



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:05 AM UTC

PDB ID : 1V10 / pdb_00001v10
Title : Structure of Rigidoporus lignosus laccase from hemihedrally twinned crystals
Authors : Rizzi, M.; Garavaglia, S.; Palmieri, F.; Cambria, A.
Deposited on : 2004-04-02
Resolution : 1.70 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

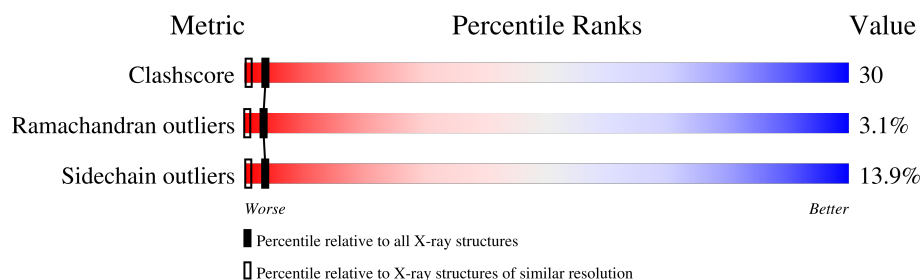
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

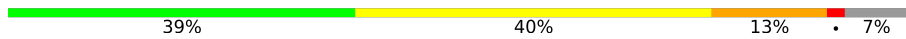
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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	521	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3769 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 LACCASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3684	2328	645	703	8			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cu	0	0
			4	4		

- Molecule 3 is water.

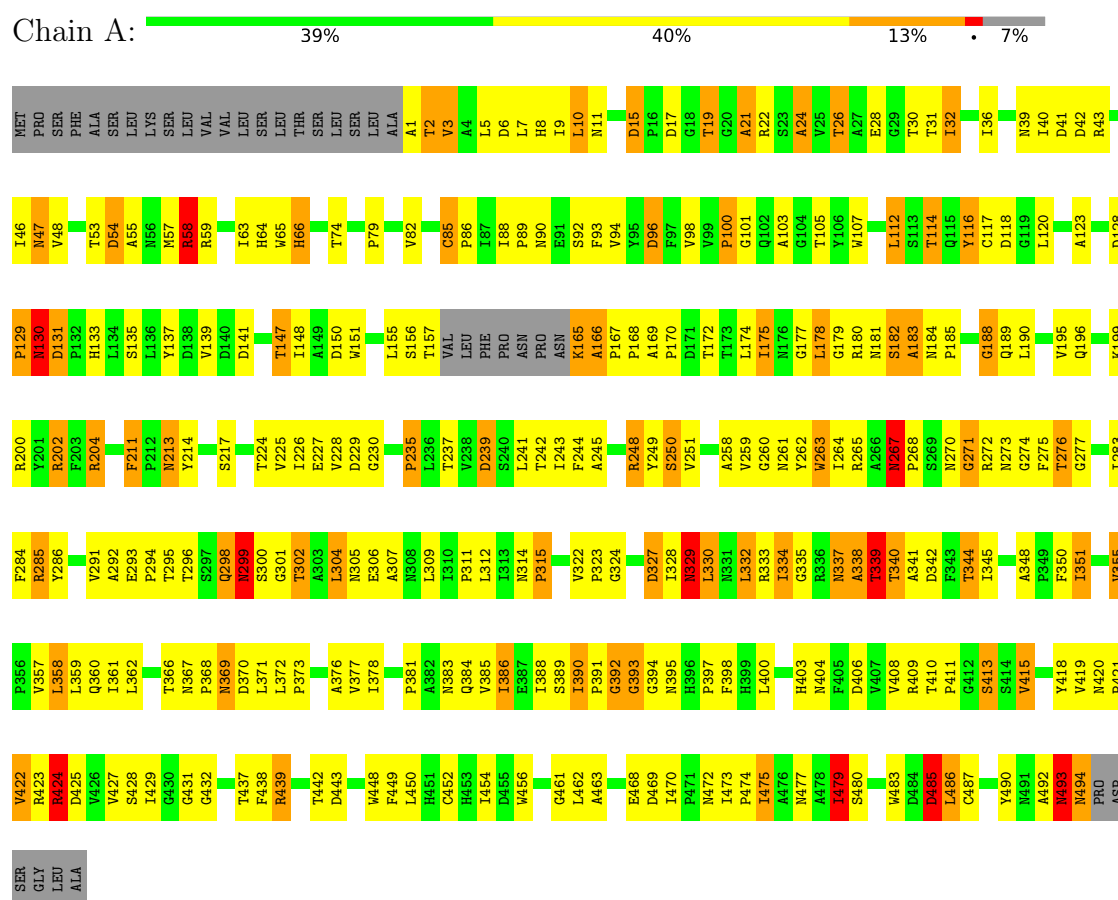
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		

