



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:02 AM UTC

PDB ID : 5CPA / pdb_00005cpa
Title : REFINED CRYSTAL STRUCTURE OF CARBOXYPEPTIDASE A AT 1.54
ANGSTROMS RESOLUTION.
Authors : Lipscomb, W.N.
Deposited on : 1982-05-06
Resolution : 1.54 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

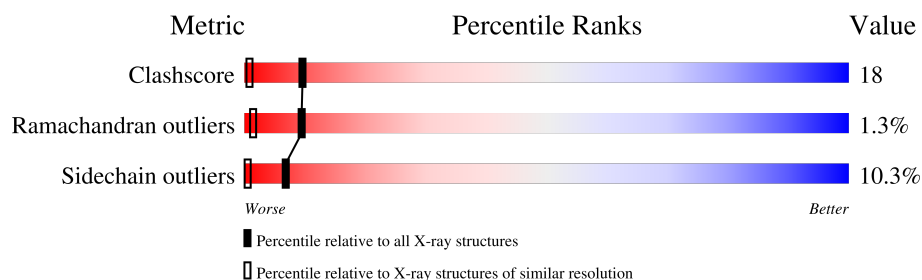
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	307	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2753 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 CARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2437	1561	406	465	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLN	GLU	conflict	UNP P00730
A	31	GLU	GLN	conflict	UNP P00730
A	89	ASN	ASP	conflict	UNP P00730
A	93	ASN	ASP	conflict	UNP P00730
A	114	ASN	ASP	conflict	UNP P00730
A	122	GLU	GLN	conflict	UNP P00730
A	185	ASN	ASP	conflict	UNP P00730
A	228	ALA	GLU	conflict	UNP P00730
A	305	VAL	LEU	conflict	UNP P00730

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

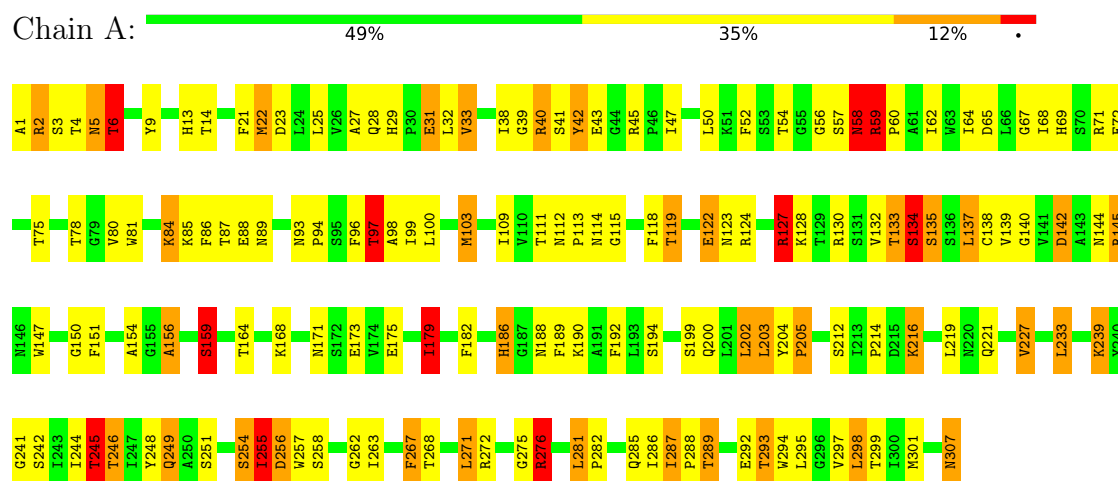
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	315	Total	O	0	0
			315	315		

3 Residue-property plots

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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.60Å 60.27Å 47.25Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.54	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.54)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2753	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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	1.77	29/2503 (1.2%)	2.28	105/3402 (3.1%)

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	5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	SER	CA-CB	8.16	1.66	1.53
1	A	263	ILE	N-CA	6.81	1.54	1.46
1	A	245	THR	N-CA	6.32	1.54	1.46
1	A	293	THR	CB-OG1	6.20	1.53	1.43
1	A	40	ARG	NE-CZ	6.04	1.39	1.33
1	A	299	THR	CA-CB	5.96	1.62	1.53
1	A	42	TYR	C-O	5.94	1.31	1.24
1	A	262	GLY	C-O	5.81	1.31	1.23
1	A	87	THR	C-O	5.81	1.31	1.24
1	A	299	THR	C-O	5.67	1.30	1.24
1	A	13	HIS	ND1-CE1	-5.63	1.26	1.32
1	A	214	PRO	C-O	5.49	1.31	1.24
1	A	29	HIS	CA-CB	5.49	1.59	1.53
1	A	124	ARG	NE-CZ	5.48	1.39	1.33
1	A	289	THR	N-CA	5.46	1.52	1.46
1	A	142	ASP	CA-C	5.41	1.59	1.52
1	A	256	ASP	N-CA	5.36	1.52	1.46
1	A	119	THR	CA-CB	5.31	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	THR	CA-CB	5.27	1.61	1.53
1	A	186	HIS	N-CA	5.25	1.52	1.46
1	A	98	ALA	N-CA	5.25	1.53	1.46
1	A	297	VAL	C-O	-5.22	1.18	1.24
1	A	23	ASP	N-CA	5.22	1.52	1.46
1	A	80	VAL	N-CA	5.21	1.52	1.46
1	A	75	THR	CA-C	5.20	1.59	1.52
1	A	147	TRP	NE1-CE2	5.15	1.43	1.37
1	A	258	SER	CB-OG	-5.14	1.31	1.42
1	A	64	ILE	CA-C	5.09	1.58	1.52
1	A	286	ILE	CA-CB	5.09	1.59	1.54

