



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:10 AM EDT

PDB ID : 1DAB
Title : The Structure of Bordetella Pertussis Virulence Factor P.69 Pertactin
Authors : Emsley, P.; Charles, I.G.; Fairweather, N.F.; Isaacs, N.W.
Deposited on : 1999-10-31
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

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 : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

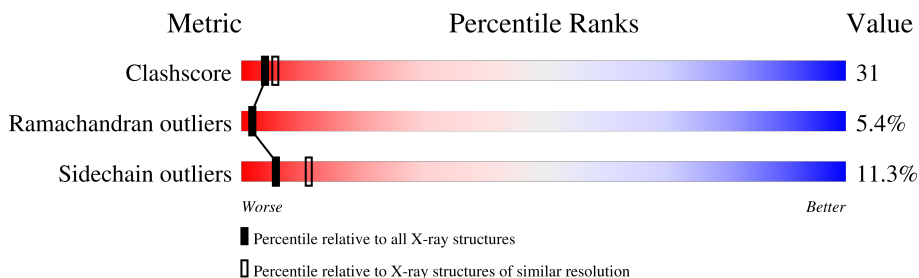
1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 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	539	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4124 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 P.69 PERTACTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			3847	2381	708	754	4			

- Molecule 2 is water.

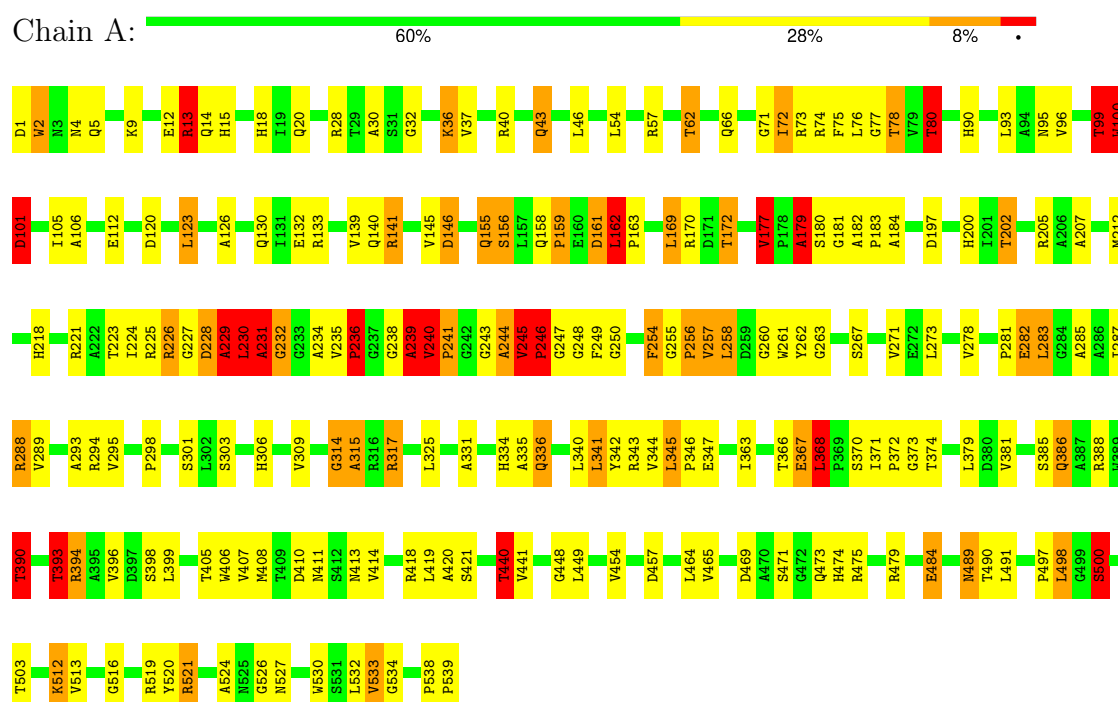
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	277	Total	O	0	0
			277	277		

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: P.69 PERTACTIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	176.20Å 176.20Å 104.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.4 (20.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.250 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4124	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.50	1/3911 (0.0%)	1.61	65/5328 (1.2%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	539	PRO	N-CD	5.69	1.55	1.47

