



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:40 PM UTC

PDB ID : 4OOU / pdb_00004oou
Title : Crystal structure of beta-1,4-D-mannanase from *Cryptopygus antarcticus*
Authors : Kim, M.-K.; An, Y.J.; Jeong, C.-S.; Cha, S.-S.
Deposited on : 2014-02-04
Resolution : 2.36 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

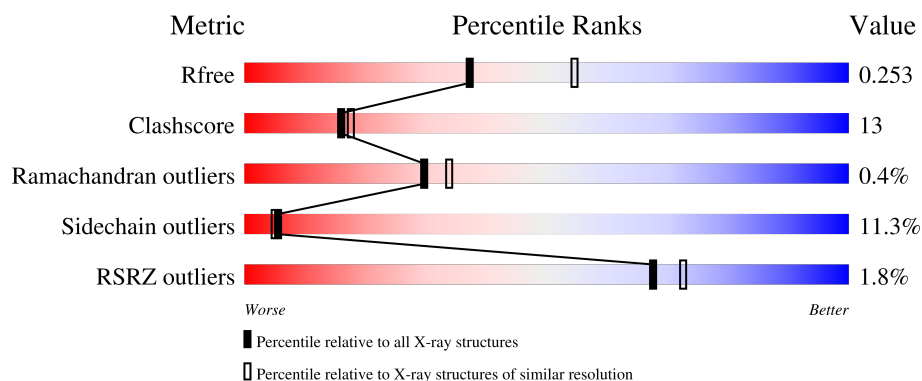
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	388	2% 72% 19% •• 6%
1	B	388	2% 67% 22% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5746 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 Beta-1,4-mannanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	367	Total	C	N	O	S	0	0	0
			2818	1773	487	548	10			
1	A	364	Total	C	N	O	S	0	0	0
			2787	1755	478	544	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	383	HIS	-	expression tag	UNP B4XC07
B	384	HIS	-	expression tag	UNP B4XC07
B	385	HIS	-	expression tag	UNP B4XC07
B	386	HIS	-	expression tag	UNP B4XC07
B	387	HIS	-	expression tag	UNP B4XC07
B	388	HIS	-	expression tag	UNP B4XC07
A	383	HIS	-	expression tag	UNP B4XC07
A	384	HIS	-	expression tag	UNP B4XC07
A	385	HIS	-	expression tag	UNP B4XC07
A	386	HIS	-	expression tag	UNP B4XC07
A	387	HIS	-	expression tag	UNP B4XC07
A	388	HIS	-	expression tag	UNP B4XC07

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			8	4	1	3		
2	A	1	Total	C	N	O	0	0
			8	4	1	3		

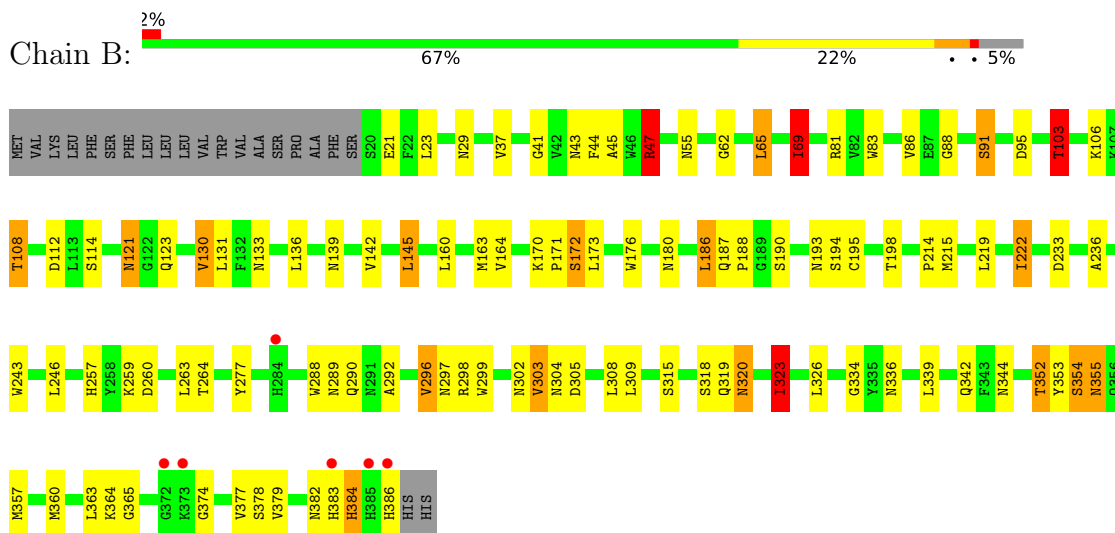
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	66	Total	O	0	0
			66	66		
3	A	59	Total	O	0	0
			59	59		

