:A:299:SER:O	2.17	0.45
1:A:358:ARG:O	1:A:368:LYS:HD2	2.15	0.45
1:A:284:PHE:CD2	1:A:288:GLU:HB2	2.32	0.45
1:A:377:TYR:OH	1:A:462:ARG:HD3	2.17	0.45
1:A:152:ARG:NH2	1:A:173:ILE:O	2.50	0.45
1:A:193:VAL:HG13	1:A:197:LEU:HD22	1.99	0.45
1:A:297:ARG:HB3	1:A:297:ARG:HH11	1.80	0.45
1:A:261:PHE:CE1	1:A:310:LEU:HD13	2.52	0.45
1:A:9:SER:HB3	1:A:41:GLU:O	2.16	0.45
1:A:387:LEU:O	1:A:387:LEU:HD12	2.17	0.45
1:A:314:ASN:OD1	1:A:360:ASP:O	2.35	0.44
1:A:398:TYR:CE2	1:A:402:ARG:HD2	2.53	0.44
1:A:203:VAL:HG12	1:A:205:ARG:HD2	2.00	0.44
1:A:434:LEU:HD21	1:A:451:LEU:HD11	2.00	0.44
1:A:182:ASP:C	1:A:182:ASP:OD1	2.56	0.44
1:A:129:ILE:O	1:A:130:PRO:C	2.56	0.44
1:A:297:ARG:HB3	1:A:297:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LYS:HZ3	1:A:91:LYS:CB	2.28	0.44
1:A:274:GLY:HA2	2:A:832:HOH:O	2.18	0.43
1:A:1:MET:O	1:A:2:VAL:C	2.56	0.43
1:A:162:LEU:HD21	1:A:295:TRP:CE3	2.53	0.43
1:A:15:HIS:CE1	1:A:244:ILE:HD12	2.48	0.43
1:A:44:ASP:OD1	1:A:46:ALA:HB3	2.18	0.43
1:A:463:LEU:O	1:A:467:LEU:HG	2.19	0.43
1:A:435:ARG:NH1	1:A:447:LEU:HB2	2.34	0.43
1:A:240:ASP:O	1:A:241:LYS:O	2.37	0.43
1:A:284:PHE:CD2	1:A:288:GLU:HG3	2.53	0.43
1:A:391:LEU:HD23	1:A:394:LEU:HD12	2.00	0.43
1:A:94:GLU:HG3	1:A:98:LYS:CD	2.48	0.43
1:A:281:ARG:NH1	1:A:288:GLU:OE1	2.50	0.43
1:A:417:ARG:HH11	1:A:417:ARG:HB3	1.84	0.43
1:A:372:LEU:CD2	1:A:454:LEU:HD21	2.49	0.42
1:A:152:ARG:HH11	1:A:152:ARG:HG3	1.83	0.42
1:A:237:ARG:O	1:A:244:ILE:HG23	2.19	0.42
1:A:109:PRO:HD2	1:A:110:GLU:OE1	2.19	0.42
1:A:77:THR:HG21	1:A:198:MET:CG	2.49	0.42
1:A:69:GLU:HG2	1:A:75:ALA:CB	2.50	0.42
1:A:137:ARG:O	1:A:142:GLU:HB2	2.19	0.42
1:A:425:VAL:HG13	1:A:429:GLN:HB2	2.00	0.42
1:A:127:ARG:HH12	1:A:152:ARG:HD3	1.84	0.42
1:A:262:LEU:HD23	1:A:317:TYR:HB3	2.01	0.42
1:A:4:THR:HB	1:A:25:ASN:ND2	2.24	0.42
1:A:294:THR:C	1:A:296:GLU:N	2.71	0.42
1:A:180:LYS:HG3	1:A:184:TYR:O	2.19	0.42
1:A:391:LEU:HD23	1:A:391:LEU:HA	1.93	0.42
1:A:150:VAL:HA	1:A:151:PRO:HD3	1.78	0.42
1:A:45:ARG:HH12	1:A:83:SER:HB2	1.84	0.42
1:A:31:ARG:HD2	1:A:31:ARG:O	2.19	0.42
1:A:101:TRP:C	1:A:149:LYS:HB3	2.40	0.42
1:A:284:PHE:CD2	1:A:288:GLU:CG	3.03	0.42
1:A:221:ARG:CB	1:A:221:ARG:NH1	2.82	0.42
1:A:256:TYR:O	1:A:261:PHE:HB2	2.19	0.42
1:A:38:VAL:O	1:A:70:GLY:HA2	2.20	0.42
1:A:13:ASP:HB3	2:A:613:HOH:O	2.20	0.42
1:A:398:TYR:CD2	1:A:402:ARG:HD2	2.54	0.42
1:A:104:ARG:HA	1:A:145:VAL:O	2.20	0.42
1:A:152:ARG:HH11	1:A:152:ARG:CG	2.33	0.41
1:A:207:GLU:HB2	1:A:233:MET:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:C	1:A:73:VAL:HG23	2.41	0.41
1:A:391:LEU:N	1:A:392:PRO:CD	2.83	0.41
1:A:454:LEU:HD23	1:A:454:LEU:N	2.35	0.41
1:A:284:PHE:HD2	1:A:288:GLU:CG	2.34	0.41
1:A:188:HIS:HD2	1:A:216:HIS:CE1	2.37	0.41
1:A:30:ARG:HB2	1:A:290:ILE:HD12	2.03	0.41
1:A:212:SER:HA	1:A:215:ILE:HD12	2.02	0.41
1:A:156:THR:OG1	1:A:170:ASN:ND2	2.52	0.41
1:A:92:TYR:HB3	1:A:223:PHE:HE1	1.79	0.41
1:A:47:ARG:HD2	1:A:47:ARG:HH11	1.73	0.41
1:A:104:ARG:HG2	1:A:144:HIS:CD2	2.55	0.41
1:A:108:THR:OG1	1:A:111:GLU:HB2	2.19	0.41
1:A:158:VAL:HG11	1:A:213:THR:HB	2.03	0.41
1:A:316:LYS:NZ	2:A:630:HOH:O	2.39	0.41
1:A:273:MET:CE	1:A:273:MET:HA	2.50	0.41
1:A:152:ARG:HA	1:A:152:ARG:HD2	1.75	0.41
1:A:274:GLY:O	1:A:275:PHE:HB2	2.20	0.41
1:A:95:GLU:HG2	1:A:99:ARG:NH2	2.34	0.41
1:A:398:TYR:N	1:A:399:PRO:CD	2.82	0.41
1:A:139:ARG:C	1:A:141:GLY:N	2.74	0.41
1:A:383:ALA:HA	1:A:442:LEU:HD22	2.02	0.41
1:A:442:LEU:HD12	1:A:442:LEU:HA	1.89	0.41
1:A:406:GLU:HG2	1:A:408:THR:CG2	2.48	0.41
1:A:1:MET:SD	1:A:34:GLY:HA2	2.61	0.41
1:A:72:ASP:OD1	1:A:73:VAL:HG23	2.21	0.41
1:A:105:ALA:HB1	1:A:107:GLU:OE1	2.21	0.41
1:A:420:ALA:HB1	1:A:425:VAL:O	2.20	0.41
1:A:262:LEU:CD1	1:A:362:LEU:HD11	2.51	0.40
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.56	0.40
1:A:282:GLU:O	1:A:313:MET:HE1	2.21	0.40
1:A:173:ILE:HA	1:A:174:PRO:HD3	1.88	0.40
1:A:15:HIS:HE1	1:A:244:ILE:CD1	2.31	0.40
1:A:426:LYS:HD2	1:A:428:GLY:H	1.86	0.40
1:A:152:ARG:N	1:A:153:PRO:HD2	2.37	0.40
1:A:417:ARG:CB	1:A:417:ARG:HH11	2.35	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	466/468 (100%)	394 (84%)	53 (11%)	19 (4%)	<b>3</b> <b>4</b>

