Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:44 PM GMT

PDB ID	:	1V10
Title	:	STRUCTURE OF RIGIDOPORUS LIGNOSUS LACCASE FROM HEMI-HEDRALLY TWINNED CRYSTALS
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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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

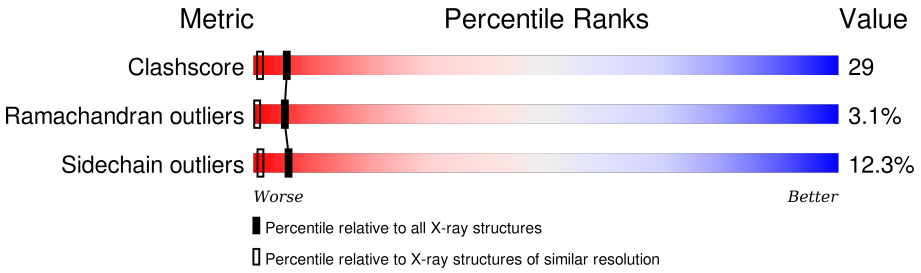
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	521	44% 39% 10% • 7%

2 Entry composition (i)

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 (three-letter code: 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		

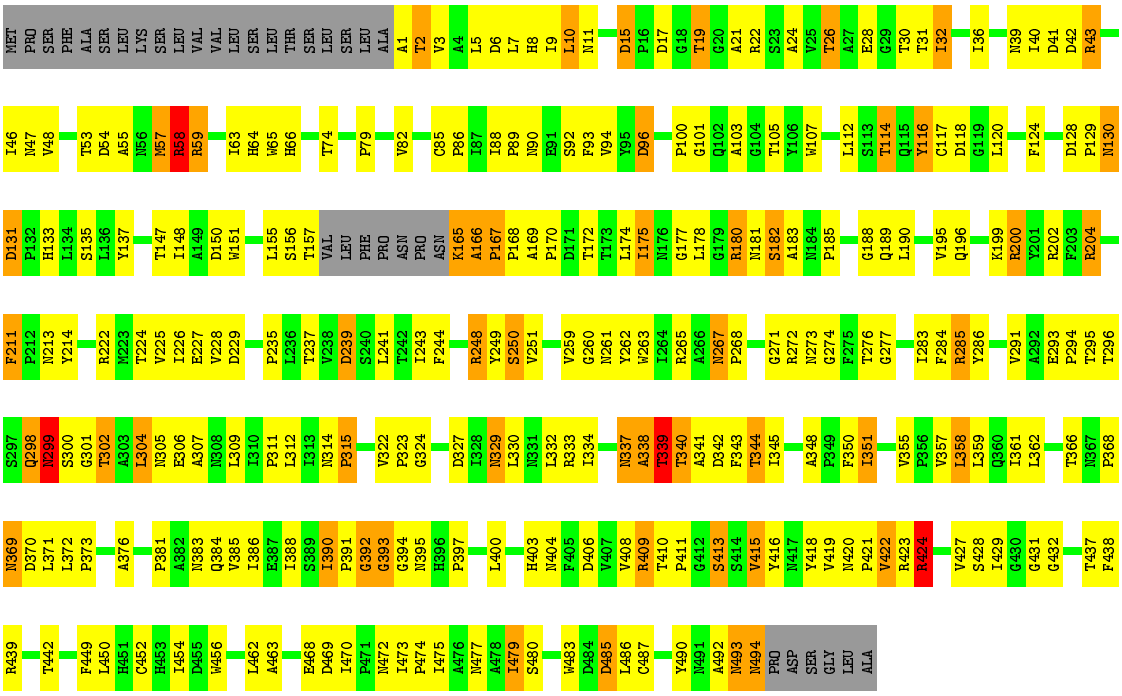
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	0.48	1/3786 (0.0%)	1.34	29/5200 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	ASN	C-O	-10.03	1.04	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	494	ASN	CA-C-O	14.64	150.84	120.10
1	A	424	ARG	NE-CZ-NH2	10.97	125.78	120.30
1	A	416	TYR	CB-CG-CD1	-8.91	115.65	121.00
1	A	424	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	A	204	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	222	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	A	116	TYR	CA-CB-CG	8.01	128.61	113.40
1	A	200	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	A	299	ASN	O-C-N	7.03	133.95	122.70
1	A	58	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	A	43	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	298	GLN	O-C-N	6.59	133.24	122.70
1	A	180	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	A	211	PHE	CB-CG-CD2	6.55	125.39	120.80
1	A	96	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	204	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	59	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	A	57	MET	CG-SD-CE	5.88	109.61	100.20
1	A	156	SER	C-N-CA	5.80	136.21	121.70
1	A	299	ASN	CA-C-N	-5.72	104.61	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	416	TYR	CB-CG-CD2	5.63	124.38	121.00
1	A	409	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	314	ASN	O-C-N	5.46	131.47	121.10
1	A	492	ALA	C-N-CA	5.29	134.91	121.70
1	A	285	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	333	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	166	ALA	O-C-N	5.09	130.77	121.10
1	A	131	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	222	ARG	CD-NE-CZ	5.04	130.65	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	210	0
2	A	4	0	0	0	0
3	A	81	0	0	5	0
All	All	3769	0	3529	210	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 29.

