



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:45 PM UTC

PDB ID : 1Y79 / pdb_00001y79
Title : Crystal Structure of the E.coli Dipeptidyl Carboxypeptidase Dcp in Complex with a Peptidic Inhibitor
Authors : Comellas-Bigler, M.; Lang, R.; Bode, W.; Maskos, K.
Deposited on : 2004-12-08
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

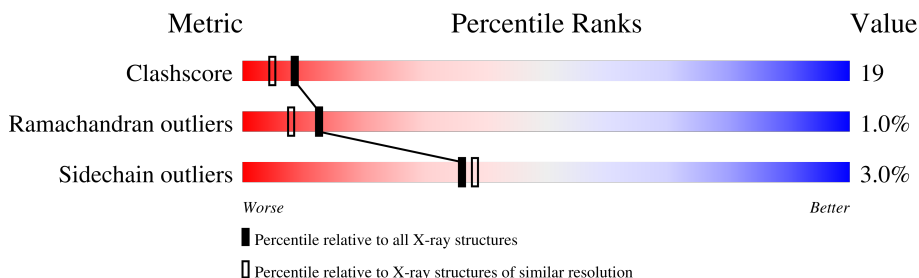
1 Overall quality at a glance

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	1	680	 66% 30% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6135 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.

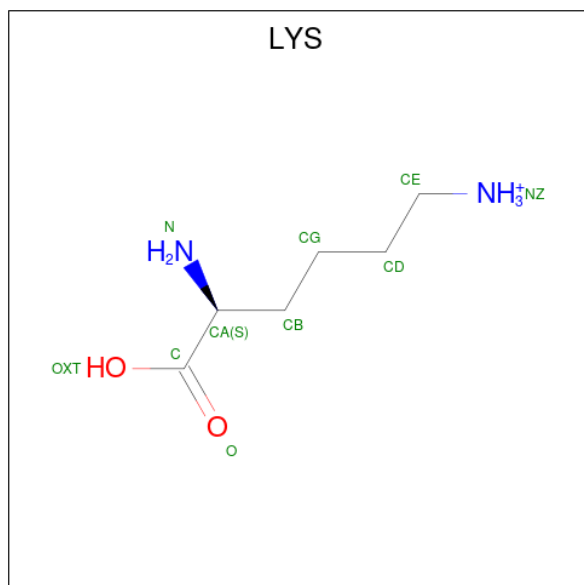
- Molecule 1 is a protein called Peptidyl-Dipeptidase Dcp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	680	Total	C	N	O	S	106	0	0
			5468	3477	963	1008	20			

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

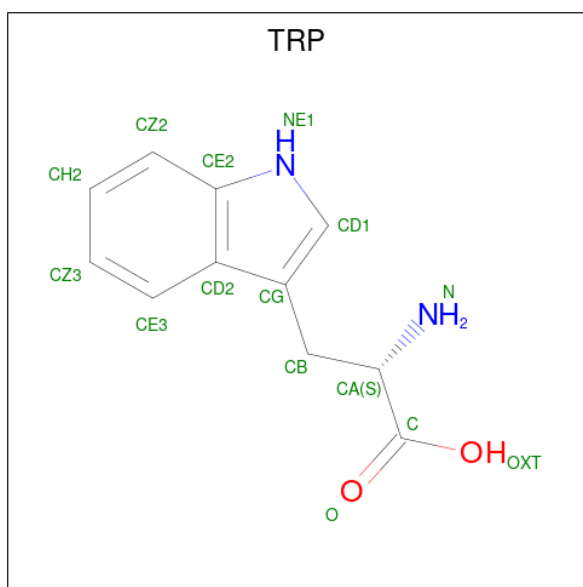
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	1	Total	Zn	0	0
			1	1		