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ALA
1	A	99	ARG
1	A	241	LYS
1	A	242	THR
1	A	248	LYS
1	A	249	SER
1	A	275	PHE
1	A	284	PHE
1	A	286	LEU
1	A	29	ALA
1	A	274	GLY
1	A	285	THR
1	A	446	GLY
1	A	117	LYS
1	A	244	ILE
1	A	290	ILE
1	A	78	GLY
1	A	291	GLN
1	A	234	PRO

### 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	393/393 (100%)	334 (85%)	59 (15%)	<b>3</b> <b>6</b>

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	9	SER
1	A	43	THR
1	A	49	VAL
1	A	50	PRO
1	A	54	GLU
1	A	60	LEU
1	A	66	SER
1	A	68	ASP
1	A	81	ARG
1	A	91	LYS
1	A	101	TRP
1	A	111	GLU
1	A	136	GLU
1	A	140	ARG
1	A	142	GLU
1	A	152	ARG
1	A	155	THR
1	A	163	ARG
1	A	179	LEU
1	A	181	SER
1	A	189	LEU
1	A	191	ASN
1	A	197	LEU
1	A	200	VAL
1	A	205	ARG
1	A	210	LEU
1	A	218	LEU
1	A	221	ARG
1	A	225	TRP
1	A	247	ARG
1	A	262	LEU
1	A	266	LEU
1	A	268	ASN
1	A	270	LEU
1	A	281	ARG
1	A	285	THR
1	A	299	SER

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Mol	Chain	Res	Type
1	A	304	VAL
1	A	309	LYS
1	A	310	LEU
1	A	311	ARG
1	A	313	MET
1	A	331	VAL
1	A	337	GLU
1	A	350	ARG
1	A	367	GLU
1	A	375	GLU
1	A	391	LEU
1	A	409	GLU
1	A	412	LEU
1	A	416	LEU
1	A	423	LYS
1	A	425	VAL
1	A	426	LYS
1	A	443	GLU
1	A	444	THR
1	A	464	GLU
1	A	467	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	32	ASN
1	A	82	GLN
1	A	170	ASN
1	A	171	GLN
1	A	188	HIS
1	A	191	ASN
1	A	196	HIS
1	A	216	HIS
1	A	232	HIS
1	A	291	GLN
1	A	314	ASN
1	A	404	GLN

### 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 will therefore be empty.

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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