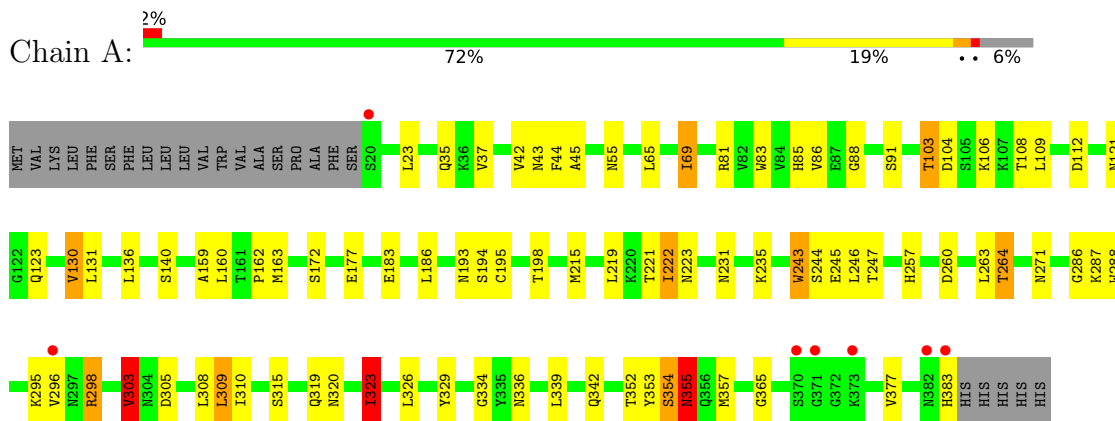
3 Residue-property plots

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 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.

• Molecule 1: Beta-1,4-mannanase



• Molecule 1: Beta-1,4-mannanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.24Å 84.48Å 164.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.16 – 2.36 46.16 – 2.36	Depositor EDS
% Data completeness (in resolution range)	86.9 (46.16-2.36) 86.9 (46.16-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.7.0029, PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.190 , 0.249 0.196 , 0.253	Depositor DCC
R_{free} test set	1895 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.992	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5746	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.87	0/2858	1.06	6/3883 (0.2%)
1	B	0.89	0/2892	1.10	8/3929 (0.2%)
All	All	0.88	0/5750	1.08	14/7812 (0.2%)

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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	ILE	CB-CA-C	-6.49	100.65	111.29
1	A	323	ILE	CB-CA-C	-6.34	103.73	112.04
1	A	334	GLY	N-CA-C	5.93	121.74	114.69
1	B	69	ILE	N-CA-CB	5.90	118.57	110.54
1	B	69	ILE	CA-CB-CG2	5.69	120.18	110.50
1	B	320	ASN	N-CA-C	5.62	119.31	111.90
1	A	377	VAL	CB-CA-C	-5.60	106.12	111.44
1	B	47	ARG	N-CA-C	-5.54	104.54	112.13
1	A	35	GLN	N-CA-C	5.40	118.25	109.24
1	A	355	ASN	CB-CA-C	5.20	119.71	109.72
1	B	103	THR	CB-CA-C	5.08	118.93	110.90
1	B	29	ASN	N-CA-C	5.08	117.52	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	374	GLY	N-CA-C	5.07	121.46	113.86
1	A	221	THR	N-CA-C	-5.06	105.65	111.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	365	GLY	Peptide
1	B	365	GLY	Peptide
1	B	383	HIS	Peptide

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	2787	0	2588	69	0
1	B	2818	0	2612	74	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
3	A	59	0	0	6	0
3	B	66	0	0	6	0
All	All	5746	0	5224	143	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 13.