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	ARG	NE-CZ-NH2	-46.02	97.29	120.30
1	A	317	ARG	NH1-CZ-NH2	16.25	137.28	119.40
1	A	235	VAL	CA-CB-CG1	-14.86	88.62	110.90
1	A	245	VAL	CG1-CB-CG2	14.08	133.44	110.90
1	A	245	VAL	N-CA-C	13.86	148.42	111.00
1	A	245	VAL	CB-CA-C	-12.99	86.71	111.40
1	A	245	VAL	CA-C-O	-12.72	93.38	120.10
1	A	258	LEU	CA-CB-CG	11.37	141.45	115.30
1	A	100	TRP	CB-CA-C	10.22	130.83	110.40
1	A	317	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	A	246	PRO	CA-CB-CG	-10.11	84.79	104.00
1	A	288	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	521	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	235	VAL	CA-CB-CG2	-8.34	98.39	110.90
1	A	368	LEU	CA-CB-CG	8.24	134.25	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	A	245	VAL	CA-C-N	7.87	139.12	117.10
1	A	231	ALA	N-CA-CB	7.81	121.03	110.10
1	A	240	VAL	CB-CA-C	7.67	125.97	111.40
1	A	99	THR	CA-C-N	-7.59	100.50	117.20
1	A	141	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	521	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	230	LEU	CB-CA-C	-7.38	96.18	110.20
1	A	246	PRO	N-CA-CB	7.26	112.02	103.30
1	A	260	GLY	CA-C-O	-7.12	107.79	120.60
1	A	123	LEU	CA-CB-CG	7.08	131.59	115.30
1	A	232	GLY	N-CA-C	7.07	130.78	113.10
1	A	533	VAL	CA-C-N	7.02	130.23	116.20
1	A	254	PHE	N-CA-C	6.98	129.85	111.00
1	A	146	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	246	PRO	CA-N-CD	-6.72	102.08	111.50
1	A	28	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	393	THR	CB-CA-C	-6.55	93.91	111.60
1	A	230	LEU	CB-CG-CD1	6.55	122.13	111.00
1	A	226	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	229	ALA	C-N-CA	6.43	137.76	121.70
1	A	245	VAL	CA-CB-CG2	-6.30	101.46	110.90
1	A	235	VAL	CG1-CB-CG2	6.23	120.87	110.90
1	A	258	LEU	CB-CA-C	6.09	121.78	110.20
1	A	260	GLY	CA-C-N	6.06	130.53	117.20
1	A	226	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	162	LEU	N-CA-C	5.94	127.05	111.00
1	A	390	THR	N-CA-CB	5.82	121.36	110.30
1	A	40	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	179	ALA	CB-CA-C	-5.74	101.49	110.10
1	A	99	THR	CB-CA-C	-5.72	96.17	111.60
1	A	177	VAL	N-CA-CB	-5.65	99.07	111.50
1	A	169	LEU	CA-CB-CG	5.61	128.21	115.30
1	A	457	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	479	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	475	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	239	ALA	CA-C-O	-5.46	108.64	120.10
1	A	236	PRO	CA-N-CD	-5.45	103.87	111.50
1	A	258	LEU	CA-C-N	5.42	129.13	117.20
1	A	101	ASP	N-CA-C	5.37	125.49	111.00
1	A	80	THR	N-CA-CB	5.36	120.48	110.30
1	A	538	PRO	C-N-CD	5.36	139.65	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ARG	N-CA-CB	-5.35	100.97	110.60
1	A	146	ASP	CB-CA-C	-5.27	99.85	110.40
1	A	260	GLY	N-CA-C	-5.26	99.95	113.10
1	A	440	THR	N-CA-CB	5.24	120.26	110.30
1	A	336	GLN	CA-CB-CG	5.15	124.72	113.40
1	A	100	TRP	CA-CB-CG	5.14	123.46	113.70
1	A	449	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	288	ARG	N-CA-CB	5.04	119.67	110.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	TRP	Mainchain
1	A	179	ALA	Mainchain
1	A	241	PRO	Mainchain
1	A	245	VAL	Mainchain
1	A	246	PRO	Mainchain
1	A	99	THR	Mainchain

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	3847	0	3837	235	0
2	A	277	0	0	33	1
All	All	4124	0	3837	235	1

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 31.

