



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:26 PM UTC

PDB ID : 1DDZ / pdb_00001ddz
Title : X-RAY STRUCTURE OF A BETA-CARBONIC ANHYDRASE FROM THE RED ALGA, PORPHYRIDIUM PURPUREUM R-1
Authors : Mitsuhashi, S.; Mizushima, T.; Yamashita, E.; Miyachi, S.; Tsukihara, T.
Deposited on : 1999-11-12
Resolution : 2.20 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

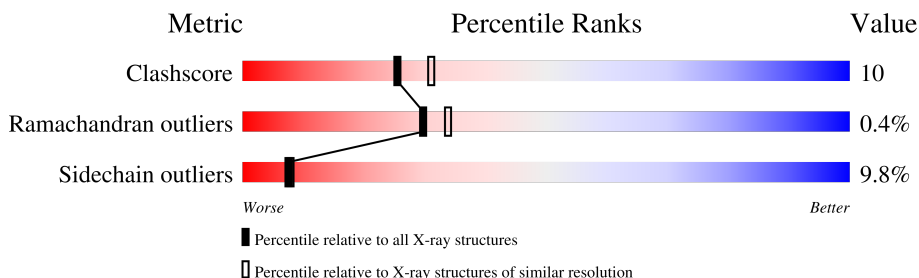
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	496	 70% 24% . .
1	B	496	 70% 23% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8100 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 CARBONIC ANHYDRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3742	2339	676	706	21			
1	B	481	Total	C	N	O	S	0	0	0
			3742	2339	676	706	21			

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	310	Total	O	0	0
			310	310		
3	B	302	Total	O	0	0
			302	302		

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	63.50Å 112.80Å 73.20Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.208 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8100	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	0.69	1/3807 (0.0%)	1.06	17/5153 (0.3%)
1	B	0.69	2/3807 (0.1%)	1.07	16/5153 (0.3%)
All	All	0.69	3/7614 (0.0%)	1.07	33/10306 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	MET	SD-CE	9.13	2.02	1.79
1	A	108	MET	SD-CE	6.52	1.95	1.79
1	B	421	VAL	CA-CB	5.09	1.61	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	SER	CB-CA-C	-8.01	96.32	109.46
1	B	169	VAL	N-CA-C	7.60	119.55	108.53
1	A	423	VAL	N-CA-C	7.52	119.31	108.48
1	B	423	VAL	N-CA-C	7.44	119.20	108.48
1	A	288	VAL	CB-CA-C	-7.43	98.86	110.52
1	B	500	ASP	CA-C-N	7.38	126.92	119.24
1	B	500	ASP	C-N-CA	7.38	126.92	119.24
1	A	169	VAL	N-CA-C	7.31	119.13	108.53
1	B	288	VAL	CB-CA-C	-7.30	99.06	110.52
1	A	500	ASP	CA-C-N	7.15	126.67	119.24
1	A	500	ASP	C-N-CA	7.15	126.67	119.24
1	B	245	LYS	N-CA-C	6.86	119.78	111.82
1	A	532	ALA	N-CA-C	-6.37	105.15	113.17
1	A	245	LYS	N-CA-C	6.30	119.13	111.82
1	B	532	ALA	N-CA-C	-6.26	105.28	113.17
1	A	141	SER	CA-CB-OG	6.25	123.59	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	416	LEU	CA-C-N	6.20	126.15	119.76
1	B	416	LEU	C-N-CA	6.20	126.15	119.76
1	A	363	GLU	N-CA-C	-6.18	101.37	110.52
1	A	145	LEU	N-CA-C	-6.07	99.29	109.07
1	B	363	GLU	N-CA-C	-5.94	101.73	110.52
1	B	145	LEU	N-CA-C	-5.86	99.63	109.07
1	A	475	GLY	N-CA-C	5.78	119.88	112.83
1	B	141	SER	CA-CB-OG	5.74	122.58	111.10
1	A	141	SER	N-CA-CB	5.64	118.34	110.11
1	A	192	VAL	N-CA-C	5.44	116.09	110.82
1	A	399	LEU	N-CA-C	-5.42	100.34	109.07
1	B	192	VAL	N-CA-C	5.38	116.04	110.82
1	B	406	SER	N-CA-C	5.38	122.25	110.80
1	B	290	GLY	N-CA-C	-5.23	101.40	110.71
1	A	226	TRP	N-CA-C	-5.17	105.55	111.14
1	A	416	LEU	CA-C-N	5.15	125.06	119.76
1	A	416	LEU	C-N-CA	5.15	125.06	119.76