- Molecule 3 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



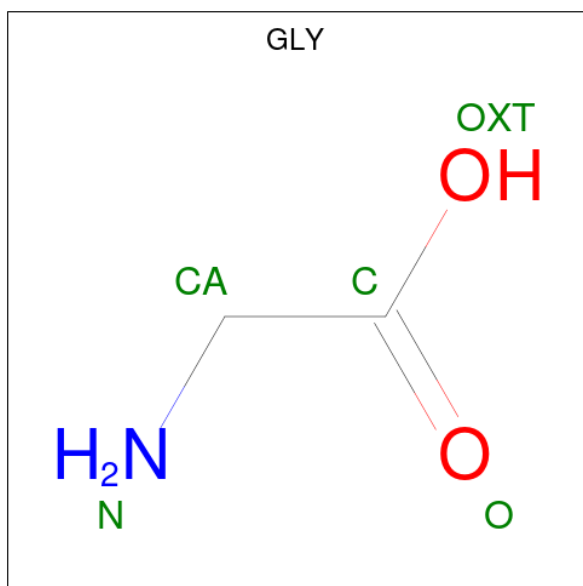
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1	1	Total	C	N	O	4	0
			9	6	2	1		

- Molecule 4 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂).



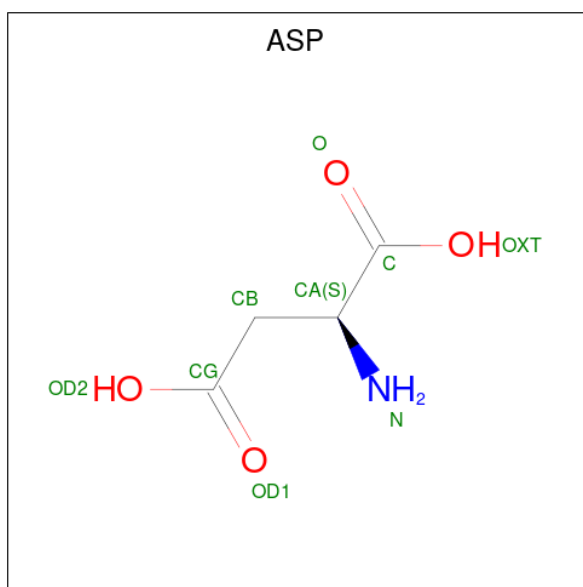
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	1	1	Total	C	N	O	8	0
			15	11	2	2		

- Molecule 5 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	1	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 6 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	1	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 7 is water.

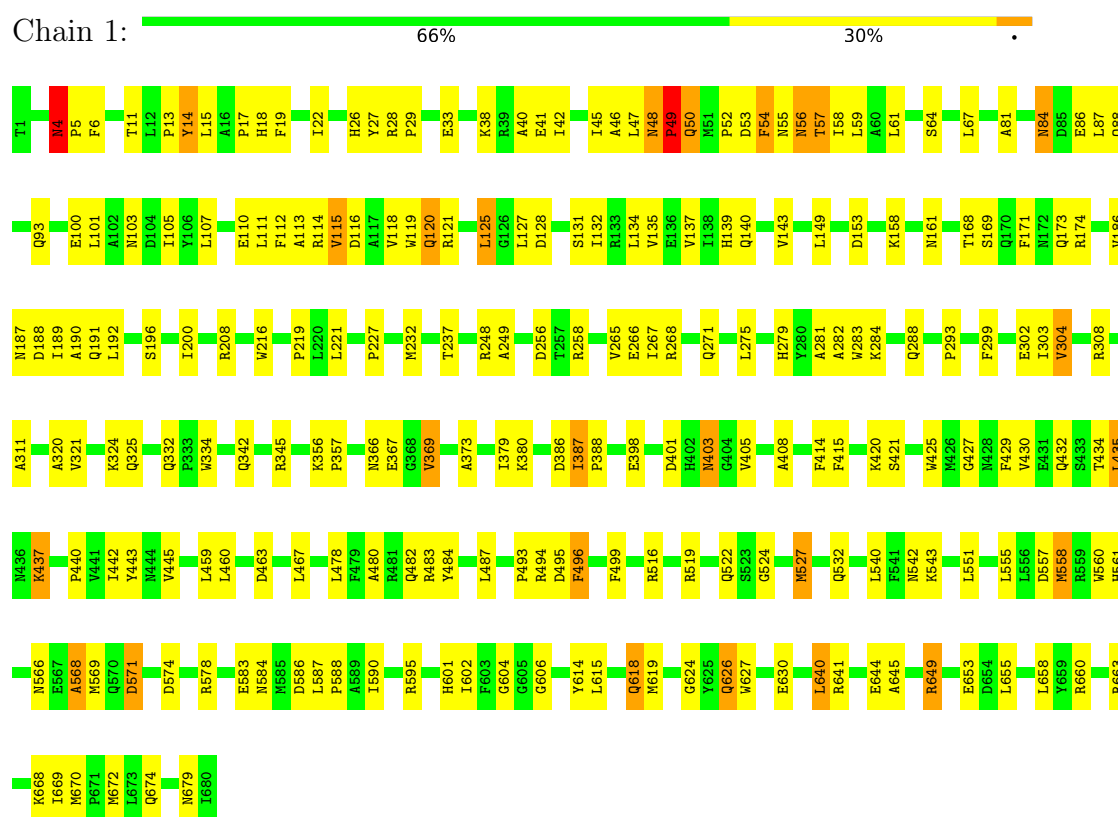
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	1	629	Total	O	0	0
			629	629		

