



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:07 AM UTC

PDB ID : 3CPA / pdb_00003cpa
Title : X-RAY CRYSTALLOGRAPHIC INVESTIGATION OF SUBSTRATE BINDING TO CARBOXYPEPTIDASE A AT SUBZERO TEMPERATURE
Authors : Lipscomb, W.N.
Deposited on : 1982-03-24
Resolution : 2.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

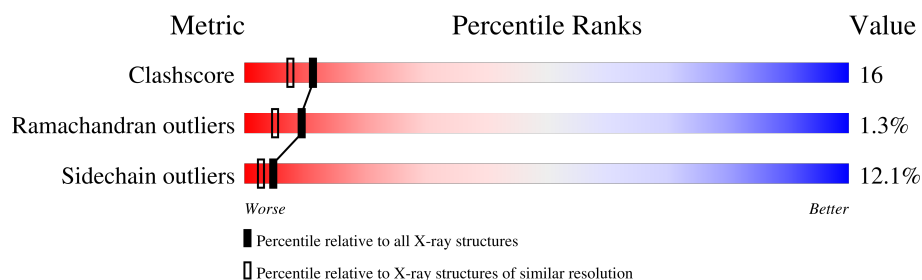
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2455 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.

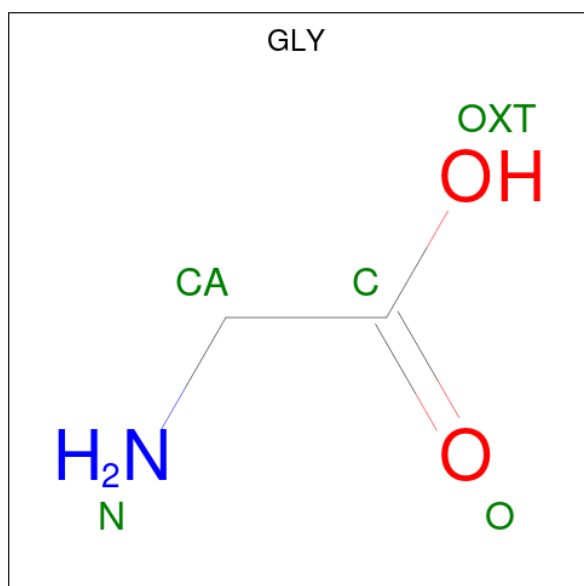
- Molecule 1 is a protein called CARBOXYPEPTIDASE A.

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:

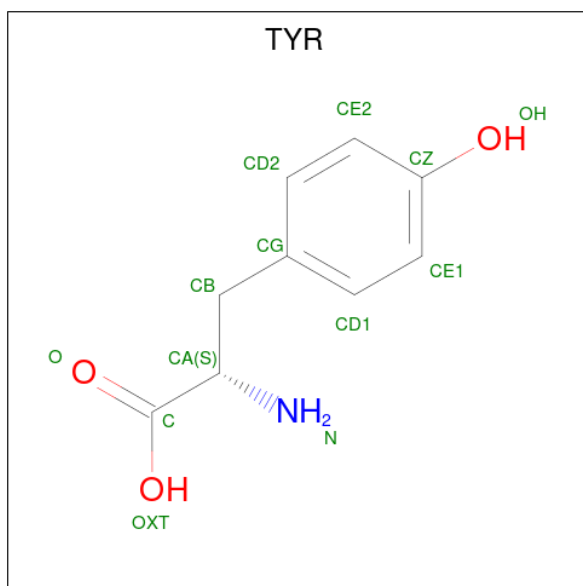
Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLN	GLU	conflict	UNP P00730
A	31	GLU	GLN	conflict	UNP P00730
A	89	ASN	ASP	conflict	UNP P00730
A	93	ASN	ASP	conflict	UNP P00730
A	114	ASN	ASP	conflict	UNP P00730
A	122	GLU	GLN	conflict	UNP P00730
A	185	ASN	ASP	conflict	UNP P00730
A	228	ALA	GLU	conflict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