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	3742	0	3705	74	0
1	B	3742	0	3705	75	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	310	0	0	9	0
3	B	302	0	0	15	0
All	All	8100	0	7410	143	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 10.

All (143) 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:B:108:MET:SD	1:B:108:MET:CE	2.02	1.47
1:A:288:VAL:HG22	1:A:299:LEU:HD21	1.57	0.86
1:B:288:VAL:HG22	1:B:299:LEU:HD21	1.58	0.85
1:B:367:ARG:HA	1:B:370:VAL:HG12	1.60	0.84
1:A:367:ARG:HA	1:A:370:VAL:HG12	1.59	0.83
1:A:381:LYS:HA	1:A:381:LYS:HE2	1.66	0.78
1:B:381:LYS:HA	1:B:381:LYS:HE2	1.66	0.77
1:B:179:HIS:HD2	3:B:607:HOH:O	1.68	0.76
1:B:285:GLN:HB2	1:B:301:VAL:HG22	1.74	0.69
1:A:201:LEU:HD23	1:A:285:GLN:HG2	1.75	0.66
1:A:288:VAL:HG22	1:A:299:LEU:CD2	2.25	0.65
1:B:261:GLU:HG3	3:B:752:HOH:O	1.97	0.65
1:B:288:VAL:HG22	1:B:299:LEU:CD2	2.25	0.64
1:A:285:GLN:HB2	1:A:301:VAL:HG22	1.78	0.64
1:B:367:ARG:HA	1:B:370:VAL:CG1	2.29	0.63
1:A:323:LYS:HG3	3:A:730:HOH:O	1.99	0.62
1:B:201:LEU:HD23	1:B:285:GLN:HG2	1.81	0.62
1:A:264:HIS:HD2	1:A:346:MET:HG3	1.63	0.62
1:B:314:ARG:HH21	1:B:329:ALA:HB3	1.64	0.62
1:B:264:HIS:HD2	1:B:346:MET:HG3	1.65	0.61
1:A:367:ARG:HA	1:A:370:VAL:CG1	2.29	0.60
1:A:563:ILE:HG13	1:A:564:GLY:N	2.17	0.60
1:B:313:TYR:HB3	1:B:331:LEU:HD22	1.83	0.60
1:B:260:LEU:HD22	1:B:346:MET:HE1	1.83	0.59
1:A:512:ASN:O	1:A:516:GLN:HG2	2.02	0.59
1:B:563:ILE:HG13	1:B:564:GLY:N	2.18	0.59
1:A:314:ARG:HH21	1:A:329:ALA:HB3	1.67	0.59
1:A:453:ARG:HG3	1:A:537:GLU:HB3	1.84	0.59
1:B:383:ASP:HB3	1:B:386:PHE:HB2	1.85	0.59
1:B:512:ASN:O	1:B:516:GLN:HG2	2.03	0.59
1:A:201:LEU:CD2	1:A:285:GLN:HG2	2.33	0.58
1:B:199:HIS:HD2	1:B:283:THR:OG1	1.85	0.58
1:A:376:ARG:O	1:A:380:LEU:HD22	2.03	0.58
1:B:552:ASP:O	1:B:553:MET:HE2	2.03	0.58
1:A:136:LEU:O	1:A:407:ARG:HD3	2.03	0.58
1:A:199:HIS:HD2	1:A:283:THR:OG1	1.86	0.58
1:A:179:HIS:HD2	3:A:596:HOH:O	1.85	0.58
1:A:260:LEU:HD22	1:A:346:MET:HE1	1.86	0.57
1:A:331:LEU:HD12	1:B:251:LEU:HG	1.86	0.57
1:A:483:HIS:HD2	3:A:717:HOH:O	1.86	0.57
1:B:376:ARG:O	1:B:380:LEU:HD22	2.04	0.57
1:A:434:SER:OG	1:B:483:HIS:HE1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASP:HB3	1:A:386:PHE:HB2	1.86	0.56
1:A:313:TYR:HB3	1:A:331:LEU:HD22	1.86	0.55
1:A:105:GLY:HA2	1:A:460:TYR:CZ	2.41	0.55
1:B:136:LEU:O	1:B:407:ARG:HD3	2.07	0.55