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: Peptidyl-Dipeptidase Dcp



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.41Å 67.92Å 153.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6135	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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	1	0.60	3/5602 (0.1%)	0.97	24/7597 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	527	MET	SD-CE	-8.04	1.59	1.79
1	1	304	VAL	CA-CB	6.61	1.57	1.54
1	1	558	MET	SD-CE	-6.13	1.64	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	414	PHE	N-CA-C	9.88	125.54	113.38
1	1	649	ARG	N-CA-C	7.01	121.07	112.23
1	1	571	ASP	N-CA-C	-6.97	97.88	108.96
1	1	429	PHE	N-CA-C	-6.46	104.44	112.90
1	1	27	TYR	N-CA-C	6.39	117.93	110.97
1	1	460	LEU	N-CA-C	-6.36	101.97	110.55
1	1	81	ALA	N-CA-C	6.04	120.78	113.41
1	1	11	THR	N-CA-C	-5.97	106.04	113.38
1	1	258	ARG	N-CA-C	5.90	117.72	111.28
1	1	568	ALA	N-CA-C	5.78	118.36	111.71
1	1	618	GLN	N-CA-C	-5.75	105.10	111.36
1	1	366	ASN	N-CA-C	5.74	117.33	111.14
1	1	415	PHE	N-CA-C	5.65	118.94	109.95
1	1	442	ILE	N-CA-C	5.60	117.40	108.89
1	1	602	ILE	N-CA-C	5.49	119.84	113.42
1	1	595	ARG	N-CA-C	-5.46	102.45	110.52
1	1	248	ARG	N-CA-C	5.42	117.89	111.33
1	1	496	PHE	N-CA-C	-5.39	106.01	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	478	LEU	N-CA-C	5.12	116.94	111.36
1	1	369	VAL	N-CA-C	5.08	115.29	110.42
1	1	387	ILE	CA-C-N	5.05	124.96	119.76
1	1	387	ILE	C-N-CA	5.05	124.96	119.76
1	1	398	GLU	N-CA-C	-5.03	101.52	109.76
1	1	4	ASN	N-CA-C	5.01	120.88	109.81

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	1	5468	0	5304	199	0
2	1	1	0	0	0	0
3	1	9	0	12	0	0
4	1	15	0	10	0	0
5	1	4	0	2	0	0
6	1	9	0	4	1	0
7	1	629	0	0	35	0
All	All	6135	0	5332	199	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 19.