All (143) 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:65:LEU:HD23	3:A:511:HOH:O	1.57	1.03
1:B:69:ILE:HD11	1:B:123:GLN:HB2	1.50	0.91
1:B:69:ILE:HD11	1:B:123:GLN:CB	2.08	0.82
1:A:108:THR:HG22	1:A:112:ASP:OD2	1.80	0.81
1:A:103:THR:HG22	1:A:104:ASP:OD1	1.80	0.81
1:B:21:GLU:H	1:B:382:ASN:HD21	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ILE:HD11	1:A:123:GLN:HB2	1.60	0.80
1:A:103:THR:CG2	1:A:104:ASP:OD1	2.32	0.78
1:A:160:LEU:HA	1:A:163:MET:HE3	1.66	0.77
1:B:103:THR:HG21	3:B:504:HOH:O	1.86	0.75
1:A:108:THR:CG2	1:A:112:ASP:OD2	2.36	0.73
1:A:69:ILE:HD11	1:A:123:GLN:CB	2.23	0.69
1:A:222:ILE:HD11	1:A:263:LEU:HD13	1.74	0.69
1:B:45:ALA:H	1:B:342:GLN:HE21	1.41	0.68
1:A:65:LEU:HB3	3:A:511:HOH:O	1.93	0.68
1:A:222:ILE:C	1:A:222:ILE:HD13	2.19	0.68
1:B:43:ASN:OD1	1:B:81:ARG:HD3	1.95	0.67
1:A:215:MET:HE2	1:A:219:LEU:HD21	1.77	0.67
1:A:286:GLY:O	1:A:319:GLN:HG2	1.95	0.67
1:B:277:TYR:CE2	1:B:303:VAL:HG22	2.31	0.65
1:A:308:LEU:H	1:A:336:ASN:HD22	1.44	0.65
1:B:160:LEU:HA	1:B:163:MET:HE3	1.79	0.64
1:B:193:ASN:HD22	1:B:194:SER:N	1.96	0.64
1:B:222:ILE:HD13	1:B:263:LEU:HD22	1.79	0.64
1:B:193:ASN:HD22	1:B:193:ASN:C	2.07	0.62
1:A:55:ASN:HA	1:A:106:LYS:HB2	1.80	0.62
1:A:222:ILE:CD1	1:A:263:LEU:HD22	2.29	0.62
1:A:231:ASN:ND2	1:A:271:ASN:HD21	1.97	0.62
1:B:308:LEU:H	1:B:336:ASN:HD22	1.46	0.62
1:A:43:ASN:OD1	1:A:81:ARG:HD3	2.02	0.60
1:A:222:ILE:HD11	1:A:263:LEU:CD1	2.31	0.60
1:A:45:ALA:H	1:A:342:GLN:HE21	1.50	0.60
1:B:298:ARG:HG3	1:B:299:TRP:N	2.15	0.59
1:B:384:HIS:HB2	3:B:516:HOH:O	2.02	0.59
1:B:195:CYS:O	1:B:257:HIS:HD2	1.87	0.58
1:A:83:TRP:CD1	1:A:130:VAL:HG13	2.39	0.58
1:B:108:THR:CG2	1:B:112:ASP:OD2	2.53	0.57
1:B:83:TRP:CD1	1:B:130:VAL:CG1	2.88	0.56
1:B:88:GLY:HA2	1:B:91:SER:O	2.05	0.55
1:B:315:SER:O	1:B:318:SER:OG	2.15	0.55
1:A:303:VAL:CG1	1:A:303:VAL:O	2.54	0.55
1:B:298:ARG:HD2	1:B:334:GLY:O	2.06	0.55
1:A:298:ARG:NH2	1:A:303:VAL:O	2.39	0.55
1:A:108:THR:HG22	1:A:112:ASP:CG	2.32	0.55
1:A:121:ASN:HD22	1:A:121:ASN:C	2.15	0.54
1:A:329:TYR:C	1:A:329:TYR:CD1	2.85	0.54
1:B:69:ILE:C	1:B:69:ILE:HD12	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:H	1:A:342:GLN:NE2	2.04	0.54