1:B:453:ARG:HG3	1:B:537:GLU:HB3	1.89	0.55
1:B:185:LEU:HD13	1:B:476:LEU:HD22	1.87	0.55
1:A:216:GLY:HA3	1:B:314:ARG:HH11	1.71	0.55
1:A:483:HIS:HE1	1:B:434:SER:OG	1.90	0.55
1:A:485:ARG:NH2	1:B:561:ASP:O	2.38	0.54
1:B:407:ARG:HB2	3:B:787:HOH:O	2.07	0.54
1:A:552:ASP:O	1:A:553:MET:HE2	2.07	0.54
1:B:201:LEU:CD2	1:B:285:GLN:HG2	2.37	0.54
1:B:105:GLY:HA2	1:B:460:TYR:CZ	2.43	0.54
1:A:185:LEU:HD13	1:A:476:LEU:HD22	1.89	0.54
1:A:170:HIS:HB2	1:A:187:VAL:HG11	1.90	0.53
1:B:218:SER:HA	3:B:758:HOH:O	2.08	0.53
1:A:263:VAL:HG11	3:A:793:HOH:O	2.08	0.53
1:A:314:ARG:HH11	1:B:216:GLY:HA3	1.74	0.53
1:A:264:HIS:CD2	1:A:346:MET:HG3	2.43	0.52
1:A:288:VAL:CG2	1:A:299:LEU:HD21	2.35	0.52
3:A:857:HOH:O	1:B:84:VAL:HG21	2.08	0.52
1:B:407:ARG:HB3	3:B:663:HOH:O	2.09	0.52
1:A:295:LYS:HA	1:A:372:ASN:HD21	1.75	0.51
1:A:260:LEU:HD22	1:A:346:MET:CE	2.41	0.51
1:A:338:GLY:HA2	3:A:776:HOH:O	2.10	0.51
1:A:379:MET:HB3	1:A:386:PHE:CD1	2.45	0.51
1:A:517:MET:SD	1:A:540:GLY:HA3	2.50	0.51
1:B:379:MET:HB3	1:B:386:PHE:CD1	2.46	0.51
1:B:264:HIS:CD2	1:B:346:MET:HG3	2.46	0.50
1:A:108:MET:HE3	1:A:109:PRO:HD2	1.94	0.49
1:A:432:ILE:HB	1:A:435:ASP:HB2	1.94	0.49
1:B:517:MET:SD	1:B:540:GLY:HA3	2.52	0.49
1:A:296:LEU:H	1:A:372:ASN:ND2	2.11	0.49
1:A:325:GLY:O	1:A:327:PRO:HD3	2.13	0.49
1:B:260:LEU:HD22	1:B:346:MET:CE	2.42	0.49
1:B:118:ASN:O	1:B:122:ARG:HG3	2.14	0.48
1:B:502:LYS:HE2	1:B:503:ASP:OD1	2.13	0.48
1:A:111:LYS:HD3	3:A:751:HOH:O	2.13	0.48
1:B:295:LYS:HA	1:B:372:ASN:HD21	1.78	0.48
1:B:99:LEU:HD12	3:B:810:HOH:O	2.13	0.47
1:A:118:ASN:O	1:A:122:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLN:HG3	1:B:193:GLN:OE1	2.15	0.47
1:B:381:LYS:HA	1:B:381:LYS:CE	2.43	0.47
1:B:311:LYS:HE3	1:B:312:PHE:CZ	2.49	0.47
1:A:381:LYS:HA	1:A:381:LYS:CE	2.42	0.47
1:A:189:GLN:HG3	1:A:193:GLN:OE1	2.15	0.46
1:A:353:LEU:C	1:A:353:LEU:HD22	2.40	0.46
1:A:312:PHE:HD2	1:A:335:THR:HG23	1.81	0.46
1:A:557:ALA:O	1:A:558:LYS:HB2	2.15	0.46
1:B:151:ASP:HB3	1:B:422:PHE:HE1	1.81	0.46
1:B:347:GLU:HA	3:B:830:HOH:O	2.16	0.46
1:A:563:ILE:HG13	1:A:564:GLY:H	1.81	0.46
1:B:424:HIS:HB2	1:B:441:VAL:HG11	1.98	0.46
1:A:139:GLY:HA3	1:A:407:ARG:NH1	2.31	0.45
1:A:151:ASP:HB3	1:A:422:PHE:HE1	1.81	0.45
1:B:170:HIS:HB2	1:B:187:VAL:HG11	1.97	0.45
1:A:297:ARG:HB3	1:A:361:LEU:HB2	1.98	0.45
1:B:154:VAL:HG22	1:B:390:LEU:HD21	1.98	0.45
