



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:42 AM UTC

PDB ID : 4OK2 / pdb_00004ok2
Title : Crystal Structure of Alg17c Mutant Y258A
Authors : Nair, S.K.; Park, D.S.
Deposited on : 2014-01-21
Resolution : 2.45 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)	:	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

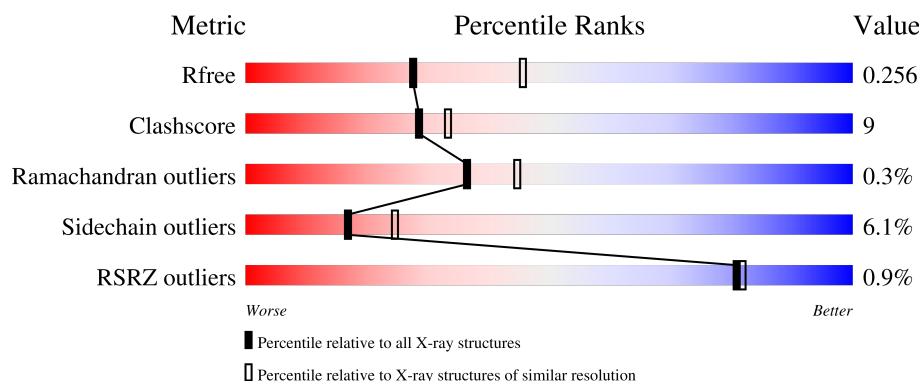
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	736	77% 16% • •
1	B	736	77% 17% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11521 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 Putative alginate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	0	0	0
			5549	3531	938	1067	13			
1	B	705	Total	C	N	O	S	0	0	0
			5539	3525	935	1066	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	ALA	TYR	engineered mutation	UNP Q21FJ0
B	258	ALA	TYR	engineered mutation	UNP Q21FJ0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

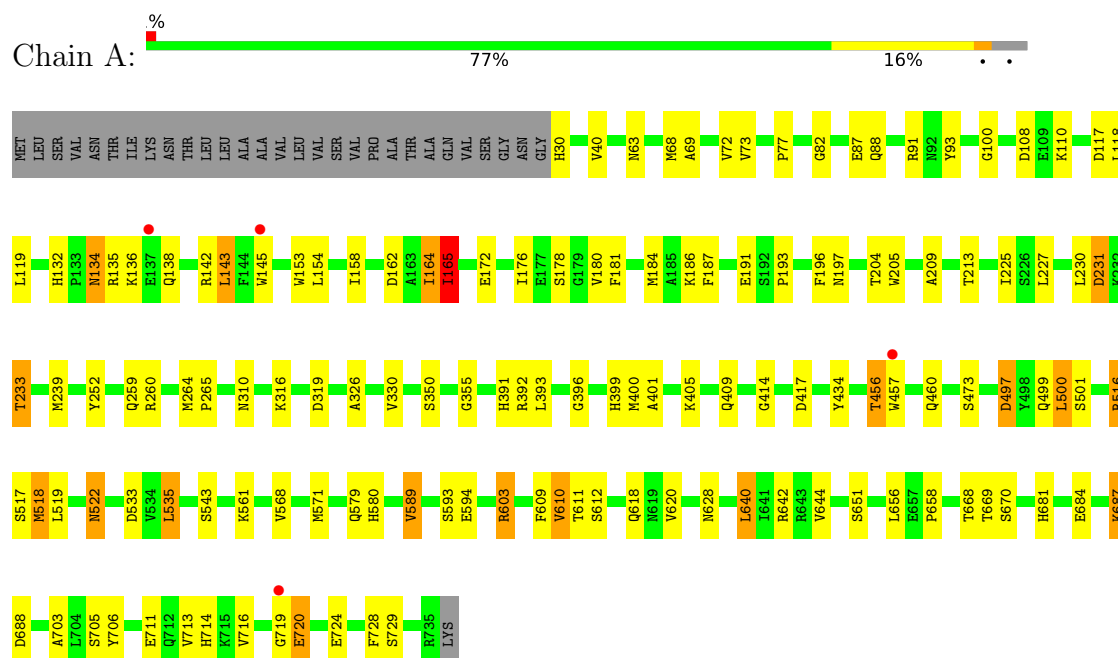
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	245	Total	O	0	0
			245	245		
3	B	186	Total	O	0	0
			186	186		

