



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:51 AM UTC

PDB ID : 4AE1 / pdb_00004ae1
Title : Crystal structure of diphtheria toxin mutant CRM197 in complex with nicotinamide
Authors : Malito, E.; Spraggon, G.
Deposited on : 2012-01-04
Resolution : 2.08 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

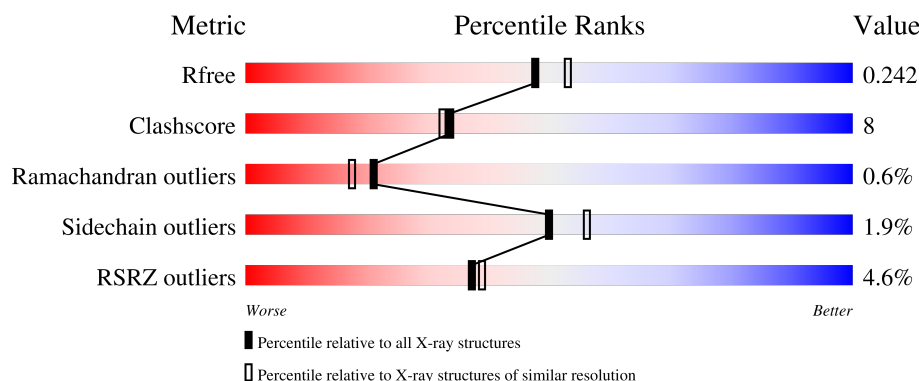
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	535	4% 82% 10% 6%
1	B	535	4% 80% 13% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NCA	A	1536	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7722 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.

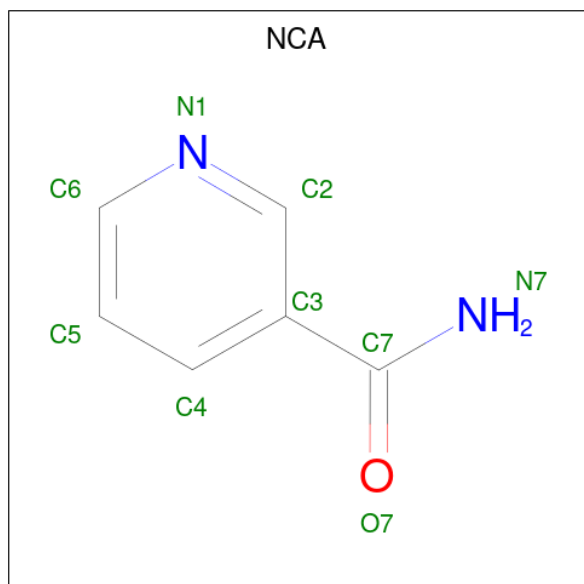
- Molecule 1 is a protein called DIPHTHERIA TOXIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3708	2336	629	731	12			
1	B	501	Total	C	N	O	S	0	1	0
			3744	2358	635	739	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	GLU	GLY	engineered mutation	UNP P00588
B	52	GLU	GLY	engineered mutation	UNP P00588

- Molecule 2 is NICOTINAMIDE (CCD ID: NCA) (formula: C₆H₆N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	6	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			9	6	2	1		

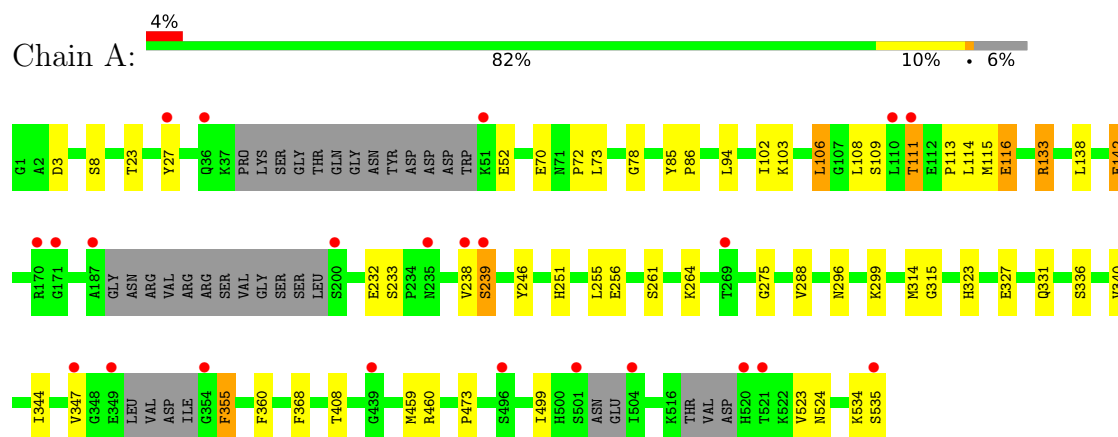
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	154	Total	O	0	0
			154	154		
3	B	98	Total	O	0	0
			98	98		