1:A:215:MET:CE	1:A:219:LEU:HD21	2.37	0.54
1:A:108:THR:CG2	1:A:112:ASP:CG	2.80	0.54
1:A:222:ILE:HD13	1:A:223:ASN:N	2.22	0.54
1:B:173:LEU:HD21	1:B:176:TRP:CZ2	2.41	0.54
1:A:65:LEU:CD2	3:A:511:HOH:O	2.34	0.54
1:B:233:ASP:OD2	1:B:236:ALA:HB2	2.09	0.53
1:A:195:CYS:O	1:A:257:HIS:HD2	1.91	0.53
1:A:315:SER:HB3	3:A:515:HOH:O	2.08	0.53
1:A:323:ILE:HD11	1:A:355:ASN:OD1	2.08	0.53
1:B:69:ILE:HD12	1:B:69:ILE:O	2.09	0.53
1:A:257:HIS:HE1	3:A:536:HOH:O	1.92	0.53
1:B:186:LEU:HD22	1:B:187:GLN:N	2.24	0.53
1:A:353:TYR:CD2	1:A:357:MET:HE2	2.45	0.52
1:B:352:THR:HG22	1:B:354:SER:N	2.25	0.51
1:A:193:ASN:HD22	1:A:194:SER:N	2.09	0.51
1:A:287:LYS:HA	1:A:319:GLN:HE21	1.76	0.51
1:A:81:ARG:HH21	1:A:177:GLU:CD	2.19	0.50
1:B:302:ASN:HB3	3:B:525:HOH:O	2.11	0.50
1:B:219:LEU:HD22	1:B:263:LEU:HD23	1.93	0.50
1:B:45:ALA:H	1:B:342:GLN:NE2	2.07	0.50
1:A:222:ILE:HD12	1:A:263:LEU:HD22	1.94	0.50
1:B:344:ASN:C	1:B:344:ASN:OD1	2.55	0.49
1:B:172:SER:HB2	3:B:507:HOH:O	2.12	0.49
1:B:121:ASN:C	1:B:121:ASN:HD22	2.20	0.49
1:B:288:TRP:H	1:B:319:GLN:HE21	1.61	0.49
1:A:83:TRP:CD1	1:A:130:VAL:CG1	2.96	0.49
1:B:298:ARG:NH2	1:B:304:ASN:HA	2.28	0.48
1:B:352:THR:CG2	1:B:354:SER:HB2	2.42	0.48
1:B:353:TYR:HD1	1:B:357:MET:HE2	1.77	0.48
1:A:352:THR:HG22	1:A:354:SER:N	2.28	0.48
1:A:288:TRP:H	1:A:319:GLN:HE21	1.60	0.48
1:B:289:ASN:HB2	1:B:292:ALA:HB2	1.95	0.48
1:B:83:TRP:CD1	1:B:130:VAL:HG11	2.49	0.48
1:A:198:THR:HA	3:A:517:HOH:O	2.13	0.48
1:B:308:LEU:H	1:B:336:ASN:ND2	2.12	0.48
1:A:298:ARG:NH1	1:A:336:ASN:HD21	2.12	0.48
1:B:55:ASN:HA	1:B:106:LYS:HB2	1.95	0.47
1:B:45:ALA:HB1	1:B:83:TRP:CD1	2.50	0.47
1:B:296:VAL:HG13	1:B:297:ASN:N	2.30	0.47
1:A:69:ILE:CD1	1:A:123:GLN:HB2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TRP:CE3	1:A:244:SER:HB3	2.49	0.47
1:A:44:PHE:HZ	1:A:69:ILE:HG22	1.80	0.47
1:A:159:ALA:C	1:A:162:PRO:HD2	2.40	0.47
1:A:193:ASN:HD22	1:A:193:ASN:C	2.22	0.46
1:B:108:THR:HG22	1:B:112:ASP:OD2	2.14	0.46
1:B:298:ARG:NH1	1:B:336:ASN:HD21	2.13	0.46
1:A:130:VAL:HB	1:A:177:GLU:HB3	1.97	0.46
1:B:352:THR:HG22	1:B:355:ASN:H	1.80	0.46
1:B:41:GLY:HA2	1:B:360:MET:SD	2.55	0.46
1:B:83:TRP:CD1	1:B:130:VAL:HG13	2.50	0.46