- Molecule 2 is GLYCINE (CCD ID: GLY) (formula: C₂H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 3 is TYROSINE (CCD ID: TYR) (formula: $C_9H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

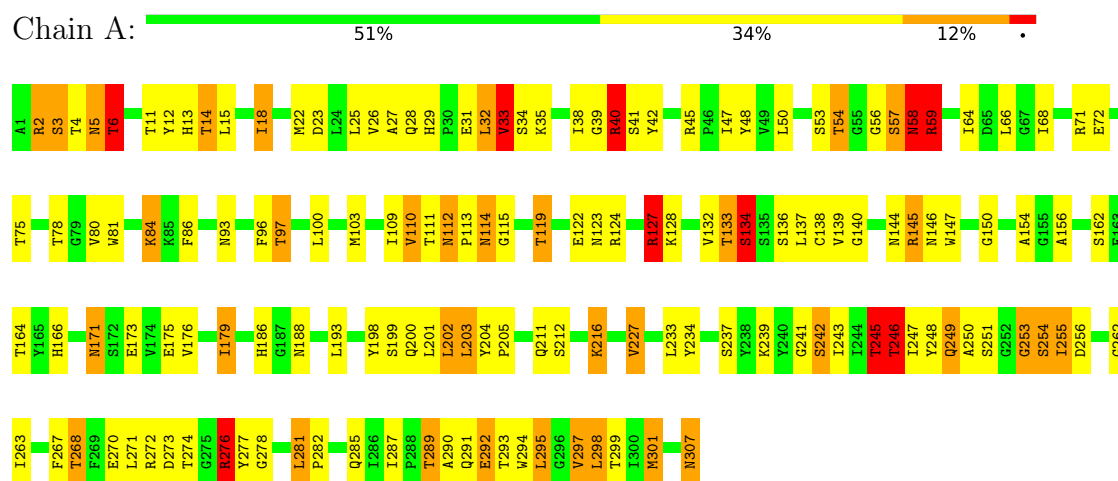
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

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) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	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	2455	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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	1.72	29/2503 (1.2%)	2.19	96/3402 (2.8%)