All (235) 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:230:LEU:HD13	1:A:231:ALA:HA	1.20	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:N	2:A:776:HOH:O	1.84	1.08
1:A:145:VAL:HG12	1:A:231:ALA:HB2	1.39	1.02
1:A:100:TRP:HA	1:A:245:VAL:HG21	1.45	0.97
1:A:100:TRP:HA	1:A:245:VAL:CG2	1.95	0.97
1:A:230:LEU:HD13	1:A:231:ALA:CA	1.93	0.96
1:A:245:VAL:HG12	1:A:246:PRO:CD	1.97	0.94
1:A:202:THR:OG1	1:A:228:ASP:HB3	1.67	0.94
1:A:393:THR:HG21	1:A:396:VAL:HG23	1.50	0.91
1:A:368:LEU:HB2	2:A:781:HOH:O	1.69	0.91
1:A:100:TRP:HB2	1:A:245:VAL:HG13	1.53	0.91
1:A:146:ASP:HB3	1:A:231:ALA:HB3	1.51	0.90
1:A:202:THR:HG1	1:A:228:ASP:HB3	1.35	0.89
1:A:230:LEU:CD1	1:A:231:ALA:HA	2.05	0.85
1:A:100:TRP:HB2	1:A:245:VAL:CG1	2.07	0.85
1:A:317:ARG:NH2	2:A:723:HOH:O	2.08	0.85
1:A:145:VAL:CG1	1:A:231:ALA:HB2	2.07	0.84
1:A:2:TRP:HB3	2:A:722:HOH:O	1.77	0.83
1:A:390:THR:HB	1:A:407:VAL:HB	1.61	0.83
1:A:76:LEU:HB3	1:A:80:THR:HG21	1.59	0.83
1:A:230:LEU:HD11	2:A:681:HOH:O	1.78	0.82
1:A:289:VAL:HG13	1:A:293:ALA:HB3	1.61	0.82
1:A:245:VAL:HG12	1:A:246:PRO:N	1.91	0.81
1:A:240:VAL:CB	1:A:241:PRO:HA	2.09	0.81
1:A:100:TRP:C	1:A:245:VAL:HG11	2.01	0.81
1:A:240:VAL:HB	1:A:241:PRO:HA	1.62	0.81
1:A:146:ASP:CB	1:A:231:ALA:HB3	2.13	0.78
1:A:232:GLY:HA2	2:A:554:HOH:O	1.86	0.76
1:A:240:VAL:HB	1:A:241:PRO:CA	2.15	0.76
1:A:101:ASP:HA	1:A:246:PRO:O	1.85	0.76
1:A:36:LYS:HE2	2:A:647:HOH:O	1.85	0.76
1:A:162:LEU:HB2	1:A:163:PRO:CD	2.17	0.74
1:A:139:VAL:HB	1:A:169:LEU:HD22	1.69	0.73
1:A:239:ALA:O	1:A:240:VAL:C	2.26	0.73
1:A:317:ARG:CZ	2:A:723:HOH:O	2.37	0.72
1:A:172:THR:HB	2:A:665:HOH:O	1.88	0.72
1:A:261:TRP:HB3	1:A:281:PRO:HG3	1.71	0.72
1:A:73:ARG:HA	1:A:249:PHE:HB3	1.71	0.72
1:A:363:ILE:HB	1:A:393:THR:HG23	1.72	0.72
1:A:230:LEU:HD13	1:A:231:ALA:N	2.04	0.71
1:A:99:THR:HA	2:A:637:HOH:O	1.90	0.71
1:A:230:LEU:HA	2:A:776:HOH:O	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:N	1:A:245:VAL:HG11	2.05	0.70
1:A:298:PRO:HD3	2:A:679:HOH:O	1.90	0.69
1:A:202:THR:HG23	2:A:682:HOH:O	1.92	0.68
1:A:230:LEU:CA	2:A:776:HOH:O	2.33	0.68
1:A:245:VAL:HG12	1:A:246:PRO:HD2	1.76	0.67
1:A:519:ARG:O	1:A:534:GLY:HA2	1.95	0.66
1:A:66:GLN:NE2	1:A:247:GLY:HA2	2.10	0.66
1:A:179:ALA:CB	1:A:239:ALA:HA	2.26	0.66
1:A:12:GLU:HG2	1:A:13:ARG:HD3	1.77	0.66
1:A:183:PRO:HG3	1:A:205:ARG:HH22	1.60	0.66
1:A:177:VAL:HG22	1:A:229:ALA:HA	1.78	0.65
1:A:390:THR:HG23	2:A:578:HOH:O	1.96	0.65
1:A:162:LEU:CB	1:A:163:PRO:CD	2.75	0.65
1:A:234:ALA:O	1:A:236:PRO:HD3	1.97	0.64
1:A:261:TRP:HE3	1:A:281:PRO:HD3	1.62	0.64