All (210) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:311:PRO:HB2	1:A:315:PRO:HG3	1.62	0.81
1:A:260:GLY:H	1:A:286:TYR:HB2	1.44	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
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:HE	1.96	0.64
1:A:261:ASN:ND2	1:A:285:ARG:HB2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:332:LEU:HB2	1:A:390:ILE:HG23	1.85	0.59
1:A:165:LYS:HZ2	1:A:339:THR:HB	1.67	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
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:227:GLU:HB3	1:A:250:SER:HB2	1.87	0.55
1:A:150:ASP:HB2	1:A:170:PRO:HB3	1.88	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:429:ILE:O	1:A:429:ILE:HG22	2.08	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:305:ASN:OD1	1:A:307:ALA:HB3	2.08	0.52
1:A:40:ILE:HD11	1:A:101:GLY:HA2	1.91	0.52
1:A:327:ASP:N	1:A:385:VAL:HG23	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:479:ILE:HG22	1:A:479:ILE:O	2.10	0.52
1:A:228:VAL:HG21	1:A:309:LEU:HD13	1.91	0.51
1:A:474:PRO:HG2	1:A:475:ILE:HG13	1.93	0.51
1:A:261:ASN:HD22	1:A:285:ARG:HB2	1.73	0.51
1:A:195:VAL:HG11	1:A:284:PHE:CZ	2.44	0.51
1:A:196:GLN:HB2	1:A:199:LYS:CD	2.40	0.51
1:A:130:ASN:N	1:A:130:ASN:HD22	2.08	0.51
1:A:408:VAL:HG11	1:A:418:TYR:CZ	2.45	0.51
1:A:302:THR:O	1:A:302:THR:HG22	2.11	0.51
1:A:6:ASP:HA	1:A:47:ASN:HB3	1.92	0.51
1:A:182:SER:HA	1:A:185:PRO:HD3	1.92	0.51
1:A:454:ILE:HG22	1:A:454:ILE:O	2.10	0.51
1:A:58:ARG:CZ	1:A:112:LEU:HD11	2.40	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:239:ASP:OD1	1:A:302:THR:O	2.30	0.50
1:A:57:MET:HG3	1:A:155:LEU:HD13	1.93	0.50
1:A:8:HIS:O	1:A:9:ILE:HD13	2.11	0.50
1:A:261:ASN:HD21	1:A:285:ARG:NE	2.06	0.50
1:A:165:LYS:O	1:A:340:THR:HG21	2.12	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:410:THR:HG22	1:A:411:PRO:O	2.13	0.49
1:A:345:ILE:HD11	1:A:462:LEU:HD12	1.95	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:404:ASN:CG	1:A:423:ARG:HE	2.16	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:337:ASN:ND2	1:A:342:ASP:HB3	2.28	0.48
1:A:168:PRO:O	1:A:169:ALA:HB2	2.13	0.48
1:A:358:LEU:HD22	1:A:362:LEU:CD1	2.44	0.48
1:A:473:ILE:N	1:A:474:PRO:HD2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HB2	1:A:450:LEU:CD1	2.43	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: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
1:A:324:GLY:HA2	1:A:329:ASN:ND2	2.20	0.46
1:A:213:ASN:HB3	1:A:244:PHE:CD2	2.51	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:189:GLN:NE2	1:A:190:LEU:O	2.50	0.45