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	6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	ALA	N-CA	-12.06	1.31	1.46
1	A	246	THR	CA-C	-10.84	1.38	1.52
1	A	71	ARG	CD-NE	-7.46	1.35	1.46
1	A	242	SER	N-CA	6.82	1.54	1.45
1	A	124	ARG	NE-CZ	6.79	1.40	1.33
1	A	64	ILE	C-O	-6.32	1.17	1.24
1	A	59	ARG	CD-NE	-6.14	1.37	1.46
1	A	227	VAL	N-CA	6.13	1.53	1.46
1	A	262	GLY	C-O	5.83	1.31	1.24
1	A	29	HIS	CA-CB	5.77	1.60	1.53
1	A	290	ALA	C-O	5.76	1.30	1.24
1	A	147	TRP	NE1-CE2	5.72	1.43	1.37
1	A	3	SER	N-CA	5.63	1.52	1.45
1	A	6	THR	CA-CB	5.61	1.62	1.53
1	A	263	ILE	N-CA	5.60	1.52	1.46
1	A	53	SER	N-CA	5.59	1.52	1.45
1	A	289	THR	N-CA	5.48	1.52	1.46
1	A	299	THR	CA-CB	5.46	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	ARG	C-O	5.35	1.30	1.24
1	A	110	VAL	CA-C	5.34	1.57	1.53
1	A	212	SER	CA-CB	5.29	1.60	1.53
1	A	119	THR	CA-CB	5.28	1.61	1.53
1	A	68	ILE	N-CA	5.21	1.53	1.46
1	A	164	THR	CA-CB	5.16	1.60	1.53
1	A	78	THR	CA-CB	5.08	1.61	1.53
1	A	34	SER	CB-OG	-5.04	1.32	1.42
1	A	171	ASN	C-O	5.03	1.32	1.24
1	A	243	ILE	CA-CB	5.02	1.59	1.54
1	A	254	SER	CA-CB	5.01	1.61	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	CD-NE-CZ	13.18	142.85	124.40
1	A	71	ARG	CD-NE-CZ	12.44	141.81	124.40
1	A	255	ILE	CA-CB-CG2	12.12	131.10	110.50
1	A	307	ASN	CA-CB-CG	10.77	123.37	112.60
1	A	40	ARG	NE-CZ-NH2	-10.14	110.07	119.20
1	A	47	ILE	O-C-N	10.06	134.88	123.10
1	A	274	THR	N-CA-C	9.98	125.00	113.02
1	A	58	ASN	CA-CB-CG	9.57	122.17	112.60
1	A	97	THR	CA-CB-CG2	9.32	126.34	110.50
1	A	5	ASN	CA-CB-CG	-9.01	103.59	112.60
1	A	292	GLU	CB-CG-CD	8.75	127.48	112.60
1	A	56	GLY	CA-C-N	8.63	138.03	121.54
1	A	56	GLY	C-N-CA	8.63	138.03	121.54
1	A	39	GLY	O-C-N	8.49	132.30	123.81
1	A	249	GLN	OE1-CD-NE2	-8.38	114.22	122.60
1	A	40	ARG	NH1-CZ-NH2	8.27	130.05	119.30
1	A	140	GLY	CA-C-O	8.06	129.25	122.24
1	A	27	ALA	CA-C-N	7.71	132.02	120.31
1	A	27	ALA	C-N-CA	7.71	132.02	120.31
1	A	59	ARG	NE-CZ-NH1	7.71	129.21	121.50
1	A	245	THR	OG1-CB-CG2	7.66	124.61	109.30
1	A	59	ARG	CG-CD-NE	7.65	128.83	112.00
1	A	33	VAL	CB-CA-C	7.48	121.25	110.33
1	A	200	GLN	OE1-CD-NE2	-7.47	115.13	122.60
1	A	138	CYS	O-C-N	7.41	131.76	123.16
1	A	6	THR	N-CA-CB	-7.32	99.78	110.47
1	A	205	PRO	O-C-N	-7.30	114.09	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	SER	CA-CB-OG	-7.23	96.63	111.10
1	A	136	SER	CA-C-N	6.97	134.32	122.26
1	A	136	SER	C-N-CA	6.97	134.32	122.26
1	A	119	THR	N-CA-CB	6.96	120.93	110.22
1	A	23	ASP	CA-C-O	-6.71	113.78	120.82
1	A	256	ASP	CA-C-O	6.60	127.42	120.42
1	A	13	HIS	CA-CB-CG	-6.41	107.39	113.80