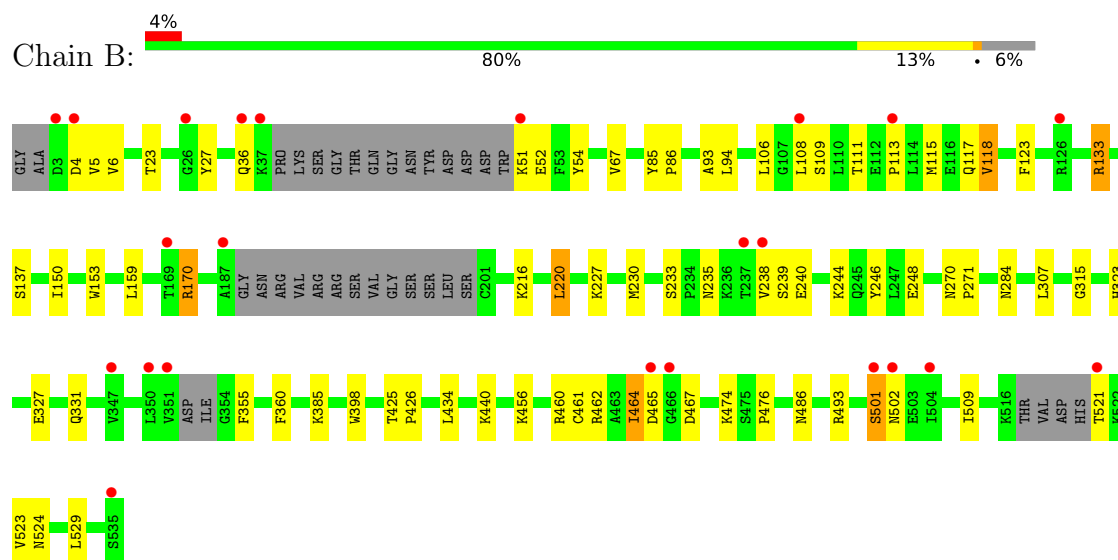
3 Residue-property plots

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: DIPHTHERIA TOXIN



• Molecule 1: DIPHTHERIA TOXIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.65Å 69.26Å 69.68Å 98.36° 99.57° 97.76°	Depositor
Resolution (Å)	52.56 – 2.08 52.56 – 2.08	Depositor EDS
% Data completeness (in resolution range)	83.7 (52.56-2.08) 90.3 (52.56-2.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.08Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.196 , 0.244 0.198 , 0.242	Depositor DCC
R_{free} test set	3257 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7722	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: NCA

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	0.49	0/3780	0.80	0/5138
1	B	0.49	0/3818	0.81	5/5185 (0.1%)
All	All	0.49	0/7598	0.81	5/10323 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	VAL	N-CA-C	-11.81	101.56	112.43
1	B	4	ASP	N-CA-C	6.28	119.04	108.23
1	B	385	LYS	CB-CA-C	-5.16	110.61	116.54
1	B	67	VAL	N-CA-C	5.04	115.54	108.89
1	B	467	ASP	N-CA-C	-5.03	107.19	113.72

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	3708	0	3498	47	1
1	B	3744	0	3564	72	1
2	A	9	0	6	0	0
2	B	9	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	154	0	0	2	0
3	B	98	0	0	1	0
All	All	7722	0	7074	112	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 8.