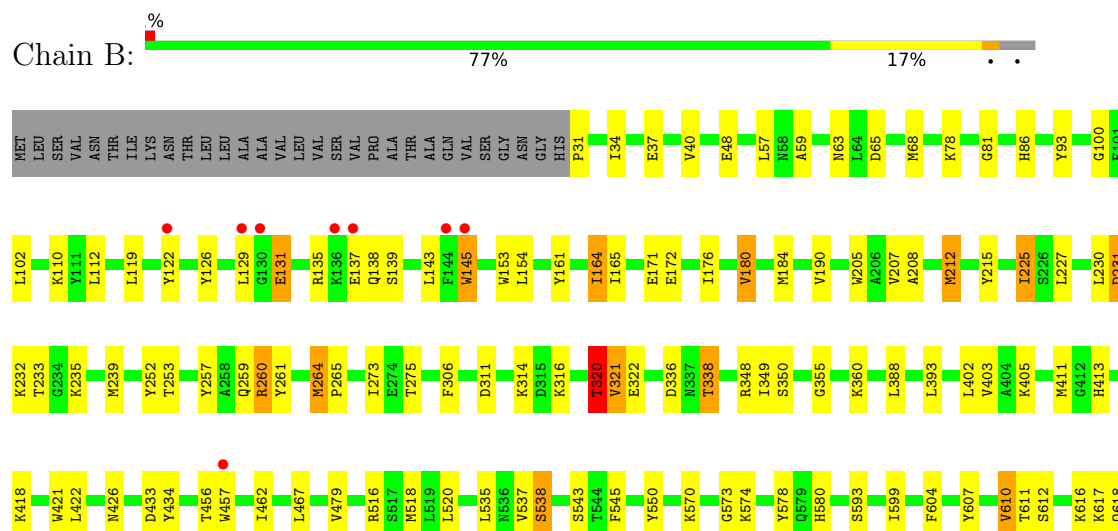
3 Residue-property plots

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: Putative alginate lyase



• Molecule 1: Putative alginate lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.95Å 136.63Å 88.86Å 90.00° 107.11° 90.00°	Depositor
Resolution (Å)	25.00 – 2.45 25.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.2 (25.00-2.45) 93.2 (25.00-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.256 0.192 , 0.256	Depositor DCC
R_{free} test set	3338 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 20.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11521	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 14.29% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/5677	0.89	2/7705 (0.0%)
1	B	0.62	0/5666	0.89	4/7689 (0.1%)
All	All	0.62	0/11343	0.89	6/15394 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	639	VAL	CB-CA-C	-6.67	100.23	110.50
1	B	639	VAL	N-CA-C	5.76	117.05	108.46
1	A	181	PHE	N-CA-C	5.64	117.12	110.97
1	A	165	ILE	N-CA-C	5.61	115.81	110.42
1	B	320	THR	CB-CA-C	-5.06	101.55	109.70
1	B	467	LEU	N-CA-C	5.02	117.48	109.96

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	5549	0	5388	101	0
1	B	5539	0	5382	93	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	245	0	0	4	0
3	B	186	0	0	10	0
All	All	11521	0	10770	193	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 9.