1	A	64	ILE	O-C-N	6.41	129.63	123.03
1	A	103	MET	CA-C-O	-6.38	113.97	121.44
1	A	14	THR	CA-CB-OG1	-6.35	100.07	109.60
1	A	245	THR	CA-CB-CG2	6.25	121.13	110.50
1	A	109	ILE	CA-C-N	-6.25	117.03	122.96
1	A	109	ILE	C-N-CA	-6.25	117.03	122.96
1	A	71	ARG	CG-CD-NE	6.24	125.72	112.00
1	A	138	CYS	CA-C-O	-6.23	113.75	120.92
1	A	233	LEU	O-C-N	6.13	130.58	122.30
1	A	97	THR	N-CA-CB	6.04	119.00	110.12
1	A	245	THR	N-CA-CB	-6.00	100.97	110.28
1	A	249	GLN	CB-CG-CD	5.98	122.77	112.60
1	A	173	GLU	CA-C-O	5.96	127.28	120.54
1	A	253	GLY	CA-C-N	5.88	130.54	121.19
1	A	253	GLY	C-N-CA	5.88	130.54	121.19
1	A	255	ILE	CA-CB-CG1	-5.87	100.43	110.40
1	A	227	VAL	N-CA-CB	-5.83	102.61	110.54
1	A	72	GLU	CG-CD-OE1	5.80	131.74	118.40
1	A	78	THR	CA-CB-OG1	-5.75	100.98	109.60
1	A	291	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	A	290	ALA	CB-CA-C	5.71	119.84	110.88
1	A	205	PRO	CA-C-N	5.70	131.96	121.70
1	A	205	PRO	C-N-CA	5.70	131.96	121.70
1	A	211	GLN	OE1-CD-NE2	5.70	128.29	122.60
1	A	162	SER	N-CA-CB	-5.69	101.60	109.97
1	A	278	GLY	O-C-N	5.69	129.69	122.58
1	A	119	THR	CA-C-O	-5.62	113.75	120.10
1	A	84	LYS	CA-C-O	5.60	126.35	120.42
1	A	292	GLU	CA-C-N	5.59	128.33	120.28
1	A	292	GLU	C-N-CA	5.59	128.33	120.28
1	A	25	LEU	O-C-N	5.58	128.04	122.12
1	A	119	THR	OG1-CB-CG2	5.57	120.44	109.30
1	A	32	LEU	O-C-N	5.54	128.90	122.25
1	A	12	TYR	O-C-N	5.45	129.16	123.06
1	A	54	THR	N-CA-CB	5.44	118.55	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	MET	O-C-N	5.42	127.87	122.12
1	A	295	LEU	N-CA-C	-5.39	105.56	111.82
1	A	297	VAL	O-C-N	5.37	127.18	121.91
1	A	11	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	144	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	234	TYR	O-C-N	5.32	128.03	122.23
1	A	68	ILE	O-C-N	5.30	127.23	121.87
1	A	193	LEU	O-C-N	5.30	129.42	123.27
1	A	227	VAL	CA-CB-CG1	5.29	119.38	110.40
1	A	97	THR	CA-C-O	-5.28	114.95	120.55
1	A	134	SER	CA-C-N	5.27	131.02	123.17
1	A	134	SER	C-N-CA	5.27	131.02	123.17
1	A	35	LYS	CG-CD-CE	5.27	123.42	111.30
1	A	216	LYS	CA-CB-CG	-5.27	103.57	114.10
1	A	254	SER	CA-C-N	5.23	127.85	120.42
1	A	254	SER	C-N-CA	5.23	127.85	120.42
1	A	110	VAL	CA-CB-CG2	5.17	119.19	110.40
1	A	249	GLN	CG-CD-NE2	5.13	124.10	116.40
1	A	103	MET	O-C-N	5.12	129.81	123.15
1	A	109	ILE	CB-CG1-CD1	-5.12	103.05	113.80
1	A	298	LEU	O-C-N	5.10	127.53	122.12
1	A	6	THR	CB-CA-C	5.10	118.16	109.24
1	A	171	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	A	56	GLY	CA-C-O	5.06	127.09	122.39
1	A	33	VAL	CA-C-O	5.04	125.70	120.36
1	A	114	ASN	O-C-N	5.04	127.53	122.09
1	A	80	VAL	N-CA-CB	-5.02	103.72	110.54