1:A:258:LEU:HB3	1:A:288:ARG:NH2	2.12	0.64
1:A:146:ASP:HB3	1:A:230:LEU:O	1.98	0.63
1:A:15:HIS:HD2	1:A:43:GLN:H	1.45	0.63
1:A:245:VAL:HG12	1:A:246:PRO:CG	2.28	0.63
1:A:183:PRO:HB3	1:A:256:PRO:HG3	1.81	0.62
1:A:101:ASP:OD1	1:A:246:PRO:HG2	2.00	0.61
1:A:227:GLY:HA2	2:A:693:HOH:O	1.98	0.61
1:A:240:VAL:HG11	1:A:243:GLY:HA3	1.82	0.61
1:A:75:PHE:CD1	1:A:250:GLY:HA3	2.35	0.61
1:A:73:ARG:CA	1:A:249:PHE:HB3	2.31	0.60
1:A:162:LEU:HB2	1:A:163:PRO:HD2	1.83	0.60
1:A:72:ILE:O	1:A:73:ARG:HB2	2.02	0.60
1:A:484:GLU:HB3	2:A:798:HOH:O	2.01	0.60
1:A:240:VAL:CB	1:A:241:PRO:CA	2.78	0.60
1:A:261:TRP:CE3	1:A:281:PRO:HD3	2.36	0.60
1:A:394:ARG:NE	1:A:413:ASN:ND2	2.50	0.60
1:A:78:THR:HG22	1:A:95:ASN:HB2	1.84	0.59
1:A:169:LEU:HD13	1:A:172:THR:CG2	2.33	0.58
1:A:9:LYS:HB3	1:A:14:GLN:HG2	1.85	0.58
1:A:169:LEU:HB3	1:A:172:THR:CG2	2.34	0.58
1:A:230:LEU:HB3	2:A:778:HOH:O	2.03	0.58
1:A:381:VAL:HG22	1:A:399:LEU:HD13	1.84	0.58
1:A:238:GLY:O	1:A:239:ALA:HB3	2.03	0.58
1:A:169:LEU:HD13	1:A:172:THR:HG23	1.86	0.57
1:A:343:ARG:HD2	1:A:379:LEU:HD22	1.85	0.57
1:A:283:LEU:HD12	1:A:283:LEU:H	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TRP:CA	1:A:245:VAL:HG11	2.35	0.57
1:A:273:LEU:O	1:A:298:PRO:HD2	2.05	0.57
1:A:100:TRP:HA	1:A:245:VAL:CB	2.34	0.56
1:A:202:THR:HA	1:A:225:ARG:O	2.05	0.56
1:A:282:GLU:HA	1:A:306:HIS:HB2	1.86	0.56
1:A:345:LEU:HB3	1:A:346:PRO:HD2	1.87	0.56
1:A:245:VAL:CG1	1:A:246:PRO:HD2	2.35	0.56
1:A:75:PHE:HD1	1:A:250:GLY:HA3	1.71	0.55
1:A:172:THR:CB	2:A:665:HOH:O	2.48	0.55
1:A:229:ALA:HB1	2:A:776:HOH:O	2.07	0.55
1:A:289:VAL:HG12	1:A:325:LEU:HD22	1.88	0.55
1:A:248:GLY:O	1:A:249:PHE:HB2	2.06	0.55
1:A:469:ASP:C	1:A:469:ASP:OD1	2.44	0.55
1:A:245:VAL:HG12	1:A:246:PRO:HG2	1.89	0.55
1:A:448:GLY:H	1:A:474:HIS:HD2	1.55	0.55
1:A:78:THR:HG23	1:A:106:ALA:HA	1.88	0.54
1:A:4:ASN:HA	1:A:32:GLY:O	2.08	0.54
1:A:240:VAL:CG2	1:A:241:PRO:HA	2.38	0.54
1:A:77:GLY:H	1:A:80:THR:HG22	1.73	0.53
1:A:112:GLU:HG2	1:A:163:PRO:HG2	1.90	0.53
1:A:184:ALA:HA	1:A:207:ALA:O	2.08	0.53
1:A:100:TRP:CA	1:A:245:VAL:HG21	2.29	0.53
1:A:228:ASP:O	1:A:229:ALA:CB	2.55	0.53
1:A:36:LYS:HB2	1:A:36:LYS:NZ	2.23	0.53
1:A:105:ILE:HD13	1:A:130:GLN:HG3	1.90	0.53
1:A:239:ALA:O	1:A:240:VAL:O	2.27	0.52
1:A:101:ASP:OD1	1:A:246:PRO:CG	2.57	0.52
1:A:314:GLY:O	1:A:315:ALA:CB	2.58	0.52
1:A:227:GLY:O	1:A:228:ASP:HB3	2.10	0.52
1:A:520:TYR:HB3	1:A:532:LEU:HG	1.91	0.52
1:A:146:ASP:CG	1:A:231:ALA:HB3	2.30	0.52
1:A:161:ASP:OD1	1:A:162:LEU:HG	2.10	0.52
1:A:146:ASP:OD1	1:A:231:ALA:HB3	2.09	0.51