All (193) 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:603:ARG:HH11	1:A:603:ARG:HG3	1.01	1.15
1:A:456:THR:CG2	1:A:580:HIS:NE2	2.17	1.08
1:B:612:SER:OG	1:B:681:HIS:HD2	1.50	0.92
1:A:393:LEU:HD21	1:A:522:ASN:HD21	1.33	0.91
1:A:603:ARG:HG3	1:A:603:ARG:NH1	1.81	0.88
1:B:68:MET:HE1	1:B:110:LYS:HD3	1.59	0.84
1:B:100:GLY:HA2	1:B:164:ILE:HD13	1.59	0.82
1:B:260:ARG:HG3	1:B:261:TYR:N	1.95	0.81
1:B:154:LEU:HB2	1:B:184:MET:HE2	1.62	0.80
1:A:456:THR:HG23	1:A:580:HIS:NE2	1.98	0.78
1:B:208:ALA:O	1:B:212:MET:CG	2.34	0.76
1:A:400:MET:HE1	1:A:658:PRO:HG2	1.68	0.75
1:A:393:LEU:HD21	1:A:522:ASN:ND2	2.00	0.75
1:A:571:MET:CE	1:A:628:ASN:OD1	2.33	0.75
1:A:612:SER:OG	1:A:681:HIS:HD2	1.69	0.75
1:B:456:THR:HG22	1:B:580:HIS:NE2	2.03	0.74
1:A:571:MET:HE1	1:A:628:ASN:OD1	1.88	0.73
1:A:132:HIS:CD2	1:A:134:ASN:H	2.07	0.73
1:B:208:ALA:O	1:B:212:MET:HG2	1.91	0.71
1:B:316:LYS:HZ3	1:B:320:THR:HG23	1.54	0.70
1:B:418:LYS:HE2	3:B:986:HOH:O	1.90	0.70
1:A:392:ARG:HH11	1:A:399:HIS:HE1	1.38	0.70
1:A:603:ARG:HH11	1:A:603:ARG:CG	1.92	0.69
1:B:336:ASP:OD1	1:B:338:THR:HB	1.91	0.69
1:A:456:THR:HG22	1:A:580:HIS:NE2	2.06	0.68
1:B:421:TRP:HB3	1:B:518:MET:CE	2.24	0.68
1:A:589:VAL:HG22	1:A:594:GLU:HG3	1.75	0.67
1:B:421:TRP:HB3	1:B:518:MET:HE3	1.77	0.67
1:A:153:TRP:CE3	1:A:184:MET:HE1	2.29	0.67
1:B:253:THR:HG22	3:B:916:HOH:O	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLY:HA2	1:A:164:ILE:HD13	1.78	0.65
1:B:208:ALA:O	1:B:212:MET:HG3	1.96	0.65
1:B:612:SER:OG	1:B:681:HIS:CD2	2.42	0.65
1:B:31:PRO:HD2	1:B:37:GLU:HG3	1.80	0.64
1:B:100:GLY:HA2	1:B:164:ILE:CD1	2.28	0.64
1:B:516:ARG:HD3	1:B:518:MET:HE2	1.79	0.63
1:B:338:THR:HG21	3:B:963:HOH:O	2.00	0.62
1:B:227:LEU:HD22	1:B:239:MET:HE3	1.81	0.62
1:A:434:TYR:CD2	1:A:457:TRP:HZ3	2.18	0.62
1:B:316:LYS:NZ	1:B:320:THR:HG23	2.13	0.62
1:B:112:LEU:HD12	1:B:164:ILE:HG13	1.81	0.61
1:A:154:LEU:HB2	1:A:184:MET:HE3	1.82	0.61
1:B:456:THR:CG2	1:B:580:HIS:NE2	2.63	0.61
1:A:154:LEU:HD13	1:A:184:MET:CE	2.29	0.61
1:A:522:ASN:N	1:A:522:ASN:HD22	1.98	0.61
1:A:119:LEU:HB3	1:A:176:ILE:HD12	1.83	0.60
1:A:30:HIS:N	3:A:953:HOH:O	2.34	0.60
1:A:227:LEU:HD22	1:A:239:MET:HE2	1.83	0.60
1:A:310:ASN:OD1	1:A:405:LYS:NZ	2.34	0.60
1:A:687:LYS:HG3	1:A:705:SER:HA	1.83	0.60
1:A:620:VAL:HG13	1:A:640:LEU:HD13	1.83	0.60
1:A:136:LYS:HB2	1:A:138:GLN:HG2	1.84	0.60
1:A:456:THR:HG21	1:A:580:HIS:NE2	2.13	0.59
1:A:205:TRP:CZ2	1:A:265:PRO:HD3	2.37	0.59
1:B:34:ILE:HD11	1:B:212:MET:HE1	1.85	0.58
1:A:392:ARG:HH11	1:A:399:HIS:CE1	2.20	0.58
1:A:132:HIS:HD2	1:A:134:ASN:H	1.49	0.58
1:B:119:LEU:HB3	1:B:176:ILE:HD12	1.85	0.58
1:B:714:HIS:O	1:B:724:GLU:HA	2.03	0.57
1:A:593:SER:HA	1:A:610:VAL:HG13	1.86	0.57
1:A:400:MET:CE	1:A:658:PRO:HG2	2.34	0.57
1:A:350:SER:O	1:A:355:GLY:HA3	2.04	0.57
1:B:421:TRP:CG	1:B:518:MET:HE1	2.40	0.57
1:B:456:THR:HG22	1:B:580:HIS:CD2	2.40	0.56
1:A:178:SER:HB2	3:A:1120:HOH:O	2.04	0.56