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	145	ARG	Sidechain
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	78	0
2	A	4	0	2	0	0
3	A	13	0	9	3	0
4	A	1	0	0	0	0
All	All	2455	0	2363	78	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 16.

All (78) 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:247:ILE:HG22	1:A:248:TYR:CD1	1.20	1.65
1:A:247:ILE:CG2	1:A:248:TYR:CE1	2.04	1.39
1:A:247:ILE:HG22	1:A:248:TYR:CE1	1.56	1.36
1:A:247:ILE:CG2	1:A:248:TYR:CD1	2.15	1.25
1:A:203:LEU:CD2	1:A:247:ILE:HD11	1.72	1.19
1:A:203:LEU:HD21	1:A:247:ILE:HD11	1.09	1.09
1:A:247:ILE:HG21	1:A:248:TYR:CE1	1.89	1.02
1:A:247:ILE:CG2	1:A:248:TYR:HE1	1.76	0.94
1:A:253:GLY:HA3	3:A:502:TYR:OH	1.67	0.93
1:A:272:ARG:HH21	1:A:292:GLU:CD	1.78	0.91
1:A:4:THR:H	1:A:28:GLN:HE22	1.17	0.88
1:A:272:ARG:NH2	1:A:292:GLU:OE2	2.05	0.88
1:A:247:ILE:HG22	1:A:248:TYR:HD1	1.04	0.85
1:A:154:ALA:O	1:A:249:GLN:OE1	1.99	0.80
1:A:145:ARG:HH11	1:A:145:ARG:HG3	1.49	0.76
1:A:203:LEU:HD21	1:A:247:ILE:CD1	2.05	0.70
1:A:253:GLY:HA3	3:A:502:TYR:CZ	2.27	0.69
1:A:93:ASN:ND2	1:A:96:PHE:H	1.90	0.69
1:A:186:HIS:HD2	1:A:188:ASN:H	1.41	0.67
1:A:242:SER:O	1:A:246:THR:HG23	1.97	0.64
1:A:272:ARG:NH2	1:A:292:GLU:CD	2.55	0.62
1:A:14:THR:O	1:A:18:ILE:HG22	2.01	0.59
1:A:246:THR:OG1	1:A:247:ILE:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:O	1:A:179:ILE:HD13	2.04	0.57
1:A:127:ARG:HG3	1:A:128:LYS:N	2.20	0.57
1:A:45:ARG:HH11	1:A:114:ASN:ND2	2.02	0.56
1:A:203:LEU:CD2	1:A:247:ILE:CD1	2.66	0.55
1:A:32:LEU:HD11	1:A:100:LEU:HD13	1.89	0.55
1:A:242:SER:OG	1:A:245:THR:HB	2.06	0.55
1:A:54:THR:OG1	1:A:59:ARG:NH2	2.39	0.55
1:A:58:ASN:HD21	1:A:188:ASN:HB2	1.70	0.55
1:A:45:ARG:HD2	1:A:114:ASN:HD22	1.74	0.53
1:A:247:ILE:CG2	1:A:248:TYR:HD1	1.91	0.53
1:A:5:ASN:HD21	1:A:84:LYS:NZ	2.08	0.52
1:A:119:THR:HA	1:A:123:ASN:O	2.09	0.51
1:A:18:ILE:HD12	1:A:110:VAL:HG23	1.91	0.51
1:A:201:LEU:HB2	1:A:270:GLU:HG3	1.93	0.51
1:A:150:GLY:O	1:A:251:SER:HB2	2.10	0.51
1:A:276:ARG:HD3	1:A:277:TYR:CE2	2.46	0.50
1:A:22:MET:HE2	1:A:50:LEU:HG	1.93	0.50
1:A:5:ASN:ND2	1:A:84:LYS:NZ	2.60	0.49
1:A:2:ARG:H	1:A:6:THR:HG21	1.77	0.49
1:A:198:TYR:HB2	1:A:273:ASP:N	2.27	0.49
1:A:281:LEU:HD13	1:A:285:GLN:HB2	1.95	0.49
1:A:22:MET:HE1	1:A:48:TYR:HB3	1.95	0.49
1:A:203:LEU:HD23	1:A:247:ILE:HD11	1.82	0.48
1:A:203:LEU:HA	1:A:241:GLY:O	2.12	0.48
1:A:202:LEU:HD12	1:A:227:VAL:HG23	1.95	0.48
1:A:112:ASN:ND2	1:A:115:GLY:H	2.11	0.48
1:A:4:THR:N	1:A:28:GLN:HE22	1.98	0.47
1:A:5:ASN:HD21	1:A:84:LYS:HZ1	1.61	0.47
1:A:26:VAL:HG22	1:A:33:VAL:HG22	1.95	0.47
1:A:186:HIS:HD2	1:A:188:ASN:N	2.10	0.46
1:A:133:THR:O	1:A:134:SER:HB3	2.16	0.45
1:A:146:ASN:HB3	1:A:176:VAL:HG21	1.98	0.45
1:A:281:LEU:HD22	1:A:282:PRO:HD2	1.99	0.45
1:A:281:LEU:HA	1:A:282:PRO:HD3	1.75	0.45
1:A:297:VAL:HG12	1:A:301:MET:HE3	1.98	0.45
1:A:42:TYR:OH	1:A:132:VAL:HG22	2.17	0.45
1:A:45:ARG:HH11	1:A:114:ASN:HD22	1.63	0.44
1:A:255:ILE:HG13	1:A:268:THR:OG1	2.17	0.44
1:A:22:MET:CE	1:A:50:LEU:HG	2.48	0.43
1:A:38:ILE:HD11	1:A:179:ILE:HD12	2.00	0.43
1:A:255:ILE:HD12	1:A:267:PHE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:THR:O	1:A:293:THR:HG22	2.19	0.42
1:A:204:TYR:O	1:A:242:SER:HA	2.19	0.42
1:A:86:PHE:HE1	1:A:294:TRP:CZ3	2.37	0.42
1:A:247:ILE:HG21	1:A:248:TYR:HE1	1.51	0.42
1:A:5:ASN:ND2	1:A:84:LYS:HZ3	2.18	0.42
1:A:111:THR:C	1:A:113:PRO:HD3	2.45	0.42
1:A:156:ALA:HB1	1:A:166:HIS:HB3	2.02	0.42
1:A:81:TRP:CD1	1:A:287:ILE:HD12	2.54	0.42
1:A:41:SER:OG	1:A:45:ARG:HB2	2.19	0.41
1:A:272:ARG:HA	1:A:273:ASP:HA	1.62	0.41
1:A:253:GLY:CA	3:A:502:TYR:OH	2.55	0.41
1:A:93:ASN:HD22	1:A:96:PHE:HB2	1.86	0.41
1:A:66:LEU:HD22	1:A:75:THR:O	2.21	0.40
1:A:171:ASN:HD22	1:A:176:VAL:HG12	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	305/307 (99%)	287 (94%)	14 (5%)	4 (1%)	9 5