All (199) 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)
1:1:432:GLN:HB2	1:1:440:PRO:HG3	1.49	0.94
1:1:578:ARG:HD3	7:1:862:HOH:O	1.74	0.86
1:1:53:ASP:HB3	7:1:1309:HOH:O	1.75	0.84
1:1:670:MET:HE1	1:1:679:ASN:CG	2.02	0.84
1:1:48:ASN:HB3	1:1:49:PRO:HD2	1.64	0.77
1:1:527:MET:HE2	1:1:532:GLN:HA	1.66	0.77
1:1:188:ASP:H	1:1:191:GLN:HE21	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:131:SER:O	1:1:135:VAL:HG23	1.84	0.77
1:1:345:ARG:HD2	7:1:1005:HOH:O	1.84	0.76
1:1:527:MET:HE2	1:1:532:GLN:CA	2.16	0.75
1:1:670:MET:HE3	1:1:674:GLN:HG3	1.68	0.75
1:1:208:ARG:HD2	7:1:1317:HOH:O	1.88	0.73
1:1:495:ASP:OD1	7:1:864:HOH:O	2.06	0.72
1:1:281:ALA:HB1	1:1:558:MET:HE1	1.72	0.72
1:1:434:THR:OG1	1:1:483:ARG:HA	1.90	0.72
1:1:268:ARG:HH11	1:1:561:HIS:HE1	1.36	0.71
1:1:103:ASN:HD21	1:1:161:ASN:HD22	1.39	0.71
1:1:107:LEU:HD22	1:1:158:LYS:HG3	1.71	0.71
1:1:48:ASN:O	1:1:49:PRO:C	2.35	0.69
1:1:640:LEU:HD23	1:1:641:ARG:N	2.08	0.68
1:1:84:ASN:ND2	1:1:87:LEU:H	1.91	0.68
1:1:125:LEU:HB2	1:1:127:LEU:HG	1.75	0.68
1:1:640:LEU:O	1:1:644:GLU:HG3	1.96	0.66
1:1:219:PRO:HD3	7:1:1117:HOH:O	1.96	0.64
1:1:281:ALA:HB1	1:1:558:MET:CE	2.27	0.64
1:1:325:GLN:HE22	1:1:342:GLN:HE22	1.43	0.64
1:1:84:ASN:HD22	1:1:86:GLU:N	1.96	0.63
1:1:84:ASN:HD22	1:1:86:GLU:H	1.45	0.63
1:1:670:MET:HE1	1:1:679:ASN:ND2	2.12	0.63
1:1:663:ARG:HD3	1:1:663:ARG:O	1.99	0.62
1:1:28:ARG:HB3	1:1:29:PRO:HD3	1.82	0.62
1:1:28:ARG:HH21	1:1:93:GLN:NE2	1.97	0.62
1:1:483:ARG:NH2	7:1:784:HOH:O	2.33	0.61
1:1:128:ASP:HA	7:1:1214:HOH:O	2.00	0.61
1:1:356:LYS:HG3	7:1:1042:HOH:O	2.01	0.61
1:1:321:VAL:O	1:1:325:GLN:HG3	2.01	0.61
1:1:288:GLN:OE1	7:1:864:HOH:O	2.16	0.60
1:1:626:GLN:O	1:1:630:GLU:HG3	2.01	0.60
1:1:574:ASP:HB2	7:1:989:HOH:O	2.00	0.60
1:1:189:ILE:HG12	1:1:216:TRP:CZ2	2.37	0.60
1:1:61:LEU:O	1:1:64:SER:HB3	2.02	0.60
1:1:493:PRO:CB	7:1:864:HOH:O	2.50	0.60
1:1:84:ASN:HD21	1:1:87:LEU:H	1.50	0.59
1:1:373:ALA:HB1	1:1:379:ILE:HD11	1.85	0.59
1:1:641:ARG:O	1:1:641:ARG:HD3	2.02	0.59
1:1:45:ILE:HA	1:1:48:ASN:HD22	1.68	0.59
1:1:56:ASN:HB3	7:1:1309:HOH:O	2.02	0.58
1:1:110:GLU:O	1:1:114:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:149:LEU:HG	1:1:153:ASP:HB2	1.85	0.58