1:A:312:PHE:HD2	1:A:335:THR:CG2	2.30	0.45
1:B:325:GLY:O	1:B:327:PRO:HD3	2.16	0.45
1:B:108:MET:HE3	1:B:109:PRO:HD2	1.98	0.45
1:B:285:GLN:NE2	1:B:298:ASP:OD1	2.50	0.45
1:B:288:VAL:CG2	1:B:299:LEU:HD21	2.38	0.44
1:B:507:ARG:HD3	1:B:510:GLU:OE1	2.16	0.44
1:B:353:LEU:HA	3:B:606:HOH:O	2.18	0.44
1:A:271:ILE:HD11	1:A:476:LEU:HD13	2.00	0.44
1:B:297:ARG:HB3	1:B:361:LEU:HB2	2.00	0.44
1:B:432:ILE:HB	1:B:435:ASP:HB2	1.98	0.44
1:B:363:GLU:H	1:B:363:GLU:CD	2.26	0.43
1:B:187:VAL:HG23	3:B:629:HOH:O	2.18	0.43
1:A:311:LYS:HE3	1:A:312:PHE:CZ	2.53	0.43
1:B:165:GLY:N	3:B:711:HOH:O	2.49	0.43
1:B:452:LYS:HG2	3:B:773:HOH:O	2.18	0.43
1:B:296:LEU:H	1:B:372:ASN:ND2	2.16	0.43
1:B:544:GLY:HA3	3:B:659:HOH:O	2.18	0.43
1:A:507:ARG:HD3	1:A:510:GLU:OE1	2.19	0.42
1:A:363:GLU:H	1:A:363:GLU:CD	2.26	0.42
1:B:312:PHE:HD2	1:B:335:THR:CG2	2.32	0.42
1:A:154:VAL:HG22	1:A:390:LEU:HD21	2.02	0.42
1:B:103:PRO:HD2	1:B:106:GLN:HB2	2.02	0.42
1:A:219:ARG:HG2	3:B:599:HOH:O	2.19	0.42
1:B:249:GLU:HG3	1:B:358:PRO:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASP:HA	1:A:130:PRO:HD2	1.89	0.41
1:A:424:HIS:HB2	1:A:441:VAL:HG11	2.01	0.41
1:B:312:PHE:HD2	1:B:335:THR:HG23	1.86	0.41
1:B:398:ILE:HD11	1:B:416:LEU:CD1	2.50	0.41
1:A:378:LYS:O	1:A:382:GLN:HG2	2.20	0.41
1:A:506:ASN:ND2	3:A:614:HOH:O	2.53	0.41
1:B:331:LEU:HD23	1:B:331:LEU:HA	1.86	0.41
1:A:249:GLU:HG3	1:A:358:PRO:HB2	2.03	0.41
1:B:205:HIS:HE1	3:B:822:HOH:O	2.03	0.41
1:A:398:ILE:HD11	1:A:416:LEU:CD1	2.51	0.41
1:A:85:MET:HG2	3:B:581:HOH:O	2.20	0.40
1:A:172:ASN:OD1	1:A:172:ASN:C	2.64	0.40
1:B:500:ASP:HA	1:B:501:PRO:HD3	1.86	0.40
1:A:198:LYS:HG2	3:A:760:HOH:O	2.20	0.40
1:B:557:ALA:O	1:B:558:LYS:HB2	2.21	0.40
1:A:241:LEU:HD13	1:A:253:ARG:HG2	2.03	0.40
1:A:502:LYS:HE2	1:A:503:ASP:OD1	2.22	0.40
1:B:563:ILE:HG13	1:B:564:GLY:H	1.85	0.40
1:A:331:LEU:HD23	1:A:331:LEU:HA	1.85	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	479/496 (97%)	460 (96%)	17 (4%)	2 (0%)	30	34
1	B	479/496 (97%)	459 (96%)	18 (4%)	2 (0%)	30	34
All	All	958/992 (97%)	919 (96%)	35 (4%)	4 (0%)	30	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	336	LYS
1	A	336	LYS
1	B	112	SER
1	A	112	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	403/414 (97%)	364 (90%)	39 (10%)	8	8
1	B	403/414 (97%)	363 (90%)	40 (10%)	7	8
All	All	806/828 (97%)	727 (90%)	79 (10%)	7	8