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: LACCASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	124.91Å 124.91Å 95.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.70	Depositor
% Data completeness (in resolution range)	99.0 (20.00-1.70)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.226 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3769	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: CU

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	0.62	4/3786 (0.1%)	1.89	100/5200 (1.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	ASN	C-O	-9.63	1.04	1.23
1	A	179	GLY	N-CA	6.61	1.52	1.45
1	A	179	GLY	CA-C	5.89	1.57	1.51
1	A	178	LEU	CA-C	5.06	1.58	1.52

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	494	ASN	CA-C-O	17.67	150.84	120.80
1	A	166	ALA	O-C-N	11.39	130.77	121.20
1	A	329	ASN	CA-CB-CG	10.32	122.92	112.60
1	A	443	ASP	CA-C-N	9.14	133.67	122.42
1	A	443	ASP	C-N-CA	9.14	133.67	122.42
1	A	298	GLN	O-C-N	8.95	133.24	122.68
1	A	314	ASN	O-C-N	8.82	131.47	121.32
1	A	299	ASN	O-C-N	8.54	133.95	122.59
1	A	211	PHE	CA-CB-CG	8.24	122.04	113.80
1	A	235	PRO	CA-C-O	-8.21	112.65	121.27
1	A	493	ASN	CA-CB-CG	-8.19	104.41	112.60
1	A	116	TYR	CA-CB-CG	8.17	128.61	113.90
1	A	156	SER	CA-C-N	8.06	136.21	121.70
1	A	156	SER	C-N-CA	8.06	136.21	121.70
1	A	314	ASN	CA-C-N	8.05	129.91	119.84
1	A	314	ASN	C-N-CA	8.05	129.91	119.84
1	A	230	GLY	CA-C-N	-7.88	113.42	123.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	GLY	C-N-CA	-7.88	113.42	123.19
1	A	424	ARG	NE-CZ-NH2	7.31	125.78	119.20
1	A	398	PHE	CA-CB-CG	-7.11	106.69	113.80
1	A	130	ASN	CA-CB-CG	7.07	119.67	112.60
1	A	492	ALA	CA-C-N	7.00	134.91	121.54
1	A	492	ALA	C-N-CA	7.00	134.91	121.54
1	A	235	PRO	O-C-N	6.88	130.48	122.98
1	A	47	ASN	CA-C-N	-6.68	114.02	122.37
1	A	47	ASN	C-N-CA	-6.68	114.02	122.37
1	A	335	GLY	CA-C-N	-6.68	113.34	122.16
1	A	335	GLY	C-N-CA	-6.68	113.34	122.16
1	A	276	THR	CA-C-O	6.62	128.25	120.58
1	A	204	ARG	O-C-N	6.54	130.68	123.22
1	A	96	ASP	CA-CB-CG	6.47	119.07	112.60
1	A	131	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	129	PRO	CA-C-N	6.38	132.81	122.67
1	A	129	PRO	C-N-CA	6.38	132.81	122.67
1	A	271	GLY	CA-C-O	-6.33	115.18	122.78
1	A	202	ARG	CA-C-O	-6.32	114.27	121.66
1	A	367	ASN	O-C-N	6.28	126.64	121.31
1	A	267	ASN	O-C-N	6.26	126.30	121.23
1	A	275	PHE	CA-CB-CG	-6.24	107.56	113.80
1	A	217	SER	O-C-N	6.23	129.62	123.46
1	A	166	ALA	CA-C-O	-6.15	115.02	121.29
1	A	139	VAL	CA-C-N	6.14	129.92	121.33
1	A	139	VAL	C-N-CA	6.14	129.92	121.33
1	A	333	ARG	CA-C-N	6.14	130.29	122.37