1:1:527:MET:HE2	1:1:532:GLN:N	2.17	0.58
1:1:42:ILE:HD13	1:1:105:ILE:HG12	1.84	0.58
1:1:356:LYS:HB3	1:1:357:PRO:HD3	1.84	0.58
1:1:279:HIS:HD2	1:1:282:ALA:H	1.52	0.57
1:1:84:ASN:HD22	1:1:84:ASN:C	2.12	0.57
1:1:38:LYS:HA	1:1:41:GLU:OE1	2.04	0.57
1:1:46:ALA:O	1:1:47:LEU:HD23	2.05	0.57
1:1:188:ASP:H	1:1:191:GLN:NE2	2.02	0.57
1:1:555:LEU:HB3	1:1:583:GLU:HG2	1.86	0.56
1:1:268:ARG:HH11	1:1:561:HIS:CE1	2.21	0.56
1:1:619:MET:HE3	1:1:668:LYS:C	2.30	0.56
1:1:54:PHE:HE1	1:1:135:VAL:HG22	1.71	0.56
1:1:401:ASP:HB3	1:1:403:ASN:ND2	2.20	0.56
1:1:275:LEU:HD13	1:1:283:TRP:CE2	2.41	0.56
1:1:40:ALA:HA	7:1:958:HOH:O	2.05	0.56
1:1:101:LEU:O	1:1:105:ILE:HG13	2.06	0.56
1:1:619:MET:HE3	1:1:669:ILE:N	2.21	0.56
1:1:88:GLN:NE2	7:1:1047:HOH:O	2.38	0.56
1:1:84:ASN:HD21	1:1:86:GLU:HB3	1.72	0.55
1:1:403:ASN:ND2	1:1:405:VAL:H	2.05	0.55
1:1:367:GLU:HG3	7:1:1288:HOH:O	2.07	0.55
1:1:105:ILE:O	1:1:111:LEU:HD23	2.07	0.55
1:1:107:LEU:CD2	1:1:158:LYS:HG3	2.37	0.54
1:1:48:ASN:ND2	7:1:1161:HOH:O	2.39	0.54
1:1:527:MET:CE	1:1:532:GLN:HA	2.36	0.54
1:1:434:THR:HA	7:1:1090:HOH:O	2.08	0.54
1:1:557:ASP:O	1:1:561:HIS:HD2	1.91	0.54
1:1:432:GLN:HG3	1:1:480:ALA:O	2.08	0.54
1:1:614:TYR:O	1:1:618:GLN:HG3	2.08	0.54
1:1:4:ASN:HD21	1:1:6:PHE:HD1	1.54	0.54
1:1:403:ASN:HD22	1:1:403:ASN:C	2.15	0.54
1:1:569:MET:HE2	7:1:1053:HOH:O	2.08	0.54
1:1:121:ARG:O	1:1:125:LEU:HG	2.08	0.54
1:1:267:ILE:O	1:1:271:GLN:HG3	2.07	0.54
1:1:84:ASN:ND2	1:1:86:GLU:H	2.07	0.53
1:1:38:LYS:HE3	1:1:42:ILE:HD11	1.91	0.53
1:1:408:ALA:HB1	1:1:440:PRO:O	2.09	0.53
1:1:320:ALA:O	1:1:324:LYS:HG3	2.08	0.52
1:1:116:ASP:O	1:1:120:GLN:NE2	2.43	0.52
1:1:325:GLN:HE22	1:1:342:GLN:NE2	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:103:ASN:ND2	1:1:161:ASN:HD22	2.06	0.52
1:1:5:PRO:HD3	1:1:26:HIS:CE1	2.44	0.52
1:1:50:GLN:O	1:1:52:PRO:HD3	2.09	0.51
1:1:284:LYS:HE2	1:1:494:ARG:NH1	2.24	0.51
1:1:494:ARG:NH2	7:1:953:HOH:O	2.38	0.51
1:1:103:ASN:HB3	1:1:158:LYS:HG2	1.92	0.51
1:1:45:ILE:HA	1:1:48:ASN:ND2	2.25	0.51
1:1:118:VAL:HG13	1:1:125:LEU:CD1	2.40	0.51
1:1:284:LYS:HE2	1:1:494:ARG:CZ	2.41	0.51
1:1:28:ARG:NH2	1:1:93:GLN:NE2	2.58	0.51
1:1:84:ASN:ND2	1:1:86:GLU:N	2.59	0.51
1:1:522:GLN:HG3	7:1:1105:HOH:O	2.10	0.51