1:B:303:VAL:HG13	1:B:303:VAL:O	2.15	0.46
1:A:308:LEU:N	1:A:336:ASN:HD22	2.11	0.46
1:B:323:ILE:HD13	1:B:355:ASN:O	2.16	0.46
1:B:171:PRO:HD2	3:B:507:HOH:O	2.16	0.46
1:B:47:ARG:HG3	1:B:47:ARG:HH11	1.81	0.45
1:A:103:THR:HG23	1:A:109:LEU:CB	2.46	0.45
1:A:308:LEU:H	1:A:336:ASN:ND2	2.12	0.45
1:A:303:VAL:O	1:A:303:VAL:HG13	2.16	0.45
1:A:309:LEU:HD22	1:A:310:ILE:C	2.41	0.45
1:B:62:GLY:HA2	1:B:65:LEU:HD11	1.99	0.45
1:A:354:SER:HA	1:A:357:MET:HE3	1.99	0.45
1:B:139:ASN:OD1	1:B:139:ASN:C	2.60	0.45
1:B:21:GLU:H	1:B:382:ASN:ND2	2.06	0.45
1:B:83:TRP:HA	1:B:130:VAL:HG13	1.98	0.44
1:B:193:ASN:C	1:B:193:ASN:ND2	2.72	0.44
1:B:160:LEU:O	1:B:164:VAL:HG23	2.18	0.44
1:B:222:ILE:HD13	1:B:263:LEU:CD2	2.47	0.44
1:A:69:ILE:C	1:A:69:ILE:HD12	2.43	0.44
1:A:260:ASP:O	1:A:264:THR:HB	2.18	0.44
1:B:121:ASN:C	1:B:121:ASN:ND2	2.76	0.44
1:A:219:LEU:HD22	1:A:263:LEU:HD23	2.00	0.44
1:B:363:LEU:O	1:B:364:LYS:C	2.61	0.44
1:B:133:ASN:ND2	1:B:180:ASN:HD22	2.15	0.43
1:B:222:ILE:CD1	1:B:263:LEU:CD2	2.97	0.43
1:A:183:GLU:OE2	1:A:247:THR:HG21	2.18	0.43
1:A:245:GLU:C	1:A:247:THR:H	2.27	0.43
1:B:259:LYS:O	1:B:260:ASP:C	2.61	0.43
1:A:323:ILE:CD1	1:A:355:ASN:OD1	2.67	0.43
1:B:103:THR:HB	3:B:509:HOH:O	2.18	0.43
1:A:69:ILE:HD11	1:A:123:GLN:CG	2.49	0.43
1:B:353:TYR:CD1	1:B:357:MET:HE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ARG:HH11	1:B:47:ARG:CG	2.32	0.42
1:B:188:PRO:HA	1:B:198:THR:OG1	2.20	0.42
1:B:377:VAL:O	1:B:379:VAL:HG23	2.20	0.42
1:A:88:GLY:HA2	1:A:91:SER:O	2.20	0.42
1:A:69:ILE:HD12	1:A:69:ILE:O	2.20	0.41
1:B:214:PRO:O	1:B:215:MET:C	2.63	0.41
1:B:44:PHE:N	1:B:45:ALA:HA	2.34	0.41
1:A:222:ILE:CD1	1:A:263:LEU:CD2	2.97	0.41
1:B:315:SER:OG	1:B:323:ILE:HG23	2.21	0.41
1:A:65:LEU:O	1:A:69:ILE:HG23	2.21	0.40
1:B:95:ASP:C	1:B:95:ASP:OD1	2.65	0.40
1:B:142:VAL:O	1:B:145:LEU:HB2	2.21	0.40
1:B:186:LEU:HD22	1:B:187:GLN:C	2.47	0.40
1:A:85:HIS:NE2	1:A:163:MET:HE1	2.35	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	A	362/388 (93%)	344 (95%)	16 (4%)	2 (1%)	21	24
1	B	365/388 (94%)	339 (93%)	25 (7%)	1 (0%)	36	43
All	All	727/776 (94%)	683 (94%)	41 (6%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	86	VAL
1	A	86	VAL
1	A	303	VAL

