WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 01:45 PM EST

PDB ID	:	1LWH
Title	:	CRYSTAL STRUCTURE OF T. MARITIMA 4-ALPHA-GLUCANOTRANS FERASE
Authors	:	Roujeinikova, A.; Raasch, C.; Sedelnikova, S.; Liebl, W.; Rice, D.W.
Deposited on	:	2002-05-31
Resolution	:	2.60 Å(reported)

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

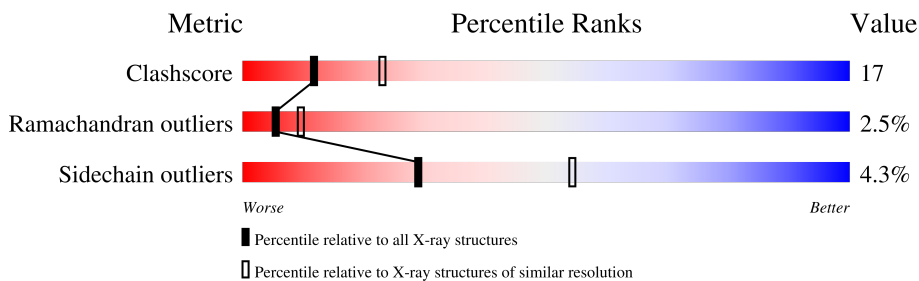|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	Percentile Ranks	Value
Clashscore		17
Ramachandran outliers		2.5%
Sidechain outliers		4.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

◻ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	441	70% 25% 5%
1	B	441	64% 32% •

WORLDWIDE

PDB

PROTEIN DATA BANK

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7462 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 4-alpha-glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total 3646	C 2376	N 603	O 652	S 15	0	0	0
1	B	441	Total 3640	C 2369	N 603	O 653	S 15	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	101	Total 101	O 101	0	0
3	B	73	Total 73	O 73	0	0

3 Residue-property plots (i)

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: 4-alpha-glucanotransferase

Chain A:

• Molecule 1: 4-alpha-glucanotransferase

Chain B:
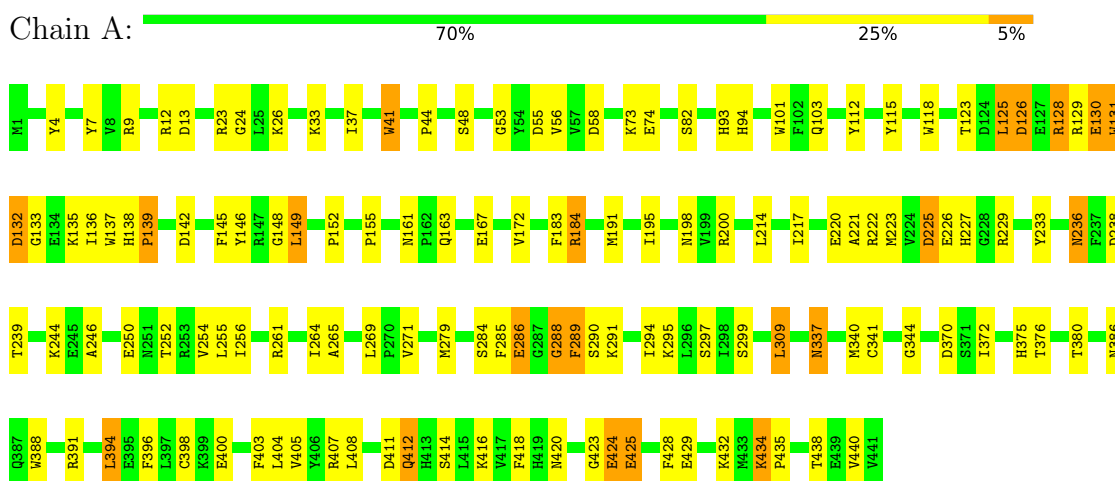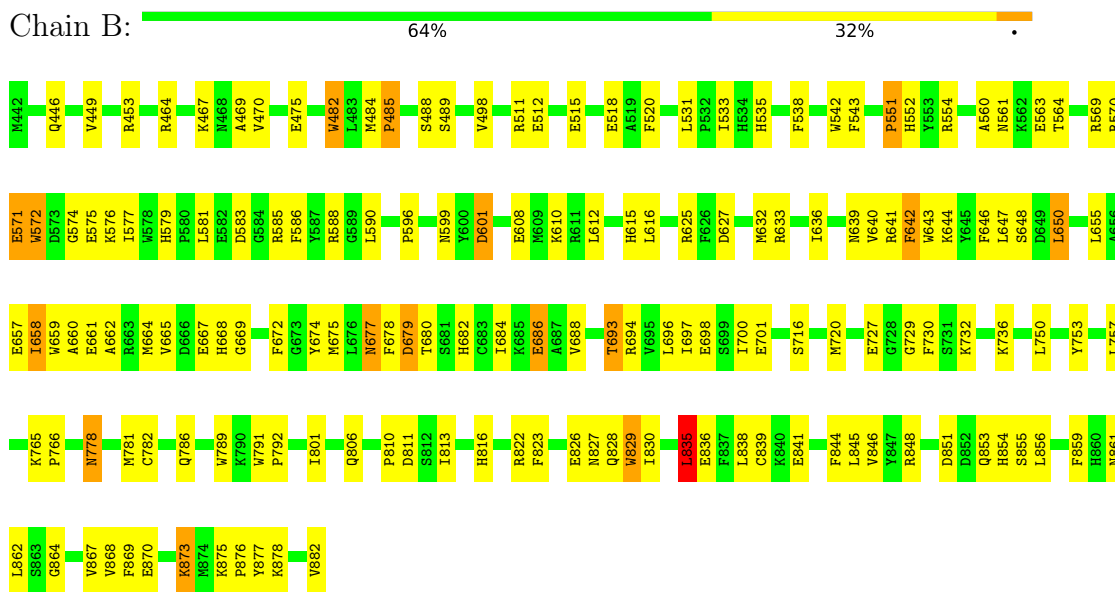
4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	92.57Å 180.28Å 199.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	89.0 (10.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.224 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7462	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.54	0/3759	0.73	2/5083 (0.0%)
1	B	0.51	0/3751	0.69	1/5071 (0.0%)
All	All	0.52	0/7510	0.71	3/10154 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	309	LEU	CA-CB-CG	6.36	129.92	115.30
1	B	835	LEU	CA-CB-CG	6.11	129.34	115.30
1	A	394	LEU	CA-CB-CG	5.21	127.28	115.30