1:A:256:PRO:CG	1:A:257:VAL:H	2.24	0.51
1:A:177:VAL:HG13	2:A:804:HOH:O	2.09	0.51
1:A:100:TRP:CB	1:A:245:VAL:CG1	2.86	0.51
1:A:484:GLU:HB2	1:A:516:GLY:HA3	1.92	0.50
1:A:162:LEU:HB2	1:A:163:PRO:HD3	1.93	0.50
1:A:314:GLY:O	1:A:347:GLU:OE1	2.29	0.50
1:A:381:VAL:HG22	1:A:399:LEU:CD1	2.41	0.50
1:A:146:ASP:HB3	1:A:231:ALA:CB	2.34	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:HB3	2:A:704:HOH:O	2.11	0.50
1:A:448:GLY:H	1:A:474:HIS:CD2	2.30	0.49
1:A:18:HIS:CE1	1:A:20:GLN:HG2	2.48	0.49
1:A:77:GLY:O	1:A:80:THR:HG22	2.12	0.49
1:A:440:THR:HB	1:A:465:VAL:HB	1.93	0.49
1:A:230:LEU:CG	1:A:231:ALA:N	2.76	0.49
1:A:15:HIS:CD2	1:A:43:GLN:H	2.28	0.49
1:A:228:ASP:O	1:A:229:ALA:HB2	2.12	0.49
1:A:256:PRO:HG2	1:A:257:VAL:H	1.77	0.49
1:A:342:TYR:CE2	1:A:344:VAL:HG22	2.47	0.49
1:A:341:LEU:HD13	1:A:342:TYR:N	2.27	0.49
1:A:240:VAL:HB	1:A:241:PRO:C	2.33	0.48
1:A:240:VAL:HG23	1:A:241:PRO:HA	1.94	0.48
1:A:298:PRO:HB3	1:A:331:ALA:HB3	1.96	0.48
1:A:398:SER:HB2	2:A:800:HOH:O	2.13	0.48
1:A:234:ALA:HA	2:A:771:HOH:O	2.13	0.48
1:A:262:TYR:HA	1:A:285:ALA:O	2.13	0.48
1:A:498:LEU:HD12	1:A:498:LEU:O	2.14	0.48
1:A:43:GLN:HE21	1:A:46:LEU:HD22	1.79	0.47
1:A:224:ILE:HG22	1:A:224:ILE:O	2.14	0.47
1:A:230:LEU:CD1	1:A:231:ALA:N	2.75	0.47
1:A:180:SER:O	1:A:182:ALA:N	2.39	0.47
1:A:100:TRP:CA	1:A:245:VAL:CG1	2.93	0.47
1:A:177:VAL:CG2	1:A:230:LEU:H	2.28	0.47
1:A:258:LEU:CB	1:A:288:ARG:NH2	2.76	0.47
1:A:273:LEU:O	1:A:298:PRO:CD	2.62	0.47
1:A:2:TRP:CD1	1:A:30:ALA:HB2	2.50	0.47
1:A:126:ALA:O	1:A:180:SER:HB2	2.14	0.47
1:A:521:ARG:HD2	2:A:805:HOH:O	2.13	0.47
1:A:342:TYR:HE2	1:A:344:VAL:HG22	1.78	0.47
1:A:406:TRP:CZ2	1:A:408:MET:HG3	2.50	0.47
1:A:71:GLY:O	1:A:72:ILE:C	2.53	0.47
1:A:489:ASN:C	1:A:489:ASN:HD22	2.18	0.47
1:A:243:GLY:O	1:A:244:ALA:CB	2.63	0.47
1:A:281:PRO:HG2	1:A:283:LEU:O	2.15	0.47
1:A:334:HIS:HB2	2:A:770:HOH:O	2.14	0.47
1:A:183:PRO:HG3	1:A:205:ARG:NH2	2.28	0.46
1:A:224:ILE:HB	1:A:278:VAL:HG22	1.96	0.46
1:A:490:THR:HG22	1:A:533:VAL:HA	1.97	0.46
1:A:524:ALA:HB2	1:A:530:TRP:CE3	2.51	0.46
1:A:317:ARG:NH1	2:A:723:HOH:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:TYR:HA	1:A:534:GLY:HA2	1.97	0.46
1:A:309:VAL:HG11	1:A:335:ALA:HB1	1.98	0.46
1:A:271:VAL:HG12	1:A:273:LEU:HD12	1.97	0.46
1:A:183:PRO:HG2	1:A:255:GLY:O	2.16	0.46
1:A:12:GLU:HG2	1:A:13:ARG:CD	2.45	0.45
1:A:90:HIS:HA	1:A:120:ASP:O	2.16	0.45
1:A:182:ALA:HA	1:A:183:PRO:HD3	1.82	0.45
1:A:177:VAL:CG2	1:A:230:LEU:N	2.79	0.45
1:A:420:ALA:O	1:A:421:SER:C	2.55	0.45
1:A:120:ASP:HA	1:A:141:ARG:O	2.17	0.45