1	A	333	ARG	C-N-CA	6.14	130.29	122.37
1	A	475	ILE	CA-C-N	6.09	128.44	120.28
1	A	475	ILE	C-N-CA	6.09	128.44	120.28
1	A	479	ILE	N-CA-C	6.07	116.10	106.88
1	A	285	ARG	CA-C-N	6.01	130.02	121.42
1	A	285	ARG	C-N-CA	6.01	130.02	121.42
1	A	184	ASN	CA-CB-CG	6.00	118.60	112.60
1	A	213	ASN	CA-C-O	-5.99	114.18	121.36
1	A	377	VAL	N-CA-C	5.94	116.41	107.80
1	A	217	SER	CA-C-N	5.86	130.98	123.13
1	A	217	SER	C-N-CA	5.86	130.98	123.13
1	A	24	ALA	CA-C-N	5.82	129.65	122.37
1	A	24	ALA	C-N-CA	5.82	129.65	122.37
1	A	183	ALA	N-CA-C	-5.81	104.95	111.28
1	A	242	THR	CA-C-N	-5.79	116.01	123.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	THR	C-N-CA	-5.79	116.01	123.19
1	A	123	ALA	O-C-N	5.79	129.50	122.96
1	A	213	ASN	O-C-N	5.76	129.51	123.06
1	A	485	ASP	CA-CB-CG	5.75	118.35	112.60
1	A	270	ASN	CA-CB-CG	-5.74	106.86	112.60
1	A	130	ASN	CA-C-N	5.72	128.43	120.65
1	A	130	ASN	C-N-CA	5.72	128.43	120.65
1	A	54	ASP	O-C-N	5.62	130.13	122.82
1	A	461	GLY	CA-C-O	5.56	124.51	118.95
1	A	264	ILE	N-CA-CB	5.53	117.69	111.21
1	A	141	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	213	ASN	CA-C-N	5.48	130.72	122.99
1	A	213	ASN	C-N-CA	5.48	130.72	122.99
1	A	248	ARG	CA-C-N	5.48	131.16	122.94
1	A	248	ARG	C-N-CA	5.48	131.16	122.94
1	A	147	THR	CA-C-N	5.47	130.16	123.10
1	A	147	THR	C-N-CA	5.47	130.16	123.10
1	A	21	ALA	O-C-N	5.46	129.53	122.81
1	A	299	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	258	ALA	CA-C-O	-5.41	115.11	121.16
1	A	298	GLN	CA-C-N	5.40	131.85	121.54
1	A	298	GLN	C-N-CA	5.40	131.85	121.54
1	A	425	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	424	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	A	263	TRP	CA-C-N	5.35	129.75	122.90
1	A	263	TRP	C-N-CA	5.35	129.75	122.90
1	A	292	ALA	CA-C-N	5.34	127.83	120.67
1	A	292	ALA	C-N-CA	5.34	127.83	120.67
1	A	327	ASP	CA-C-O	5.28	125.78	119.60
1	A	448	TRP	CA-C-N	5.23	128.65	120.75
1	A	448	TRP	C-N-CA	5.23	128.65	120.75
1	A	327	ASP	N-CA-C	-5.22	106.06	112.90
1	A	389	SER	O-C-N	-5.21	117.10	123.30
1	A	188	GLY	N-CA-C	5.19	120.54	111.25
1	A	335	GLY	O-C-N	-5.16	118.80	123.29
1	A	85	CYS	N-CA-CB	5.14	116.25	110.03
1	A	66	HIS	CA-CB-CG	5.09	118.89	113.80
1	A	439	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	A	58	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	A	264	ILE	CA-C-O	-5.04	115.09	120.59
1	A	245	ALA	CA-C-O	5.03	126.23	120.80

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	3684	0	3529	215	0
2	A	4	0	0	0	0
3	A	81	0	0	5	0
All	All	3769	0	3529	215	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 30.