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ILE	CA-CB-CG2	15.10	136.18	110.50
1	A	59	ARG	CD-NE-CZ	13.52	143.33	124.40
1	A	140	GLY	CA-C-O	10.08	130.45	122.29
1	A	245	THR	OG1-CB-CG2	10.07	129.44	109.30
1	A	245	THR	N-CA-CB	-10.04	94.84	110.30
1	A	40	ARG	NE-CZ-NH2	-9.75	110.43	119.20
1	A	39	GLY	O-C-N	9.68	133.49	123.81
1	A	307	ASN	CA-CB-CG	9.02	121.62	112.60
1	A	254	SER	CA-CB-OG	-8.89	93.31	111.10
1	A	5	ASN	CA-CB-CG	-8.73	103.87	112.60
1	A	23	ASP	CA-C-O	-8.59	111.45	120.55
1	A	6	THR	N-CA-CB	-8.19	98.49	110.53
1	A	249	GLN	CB-CG-CD	8.17	126.49	112.60
1	A	97	THR	CA-C-O	-8.14	110.61	119.97
1	A	216	LYS	CA-CB-CG	-8.07	97.97	114.10
1	A	56	GLY	CA-C-N	7.88	136.59	121.54
1	A	56	GLY	C-N-CA	7.88	136.59	121.54
1	A	13	HIS	CA-CB-CG	-7.64	106.16	113.80
1	A	33	VAL	CB-CA-C	7.61	121.90	110.63
1	A	256	ASP	CA-C-O	7.50	128.37	120.42
1	A	145	ARG	CD-NE-CZ	-7.47	113.94	124.40
1	A	64	ILE	O-C-N	7.36	130.61	123.03
1	A	200	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	A	221	GLN	N-CA-CB	7.08	120.63	110.16
1	A	27	ALA	CA-C-N	7.06	131.04	120.31
1	A	27	ALA	C-N-CA	7.06	131.04	120.31
1	A	221	GLN	OE1-CD-NE2	-7.03	115.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ARG	CD-NE-CZ	-6.99	114.61	124.40
1	A	103	MET	CA-C-O	-6.96	113.30	121.44
1	A	144	ASN	CA-CB-CG	-6.93	105.67	112.60
1	A	59	ARG	N-CA-C	-6.88	100.28	109.84
1	A	156	ALA	CA-C-O	-6.78	113.64	121.10
1	A	227	VAL	N-CA-CB	-6.74	101.38	110.54
1	A	58	ASN	CA-CB-CG	6.73	119.33	112.60
1	A	68	ILE	O-C-N	6.71	128.64	121.87
1	A	40	ARG	NH1-CZ-NH2	6.68	127.99	119.30
1	A	159	SER	N-CA-CB	-6.58	101.61	110.23
1	A	22	MET	O-C-N	6.58	128.85	122.07
1	A	298	LEU	O-C-N	6.39	128.74	122.09
1	A	249	GLN	N-CA-CB	6.36	119.07	109.34
1	A	244	ILE	CA-C-O	-6.30	114.40	120.95
1	A	130	ARG	NE-CZ-NH2	-6.27	113.56	119.20
1	A	258	SER	O-C-N	6.22	129.92	122.27
1	A	173	GLU	CA-C-O	6.14	127.69	120.69
1	A	257	TRP	O-C-N	6.13	128.41	122.03
1	A	122	GLU	CA-CB-CG	6.12	126.34	114.10
1	A	47	ILE	O-C-N	6.11	130.24	123.10
1	A	59	ARG	O-C-N	6.10	128.26	121.43
1	A	119	THR	CA-C-O	-6.05	113.02	119.97
1	A	301	MET	O-C-N	5.93	128.40	122.12
1	A	71	ARG	NE-CZ-NH1	-5.87	115.63	121.50
1	A	14	THR	CA-CB-OG1	-5.86	100.82	109.60