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	3646	0	3496	115	1
1	B	3640	0	3489	134	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	101	0	0	4	0
3	B	73	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7462	0	6985	248	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 17.

All (248) 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:291:LYS:HG3	1:A:372:ILE:HD11	1.44	0.99
1:B:716:SER:HA	1:B:720:MET:HE2	1.47	0.96
1:B:868:VAL:HG22	1:B:873:LYS:HB3	1.46	0.94
1:A:423:GLY:HA2	1:A:435:PRO:HB3	1.50	0.93
1:B:570:ARG:HB2	1:B:577:ILE:HD11	1.52	0.91
1:A:386:ASN:HD22	1:A:388:TRP:HE1	1.20	0.90
1:B:836:GLU:OE1	1:B:848:ARG:NH1	2.09	0.85
1:A:73:LYS:NZ	3:A:1048:HOH:O	2.11	0.83
1:B:570:ARG:O	1:B:574:GLY:HA2	1.80	0.81
1:A:434:LYS:HD2	1:A:434:LYS:N	1.98	0.79
1:B:531:LEU:HG	1:B:533:ILE:HG23	1.63	0.79
1:A:118:TRP:CZ3	1:A:146:TYR:HB3	2.19	0.78
1:A:434:LYS:HD2	1:A:434:LYS:H	1.48	0.78
1:B:554:ARG:HH22	1:B:585:ARG:HD2	1.50	0.77
1:A:128:ARG:HG2	1:A:133:GLY:O	1.89	0.72
1:B:873:LYS:HD2	1:B:873:LYS:O	1.89	0.72
1:A:420:ASN:ND2	1:A:435:PRO:HA	2.06	0.70
1:A:423:GLY:O	1:A:424:GLU:HB3	1.90	0.70
1:B:610:LYS:HE2	1:B:646:PHE:O	1.93	0.69
1:A:225:ASP:O	1:A:229:ARG:HG2	1.94	0.68
1:B:657:GLU:HG3	1:B:678:PHE:CD1	2.29	0.68
1:A:101:TRP:CH2	1:A:167:GLU:HG2	2.30	0.66
1:B:657:GLU:HG3	1:B:678:PHE:CE1	2.28	0.66
1:A:285:PHE:O	1:A:288:GLY:N	2.29	0.66
1:A:131:TRP:HH2	1:A:149:LEU:HD21	1.60	0.66
1:B:641:ARG:NH2	1:B:644:LYS:HD3	2.11	0.66
1:B:694:ARG:O	1:B:698:GLU:HG2	1.96	0.66
1:B:835:LEU:HD12	1:B:835:LEU:O	1.96	0.66
1:B:551:PRO:HG2	1:B:552:HIS:H	1.59	0.65
1:B:674:TYR:O	1:B:675:MET:HE2	1.97	0.65
1:A:138:HIS:HE1	1:A:148:GLY:O	1.79	0.64
1:B:659:TRP:C	1:B:661:GLU:H	2.00	0.64
1:B:841:GLU:HG3	1:B:844:PHE:CZ	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:ALA:H	1:B:665:VAL:HG21	1.63	0.63
1:A:411:ASP:HB2	1:A:412:GLN:NE2	2.15	0.62
1:A:12:ARG:HG2	1:A:24:GLY:O	1.99	0.62
1:A:411:ASP:HB2	1:A:412:GLN:HE22	1.65	0.62
1:B:684:ILE:O	1:B:688:VAL:HG23	2.00	0.61
1:B:658:ILE:HG13	1:B:668:HIS:ND1	2.16	0.61
1:B:577:ILE:HG22	1:B:588:ARG:HG3	1.81	0.61
1:B:640:VAL:HG22	1:B:668:HIS:NE2	2.16	0.61
1:A:337:ASN:C	1:A:337:ASN:HD22	2.03	0.60
1:A:236:ASN:ND2	1:A:239:THR:H	1.99	0.60