All (215) 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:392:GLY:HA2	1:A:429:ILE:HG22	1.50	0.93
1:A:1:ALA:HB3	1:A:36:ILE:HG12	1.50	0.92
1:A:178:LEU:HD22	1:A:189:GLN:HB3	1.53	0.92
1:A:32:ILE:HD11	1:A:177:GLY:N	1.86	0.91
1:A:267:ASN:HD21	1:A:274:GLY:H	1.12	0.91
1:A:1:ALA:HB1	1:A:5:LEU:HD22	1.53	0.90
1:A:470:ILE:HA	1:A:473:ILE:HD12	1.52	0.89
1:A:180:ARG:NH1	1:A:277:GLY:O	2.05	0.88
1:A:324:GLY:HA2	1:A:329:ASN:HD22	1.40	0.85
1:A:241:LEU:HD21	1:A:304:LEU:HD13	1.58	0.85
1:A:85:CYS:HG	1:A:487:CYS:HG	0.88	0.84
1:A:7:LEU:HD12	1:A:46:ILE:HG23	1.59	0.82
1:A:180:ARG:NH2	1:A:293:GLU:OE2	2.13	0.81
1:A:260:GLY:H	1:A:286:TYR:HB2	1.44	0.81
1:A:311:PRO:HB2	1:A:315:PRO:HG3	1.62	0.81
1:A:381:PRO:HG2	1:A:384:GLN:HG3	1.63	0.80
1:A:272:ARG:HH21	1:A:276:THR:HB	1.48	0.78
1:A:411:PRO:HG3	1:A:428:SER:O	1.87	0.75
1:A:196:GLN:HB2	1:A:199:LYS:HD2	1.68	0.75
1:A:261:ASN:HD21	1:A:285:ARG:HE	1.32	0.74
1:A:11:ASN:ND2	1:A:53:THR:H	1.85	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:OD1	1:A:19:THR:HB	1.89	0.73
1:A:26:THR:HG21	1:A:30:THR:O	1.90	0.72
1:A:267:ASN:HD21	1:A:274:GLY:N	1.88	0.72
1:A:272:ARG:NH2	1:A:276:THR:HB	2.04	0.71
1:A:148:ILE:HD12	1:A:175:ILE:HD13	1.72	0.71
1:A:285:ARG:NH1	1:A:291:VAL:HG13	2.05	0.71
1:A:11:ASN:ND2	1:A:54:ASP:H	1.89	0.71
1:A:285:ARG:HH12	1:A:291:VAL:HG13	1.58	0.69
1:A:413:SER:OG	1:A:415:VAL:HG23	1.93	0.69
1:A:267:ASN:HD22	1:A:268:PRO:HD2	1.57	0.68
1:A:390:ILE:HB	1:A:429:ILE:HD13	1.76	0.67
1:A:129:PRO:HB2	1:A:130:ASN:ND2	2.10	0.67
1:A:114:THR:HG22	1:A:117:CYS:SG	2.35	0.66
1:A:493:ASN:O	1:A:494:ASN:HB2	1.95	0.66
1:A:327:ASP:H	1:A:385:VAL:HG23	1.60	0.66
1:A:7:LEU:HD11	1:A:36:ILE:HD11	1.77	0.65
1:A:298:GLN:HG2	1:A:299:ASN:N	2.12	0.64
1:A:397:PRO:HD2	1:A:452:CYS:SG	2.38	0.64
1:A:6:ASP:O	1:A:7:LEU:HG	1.98	0.64
1:A:261:ASN:ND2	1:A:285:ARG:HB2	2.13	0.64
1:A:261:ASN:ND2	1:A:285:ARG:HE	1.96	0.64
1:A:388:ILE:O	1:A:437:THR:HA	1.98	0.62
1:A:483:TRP:HA	1:A:486:LEU:HD11	1.81	0.62
1:A:88:ILE:HG22	1:A:89:PRO:O	1.99	0.62
1:A:11:ASN:HD21	1:A:54:ASP:H	1.48	0.62
1:A:114:THR:HG21	1:A:456:TRP:CE3	2.35	0.62
1:A:2:THR:HG22	1:A:3:VAL:H	1.65	0.61
1:A:128:ASP:HB3	1:A:131:ASP:HB2	1.81	0.61
1:A:259:VAL:HG13	1:A:286:TYR:HB3	1.82	0.61
1:A:11:ASN:HD21	1:A:53:THR:H	1.48	0.60
1:A:74:THR:HG23	1:A:358:LEU:HD11	1.82	0.60
1:A:268:PRO:HG2	1:A:273:ASN:ND2	2.16	0.60