1:A:229:ALA:O	1:A:230:LEU:CB	2.64	0.45
1:A:419:LEU:HD13	1:A:448:GLY:HA3	1.99	0.45
1:A:258:LEU:HB3	1:A:288:ARG:HH22	1.78	0.45
1:A:155:GLN:O	1:A:156:SER:C	2.56	0.44
1:A:161:ASP:CG	1:A:162:LEU:H	2.20	0.44
1:A:410:ASP:OD1	1:A:411:ASN:N	2.45	0.44
1:A:12:GLU:O	1:A:13:ARG:C	2.57	0.44
1:A:112:GLU:OE2	1:A:163:PRO:HD2	2.18	0.44
1:A:289:VAL:CG1	1:A:325:LEU:HD22	2.48	0.44
1:A:66:GLN:HG2	2:A:666:HOH:O	2.17	0.43
1:A:441:VAL:HG12	1:A:465:VAL:O	2.17	0.43
1:A:513:VAL:HG13	1:A:520:TYR:HB2	1.99	0.43
1:A:172:THR:CG2	2:A:665:HOH:O	2.67	0.43
1:A:343:ARG:CD	1:A:379:LEU:HD22	2.47	0.43
1:A:386:GLN:HE21	1:A:386:GLN:HA	1.82	0.43
1:A:212:MET:CE	1:A:267:SER:HB3	2.47	0.43
1:A:394:ARG:HE	1:A:413:ASN:ND2	2.15	0.43
1:A:78:THR:CG2	1:A:106:ALA:HA	2.47	0.43
1:A:388:ARG:HD3	1:A:390:THR:HG22	2.01	0.43
1:A:230:LEU:HD22	1:A:231:ALA:H	1.83	0.43
1:A:418:ARG:HD2	2:A:800:HOH:O	2.18	0.43
1:A:212:MET:HE3	1:A:267:SER:HB3	2.01	0.42
1:A:366:THR:O	1:A:368:LEU:N	2.52	0.42
1:A:179:ALA:HA	1:A:239:ALA:CB	2.49	0.42
1:A:243:GLY:O	1:A:244:ALA:HB3	2.19	0.42
1:A:414:VAL:O	1:A:441:VAL:HA	2.18	0.42
1:A:183:PRO:HD2	1:A:254:PHE:O	2.18	0.42
1:A:234:ALA:C	1:A:236:PRO:HD3	2.39	0.42
1:A:162:LEU:CB	1:A:163:PRO:HD3	2.47	0.42
1:A:245:VAL:CG1	1:A:246:PRO:CD	2.81	0.42
1:A:183:PRO:HB3	1:A:256:PRO:CG	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:HA	1:A:413:ASN:HB2	2.02	0.42
1:A:454:VAL:HG13	1:A:491:LEU:HD13	2.01	0.42
1:A:197:ASP:OD1	1:A:221:ARG:HD2	2.20	0.42
1:A:218:HIS:O	1:A:218:HIS:ND1	2.51	0.42
1:A:256:PRO:O	1:A:257:VAL:HB	2.19	0.42
1:A:512:LYS:HE2	1:A:519:ARG:NH1	2.34	0.42
1:A:177:VAL:HG21	1:A:230:LEU:N	2.35	0.41
1:A:179:ALA:HB2	1:A:239:ALA:CA	2.50	0.41
1:A:146:ASP:HB2	1:A:177:VAL:HB	2.02	0.41
1:A:497:PRO:O	1:A:500:SER:HB3	2.20	0.41
1:A:200:HIS:HD2	1:A:223:THR:OG1	2.03	0.41
1:A:238:GLY:N	2:A:809:HOH:O	2.53	0.41
1:A:498:LEU:HD13	1:A:527:ASN:HA	2.02	0.41
1:A:261:TRP:CH2	1:A:263:GLY:HA2	2.56	0.41
1:A:169:LEU:HD13	1:A:172:THR:HG21	2.02	0.41
1:A:172:THR:HG22	2:A:665:HOH:O	2.20	0.41
1:A:372:PRO:O	1:A:374:THR:N	2.53	0.41
1:A:9:LYS:HB2	1:A:37:VAL:HG22	2.04	0.40
1:A:15:HIS:HD2	1:A:43:GLN:N	2.17	0.40
1:A:287:ILE:HD13	1:A:295:VAL:HG11	2.02	0.40
1:A:2:TRP:HA	1:A:5:GLN:NE2	2.35	0.40
1:A:36:LYS:HE3	1:A:62:THR:HG23	2.04	0.40
1:A:132:GLU:HG3	1:A:133:ARG:HG3	2.03	0.40
1:A:140:GLN:HG2	1:A:170:ARG:HB3	2.04	0.40
1:A:490:THR:HG22	1:A:533:VAL:O	2.21	0.40
1:A:490:THR:HG23	2:A:602:HOH:O	2.22	0.40
1:A:158:GLN:O	1:A:159:PRO:C	2.59	0.40
1:A:227:GLY:O	1:A:228:ASP:CB	2.68	0.40
1:A:366:THR:O	1:A:367:GLU:C	2.60	0.40