1:A:88:ILE:HG23	1:A:89:PRO:HD2	1.99	0.45
1:A:239:ASP:N	1:A:239:ASP:OD1	2.49	0.45
1:A:7:LEU:HD12	1:A:46:ILE:CG2	2.40	0.45
1:A:322:VAL:O	1:A:439:ARG:NH2	2.49	0.45
1:A:8:HIS:CD2	1:A:8:HIS:H	2.34	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:271:GLY:O	1:A:273:ASN:ND2	2.50	0.44
1:A:58:ARG:CD	1:A:112:LEU:HD21	2.46	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:OD1	1:A:485:ASP:N	2.50	0.44
1:A:388:ILE:O	1:A:437:THR:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:419:VAL:HG12	1:A:420:ASN:CG	2.39	0.43
1:A:40:ILE:O	1:A:41:ASP:HB3	2.19	0.43
1:A:419:VAL:HG12	1:A:420:ASN:N	2.34	0.43
1:A:332:LEU:O	1:A:390:ILE:HG23	2.19	0.43
1:A:175:ILE:N	1:A:178:LEU:O	2.45	0.43
1:A:93:PHE:CD1	1:A:486:LEU:HD21	2.54	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:147:THR:C	1:A:148:ILE:HD13	2.40	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: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: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:400:LEU:CD2	1:A:403:HIS:HB2	2.50	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:470:ILE:HA	1:A:473:ILE:CD1	2.34	0.41
1:A:181:ASN:OD1	1:A:182:SER:N	2.49	0.41
1:A:135:SER:O	1:A:200:ARG:NH2	2.51	0.41
1:A:182:SER:HB2	1:A:272:ARG:NH1	2.35	0.41
1:A:151:TRP:HB2	1:A:174:LEU:HD11	2.03	0.41
1:A:130:ASN:N	1:A:130:ASN:ND2	2.69	0.41
1:A:10:LEU:HD13	1:A:10:LEU:N	2.36	0.40
1:A:429:ILE:HD13	1:A:429:ILE:HG21	1.66	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

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%)	5 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%)	348 (88%)	49 (12%)	6 1

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	10	LEU
1	A	15	ASP
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	114	THR
1	A	116	TYR
1	A	120	LEU
1	A	124	PHE
1	A	130	ASN
1	A	157	THR
1	A	165	LYS
1	A	167	PRO
1	A	175	ILE
1	A	182	SER
1	A	239	ASP
1	A	248	ARG
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	329	ASN
1	A	330	LEU
1	A	337	ASN
1	A	339	THR
1	A	340	THR
1	A	343	PHE
1	A	344	THR
1	A	351	ILE
1	A	358	LEU
1	A	366	THR
1	A	369	ASN
1	A	390	ILE
1	A	413	SER
1	A	415	VAL

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	ASN
1	A	13	ASN
1	A	47	ASN
1	A	70	GLN
1	A	84	GLN
1	A	130	ASN
1	A	133	HIS
1	A	213	ASN
1	A	233	HIS
1	A	234	GLN
1	A	257	GLN
1	A	261	ASN
1	A	267	ASN
1	A	273	ASN
1	A	287	GLN
1	A	298	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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 (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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.