1:B:231:ASP:O	1:B:232:LYS:HB2	2.05	0.56
1:A:204:THR:HG22	1:A:265:PRO:HB2	1.88	0.56
1:B:516:ARG:CD	1:B:518:MET:HE2	2.36	0.56
1:B:574:LYS:HG2	3:B:959:HOH:O	2.06	0.56
1:A:460:GLN:NE2	1:A:473:SER:OG	2.40	0.55
1:B:593:SER:HA	1:B:610:VAL:HG13	1.86	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LYS:NZ	1:B:320:THR:CG2	2.69	0.55
1:B:86:HIS:CE1	1:B:145:TRP:HZ3	2.23	0.55
1:B:422:LEU:HD11	1:B:433:ASP:HB2	1.89	0.55
1:B:321:VAL:HB	3:B:934:HOH:O	2.06	0.54
1:A:500:LEU:HG	1:A:501:SER:N	2.21	0.54
1:A:687:LYS:HZ3	1:A:714:HIS:HD2	1.55	0.54
1:A:687:LYS:NZ	1:A:714:HIS:HD2	2.05	0.54
1:B:57:LEU:HD11	1:B:102:LEU:HD21	1.89	0.54
1:A:252:TYR:H	1:A:259:GLN:NE2	2.06	0.54
1:A:172:GLU:O	1:A:176:ILE:HG12	2.07	0.53
1:A:568:VAL:HG23	1:B:570:LYS:HG2	1.90	0.53
1:A:405:LYS:HE2	1:A:417:ASP:OD1	2.08	0.53
1:A:714:HIS:O	1:A:724:GLU:HA	2.08	0.53
1:B:402:LEU:HD13	1:B:520:LEU:HD11	1.91	0.53
1:B:434:TYR:CD2	1:B:457:TRP:HZ3	2.27	0.53
1:A:225:ILE:HD12	1:A:230:LEU:HA	1.91	0.52
1:A:205:TRP:CH2	1:A:264:MET:HG2	2.45	0.52
1:A:714:HIS:HE1	3:A:923:HOH:O	1.92	0.51
1:A:153:TRP:HE3	1:A:184:MET:HE1	1.74	0.51
1:A:193:PRO:O	1:A:197:ASN:HB2	2.11	0.51
1:A:516:ARG:HD2	1:A:533:ASP:OD1	2.11	0.51
1:A:618:GLN:HG2	1:A:644:VAL:HG22	1.92	0.51
1:B:257:TYR:O	1:B:260:ARG:HG2	2.10	0.51
1:A:396:GLY:O	1:A:399:HIS:HD2	1.94	0.51
1:B:426:ASN:ND2	3:B:1001:HOH:O	2.44	0.51
1:A:82:GLY:HA2	1:A:87:GLU:OE2	2.11	0.50
1:A:681:HIS:HE1	1:A:688:ASP:OD1	1.95	0.50
1:A:571:MET:HE2	1:A:628:ASN:OD1	2.10	0.50
1:A:706:TYR:HA	1:A:728:PHE:CE2	2.46	0.50
1:B:537:VAL:HG22	1:B:538:SER:N	2.27	0.49
1:A:703:ALA:O	1:A:729:SER:HA	2.12	0.49
1:B:86:HIS:CE1	1:B:145:TRP:CZ3	3.00	0.49
1:A:231:ASP:OD2	1:A:233:THR:OG1	2.31	0.49
1:B:421:TRP:HB3	1:B:518:MET:HE1	1.94	0.49
1:B:607:TYR:HE1	1:B:654:SER:HB3	1.78	0.49
1:A:154:LEU:HB3	1:A:209:ALA:HB1	1.95	0.49
1:B:612:SER:HG	1:B:681:HIS:HD2	1.57	0.49
1:A:196:PHE:CZ	1:A:225:ILE:HG22	2.48	0.48
1:A:205:TRP:HH2	1:A:264:MET:HE3	1.78	0.48
1:A:497:ASP:OD2	1:A:497:ASP:N	2.43	0.48
1:A:609:PHE:HB2	1:A:642:ARG:CZ	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:TYR:H	1:B:259:GLN:NE2	2.12	0.48
1:B:709:ASN:HB2	3:B:1033:HOH:O	2.12	0.48
1:B:122:TYR:HB3	1:B:180:VAL:HG11	1.93	0.48
1:B:348:ARG:HG3	3:B:1031:HOH:O	2.13	0.48
1:A:593:SER:CA	1:A:610:VAL:HG13	2.43	0.48
1:B:231:ASP:HB2	1:B:233:THR:H	1.77	0.47
1:B:611:THR:HA	1:B:651:SER:O	2.15	0.47
1:A:326:ALA:O	1:A:330:VAL:HG23	2.14	0.47
1:B:607:TYR:CE1	1:B:654:SER:HB3	2.50	0.47
1:A:571:MET:HE2	1:A:579:GLN:O	2.14	0.47
1:B:611:THR:HB	1:B:618:GLN:OE1	2.15	0.47
1:A:88:GLN:OE1	1:A:91:ARG:NH1	2.48	0.46
1:B:172:GLU:O	1:B:176:ILE:HG12	2.14	0.46
1:B:550:TYR:CD1	1:B:639:VAL:HG13	2.49	0.46
1:B:684:GLU:HB2	1:B:716:VAL:HG13	1.97	0.46
1:B:161:TYR:CZ	1:B:165:ILE:HD11	2.50	0.46
1:A:88:GLN:HA	1:A:91:ARG:NH1	2.31	0.46
1:A:158:ILE:HG12	1:A:213:THR:HA	1.97	0.46
1:B:264:MET:HB3	1:B:265:PRO:CD	2.46	0.46