1:B:839:CYS:HB3	1:B:846:VAL:HB	1.83	0.60
1:B:827:ASN:HD22	1:B:829:TRP:HE1	1.49	0.60
1:A:128:ARG:HG2	1:A:128:ARG:HH11	1.67	0.60
1:A:214:LEU:HD21	1:A:271:VAL:HG21	1.84	0.60
1:A:33:LYS:HE2	1:A:82:SER:O	2.02	0.60
1:B:844:PHE:CD1	1:B:867:VAL:HG21	2.36	0.60
1:A:126:ASP:O	1:A:128:ARG:HD2	2.02	0.59
1:A:236:ASN:HD21	1:A:238:ASP:HB3	1.66	0.59
1:A:337:ASN:HD21	1:A:341:CYS:H	1.48	0.59
1:B:813:ILE:HD12	1:B:813:ILE:H	1.67	0.59
1:B:697:ILE:HD11	1:B:845:LEU:HD13	1.84	0.59
1:B:677:ASN:HD21	1:B:679:ASP:HB3	1.68	0.59
1:A:139:PRO:HB3	1:A:145:PHE:CZ	2.38	0.58
1:B:669:GLY:HA2	1:B:675:MET:CE	2.33	0.58
1:A:198:ASN:HD22	1:A:227:HIS:CE1	2.21	0.58
1:B:467:LYS:O	1:B:470:VAL:HG23	2.04	0.58
1:B:669:GLY:HA2	1:B:675:MET:HE3	1.86	0.58
1:B:727:GLU:C	1:B:729:GLY:H	2.06	0.58
1:A:291:LYS:HG3	1:A:372:ILE:CD1	2.25	0.58
1:A:425:GLU:HG3	1:A:434:LYS:HA	1.86	0.58
1:B:658:ILE:HD12	1:B:665:VAL:HA	1.85	0.57
1:A:291:LYS:O	1:A:295:LYS:HG3	2.03	0.57
1:B:542:TRP:CH2	1:B:608:GLU:HG2	2.40	0.57
1:B:841:GLU:HG3	1:B:844:PHE:CE1	2.39	0.57
1:A:94:HIS:HB2	1:A:155:PRO:O	2.04	0.57
1:B:561:ASN:H	1:B:564:THR:HB	1.70	0.56
1:A:172:VAL:HG13	1:A:183:PHE:CE2	2.41	0.56
1:B:554:ARG:HH12	1:B:585:ARG:HH11	1.53	0.56
1:B:813:ILE:HD12	1:B:813:ILE:N	2.20	0.56
1:B:658:ILE:HG22	1:B:675:MET:SD	2.46	0.56
1:A:408:LEU:O	1:A:414:SER:HA	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ILE:HG22	1:B:588:ARG:CG	2.36	0.55
1:B:851:ASP:OD2	1:B:854:HIS:N	2.39	0.55
1:A:56:VAL:HG12	1:A:58:ASP:H	1.71	0.55
1:B:835:LEU:HD12	1:B:835:LEU:C	2.27	0.55
1:B:757:LEU:HD13	1:B:801:ILE:O	2.07	0.55
1:B:581:LEU:HD12	1:B:585:ARG:HB2	1.88	0.55
1:A:398:CYS:HB3	1:A:405:VAL:HB	1.90	0.54
1:B:641:ARG:HH21	1:B:644:LYS:HD3	1.71	0.54
1:B:838:LEU:HB2	1:B:846:VAL:HG12	1.88	0.54
1:B:875:LYS:HB3	1:B:876:PRO:HD2	1.89	0.54
1:A:138:HIS:CD2	1:A:152:PRO:HB3	2.43	0.54
1:A:254:VAL:HG23	1:A:255:LEU:N	2.23	0.54
1:B:636:ILE:HD11	1:B:664:MET:HG2	1.89	0.54
1:B:835:LEU:HA	1:B:848:ARG:O	2.08	0.54
1:A:4:TYR:HB2	1:A:37:ILE:HD12	1.90	0.53
1:B:636:ILE:CD1	1:B:664:MET:HG2	2.38	0.53
1:A:295:LYS:O	1:A:375:HIS:HE1	1.92	0.53
1:A:223:MET:HE2	1:A:226:GLU:HG3	1.91	0.53
1:A:284:SER:HA	1:A:288:GLY:HA2	1.91	0.53
1:B:535:HIS:HB2	1:B:596:PRO:O	2.09	0.53
1:A:101:TRP:CZ2	1:A:167:GLU:HG2	2.44	0.52