1:1:196:SER:O	1:1:200:ILE:HG13	2.12	0.50
1:1:190:ALA:HB3	7:1:992:HOH:O	2.12	0.50
1:1:493:PRO:HB3	7:1:864:HOH:O	2.11	0.50
1:1:645:ALA:HB1	7:1:1115:HOH:O	2.10	0.50
1:1:168:THR:HG23	1:1:604:GLY:HA2	1.93	0.49
1:1:268:ARG:HA	1:1:271:GLN:HE21	1.76	0.49
1:1:369:VAL:HG21	1:1:467:LEU:HG	1.94	0.49
1:1:53:ASP:O	1:1:57:THR:HG23	2.12	0.49
1:1:139:HIS:O	1:1:143:VAL:HG23	2.12	0.49
1:1:494:ARG:HD3	1:1:606:GLY:O	2.13	0.49
1:1:649:ARG:HG3	1:1:658:LEU:HD11	1.94	0.49
1:1:107:LEU:HD12	1:1:107:LEU:N	2.28	0.48
1:1:187:ASN:H	1:1:191:GLN:HE22	1.61	0.48
1:1:55:ASN:HA	1:1:59:LEU:HB3	1.93	0.48
1:1:84:ASN:ND2	1:1:84:ASN:C	2.71	0.48
1:1:140:GLN:NE2	7:1:983:HOH:O	2.44	0.48
1:1:432:GLN:CD	1:1:432:GLN:C	2.81	0.48
1:1:434:THR:HG1	1:1:483:ARG:HA	1.76	0.48
1:1:48:ASN:HB3	1:1:49:PRO:CD	2.40	0.48
1:1:118:VAL:HG13	1:1:125:LEU:HD11	1.95	0.48
1:1:420:LYS:HG2	1:1:421:SER:O	2.13	0.48
1:1:540:LEU:O	1:1:543:LYS:HB2	2.14	0.48
1:1:103:ASN:HD21	1:1:161:ASN:ND2	2.09	0.47
1:1:18:HIS:O	1:1:22:ILE:HG13	2.14	0.47
1:1:221:LEU:HD22	1:1:227:PRO:CG	2.44	0.47
1:1:112:PHE:O	1:1:115:VAL:N	2.47	0.47
1:1:325:GLN:NE2	1:1:342:GLN:HE22	2.10	0.47
1:1:516:ARG:NE	7:1:1206:HOH:O	2.48	0.47
1:1:557:ASP:O	1:1:561:HIS:CD2	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:493:PRO:HD2	1:1:655:LEU:CD1	2.44	0.47
1:1:660:ARG:NH1	7:1:1249:HOH:O	2.48	0.47
1:1:601:HIS:HD2	7:1:738:HOH:O	1.97	0.47
1:1:311:ALA:HB1	1:1:590:ILE:CD1	2.44	0.46
1:1:386:ASP:C	1:1:387:ILE:HD12	2.41	0.46
1:1:103:ASN:HA	1:1:107:LEU:HD13	1.98	0.46
1:1:302:GLU:CG	1:1:303:ILE:HG23	2.44	0.46
1:1:4:ASN:HD22	1:1:6:PHE:H	1.63	0.46
1:1:186:VAL:HG21	1:1:192:LEU:HD21	1.97	0.46
1:1:266:GLU:HA	1:1:568:ALA:HB1	1.97	0.46
1:1:279:HIS:CD2	1:1:282:ALA:H	2.30	0.46
1:1:435:LEU:C	1:1:437:LYS:H	2.24	0.46
1:1:299:PHE:O	1:1:302:GLU:HG2	2.16	0.46
1:1:134:LEU:HD22	1:1:484:TYR:CD2	2.51	0.46
1:1:614:TYR:CD2	6:1:704:ASP:HB3	2.51	0.45
1:1:169:SER:O	1:1:173:GLN:HG3	2.16	0.45
1:1:571:ASP:HB3	1:1:574:ASP:HB3	1.98	0.45
1:1:459:LEU:HB3	1:1:463:ASP:HB2	1.98	0.45
1:1:293:PRO:HB3	1:1:558:MET:HE2	1.99	0.45
1:1:670:MET:CE	1:1:674:GLN:HG3	2.43	0.44
1:1:551:LEU:HD23	1:1:615:LEU:HD13	2.00	0.44
1:1:149:LEU:HG	1:1:153:ASP:CB	2.48	0.44