1:B:520:LEU:N	1:B:520:LEU:HD12	2.31	0.46
1:B:264:MET:HB3	1:B:265:PRO:HD3	1.97	0.46
1:B:306:PHE:HD2	1:B:316:LYS:HG3	1.81	0.46
1:A:186:LYS:HE3	1:A:191:GLU:OE2	2.16	0.45
1:B:543:SER:HB2	1:B:545:PHE:CE1	2.51	0.45
1:B:403:VAL:HB	1:B:422:LEU:HB2	1.99	0.45
1:B:215:TYR:HE1	1:B:273:ILE:HD13	1.82	0.45
1:A:153:TRP:CZ3	1:A:184:MET:HE1	2.51	0.45
1:B:703:ALA:O	1:B:729:SER:HA	2.16	0.45
1:A:612:SER:OG	1:A:681:HIS:CD2	2.60	0.45
1:A:603:ARG:NH1	1:A:603:ARG:CG	2.61	0.45
1:B:31:PRO:N	3:B:908:HOH:O	2.49	0.44
1:B:231:ASP:O	1:B:232:LYS:CB	2.66	0.44
1:A:589:VAL:CG2	1:A:594:GLU:HG3	2.42	0.44
1:A:72:VAL:HG13	1:A:118:LEU:HD23	1.99	0.44
1:A:93:TYR:HB3	1:A:153:TRP:CD1	2.52	0.44
1:A:108:ASP:OD1	1:A:110:LYS:HG2	2.17	0.44
1:B:260:ARG:CD	1:B:316:LYS:HD2	2.46	0.44
1:A:231:ASP:OD1	1:A:231:ASP:N	2.39	0.44
1:A:260:ARG:HD2	1:A:260:ARG:C	2.43	0.44
1:B:320:THR:HB	1:B:322:GLU:OE1	2.18	0.44
1:B:126:TYR:HA	1:B:129:LEU:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:HG21	1:A:117:ASP:HB3	2.00	0.43
1:B:734:ARG:HB3	1:B:735:ARG:H	1.72	0.43
1:A:719:GLY:O	1:A:720:GLU:HB2	2.18	0.43
1:B:311:ASP:HB2	1:B:413:HIS:HB3	2.00	0.43
1:A:77:PRO:HG3	1:A:143:LEU:HA	1.99	0.43
1:A:162:ASP:HA	1:A:165:ILE:HD11	1.99	0.43
1:A:391:HIS:O	1:A:401:ALA:HA	2.19	0.43
1:A:142:ARG:HG3	1:A:187:PHE:CE2	2.54	0.43
1:B:205:TRP:CZ2	1:B:265:PRO:HD3	2.54	0.43
1:B:350:SER:O	1:B:355:GLY:HA3	2.19	0.43
1:B:65:ASP:HA	1:B:68:MET:HE2	1.99	0.43
1:A:68:MET:HE1	1:A:110:LYS:HD2	2.00	0.43
1:B:611:THR:HG21	1:B:644:VAL:HG21	2.01	0.42
1:A:516:ARG:HD3	1:A:535:LEU:HB2	2.01	0.42
1:B:138:GLN:O	1:B:139:SER:C	2.62	0.42
1:B:599:ILE:HD13	1:B:604:PHE:CE1	2.54	0.42
1:B:225:ILE:HG13	1:B:230:LEU:HA	2.01	0.42
1:B:93:TYR:CD2	1:B:153:TRP:HA	2.54	0.42
1:B:349:ILE:HD12	3:B:936:HOH:O	2.19	0.42
1:A:93:TYR:CD1	1:A:153:TRP:HA	2.54	0.42
1:A:409:GLN:O	1:A:414:GLY:HA3	2.19	0.42
1:B:402:LEU:HD13	1:B:520:LEU:CD1	2.49	0.42
1:A:684:GLU:O	1:A:687:LYS:HB2	2.19	0.42
1:A:63:ASN:HB3	3:A:1063:HOH:O	2.19	0.41
1:A:393:LEU:HD13	1:A:499:GLN:HE21	1.85	0.41
1:B:573:GLY:HA3	1:B:578:TYR:HB3	2.01	0.41
1:A:611:THR:HA	1:A:651:SER:O	2.19	0.41
1:A:669:THR:HG22	1:A:670:SER:N	2.34	0.41
1:B:131:GLU:H	1:B:131:GLU:HG2	1.64	0.41
1:B:537:VAL:CG2	1:B:538:SER:N	2.83	0.41
1:A:518:MET:HE3	1:A:533:ASP:HB2	2.01	0.41
1:B:59:ALA:O	1:B:63:ASN:ND2	2.54	0.41
1:B:215:TYR:CE1	1:B:273:ILE:HD13	2.54	0.41
1:A:319:ASP:OD1	1:A:319:ASP:C	2.62	0.41
1:A:500:LEU:HD12	1:A:519:LEU:HG	2.03	0.41
1:B:388:LEU:HD12	1:B:405:LYS:HA	2.03	0.41
1:A:684:GLU:HB3	1:A:716:VAL:HG13	2.02	0.41
1:B:620:VAL:C	1:B:621:LEU:HD12	2.46	0.41
1:A:516:ARG:HG3	1:A:517:SER:N	2.36	0.40
1:B:153:TRP:CE3	1:B:184:MET:HE1	2.56	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	704/736 (96%)	671 (95%)	31 (4%)	2 (0%)	36	45
1	B	703/736 (96%)	659 (94%)	42 (6%)	2 (0%)	36	45
All	All	1407/1472 (96%)	1330 (94%)	73 (5%)	4 (0%)	36	45