1:A:112:TYR:O	1:A:115:TYR:HB2	2.10	0.52
1:A:299:SER:HB3	1:A:438:THR:OG1	2.09	0.52
1:B:453:ARG:HD3	1:B:469:ALA:HB2	1.93	0.51
1:B:864:GLY:C	1:B:876:PRO:HB3	2.31	0.51
1:B:658:ILE:HD13	1:B:660:ALA:H	1.75	0.51
1:A:407:ARG:NH2	3:A:1006:HOH:O	2.43	0.51
1:A:428:PHE:CD2	1:A:429:GLU:HG3	2.45	0.51
1:A:131:TRP:CH2	1:A:149:LEU:HD21	2.43	0.51
1:A:246:ALA:O	1:A:250:GLU:N	2.43	0.51
1:A:128:ARG:NH2	1:A:135:LYS:HE2	2.26	0.50
1:A:41:TRP:CD1	1:A:41:TRP:C	2.85	0.50
1:A:398:CYS:SG	1:A:400:GLU:HG2	2.51	0.50
1:A:161:ASN:OD1	1:A:163:GLN:HB2	2.10	0.50
1:A:93:HIS:HB2	1:A:191:MET:HE3	1.94	0.50
1:B:464:ARG:HD2	1:B:512:GLU:OE2	2.12	0.50
1:A:420:ASN:HD22	1:A:435:PRO:HA	1.75	0.50
1:A:238:ASP:OD2	1:A:261:ARG:HD2	2.12	0.50
1:A:129:ARG:HD2	1:A:132:ASP:CB	2.42	0.50
1:B:612:LEU:O	1:B:615:HIS:HB3	2.12	0.50
1:A:372:ILE:HD12	1:A:372:ILE:N	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ARG:HE	1:B:641:ARG:HA	1.76	0.49
1:A:428:PHE:CE2	1:A:429:GLU:HG3	2.47	0.49
1:A:229:ARG:HG3	1:A:229:ARG:HH11	1.77	0.49
1:A:252:THR:O	1:A:256:ILE:HG13	2.12	0.49
1:A:424:GLU:N	1:A:435:PRO:HG3	2.28	0.49
1:B:511:ARG:O	1:B:515:GLU:HG3	2.13	0.49
1:A:376:THR:O	1:A:380:THR:HG23	2.13	0.49
1:A:55:ASP:OD1	1:A:55:ASP:N	2.42	0.48
1:A:130:GLU:O	1:A:131:TRP:O	2.31	0.48
1:B:583:ASP:OD2	1:B:585:ARG:NE	2.45	0.48
1:B:636:ILE:O	1:B:640:VAL:HG23	2.13	0.48
1:B:682:HIS:HE1	1:B:686:GLU:HG3	1.78	0.48
1:B:449:VAL:HG23	3:B:895:HOH:O	2.12	0.48
1:B:801:ILE:HA	1:B:806:GLN:HE21	1.79	0.48
1:A:289:PHE:HB2	3:A:958:HOH:O	2.14	0.48
1:B:875:LYS:HB2	1:B:878:LYS:HD2	1.94	0.48
1:B:791:TRP:CD1	1:B:792:PRO:HD2	2.49	0.48
1:B:482:TRP:CD1	1:B:482:TRP:C	2.86	0.47
1:A:432:LYS:HB3	1:A:434:LYS:HE3	1.96	0.47
1:A:285:PHE:O	1:A:286:GLU:C	2.52	0.47
1:B:868:VAL:HG22	1:B:873:LYS:CB	2.32	0.47
1:A:236:ASN:C	1:A:236:ASN:HD22	2.18	0.47
1:B:658:ILE:O	1:B:665:VAL:HG22	2.15	0.47
1:A:236:ASN:HD21	1:A:239:THR:H	1.60	0.47
1:A:337:ASN:ND2	1:A:340:MET:H	2.12	0.47
1:B:859:PHE:HE2	1:B:882:VAL:CG2	2.28	0.47
1:B:560:ALA:CB	1:B:586:PHE:HB2	2.45	0.46
1:B:859:PHE:HE2	1:B:882:VAL:HG23	1.81	0.46
1:A:7:TYR:CE2	1:A:9:ARG:HB3	2.50	0.46
1:A:337:ASN:C	1:A:337:ASN:ND2	2.68	0.46
1:A:337:ASN:ND2	1:A:340:MET:N	2.64	0.46
1:B:647:LEU:HA	1:B:650:LEU:HD12	1.97	0.46