All (4) Ramachandran outliers are listed below:

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

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%)	231 (88%)	32 (12%)	5 3

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	6	THR
1	A	15	LEU
1	A	18	ILE
1	A	31	GLU
1	A	33	VAL
1	A	40	ARG
1	A	57	SER
1	A	58	ASN
1	A	59	ARG
1	A	97	THR
1	A	112	ASN
1	A	122	GLU
1	A	127	ARG
1	A	137	LEU
1	A	139	VAL
1	A	179	ILE
1	A	202	LEU
1	A	203	LEU
1	A	216	LYS
1	A	237	SER
1	A	239	LYS
1	A	245	THR
1	A	246	THR
1	A	254	SER
1	A	268	THR
1	A	271	LEU
1	A	276	ARG
1	A	281	LEU
1	A	295	LEU

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Mol	Chain	Res	Type
1	A	298	LEU
1	A	307	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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	93	ASN
1	A	112	ASN
1	A	114	ASN
1	A	120	HIS
1	A	171	ASN
1	A	186	HIS
1	A	221	GLN
1	A	249	GLN
1	A	307	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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
3	TYR	A	502	2	12,13,13	1.69	2 (16%)	13,17,17	1.35	3 (23%)
2	GLY	A	501	3	3,3,4	0.80	0	1,2,4	0.87	0

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
3	TYR	A	502	2	-	3/8/8/8	0/1/1/1
2	GLY	A	501	3	-	0/0/1/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	TYR	CE1-CD1	4.44	1.46	1.38
3	A	502	TYR	CE2-CD2	2.63	1.43	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	TYR	CD2-CE2-CZ	-2.75	116.97	119.88
3	A	502	TYR	CE2-CZ-CE1	2.11	123.13	119.77
3	A	502	TYR	CE1-CD1-CG	-2.08	118.26	121.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	TYR	OXT-C-CA-N
3	A	502	TYR	C-CA-CB-CG
3	A	502	TYR	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	TYR	3	0

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.