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	720	GLU
1	B	81	GLY
1	B	718	ALA
1	A	69	ALA

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	586/610 (96%)	556 (95%)	30 (5%)	21	31
1	B	585/610 (96%)	543 (93%)	42 (7%)	13	17
All	All	1171/1220 (96%)	1099 (94%)	72 (6%)	17	24

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	73	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	134	ASN
1	A	135	ARG
1	A	143	LEU
1	A	145	TRP
1	A	164	ILE
1	A	165	ILE
1	A	180	VAL
1	A	231	ASP
1	A	233	THR
1	A	316	LYS
1	A	456	THR
1	A	497	ASP
1	A	500	LEU
1	A	516	ARG
1	A	518	MET
1	A	522	ASN
1	A	535	LEU
1	A	543	SER
1	A	561	LYS
1	A	589	VAL
1	A	603	ARG
1	A	610	VAL
1	A	640	LEU
1	A	656	LEU
1	A	668	THR
1	A	687	LYS
1	A	711	GLU
1	A	713	VAL
1	B	40	VAL
1	B	48	GLU
1	B	78	LYS
1	B	131	GLU
1	B	135	ARG
1	B	137	GLU
1	B	143	LEU
1	B	145	TRP
1	B	164	ILE
1	B	171	GLU
1	B	180	VAL
1	B	190	VAL
1	B	207	VAL
1	B	212	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	225	ILE
1	B	231	ASP
1	B	235	LYS
1	B	260	ARG
1	B	264	MET
1	B	275	THR
1	B	314	LYS
1	B	320	THR
1	B	321	VAL
1	B	338	THR
1	B	360	LYS
1	B	393	LEU
1	B	411	MET
1	B	462	ILE
1	B	479	VAL
1	B	535	LEU
1	B	538	SER
1	B	610	VAL
1	B	616	LYS
1	B	617	LYS
1	B	620	VAL
1	B	621	LEU
1	B	639	VAL
1	B	649	GLN
1	B	656	LEU
1	B	670	SER
1	B	677	LYS
1	B	694	LEU