1:B:727:GLU:C	1:B:729:GLY:N	2.69	0.46
1:A:396:PHE:CE1	1:A:404:LEU:HD11	2.49	0.46
1:B:693:THR:HG21	1:B:844:PHE:O	2.15	0.46
1:B:647:LEU:HD11	1:B:672:PHE:CE2	2.50	0.46
1:B:778:ASN:HD21	1:B:782:CYS:H	1.63	0.46
1:A:396:PHE:HE1	1:A:404:LEU:HD11	1.80	0.46
1:B:781:MET:O	1:B:786:GLN:HG2	2.15	0.46
1:B:542:TRP:CZ2	1:B:608:GLU:HG2	2.51	0.45
1:A:41:TRP:CZ2	1:A:184:ARG:HG3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:ASN:ND2	1:B:679:ASP:HB3	2.30	0.45
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.82	0.45
1:B:538:PHE:CD1	1:B:543:PHE:HE2	2.34	0.45
1:B:599:ASN:OD1	1:B:601:ASP:HB2	2.16	0.45
1:A:195:ILE:HD11	1:A:227:HIS:NE2	2.32	0.45
1:B:682:HIS:HD2	3:B:1040:HOH:O	1.99	0.45
1:B:851:ASP:OD1	1:B:854:HIS:HD2	2.00	0.45
1:B:869:PHE:CD2	1:B:870:GLU:HG3	2.52	0.45
1:A:244:LYS:NZ	1:A:279:MET:CE	2.80	0.45
1:B:470:VAL:HG22	1:B:520:PHE:CE1	2.52	0.45
1:B:570:ARG:O	1:B:574:GLY:CA	2.61	0.45
1:A:198:ASN:HD22	1:A:227:HIS:HE1	1.60	0.44
1:A:200:ARG:HG3	1:A:200:ARG:HH11	1.82	0.44
1:A:418:PHE:O	1:A:438:THR:HA	2.18	0.44
1:B:639:ASN:O	1:B:642:PHE:HB3	2.17	0.44
1:B:828:GLN:O	1:B:830:ILE:N	2.50	0.44
1:A:103:GLN:HA	1:A:103:GLN:NE2	2.33	0.44
1:A:221:ALA:C	1:A:223:MET:H	2.20	0.44
1:A:9:ARG:NH2	1:B:789:TRP:O	2.51	0.44
1:A:223:MET:CE	1:A:226:GLU:HG3	2.48	0.44
1:A:93:HIS:HB2	1:A:191:MET:CE	2.48	0.44
1:B:644:LYS:O	1:B:648:SER:HB3	2.17	0.44
1:B:732:LYS:HE2	1:B:811:ASP:O	2.17	0.43
1:B:867:VAL:O	1:B:873:LYS:HA	2.19	0.43
1:B:579:HIS:O	1:B:586:PHE:HA	2.18	0.43
1:B:560:ALA:HB3	1:B:586:PHE:HB2	2.00	0.43
1:B:577:ILE:HD12	1:B:590:LEU:HD12	2.00	0.43
1:A:255:LEU:HD12	1:A:255:LEU:O	2.18	0.43
1:A:128:ARG:HG3	1:A:135:LYS:HA	1.99	0.43
1:A:131:TRP:O	1:A:133:GLY:N	2.52	0.43
1:B:778:ASN:N	1:B:778:ASN:HD22	2.16	0.43
1:A:13:ASP:O	1:A:344:GLY:HA2	2.18	0.43
1:A:223:MET:HE2	1:A:223:MET:HA	2.00	0.43
1:B:484:MET:HB3	1:B:485:PRO:HD2	2.00	0.42
1:A:23:ARG:O	1:A:26:LYS:HB3	2.19	0.42
1:A:48:SER:OG	1:A:53:GLY:HA2	2.19	0.42
1:A:391:ARG:HG3	1:A:391:ARG:NH1	2.33	0.42
1:B:625:ARG:NH1	1:B:627:ASP:HB3	2.34	0.42
1:B:633:ARG:HG3	1:B:633:ARG:HH11	1.84	0.42
1:B:778:ASN:HD22	1:B:778:ASN:H	1.65	0.42
1:B:859:PHE:CE2	1:B:882:VAL:HG23	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:HG22	1:A:265:ALA:N	2.34	0.42