1:A:394:GLY:O	1:A:395:ASN:HB2	2.00	0.60
1:A:357:VAL:O	1:A:361:ILE:HG13	2.01	0.60
1:A:369:ASN:OD1	1:A:370:ASP:OD1	2.19	0.60
1:A:165:LYS:HZ2	1:A:339:THR:HB	1.67	0.59
1:A:332:LEU:HB2	1:A:390:ILE:HG23	1.85	0.59
1:A:243:ILE:HD12	1:A:249:TYR:HD2	1.68	0.59
1:A:408:VAL:HG11	1:A:418:TYR:CE1	2.38	0.58
1:A:351:ILE:HG12	1:A:351:ILE:O	2.03	0.58
1:A:172:THR:HG23	1:A:180:ARG:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PRO:HB2	1:A:82:VAL:HB	1.86	0.58
1:A:337:ASN:CB	1:A:342:ASP:HB3	2.34	0.57
1:A:46:ILE:HG21	1:A:65:TRP:CH2	2.38	0.57
1:A:298:GLN:CG	1:A:299:ASN:N	2.67	0.57
1:A:105:THR:HG21	1:A:204:ARG:HB3	1.87	0.57
1:A:327:ASP:OD2	1:A:385:VAL:HG22	2.04	0.57
1:A:74:THR:H	1:A:477:ASN:ND2	2.03	0.57
1:A:3:VAL:HG13	1:A:43:ARG:O	2.04	0.56
1:A:383:ASN:HB3	3:A:2069:HOH:O	2.04	0.56
1:A:1:ALA:HB1	1:A:5:LEU:CD2	2.31	0.56
1:A:214:TYR:HA	1:A:267:ASN:O	2.06	0.56
1:A:89:PRO:O	1:A:90:ASN:HB2	2.06	0.56
1:A:129:PRO:HB2	1:A:130:ASN:HD22	1.70	0.56
1:A:493:ASN:O	1:A:494:ASN:CB	2.54	0.56
1:A:150:ASP:HB2	1:A:170:PRO:HB3	1.88	0.55
1:A:227:GLU:HB3	1:A:250:SER:HB2	1.87	0.55
1:A:263:TRP:CD2	1:A:294:PRO:HB2	2.42	0.55
1:A:340:THR:O	1:A:340:THR:HG22	2.06	0.55
1:A:58:ARG:HD3	1:A:112:LEU:HD21	1.89	0.54
1:A:386:ILE:O	1:A:439:ARG:HA	2.08	0.54
1:A:404:ASN:CG	1:A:423:ARG:HE	2.16	0.54
1:A:8:HIS:HD2	1:A:28:GLU:OE2	1.92	0.53
1:A:19:THR:OG1	1:A:183:ALA:HB3	2.08	0.53
1:A:322:VAL:HG22	1:A:323:PRO:O	2.09	0.53
1:A:30:THR:HG22	1:A:32:ILE:H	1.74	0.53
1:A:40:ILE:HD11	1:A:101:GLY:HA2	1.91	0.52
1:A:305:ASN:OD1	1:A:307:ALA:HB3	2.08	0.52
1:A:327:ASP:N	1:A:385:VAL:HG23	2.24	0.52
1:A:225:VAL:O	1:A:235:PRO:HA	2.10	0.52
1:A:239:ASP:OD1	1:A:302:THR:HB	2.09	0.52
1:A:373:PRO:HG2	1:A:376:ALA:HB3	1.92	0.52
1:A:429:ILE:HG22	1:A:429:ILE:O	2.08	0.52
1:A:479:ILE:O	1:A:479:ILE:HG22	2.10	0.52
1:A:228:VAL:HG21	1:A:309:LEU:HD13	1.91	0.51
1:A:195:VAL:HG11	1:A:284:PHE:CZ	2.44	0.51
1:A:261:ASN:HD22	1:A:285:ARG:HB2	1.73	0.51
1:A:474:PRO:HG2	1:A:475:ILE:HG13	1.93	0.51
1:A:130:ASN:HD22	1:A:130:ASN:N	2.08	0.51
1:A:196:GLN:HB2	1:A:199:LYS:CD	2.40	0.51
1:A:302:THR:HG22	1:A:302:THR:O	2.11	0.51
1:A:408:VAL:HG11	1:A:418:TYR:CZ	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ASP:HA	1:A:47:ASN:HB3	1.92	0.51
1:A:58:ARG:CZ	1:A:112:LEU:HD11	2.40	0.51
1:A:182:SER:HA	1:A:185:PRO:HD3	1.92	0.51
1:A:454:ILE:O	1:A:454:ILE:HG22	2.10	0.51