1	A	194	SER	CA-C-O	-5.80	114.56	120.71
1	A	25	LEU	CA-C-O	-5.79	114.28	120.42
1	A	94	PRO	CA-C-N	5.75	128.26	120.44
1	A	94	PRO	C-N-CA	5.75	128.26	120.44
1	A	33	VAL	CA-C-O	5.73	126.41	120.39
1	A	289	THR	O-C-N	5.73	127.97	122.07
1	A	271	LEU	N-CA-CB	-5.71	102.22	110.45
1	A	118	PHE	CA-C-N	5.69	128.96	120.31
1	A	118	PHE	C-N-CA	5.69	128.96	120.31
1	A	78	THR	CA-CB-OG1	-5.65	101.12	109.60
1	A	233	LEU	O-C-N	5.62	129.89	122.30
1	A	119	THR	N-CA-CB	5.58	118.93	110.28
1	A	109	ILE	CB-CG1-CD1	-5.56	102.13	113.80
1	A	25	LEU	O-C-N	5.56	128.48	122.15
1	A	164	THR	CA-C-O	-5.55	113.84	120.55
1	A	205	PRO	CA-C-N	5.54	131.68	121.70
1	A	205	PRO	C-N-CA	5.54	131.68	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ARG	CA-CB-CG	-5.52	103.06	114.10
1	A	58	ASN	CB-CA-C	5.51	119.97	112.09
1	A	84	LYS	CA-C-O	5.47	126.22	120.42
1	A	179	ILE	N-CA-CB	5.47	117.57	110.57
1	A	212	SER	CA-CB-OG	-5.47	100.17	111.10
1	A	295	LEU	O-C-N	5.46	128.99	122.27
1	A	254	SER	CB-CA-C	-5.46	101.78	110.84
1	A	292	GLU	CB-CG-CD	5.43	121.83	112.60
1	A	62	ILE	CA-C-O	-5.39	114.77	120.48
1	A	186	HIS	CA-C-O	5.39	126.25	120.70
1	A	97	THR	CB-CA-C	5.36	120.96	110.67
1	A	21	PHE	CZ-CE2-CD2	-5.35	110.37	120.00
1	A	221	GLN	N-CA-C	-5.34	105.54	111.36
1	A	267	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	138	CYS	CA-C-O	-5.32	114.80	120.92
1	A	189	PHE	CA-CB-CG	-5.31	108.49	113.80
1	A	275	GLY	CA-C-O	-5.30	111.34	120.57
1	A	43	GLU	CA-C-N	5.28	129.54	121.51
1	A	43	GLU	C-N-CA	5.28	129.54	121.51
1	A	276	ARG	O-C-N	5.26	127.57	122.09
1	A	268	THR	CA-C-O	-5.24	115.05	120.70
1	A	119	THR	OG1-CB-CG2	5.12	119.55	109.30
1	A	151	PHE	CA-C-O	-5.12	115.38	120.96
1	A	292	GLU	CA-C-N	5.12	127.14	120.28
1	A	292	GLU	C-N-CA	5.12	127.14	120.28
1	A	1	ALA	CB-CA-C	5.12	118.17	110.50
1	A	298	LEU	CA-C-N	-5.11	113.80	120.44
1	A	298	LEU	C-N-CA	-5.11	113.80	120.44
1	A	171	ASN	OD1-CG-ND2	-5.09	117.50	122.60
1	A	299	THR	CA-CB-OG1	-5.09	101.97	109.60
1	A	122	GLU	CB-CG-CD	5.07	121.22	112.60
1	A	135	SER	N-CA-C	-5.05	104.03	111.81
1	A	97	THR	N-CA-CB	5.05	118.11	110.28
1	A	99	ILE	CA-C-O	-5.04	115.90	121.29
1	A	97	THR	CA-C-N	-5.01	112.69	120.31
1	A	97	THR	C-N-CA	-5.01	112.69	120.31