All (1) 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)
2:A:766:HOH:O	2:A:809:HOH:O[2_665]	2.04	0.16

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	537/539 (100%)	475 (88%)	33 (6%)	29 (5%)	2 2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ILE
1	A	100	TRP
1	A	101	ASP
1	A	162	LEU
1	A	228	ASP
1	A	229	ALA
1	A	231	ALA
1	A	236	PRO
1	A	240	VAL
1	A	244	ALA
1	A	256	PRO
1	A	257	VAL
1	A	315	ALA
1	A	367	GLU
1	A	373	GLY
1	A	155	GLN
1	A	156	SER
1	A	230	LEU
1	A	500	SER
1	A	526	GLY
1	A	74	ARG
1	A	159	PRO
1	A	161	ASP
1	A	181	GLY
1	A	239	ALA
1	A	13	ARG
1	A	385	SER
1	A	314	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	371	ILE

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	389/389 (100%)	345 (89%)	44 (11%)	6 11

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	2	TRP
1	A	13	ARG
1	A	36	LYS
1	A	43	GLN
1	A	54	LEU
1	A	62	THR
1	A	78	THR
1	A	80	THR
1	A	93	LEU
1	A	96	VAL
1	A	123	LEU
1	A	172	THR
1	A	177	VAL
1	A	202	THR
1	A	226	ARG
1	A	240	VAL
1	A	245	VAL
1	A	246	PRO
1	A	282	GLU
1	A	283	LEU
1	A	294	ARG
1	A	301	SER
1	A	303	SER
1	A	336	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	340	LEU
1	A	341	LEU
1	A	345	LEU
1	A	368	LEU
1	A	370	SER
1	A	386	GLN
1	A	390	THR
1	A	393	THR
1	A	405	THR
1	A	440	THR
1	A	464	LEU
1	A	471	SER
1	A	473	GLN
1	A	484	GLU
1	A	489	ASN
1	A	498	LEU
1	A	500	SER
1	A	503	THR
1	A	512	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	41	GLN
1	A	43	GLN
1	A	66	GLN
1	A	150	HIS
1	A	200	HIS
1	A	336	GLN
1	A	386	GLN
1	A	413	ASN
1	A	474	HIS
1	A	489	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 monosaccharides 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 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.