1:1:496:PHE:O	1:1:499:PHE:HB3	2.17	0.44
1:1:332:GLN:HG3	1:1:334:TRP:CZ2	2.53	0.44
1:1:586:ASP:HB3	7:1:819:HOH:O	2.18	0.44
1:1:427:GLY:HA3	1:1:443:TYR:CZ	2.52	0.44
1:1:555:LEU:HD13	1:1:583:GLU:HG3	2.00	0.44
1:1:103:ASN:O	1:1:107:LEU:HB2	2.17	0.43
1:1:38:LYS:HG2	1:1:101:LEU:HD21	2.00	0.43
1:1:618:GLN:HE21	1:1:672:MET:HE3	1.83	0.43
1:1:641:ARG:HD3	1:1:641:ARG:C	2.43	0.43
1:1:54:PHE:CE1	1:1:58:ILE:HG21	2.54	0.43
1:1:17:PRO:HB2	1:1:19:PHE:CE1	2.54	0.43
1:1:125:LEU:HD12	1:1:127:LEU:HD11	2.00	0.43
1:1:587:LEU:HA	1:1:588:PRO:HD2	1.91	0.43
1:1:4:ASN:HA	1:1:5:PRO:HD3	1.79	0.43
1:1:134:LEU:HD22	1:1:484:TYR:CG	2.54	0.43
1:1:57:THR:OG1	1:1:58:ILE:N	2.51	0.42
1:1:483:ARG:NE	7:1:1071:HOH:O	2.41	0.42
1:1:171:PHE:CD1	1:1:171:PHE:C	2.98	0.42
1:1:494:ARG:N	7:1:864:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:119:TRP:HE3	1:1:120:GLN:NE2	2.17	0.42
1:1:653:GLU:HG3	7:1:771:HOH:O	2.20	0.42
1:1:232:MET:HE3	1:1:237:THR:HG22	2.02	0.42
1:1:281:ALA:CB	1:1:558:MET:HE3	2.49	0.42
1:1:137:VAL:HG21	1:1:487:LEU:HD21	2.02	0.41
1:1:265:VAL:HG21	1:1:560:TRP:CE3	2.54	0.41
1:1:47:LEU:C	1:1:48:ASN:O	2.62	0.41
1:1:308:ARG:NH2	1:1:584:ASN:HB3	2.35	0.41
1:1:4:ASN:ND2	1:1:6:PHE:HB2	2.35	0.41
1:1:173:GLN:HA	7:1:903:HOH:O	2.21	0.41
1:1:112:PHE:O	1:1:113:ALA:C	2.63	0.41
1:1:53:ASP:O	1:1:54:PHE:C	2.64	0.41
1:1:100:GLU:O	1:1:103:ASN:HB2	2.20	0.41
1:1:132:ILE:HA	1:1:135:VAL:HG23	2.03	0.41
1:1:249:ALA:O	1:1:256:ASP:HA	2.21	0.41
1:1:432:GLN:NE2	1:1:482:GLN:H	2.18	0.41
1:1:624:GLY:O	1:1:627:TRP:HB3	2.21	0.41
1:1:670:MET:HE1	1:1:679:ASN:OD1	2.19	0.41
1:1:13:PRO:C	1:1:15:LEU:N	2.78	0.41
1:1:14:TYR:O	1:1:15:LEU:HB2	2.22	0.40
1:1:174:ARG:HD2	7:1:961:HOH:O	2.22	0.40
1:1:387:ILE:HD12	1:1:387:ILE:N	2.36	0.40
1:1:380:LYS:NZ	7:1:1012:HOH:O	2.54	0.40
1:1:425:TRP:CZ2	1:1:445:VAL:HG11	2.56	0.40
1:1:48:ASN:O	1:1:49:PRO:O	2.39	0.40
1:1:387:ILE:HA	1:1:388:PRO:HD3	1.82	0.40
1:1:403:ASN:ND2	1:1:403:ASN:C	2.79	0.40
1:1:519:ARG:HD3	1:1:524:GLY:O	2.22	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	1	678/680 (100%)	642 (95%)	29 (4%)	7 (1%)	12 8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	49	PRO
1	1	50	GLN
1	1	54	PHE
1	1	125	LEU
1	1	435	LEU
1	1	14	TYR
1	1	48	ASN