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2	ARG	Sidechain
1	A	276	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	59	ARG	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	2437	0	2352	85	5
2	A	1	0	0	0	0
3	A	315	0	0	24	169
All	All	2753	0	2352	85	169

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 18.

All (85) 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:4:THR:H	1:A:28:GLN:HE22	1.11	0.92
1:A:249:GLN:O	3:A:582(B):HOH:O	1.89	0.88
1:A:137:LEU:HD22	1:A:137:LEU:H	1.39	0.87
1:A:31:GLU:HB2	3:A:453(A):HOH:O	1.74	0.87
1:A:248:TYR:CD1	3:A:580(B):HOH:O	2.28	0.86
1:A:248:TYR:CE1	3:A:580(B):HOH:O	2.28	0.85
1:A:242:SER:O	1:A:246:THR:HG23	1.77	0.85
1:A:2:ARG:HD3	3:A:410(H):HOH:O	1.78	0.82
1:A:289:THR:O	1:A:293:THR:HG22	1.81	0.79
1:A:175:GLU:O	1:A:179:ILE:HD13	1.82	0.79
1:A:154:ALA:HA	3:A:542(B):HOH:O	1.84	0.77
1:A:168:LYS:HG2	3:A:380(A):HOH:O	1.83	0.77
1:A:22:MET:HE2	1:A:50:LEU:HG	1.68	0.76
1:A:133:THR:O	1:A:134:SER:HB3	1.86	0.75
1:A:159:SER:HB3	3:A:520(B):HOH:O	1.87	0.74
1:A:134:SER:OG	1:A:135:SER:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:O	3:A:463(A):HOH:O	2.06	0.73
1:A:5:ASN:HD21	1:A:84:LYS:HZ1	1.37	0.71
1:A:242:SER:OG	1:A:245:THR:HB	1.92	0.70
1:A:159:SER:CB	3:A:520(B):HOH:O	2.38	0.70
1:A:256:ASP:OD2	3:A:309(A):HOH:O	2.11	0.68
1:A:67:GLY:O	3:A:577(A):HOH:O	2.14	0.66
1:A:81:TRP:CD1	1:A:287:ILE:HD12	2.31	0.65
1:A:86:PHE:HE1	1:A:294:TRP:CZ3	2.16	0.64
1:A:4:THR:N	1:A:28:GLN:HE22	1.91	0.64
1:A:22:MET:CE	3:A:532(A):HOH:O	2.48	0.61
1:A:186:HIS:HD2	1:A:188:ASN:H	1.48	0.61
1:A:93:ASN:O	1:A:97:THR:HG23	2.03	0.59
1:A:137:LEU:H	1:A:137:LEU:CD2	2.16	0.57
1:A:93:ASN:O	1:A:97:THR:CG2	2.54	0.56
1:A:5:ASN:ND2	1:A:84:LYS:NZ	2.54	0.56
1:A:65:ASP:OD2	3:A:564(A):HOH:O	2.18	0.56
1:A:5:ASN:HD21	1:A:84:LYS:NZ	2.03	0.56
1:A:54:THR:OG1	1:A:59:ARG:NH2	2.39	0.56
1:A:119:THR:HA	1:A:123:ASN:O	2.06	0.54
1:A:42:TYR:OH	1:A:132:VAL:HG22	2.07	0.54
1:A:45:ARG:HH11	1:A:114:ASN:ND2	2.06	0.54
1:A:248:TYR:CG	3:A:580(B):HOH:O	2.58	0.53
1:A:88:GLU:OE2	3:A:448(A):HOH:O	2.18	0.53
1:A:93:ASN:ND2	1:A:96:PHE:H	2.07	0.52
1:A:6:THR:HG21	3:A:490(A):HOH:O	2.08	0.52
1:A:241:GLY:HA3	1:A:246:THR:HG21	1.91	0.52
1:A:241:GLY:HA3	1:A:246:THR:CG2	2.41	0.51
1:A:89:ASN:ND2	3:A:445(A):HOH:O	2.45	0.50
1:A:202:LEU:HD12	1:A:227:VAL:HG23	1.93	0.50
1:A:6:THR:CG2	3:A:490(A):HOH:O	2.60	0.50
1:A:204:TYR:HB2	1:A:205:PRO:CD	2.43	0.49
1:A:272:ARG:HH11	1:A:285:GLN:HE21	1.61	0.49
1:A:32:LEU:HD11	1:A:100:LEU:HD13	1.95	0.49
1:A:219:LEU:HG	1:A:267:PHE:CZ	2.49	0.48
1:A:203:LEU:HD11	1:A:246:THR:OG1	2.14	0.48
1:A:22:MET:HE2	1:A:50:LEU:CG	2.41	0.47
1:A:127:ARG:HG3	1:A:128:LYS:N	2.29	0.47
1:A:281:LEU:HA	1:A:282:PRO:HD3	1.74	0.46
1:A:112:ASN:ND2	1:A:115:GLY:H	2.13	0.46
1:A:289:THR:O	1:A:293:THR:CG2	2.60	0.46
1:A:156:ALA:CA	3:A:556(B):HOH:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASN:HD21	1:A:188:ASN:HB2	1.81	0.46
1:A:287:ILE:N	1:A:288:PRO:HD2	2.30	0.46
1:A:9:TYR:HB3	1:A:287:ILE:HD11	1.98	0.45
1:A:127:ARG:NH1	3:A:581(B):HOH:O	2.49	0.45
1:A:132:VAL:HG23	1:A:133:THR:OG1	2.16	0.45
1:A:203:LEU:HA	1:A:241:GLY:O	2.16	0.45
1:A:134:SER:HG	1:A:135:SER:H	1.60	0.44
1:A:41:SER:OG	1:A:45:ARG:HB2	2.18	0.44
1:A:192:PHE:HD1	1:A:255:ILE:HD13	1.83	0.44
1:A:69:HIS:HB2	1:A:72:GLU:CD	2.43	0.43
1:A:142:ASP:OD2	1:A:145:ARG:HD2	2.19	0.43
1:A:60:PRO:HB2	1:A:103:MET:HE3	2.01	0.43
1:A:111:THR:C	1:A:113:PRO:HD3	2.44	0.43
1:A:186:HIS:HD2	1:A:188:ASN:N	2.14	0.43
1:A:32:LEU:O	1:A:52:PHE:HA	2.17	0.43
1:A:248:TYR:CZ	3:A:580(B):HOH:O	2.62	0.43
1:A:245:THR:HG21	3:A:369(A):HOH:O	2.18	0.42
1:A:9:TYR:CB	1:A:287:ILE:HD11	2.50	0.42
1:A:132:VAL:O	1:A:133:THR:CB	2.68	0.42
1:A:233:LEU:HA	1:A:233:LEU:HD23	1.74	0.42
1:A:85:LYS:HE3	1:A:89:ASN:ND2	2.35	0.41
1:A:137:LEU:HD22	1:A:137:LEU:N	2.22	0.41
1:A:45:ARG:HH11	1:A:114:ASN:HD22	1.68	0.41
1:A:239:LYS:HZ2	1:A:239:LYS:HB2	1.85	0.41
1:A:45:ARG:HD2	1:A:114:ASN:HD22	1.86	0.41
1:A:4:THR:H	1:A:28:GLN:NE2	1.95	0.40
1:A:150:GLY:O	1:A:251:SER:HB2	2.20	0.40
1:A:22:MET:HE3	3:A:532(A):HOH:O	2.17	0.40