1:B:632:MET:HG3	1:B:643:TRP:CZ2	2.55	0.42
1:B:660:ALA:CB	1:B:664:MET:HB3	2.49	0.42
1:B:682:HIS:CE1	1:B:686:GLU:HG3	2.54	0.42
1:A:291:LYS:HE2	1:A:370:ASP:O	2.20	0.42
1:B:633:ARG:HG3	1:B:633:ARG:NH1	2.34	0.42
1:B:633:ARG:HD2	1:B:633:ARG:HA	1.75	0.42
1:B:862:LEU:N	1:B:862:LEU:HD12	2.34	0.42
1:A:74:GLU:HG2	3:A:990:HOH:O	2.19	0.42
1:A:118:TRP:CE3	1:A:146:TYR:HB3	2.55	0.42
1:A:123:THR:HG22	1:A:125:LEU:HD12	2.02	0.42
1:A:400:GLU:HG3	1:A:403:PHE:CZ	2.55	0.42
1:B:659:TRP:C	1:B:661:GLU:N	2.70	0.42
1:B:716:SER:HA	1:B:720:MET:CE	2.33	0.42
1:B:848:ARG:HE	1:B:855:SER:HG	1.66	0.42
1:B:488:SER:O	1:B:498:VAL:HG22	2.19	0.42
1:B:569:ARG:HA	1:B:575:GLU:O	2.19	0.42
1:B:861:ASN:O	1:B:877:TYR:HA	2.20	0.42
1:A:93:HIS:HA	1:A:191:MET:CE	2.50	0.42
1:B:571:GLU:O	1:B:572:TRP:C	2.58	0.42
1:B:659:TRP:CG	1:B:659:TRP:O	2.73	0.42
1:A:131:TRP:H	1:A:131:TRP:HE3	1.67	0.42
1:B:765:LYS:HB3	1:B:766:PRO:HA	2.01	0.42
1:A:217:ILE:HG21	1:A:227:HIS:CD2	2.55	0.41
1:A:294:ILE:O	1:A:297:SER:HB2	2.20	0.41
1:A:264:ILE:CG2	1:A:265:ALA:N	2.83	0.41
1:B:778:ASN:HD21	1:B:782:CYS:N	2.18	0.41
1:A:284:SER:HA	1:A:288:GLY:CA	2.50	0.41
1:A:416:LYS:O	1:A:440:VAL:HA	2.20	0.41
1:A:432:LYS:CB	1:A:434:LYS:HE3	2.49	0.41
1:B:696:LEU:O	1:B:700:ILE:HG13	2.20	0.41
1:B:446:GLN:O	1:B:753:TYR:HB3	2.21	0.41
1:B:680:THR:O	1:B:684:ILE:HG13	2.21	0.41
1:A:41:TRP:CE2	1:A:184:ARG:HG3	2.55	0.41
1:B:658:ILE:O	1:B:658:ILE:HG23	2.21	0.41
1:B:659:TRP:O	1:B:659:TRP:CD2	2.74	0.41
1:B:822:ARG:O	1:B:826:GLU:HG3	2.20	0.41
1:B:868:VAL:HG12	1:B:869:PHE:N	2.36	0.41
1:B:664:MET:SD	1:B:667:GLU:OE1	2.79	0.41
1:B:736:LYS:O	1:B:816:HIS:CE1	2.73	0.41
1:B:813:ILE:H	1:B:813:ILE:CD1	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:835:LEU:C	1:B:835:LEU:CD1	2.88	0.41
1:A:184:ARG:C	1:A:184:ARG:HD2	2.41	0.41
1:B:570:ARG:HB2	1:B:577:ILE:CD1	2.35	0.41
1:B:823:PHE:CZ	1:B:856:LEU:HD21	2.56	0.41
1:B:570:ARG:O	1:B:571:GLU:O	2.38	0.40
1:A:233:TYR:HA	1:A:269:LEU:O	2.21	0.40
1:A:284:SER:CA	1:A:288:GLY:HA2	2.52	0.40
1:B:538:PHE:CE1	1:B:543:PHE:HE2	2.40	0.40
1:A:136:ILE:HG13	1:A:137:TRP:CD1	2.56	0.40
1:B:561:ASN:HB3	1:B:563:GLU:H	1.85	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)
1:A:74:GLU:OE1	1:A:74:GLU:OE1[3_756]	1.72	0.48