1:A:262:TYR:CD2	1:A:296:THR:HG21	2.46	0.51
1:A:133:HIS:CD2	1:A:226:ILE:HB	2.46	0.51
1:A:1:ALA:CB	1:A:5:LEU:HD22	2.35	0.51
1:A:298:GLN:CG	1:A:299:ASN:H	2.22	0.51
1:A:57:MET:HG3	1:A:155:LEU:HD13	1.93	0.50
1:A:239:ASP:OD1	1:A:302:THR:O	2.30	0.50
1:A:8:HIS:O	1:A:9:ILE:HD13	2.11	0.50
1:A:165:LYS:O	1:A:340:THR:HG21	2.12	0.50
1:A:261:ASN:HD21	1:A:285:ARG:NE	2.06	0.50
1:A:400:LEU:HD21	1:A:403:HIS:HB2	1.92	0.50
1:A:338:ALA:O	1:A:339:THR:O	2.30	0.49
1:A:15:ASP:OD1	1:A:21:ALA:HB2	2.11	0.49
1:A:345:ILE:HD11	1:A:462:LEU:HD12	1.95	0.49
1:A:410:THR:HG22	1:A:411:PRO:O	2.13	0.49
1:A:74:THR:H	1:A:477:ASN:HD22	1.60	0.49
1:A:452:CYS:SG	1:A:454:ILE:HB	2.53	0.49
1:A:265:ARG:NE	1:A:298:GLN:HB2	2.28	0.48
1:A:241:LEU:HD23	1:A:304:LEU:HD22	1.95	0.48
1:A:85:CYS:CB	1:A:487:CYS:HG	2.24	0.48
1:A:283:ILE:HG12	1:A:294:PRO:HD3	1.94	0.48
1:A:168:PRO:O	1:A:169:ALA:HB2	2.13	0.48
1:A:337:ASN:ND2	1:A:342:ASP:HB3	2.28	0.48
1:A:358:LEU:HD22	1:A:362:LEU:CD1	2.44	0.48
1:A:400:LEU:HB2	1:A:450:LEU:CD1	2.43	0.48
1:A:419:VAL:HG12	1:A:420:ASN:CG	2.39	0.48
1:A:473:ILE:N	1:A:474:PRO:HD2	2.29	0.48
1:A:410:THR:HG23	1:A:411:PRO:HD2	1.96	0.47
1:A:94:VAL:HG13	1:A:94:VAL:O	2.15	0.47
1:A:24:ALA:HB1	1:A:118:ASP:O	2.14	0.47
1:A:107:TRP:CD1	1:A:248:ARG:HD2	2.50	0.47
1:A:79:PRO:HG2	3:A:2023:HOH:O	2.13	0.47
1:A:147:THR:C	1:A:148:ILE:HD13	2.40	0.47
1:A:309:LEU:HB2	1:A:422:VAL:HG13	1.96	0.47
1:A:11:ASN:HA	1:A:24:ALA:O	2.15	0.47
1:A:229:ASP:OD2	1:A:424:ARG:HB2	2.15	0.47
1:A:268:PRO:HG2	1:A:273:ASN:HD22	1.76	0.46
1:A:86:PRO:HG2	1:A:490:TYR:CE1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASN:HB3	1:A:244:PHE:CD2	2.51	0.46
1:A:324:GLY:HA2	1:A:329:ASN:ND2	2.20	0.46
1:A:241:LEU:CD2	1:A:304:LEU:HD22	2.46	0.46
1:A:334:ILE:HA	1:A:344:THR:O	2.16	0.46
1:A:406:ASP:O	1:A:438:PHE:HA	2.15	0.46
1:A:88:ILE:HD11	1:A:490:TYR:HA	1.96	0.46
1:A:182:SER:HB2	1:A:272:ARG:HH11	1.81	0.45
1:A:400:LEU:HB2	1:A:450:LEU:HD12	1.98	0.45
1:A:88:ILE:HG23	1:A:89:PRO:HD2	1.99	0.45
1:A:189:GLN:NE2	1:A:190:LEU:O	2.50	0.45
1:A:239:ASP:OD1	1:A:239:ASP:N	2.49	0.45
1:A:7:LEU:HD12	1:A:46:ILE:CG2	2.40	0.45
1:A:8:HIS:CD2	1:A:8:HIS:H	2.34	0.45
1:A:322:VAL:O	1:A:439:ARG:NH2	2.49	0.45
1:A:32:ILE:HD12	1:A:147:THR:OG1	2.15	0.45
1:A:409:ARG:NE	3:A:2074:HOH:O	2.49	0.45
1:A:469:ASP:OD1	1:A:472:ASN:ND2	2.50	0.45
1:A:344:THR:HG22	1:A:348:ALA:H	1.81	0.45