All (169) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:310(A):HOH:O	3:A:310(C):HOH:O[2_544]	0.00	2.20
3:A:311(A):HOH:O	3:A:311(B):HOH:O[2_545]	0.00	2.20
3:A:315(A):HOH:O	3:A:315(C):HOH:O[2_544]	0.00	2.20
3:A:317(A):HOH:O	3:A:317(C):HOH:O[2_544]	0.00	2.20
3:A:319(A):HOH:O	3:A:319(B):HOH:O[2_545]	0.00	2.20
3:A:323(A):HOH:O	3:A:323(C):HOH:O[2_544]	0.00	2.20
3:A:324(A):HOH:O	3:A:324(B):HOH:O[2_545]	0.00	2.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:325(A):HOH:O	3:A:325(D):HOH:O[2_555]	0.00	2.20
3:A:326(A):HOH:O	3:A:326(B):HOH:O[2_545]	0.00	2.20
3:A:328(A):HOH:O	3:A:328(B):HOH:O[2_545]	0.00	2.20
3:A:329(A):HOH:O	3:A:329(C):HOH:O[2_544]	0.00	2.20
3:A:330(A):HOH:O	3:A:330(C):HOH:O[2_544]	0.00	2.20
3:A:332(A):HOH:O	3:A:332(C):HOH:O[2_544]	0.00	2.20
3:A:335(A):HOH:O	3:A:335(B):HOH:O[2_545]	0.00	2.20
3:A:340(A):HOH:O	3:A:340(B):HOH:O[2_545]	0.00	2.20
3:A:341(A):HOH:O	3:A:341(B):HOH:O[2_545]	0.00	2.20
3:A:342(A):HOH:O	3:A:342(C):HOH:O[2_544]	0.00	2.20
3:A:344(A):HOH:O	3:A:344(C):HOH:O[2_544]	0.00	2.20
3:A:352(A):HOH:O	3:A:352(C):HOH:O[2_544]	0.00	2.20
3:A:354(A):HOH:O	3:A:354(B):HOH:O[2_545]	0.00	2.20
3:A:357(A):HOH:O	3:A:357(B):HOH:O[2_545]	0.00	2.20
3:A:359(A):HOH:O	3:A:359(B):HOH:O[2_545]	0.00	2.20
3:A:362(A):HOH:O	3:A:362(B):HOH:O[2_545]	0.00	2.20
3:A:363(A):HOH:O	3:A:363(B):HOH:O[2_545]	0.00	2.20
3:A:365(A):HOH:O	3:A:365(B):HOH:O[2_545]	0.00	2.20
3:A:366(E):HOH:O	3:A:366(I):HOH:O[2_544]	0.00	2.20
3:A:367(A):HOH:O	3:A:367(D):HOH:O[2_555]	0.00	2.20
3:A:368(E):HOH:O	3:A:368(F):HOH:O[2_545]	0.00	2.20
3:A:368(E):HOH:O	3:A:368(I):HOH:O[2_544]	0.00	2.20
3:A:368(F):HOH:O	3:A:368(I):HOH:O[1_556]	0.00	2.20
3:A:371(A):HOH:O	3:A:371(B):HOH:O[2_545]	0.00	2.20
3:A:372(A):HOH:O	3:A:372(D):HOH:O[2_555]	0.00	2.20
3:A:374(E):HOH:O	3:A:374(F):HOH:O[2_545]	0.00	2.20
3:A:375(A):HOH:O	3:A:375(B):HOH:O[2_545]	0.00	2.20
3:A:386(A):HOH:O	3:A:386(D):HOH:O[2_555]	0.00	2.20
3:A:388(A):HOH:O	3:A:388(B):HOH:O[2_545]	0.00	2.20
3:A:389(A):HOH:O	3:A:389(D):HOH:O[2_555]	0.00	2.20
3:A:390(A):HOH:O	3:A:390(D):HOH:O[2_555]	0.00	2.20
3:A:392(A):HOH:O	3:A:392(B):HOH:O[2_545]	0.00	2.20
3:A:395(A):HOH:O	3:A:395(G):HOH:O[1_554]	0.00	2.20
3:A:397(E):HOH:O	3:A:397(H):HOH:O[2_555]	0.00	2.20
3:A:402(A):HOH:O	3:A:402(D):HOH:O[2_555]	0.00	2.20
3:A:408(E):HOH:O	3:A:408(F):HOH:O[2_545]	0.00	2.20
3:A:409(E):HOH:O	3:A:409(H):HOH:O[2_555]	0.00	2.20
3:A:410(E):HOH:O	3:A:410(H):HOH:O[2_555]	0.00	2.20
3:A:412(E):HOH:O	3:A:412(F):HOH:O[2_545]	0.00	2.20