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

Mol	Chain	Res	Type
1	A	32	ASN
1	A	58	ASN
1	A	132	HIS
1	A	201	ASN
1	A	259	GLN
1	A	344	GLN
1	A	368	GLN
1	A	399	HIS
1	A	428	ASN
1	A	441	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	460	GLN
1	A	522	ASN
1	A	585	ASN
1	A	681	HIS
1	A	714	HIS
1	B	42	ASN
1	B	63	ASN
1	B	86	HIS
1	B	149	ASN
1	B	197	ASN
1	B	201	ASN
1	B	259	GLN
1	B	276	ASN
1	B	409	GLN
1	B	413	HIS
1	B	426	ASN
1	B	428	ASN
1	B	486	HIS
1	B	552	ASN
1	B	636	GLN
1	B	638	GLN
1	B	681	HIS
1	B	699	ASN
1	B	712	GLN
1	B	717	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 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

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	706/736 (95%)	-0.27	4 (0%) 85 87	17, 37, 65, 120	0
1	B	705/736 (95%)	-0.02	9 (1%) 75 77	22, 40, 77, 134	0
All	All	1411/1472 (95%)	-0.15	13 (0%) 81 82	17, 39, 72, 134	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	145	TRP	3.5
1	B	457	TRP	2.9
1	A	145	TRP	2.6
1	B	122	TYR	2.6
1	A	457	TRP	2.5
1	B	136	LYS	2.4
1	A	719	GLY	2.3
1	B	735	ARG	2.2
1	B	129	LEU	2.2
1	B	137	GLU	2.2
1	B	130	GLY	2.1
1	A	137	GLU	2.1
1	B	144	PHE	2.1

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	ZN	B	801	1/1	0.98	0.03	34,34,34,34	0
2	ZN	A	801	1/1	0.99	0.04	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.