1:A:189:GLN:HG2	1:A:190:LEU:N	2.32	0.45
1:A:263:TRP:CE2	1:A:294:PRO:HB2	2.52	0.45
1:A:43:ARG:NH1	1:A:96:ASP:OD1	2.50	0.45
1:A:58:ARG:CD	1:A:112:LEU:HD21	2.46	0.44
1:A:271:GLY:O	1:A:273:ASN:ND2	2.50	0.44
1:A:372:LEU:HB3	1:A:373:PRO:HA	1.99	0.44
1:A:32:ILE:CD1	1:A:147:THR:OG1	2.65	0.44
1:A:165:LYS:HB3	1:A:166:ALA:H	1.35	0.44
1:A:350:PHE:HB2	1:A:463:ALA:O	2.18	0.44
1:A:442:THR:HA	1:A:468:GLU:OE2	2.18	0.44
1:A:485:ASP:N	1:A:485:ASP:OD1	2.50	0.44
1:A:388:ILE:O	1:A:437:THR:HG23	2.18	0.44
1:A:406:ASP:HB3	1:A:421:PRO:CG	2.48	0.44
1:A:386:ILE:HD13	1:A:386:ILE:N	2.33	0.44
1:A:355:VAL:HG13	1:A:359:LEU:HD23	2.00	0.43
1:A:224:THR:HG23	1:A:237:THR:OG1	2.17	0.43
1:A:85:CYS:HG	1:A:487:CYS:CB	2.27	0.43
1:A:259:VAL:HG23	3:A:2046:HOH:O	2.17	0.43
1:A:48:VAL:O	1:A:92:SER:HA	2.19	0.43
1:A:393:GLY:O	1:A:431:GLY:HA2	2.19	0.43
1:A:40:ILE:O	1:A:41:ASP:HB3	2.19	0.43
1:A:337:ASN:CG	1:A:342:ASP:HB3	2.44	0.43
1:A:419:VAL:HG12	1:A:420:ASN:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:CD1	1:A:486:LEU:HD21	2.54	0.43
1:A:175:ILE:N	1:A:178:LEU:O	2.45	0.43
1:A:332:LEU:O	1:A:390:ILE:HG23	2.19	0.43
1:A:32:ILE:HD11	1:A:177:GLY:H	1.74	0.42
1:A:224:THR:O	1:A:251:VAL:HA	2.19	0.42
1:A:392:GLY:HA2	1:A:429:ILE:CG2	2.37	0.42
1:A:339:THR:HB	1:A:340:THR:H	1.55	0.42
1:A:55:ALA:HA	1:A:59:ARG:NE	2.33	0.42
1:A:385:VAL:C	1:A:386:ILE:HD13	2.44	0.42
1:A:17:ASP:O	1:A:188:GLY:HA2	2.20	0.42
1:A:137:TYR:OH	1:A:202:ARG:NH2	2.52	0.42
1:A:103:ALA:CB	1:A:128:ASP:HB2	2.50	0.41
1:A:98:VAL:C	1:A:100:PRO:HD3	2.45	0.41
1:A:483:TRP:O	1:A:486:LEU:HD12	2.20	0.41
1:A:59:ARG:O	1:A:89:PRO:HG3	2.21	0.41
1:A:167:PRO:HG2	3:A:2036:HOH:O	2.21	0.41
1:A:368:PRO:HA	1:A:371:LEU:HD12	2.03	0.41
1:A:400:LEU:CD2	1:A:403:HIS:HB2	2.50	0.41
1:A:470:ILE:HA	1:A:473:ILE:CD1	2.34	0.41
1:A:135:SER:O	1:A:200:ARG:NH2	2.51	0.41
1:A:181:ASN:OD1	1:A:182:SER:N	2.49	0.41
1:A:182:SER:HB2	1:A:272:ARG:NH1	2.35	0.41
1:A:329:ASN:C	1:A:330:LEU:HD13	2.45	0.41
1:A:151:TRP:HB2	1:A:174:LEU:HD11	2.03	0.41
1:A:130:ASN:ND2	1:A:130:ASN:N	2.69	0.41
1:A:10:LEU:HD13	1:A:10:LEU:N	2.36	0.40
1:A:469:ASP:CG	1:A:472:ASN:HB2	2.47	0.40
1:A:39:ASN:O	1:A:42:ASP:HB2	2.20	0.40
1:A:64:HIS:NE2	1:A:66:HIS:HA	2.36	0.40
1:A:429:ILE:HD13	1:A:429:ILE:HG21	1.66	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	483/521 (93%)	420 (87%)	48 (10%)	15 (3%)	3 0