3:A:413(E):HOH:O	3:A:413(H):HOH:O[2_555]	0.00	2.20
3:A:429(E):HOH:O	3:A:429(H):HOH:O[2_555]	0.00	2.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:429(E):HOH:O	3:A:429(J):HOH:O[2_554]	0.00	2.20
3:A:429(H):HOH:O	3:A:429(J):HOH:O[1_556]	0.00	2.20
3:A:446(E):HOH:O	3:A:446(H):HOH:O[2_555]	0.00	2.20
3:A:514(A):HOH:O	3:A:514(L):HOH:O[1_556]	0.00	2.20
3:A:515(A):HOH:O	3:A:515(L):HOH:O[1_556]	0.00	2.20
3:A:525(A):HOH:O	3:A:525(B):HOH:O[2_545]	0.00	2.20
3:A:533(A):HOH:O	3:A:533(B):HOH:O[2_545]	0.00	2.20
3:A:553(A):HOH:O	3:A:553(B):HOH:O[2_545]	0.00	2.20
3:A:565(A):HOH:O	3:A:565(B):HOH:O[2_545]	0.00	2.20
3:A:572(A):HOH:O	3:A:572(D):HOH:O[2_555]	0.00	2.20
3:A:576(A):HOH:O	3:A:576(L):HOH:O[1_556]	0.00	2.20
3:A:584(A):HOH:O	3:A:584(B):HOH:O[2_545]	0.00	2.20
3:A:366(A):HOH:O	3:A:366(E):HOH:O[1_455]	0.01	2.19
3:A:366(A):HOH:O	3:A:366(I):HOH:O[2_444]	0.01	2.19
3:A:368(A):HOH:O	3:A:368(E):HOH:O[1_455]	0.01	2.19
3:A:368(A):HOH:O	3:A:368(F):HOH:O[2_445]	0.01	2.19
3:A:368(A):HOH:O	3:A:368(I):HOH:O[2_444]	0.01	2.19
3:A:374(A):HOH:O	3:A:374(E):HOH:O[1_455]	0.01	2.19
3:A:374(A):HOH:O	3:A:374(F):HOH:O[2_445]	0.01	2.19
3:A:381(A):HOH:O	3:A:381(E):HOH:O[1_455]	0.01	2.19
3:A:396(A):HOH:O	3:A:396(I):HOH:O[2_444]	0.01	2.19
3:A:397(A):HOH:O	3:A:397(E):HOH:O[1_455]	0.01	2.19
3:A:397(A):HOH:O	3:A:397(H):HOH:O[2_455]	0.01	2.19
3:A:399(A):HOH:O	3:A:399(I):HOH:O[2_444]	0.01	2.19
3:A:407(A):HOH:O	3:A:407(I):HOH:O[2_444]	0.01	2.19
3:A:408(A):HOH:O	3:A:408(E):HOH:O[1_455]	0.01	2.19
3:A:408(A):HOH:O	3:A:408(F):HOH:O[2_445]	0.01	2.19
3:A:409(A):HOH:O	3:A:409(E):HOH:O[1_455]	0.01	2.19
3:A:409(A):HOH:O	3:A:409(H):HOH:O[2_455]	0.01	2.19
3:A:410(A):HOH:O	3:A:410(E):HOH:O[1_455]	0.01	2.19
3:A:410(A):HOH:O	3:A:410(H):HOH:O[2_455]	0.01	2.19
3:A:411(A):HOH:O	3:A:411(I):HOH:O[2_444]	0.01	2.19
3:A:412(A):HOH:O	3:A:412(E):HOH:O[1_455]	0.01	2.19
3:A:412(A):HOH:O	3:A:412(F):HOH:O[2_445]	0.01	2.19
3:A:413(A):HOH:O	3:A:413(E):HOH:O[1_455]	0.01	2.19
3:A:413(A):HOH:O	3:A:413(H):HOH:O[2_455]	0.01	2.19
3:A:420(A):HOH:O	3:A:420(I):HOH:O[2_444]	0.01	2.19
3:A:421(A):HOH:O	3:A:421(I):HOH:O[2_444]	0.01	2.19
3:A:429(A):HOH:O	3:A:429(E):HOH:O[1_455]	0.01	2.19
3:A:429(A):HOH:O	3:A:429(H):HOH:O[2_455]	0.01	2.19
3:A:429(A):HOH:O	3:A:429(J):HOH:O[2_454]	0.01	2.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:430(A):HOH:O	3:A:430(J):HOH:O[2_454]	0.01	2.19
3:A:433(A):HOH:O	3:A:433(F):HOH:O[2_445]	0.01	2.19
3:A:434(A):HOH:O	3:A:434(I):HOH:O[2_444]	0.01	2.19