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	1	558/558 (100%)	541 (97%)	17 (3%)	36 38

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	4	ASN
1	1	33	GLU
1	1	49	PRO
1	1	56	ASN
1	1	57	THR
1	1	67	LEU
1	1	84	ASN
1	1	115	VAL
1	1	120	GLN
1	1	304	VAL
1	1	403	ASN
1	1	430	VAL
1	1	437	LYS
1	1	542	ASN

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Mol	Chain	Res	Type
1	1	566	ASN
1	1	626	GLN
1	1	640	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	4	ASN
1	1	21	GLN
1	1	48	ASN
1	1	55	ASN
1	1	84	ASN
1	1	88	GLN
1	1	93	GLN
1	1	103	ASN
1	1	120	GLN
1	1	140	GLN
1	1	170	GLN
1	1	173	GLN
1	1	191	GLN
1	1	270	GLN
1	1	271	GLN
1	1	279	HIS
1	1	298	ASN
1	1	325	GLN
1	1	342	GLN
1	1	403	ASN
1	1	432	GLN
1	1	444	ASN
1	1	476	HIS
1	1	561	HIS
1	1	601	HIS
1	1	618	GLN
1	1	631	GLN
1	1	674	GLN
1	1	675	HIS
1	1	679	ASN

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
4	TRP	1	702	3,2	15,16,16	0.75	0	18,22,22	0.38	0
6	ASP	1	704	5	7,8,8	1.05	0	6,10,10	0.75	0
3	LYS	1	701	4	7,8,9	0.48	0	3,8,10	0.44	0
5	GLY	1	703	6	3,3,4	0.78	0	1,2,4	0.61	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
4	TRP	1	702	3,2	-	7/8/8/8	0/2/2/2
6	ASP	1	704	5	-	2/8/8/8	-
3	LYS	1	701	4	-	0/6/7/9	-
5	GLY	1	703	6	-	0/0/1/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1	702	TRP	O-C-CA-N
4	1	702	TRP	OXT-C-CA-N
4	1	702	TRP	CA-CB-CG-CD1
4	1	702	TRP	CA-CB-CG-CD2
4	1	702	TRP	N-CA-CB-CG
6	1	704	ASP	CA-CB-CG-OD1
4	1	702	TRP	O-C-CA-CB
4	1	702	TRP	OXT-C-CA-CB
6	1	704	ASP	CA-CB-CG-OD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	704	ASP	1	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.