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	PHE
1	A	299	ASN
1	A	302	THR
1	A	338	ALA
1	A	339	THR
1	A	493	ASN
1	A	301	GLY
1	A	312	LEU
1	A	392	GLY
1	A	393	GLY
1	A	432	GLY
1	A	341	ALA
1	A	315	PRO
1	A	391	PRO
1	A	100	PRO

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	397/427 (93%)	342 (86%)	55 (14%)	3 0

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	VAL
1	A	10	LEU
1	A	15	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	19	THR
1	A	22	ARG
1	A	26	THR
1	A	31	THR
1	A	32	ILE
1	A	58	ARG
1	A	63	ILE
1	A	112	LEU
1	A	114	THR
1	A	116	TYR
1	A	120	LEU
1	A	130	ASN
1	A	157	THR
1	A	165	LYS
1	A	175	ILE
1	A	182	SER
1	A	239	ASP
1	A	250	SER
1	A	267	ASN
1	A	295	THR
1	A	300	SER
1	A	304	LEU
1	A	306	GLU
1	A	328	ILE
1	A	329	ASN
1	A	330	LEU
1	A	332	LEU
1	A	334	ILE
1	A	337	ASN
1	A	339	THR
1	A	340	THR
1	A	344	THR
1	A	351	ILE
1	A	355	VAL
1	A	358	LEU
1	A	360	GLN
1	A	366	THR
1	A	369	ASN
1	A	378	ILE
1	A	386	ILE
1	A	390	ILE
1	A	413	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	415	VAL
1	A	422	VAL
1	A	424	ARG
1	A	427	VAL
1	A	449	PHE
1	A	479	ILE
1	A	480	SER
1	A	485	ASP
1	A	486	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	ASN
1	A	47	ASN
1	A	70	GLN
1	A	130	ASN
1	A	133	HIS
1	A	213	ASN
1	A	233	HIS
1	A	257	GLN
1	A	261	ASN
1	A	267	ASN
1	A	273	ASN
1	A	287	GLN
1	A	329	ASN
1	A	477	ASN

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.