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	439/441 (100%)	395 (90%)	31 (7%)	13 (3%)	4	7
1	B	439/441 (100%)	396 (90%)	34 (8%)	9 (2%)	7	13
All	All	878/882 (100%)	791 (90%)	65 (7%)	22 (2%)	5	9

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	131	TRP
1	A	424	GLU
1	B	571	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	572	TRP
1	B	829	TRP
1	A	132	ASP
1	A	290	SER
1	A	142	ASP
1	A	220	GLU
1	A	222	ARG
1	A	425	GLU
1	B	485	PRO
1	A	44	PRO
1	A	125	LEU
1	A	130	GLU
1	A	286	GLU
1	B	642	PHE
1	B	679	ASP
1	A	288	GLY
1	B	551	PRO
1	B	693	THR
1	B	810	PRO

5.3.2   Protein sidechains (i)

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	386/393 (98%)	372 (96%)	14 (4%)	35	61
1	B	386/393 (98%)	367 (95%)	19 (5%)	25	48
All	All	772/786 (98%)	739 (96%)	33 (4%)	29	54

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	TRP
1	A	126	ASP
1	A	128	ARG
1	A	139	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	149	LEU
1	A	184	ARG
1	A	225	ASP
1	A	236	ASN
1	A	289	PHE
1	A	309	LEU
1	A	337	ASN
1	A	394	LEU
1	A	412	GLN
1	A	434	LYS
1	B	475	GLU
1	B	482	TRP
1	B	489	SER
1	B	518	GLU
1	B	576	LYS
1	B	601	ASP
1	B	616	LEU
1	B	650	LEU
1	B	655	LEU
1	B	658	ILE
1	B	677	ASN
1	B	686	GLU
1	B	701	GLU
1	B	730	PHE
1	B	750	LEU
1	B	778	ASN
1	B	835	LEU
1	B	853	GLN
1	B	873	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	27	ASN
1	A	103	GLN
1	A	111	HIS
1	A	138	HIS
1	A	197	GLN
1	A	227	HIS
1	A	236	ASN
1	A	337	ASN

Continued from previous page...

Mol	Chain	Res	Type
1	A	375	HIS
1	A	386	ASN
1	A	412	GLN
1	B	446	GLN
1	B	544	GLN
1	B	677	ASN
1	B	682	HIS
1	B	778	ASN
1	B	827	ASN
1	B	853	GLN
1	B	854	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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 (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.