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	291/321 (91%)	262 (90%)	29 (10%)	7	7
1	B	295/321 (92%)	258 (88%)	37 (12%)	4	4
All	All	586/642 (91%)	520 (89%)	66 (11%)	5	5

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	LEU
1	B	37	VAL
1	B	47	ARG
1	B	65	LEU
1	B	69	ILE
1	B	91	SER
1	B	103	THR
1	B	108	THR
1	B	114	SER
1	B	121	ASN
1	B	130	VAL
1	B	131	LEU
1	B	136	LEU
1	B	145	LEU
1	B	170	LYS
1	B	172	SER
1	B	186	LEU
1	B	190	SER
1	B	222	ILE
1	B	243	TRP
1	B	246	LEU
1	B	264	THR
1	B	290	GLN
1	B	296	VAL
1	B	303	VAL
1	B	305	ASP
1	B	309	LEU

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Mol	Chain	Res	Type
1	B	320	ASN
1	B	323	ILE
1	B	326	LEU
1	B	339	LEU
1	B	352	THR
1	B	354	SER
1	B	355	ASN
1	B	378	SER
1	B	384	HIS
1	B	386	HIS
1	A	23	LEU
1	A	37	VAL
1	A	42	VAL
1	A	69	ILE
1	A	103	THR
1	A	130	VAL
1	A	131	LEU
1	A	136	LEU
1	A	140	SER
1	A	172	SER
1	A	186	LEU
1	A	222	ILE
1	A	235	LYS
1	A	243	TRP
1	A	246	LEU
1	A	264	THR
1	A	295	LYS
1	A	296	VAL
1	A	298	ARG
1	A	303	VAL
1	A	305	ASP
1	A	309	LEU
1	A	320	ASN
1	A	323	ILE
1	A	326	LEU
1	A	339	LEU
1	A	354	SER
1	A	355	ASN
1	A	383	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	ASN
1	B	55	ASN
1	B	121	ASN
1	B	123	GLN
1	B	133	ASN
1	B	143	GLN
1	B	144	ASN
1	B	193	ASN
1	B	230	HIS
1	B	231	ASN
1	B	257	HIS
1	B	291	ASN
1	B	302	ASN
1	B	332	ASN
1	B	333	ASN
1	B	336	ASN
1	B	342	GLN
1	B	382	ASN
1	B	385	HIS
1	A	35	GLN
1	A	70	ASN
1	A	121	ASN
1	A	124	ASN
1	A	133	ASN
1	A	144	ASN
1	A	187	GLN
1	A	193	ASN
1	A	230	HIS
1	A	231	ASN
1	A	257	HIS
1	A	302	ASN
1	A	319	GLN
1	A	332	ASN
1	A	336	ASN
1	A	342	GLN

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](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	TRS	B	401	-	7,7,7	0.69	0	9,9,9	1.27	0
2	TRS	A	401	-	7,7,7	0.45	0	9,9,9	1.04	1 (11%)

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
2	TRS	B	401	-	-	3/9/9/9	-
2	TRS	A	401	-	-	6/9/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	TRS	C2-C-C1	-2.23	104.71	110.66

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	TRS	C1-C-C2-O2
2	A	401	TRS	C3-C-C2-O2
2	B	401	TRS	C3-C-C2-O2
2	A	401	TRS	C2-C-C1-O1
2	A	401	TRS	N-C-C1-O1
2	A	401	TRS	C1-C-C2-O2
2	A	401	TRS	C3-C-C1-O1
2	B	401	TRS	N-C-C2-O2
2	A	401	TRS	N-C-C2-O2

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	364/388 (93%)	-0.22	7 (1%) 66 71	28, 42, 57, 95	0
1	B	367/388 (94%)	-0.18	6 (1%) 70 76	28, 41, 57, 100	0
All	All	731/776 (94%)	-0.20	13 (1%) 67 72	28, 41, 58, 100	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	GLY	3.5
1	B	373	LYS	3.4
1	A	383	HIS	3.3
1	B	385	HIS	3.1
1	A	370	SER	3.1
1	A	20	SER	2.7
1	B	383	HIS	2.6
1	A	382	ASN	2.5
1	B	386	HIS	2.4
1	A	371	GLY	2.4
1	A	373	LYS	2.3
1	A	296	VAL	2.2
1	B	284	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TRS	A	401	8/8	0.93	0.14	38,41,43,49	0
2	TRS	B	401	8/8	0.95	0.09	31,37,42,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.