3:A:438(A):HOH:O	3:A:438(I):HOH:O[2_444]	0.01	2.19
3:A:442(A):HOH:O	3:A:442(K):HOH:O[1_655]	0.01	2.19
3:A:444(A):HOH:O	3:A:444(F):HOH:O[2_445]	0.01	2.19
3:A:445(A):HOH:O	3:A:445(E):HOH:O[1_455]	0.01	2.19
3:A:446(A):HOH:O	3:A:446(E):HOH:O[1_455]	0.01	2.19
3:A:446(A):HOH:O	3:A:446(H):HOH:O[2_455]	0.01	2.19
3:A:447(A):HOH:O	3:A:447(I):HOH:O[2_444]	0.01	2.19
3:A:448(A):HOH:O	3:A:448(E):HOH:O[1_455]	0.01	2.19
3:A:451(A):HOH:O	3:A:451(J):HOH:O[2_454]	0.01	2.19
3:A:452(A):HOH:O	3:A:452(I):HOH:O[2_444]	0.01	2.19
3:A:453(A):HOH:O	3:A:453(I):HOH:O[2_444]	0.01	2.19
3:A:454(A):HOH:O	3:A:454(J):HOH:O[2_454]	0.01	2.19
3:A:455(A):HOH:O	3:A:455(F):HOH:O[2_445]	0.01	2.19
3:A:456(A):HOH:O	3:A:456(I):HOH:O[2_444]	0.01	2.19
3:A:457(A):HOH:O	3:A:457(E):HOH:O[1_455]	0.01	2.19
3:A:460(A):HOH:O	3:A:460(E):HOH:O[1_455]	0.01	2.19
3:A:463(A):HOH:O	3:A:463(I):HOH:O[2_444]	0.01	2.19
3:A:472(A):HOH:O	3:A:472(I):HOH:O[2_444]	0.01	2.19
3:A:475(A):HOH:O	3:A:475(H):HOH:O[2_455]	0.01	2.19
3:A:478(A):HOH:O	3:A:478(I):HOH:O[2_444]	0.01	2.19
3:A:490(A):HOH:O	3:A:490(F):HOH:O[2_445]	0.01	2.19
3:A:363(A):HOH:O	3:A:365(B):HOH:O[2_545]	0.79	1.41
3:A:363(B):HOH:O	3:A:365(A):HOH:O[2_555]	0.79	1.41
3:A:463(I):HOH:O	3:A:472(A):HOH:O[2_454]	0.82	1.38
3:A:463(A):HOH:O	3:A:472(I):HOH:O[2_444]	0.83	1.37
3:A:367(A):HOH:O	3:A:533(A):HOH:O[2_555]	0.96	1.24
3:A:367(D):HOH:O	3:A:533(B):HOH:O[2_545]	0.96	1.24
3:A:354(A):HOH:O	3:A:357(B):HOH:O[2_545]	0.99	1.21
3:A:354(B):HOH:O	3:A:357(A):HOH:O[2_555]	0.99	1.21
3:A:490(A):HOH:O	3:A:490(B):HOH:O[2_545]	1.00	1.20
3:A:490(B):HOH:O	3:A:490(F):HOH:O[1_655]	1.00	1.20
3:A:518(A):HOH:O	3:A:518(B):HOH:O[2_545]	1.00	1.20
3:A:520(A):HOH:O	3:A:520(B):HOH:O[2_545]	1.00	1.20
3:A:521(A):HOH:O	3:A:521(B):HOH:O[2_545]	1.00	1.20
3:A:523(A):HOH:O	3:A:523(B):HOH:O[2_545]	1.00	1.20
3:A:531(A):HOH:O	3:A:531(C):HOH:O[2_544]	1.00	1.20
3:A:535(A):HOH:O	3:A:535(B):HOH:O[2_545]	1.00	1.20
3:A:540(A):HOH:O	3:A:540(B):HOH:O[2_545]	1.00	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:542(A):HOH:O	3:A:542(B):HOH:O[2_545]	1.00	1.20
3:A:554(A):HOH:O	3:A:554(C):HOH:O[2_544]	1.00	1.20
3:A:556(A):HOH:O	3:A:556(B):HOH:O[2_545]	1.00	1.20
3:A:558(A):HOH:O	3:A:558(B):HOH:O[2_545]	1.00	1.20
3:A:559(A):HOH:O	3:A:559(C):HOH:O[2_544]	1.00	1.20
3:A:561(A):HOH:O	3:A:561(C):HOH:O[2_544]	1.00	1.20
3:A:569(A):HOH:O	3:A:569(B):HOH:O[2_545]	1.00	1.20
3:A:573(A):HOH:O	3:A:573(C):HOH:O[2_544]	1.00	1.20
3:A:575(A):HOH:O	3:A:575(B):HOH:O[2_545]	1.00	1.20
3:A:576(A):HOH:O	3:A:576(B):HOH:O[2_545]	1.00	1.20