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	108	MET
1	A	113	ASN
1	A	145	LEU
1	A	151	ASP
1	A	166	GLU
1	A	188	LEU
1	A	197	VAL
1	A	222	LEU
1	A	228	ARG
1	A	241	LEU
1	A	251	LEU
1	A	253	ARG
1	A	254	LEU
1	A	281	GLU
1	A	285	GLN
1	A	287	VAL
1	A	288	VAL
1	A	302	VAL
1	A	314	ARG

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Mol	Chain	Res	Type
1	A	335	THR
1	A	342	LEU
1	A	353	LEU
1	A	368	VAL
1	A	378	LYS
1	A	380	LEU
1	A	398	ILE
1	A	399	LEU
1	A	406	SER
1	A	421	VAL
1	A	442	LEU
1	A	453	ARG
1	A	484	ILE
1	A	499	THR
1	A	505	LEU
1	A	508	LEU
1	A	514	LEU
1	A	520	VAL
1	A	541	VAL
1	B	88	LEU
1	B	108	MET
1	B	109	PRO
1	B	113	ASN
1	B	145	LEU
1	B	151	ASP
1	B	166	GLU
1	B	188	LEU
1	B	197	VAL
1	B	222	LEU
1	B	228	ARG
1	B	241	LEU
1	B	251	LEU
1	B	253	ARG
1	B	254	LEU
1	B	281	GLU
1	B	285	GLN
1	B	287	VAL
1	B	288	VAL
1	B	302	VAL
1	B	314	ARG
1	B	335	THR
1	B	342	LEU

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Mol	Chain	Res	Type
1	B	353	LEU
1	B	368	VAL
1	B	378	LYS
1	B	380	LEU
1	B	398	ILE
1	B	399	LEU
1	B	406	SER
1	B	421	VAL
1	B	442	LEU
1	B	453	ARG
1	B	484	ILE
1	B	499	THR
1	B	505	LEU
1	B	508	LEU
1	B	514	LEU
1	B	520	VAL
1	B	541	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	138	ASN
1	A	158	GLN
1	A	179	HIS
1	A	199	HIS
1	A	355	GLN
1	A	372	ASN
1	A	374	ASN
1	A	389	ASN
1	A	394	GLN
1	A	430	GLN
1	A	483	HIS
1	A	506	ASN
1	A	512	ASN
1	A	539	GLN
1	B	138	ASN
1	B	179	HIS
1	B	199	HIS
1	B	355	GLN
1	B	372	ASN
1	B	374	ASN

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Mol	Chain	Res	Type
1	B	389	ASN
1	B	394	GLN
1	B	430	GLN
1	B	483	HIS
1	B	506	ASN
1	B	512	ASN
1	B	539	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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.