3:A:576(B):HOH:O	3:A:576(L):HOH:O[2_554]	1.00	1.20
3:A:578(A):HOH:O	3:A:578(B):HOH:O[2_545]	1.00	1.20
3:A:579(A):HOH:O	3:A:579(C):HOH:O[2_544]	1.00	1.20
3:A:580(A):HOH:O	3:A:580(B):HOH:O[2_545]	1.00	1.20
3:A:581(A):HOH:O	3:A:581(B):HOH:O[2_545]	1.00	1.20
3:A:582(A):HOH:O	3:A:582(B):HOH:O[2_545]	1.00	1.20
3:A:585(A):HOH:O	3:A:585(C):HOH:O[2_544]	1.00	1.20
3:A:586(A):HOH:O	3:A:586(B):HOH:O[2_545]	1.00	1.20
3:A:434(I):HOH:O	3:A:438(A):HOH:O[2_454]	1.13	1.07
3:A:434(A):HOH:O	3:A:438(I):HOH:O[2_444]	1.15	1.05
3:A:410(A):HOH:O	3:A:413(E):HOH:O[1_455]	1.72	0.48
3:A:410(A):HOH:O	3:A:413(H):HOH:O[2_455]	1.72	0.48
3:A:410(E):HOH:O	3:A:413(A):HOH:O[1_655]	1.72	0.48
3:A:410(E):HOH:O	3:A:413(H):HOH:O[2_555]	1.72	0.48
3:A:410(H):HOH:O	3:A:413(A):HOH:O[2_445]	1.72	0.48
3:A:410(H):HOH:O	3:A:413(E):HOH:O[2_545]	1.72	0.48
3:A:573(C):HOH:O	3:A:579(A):HOH:O[2_554]	1.74	0.46
3:A:362(A):HOH:O	3:A:374(A):HOH:O[1_655]	1.84	0.36
3:A:362(B):HOH:O	3:A:374(A):HOH:O[2_455]	1.84	0.36
3:A:362(A):HOH:O	3:A:374(F):HOH:O[2_545]	1.85	0.35
3:A:362(B):HOH:O	3:A:374(E):HOH:O[2_555]	1.85	0.35
1:A:38:ILE:O	3:A:585(C):HOH:O[2_544]	1.91	0.29
3:A:478(I):HOH:O	3:A:488(A):HOH:O[2_454]	1.97	0.23
3:A:578(B):HOH:O	3:A:580(A):HOH:O[2_555]	1.98	0.22
1:A:182:PHE:CD2	3:A:554(C):HOH:O[2_544]	2.03	0.17
1:A:100:LEU:O	3:A:463(I):HOH:O[2_444]	2.07	0.13
3:A:535(B):HOH:O	3:A:542(A):HOH:O[2_555]	2.07	0.13
1:A:182:PHE:CE2	3:A:554(C):HOH:O[2_544]	2.11	0.09
1:A:88:GLU:OE2	3:A:448(E):HOH:O[1_455]	2.18	0.02

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	305/307 (99%)	284 (93%)	17 (6%)	4 (1%)	9 1

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	133	THR
1	A	134	SER
1	A	199	SER

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	263/263 (100%)	236 (90%)	27 (10%)	7 0

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	6	THR
1	A	31	GLU
1	A	33	VAL
1	A	58	ASN
1	A	97	THR
1	A	122	GLU

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Mol	Chain	Res	Type
1	A	134	SER
1	A	137	LEU
1	A	139	VAL
1	A	159	SER
1	A	179	ILE
1	A	190	LYS
1	A	202	LEU
1	A	203	LEU
1	A	216	LYS
1	A	239	LYS
1	A	245	THR
1	A	246	THR
1	A	254	SER
1	A	255	ILE
1	A	271	LEU
1	A	276	ARG
1	A	281	LEU
1	A	287	ILE
1	A	298	LEU
1	A	307	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	28	GLN
1	A	37	GLN
1	A	58	ASN
1	A	89	ASN
1	A	93	ASN
1	A	112	ASN
1	A	171	ASN
1	A	186	HIS
1	A	285	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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.