All (112) 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:B:51:LYS:HG2	1:B:153:TRP:CD1	1.54	1.40
1:B:51:LYS:CG	1:B:153:TRP:HD1	1.51	1.23
1:B:51:LYS:O	1:B:115:MET:CB	2.02	1.07
1:B:51:LYS:C	1:B:52:GLU:HG2	1.84	1.03
1:B:51:LYS:C	1:B:52:GLU:CG	2.34	1.00
1:B:51:LYS:O	1:B:115:MET:HG3	1.71	0.89
1:B:51:LYS:O	1:B:115:MET:CG	2.21	0.87
1:A:142:GLU:H	1:A:142:GLU:CD	1.81	0.87
1:B:51:LYS:O	1:B:115:MET:HB3	1.73	0.87
1:B:51:LYS:HG2	1:B:153:TRP:HD1	0.71	0.85
1:A:52:GLU:HG2	1:A:115:MET:HG3	1.60	0.83
1:B:51:LYS:O	1:B:52:GLU:HG2	1.81	0.81
1:B:51:LYS:HA	1:B:153:TRP:CD1	2.17	0.80
1:A:85:TYR:CD1	1:A:133:ARG:HD2	2.20	0.74
1:B:51:LYS:N	1:B:52:GLU:HG3	2.02	0.74
1:A:73:LEU:HD22	1:B:476:PRO:HD3	1.70	0.73
1:B:227:LYS:HA	1:B:230:MET:HE3	1.71	0.73
1:B:51:LYS:CG	1:B:153:TRP:CD1	2.42	0.70
1:B:51:LYS:C	1:B:52:GLU:CB	2.45	0.70
1:B:460:ARG:HD2	1:B:462:ARG:NH2	2.06	0.69
1:A:142:GLU:HG3	1:B:486:ASN:HB3	1.74	0.69
1:A:142:GLU:HG3	1:B:486:ASN:CB	2.23	0.68
1:B:244:LYS:O	1:B:248:GLU:HG3	1.93	0.68
1:A:142:GLU:HG3	1:B:486:ASN:CG	2.19	0.68
1:B:113:PRO:O	1:B:117:GLN:HG3	1.95	0.67
1:A:106:LEU:HB3	1:A:108:LEU:HD13	1.77	0.65
1:B:51:LYS:HA	1:B:153:TRP:NE1	2.12	0.64
1:B:170:ARG:HH11	1:B:170:ARG:HG3	1.65	0.62
1:B:315:GLY:HA3	1:B:323:HIS:CD2	2.35	0.62
1:B:461:CYS:O	1:B:462:ARG:HD3	2.00	0.62
1:A:142:GLU:HG3	1:B:486:ASN:ND2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LEU:CB	1:B:108:LEU:HD23	2.30	0.61
1:A:133:ARG:HD3	3:A:2017:HOH:O	2.00	0.61
1:A:315:GLY:HA3	1:A:323:HIS:CD2	2.36	0.61
1:B:460:ARG:HD2	1:B:462:ARG:CZ	2.31	0.60
1:B:51:LYS:O	1:B:115:MET:HB2	1.98	0.60
1:B:86:PRO:O	1:B:133:ARG:NH2	2.34	0.58
1:A:255:LEU:HG	1:A:264:LYS:HD3	1.85	0.58
1:B:51:LYS:CB	1:B:153:TRP:HD1	2.12	0.58
1:B:238:VAL:HG22	1:B:239:SER:H	1.67	0.58
1:B:106:LEU:HB2	1:B:108:LEU:HD23	1.84	0.57
1:B:170:ARG:HG3	1:B:170:ARG:NH1	2.19	0.57
1:B:230:MET:O	1:B:233:SER:HB3	2.04	0.57
1:B:109:SER:OG	1:B:111:THR:HG22	2.04	0.57
1:A:327:GLU:HG3	1:A:331:GLN:HE21	1.70	0.57
1:B:51:LYS:CA	1:B:153:TRP:CD1	2.89	0.56
1:B:118:VAL:HA	1:B:123:PHE:CD2	2.42	0.55
1:A:232:GLU:HG2	1:A:232:GLU:O	2.04	0.55
1:A:102:ILE:O	1:A:106:LEU:HB2	2.06	0.54
1:A:113:PRO:HG2	1:A:116:GLU:HB2	1.90	0.54
1:A:327:GLU:HG3	1:A:331:GLN:NE2	2.24	0.53
1:A:238:VAL:HG22	1:A:239:SER:N	2.24	0.52
1:B:238:VAL:HG22	1:B:239:SER:N	2.25	0.52
1:A:261:SER:O	1:A:264:LYS:HB3	2.10	0.52
1:B:52:GLU:N	1:B:153:TRP:NE1	2.57	0.51
1:B:233:SER:HB2	1:B:246:TYR:CZ	2.46	0.51
1:A:408:THR:OG1	1:A:499:ILE:HG13	2.11	0.51
1:A:523:VAL:HG22	1:A:524:ASN:N	2.26	0.51
1:B:52:GLU:N	1:B:153:TRP:HE1	2.10	0.50
1:B:523:VAL:HG22	1:B:524:ASN:N	2.25	0.50
1:A:142:GLU:CG	1:B:486:ASN:HB3	2.41	0.50
1:B:51:LYS:CB	1:B:153:TRP:CD1	2.91	0.50
1:A:296:ASN:CG	1:A:299:LYS:HZ3	2.20	0.49
1:A:340:VAL:O	1:A:344:ILE:HG13	2.13	0.49
1:A:256:GLU:HG2	3:A:2043:HOH:O	2.11	0.49
1:B:464:ILE:HG22	1:B:465:ASP:N	2.27	0.49
1:A:355:PHE:CE1	1:A:360:PHE:HB2	2.48	0.49
1:B:327:GLU:HG3	1:B:331:GLN:HE21	1.78	0.48
1:B:523:VAL:HG22	1:B:524:ASN:H	1.77	0.48
1:A:534:LYS:O	1:A:535:SER:HB2	2.14	0.47
1:B:240:GLU:HG3	1:B:244:LYS:HZ2	1.79	0.47
1:B:355:PHE:CE2	1:B:360:PHE:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ARG:HD3	1:A:460:ARG:HA	1.53	0.47
1:B:85:TYR:CE2	1:B:159:LEU:HD21	2.49	0.47
1:A:85:TYR:CE1	1:A:133:ARG:HD2	2.49	0.47
1:A:94:LEU:HB2	1:A:138:LEU:CD2	2.44	0.47
1:A:251:HIS:CD2	1:A:275:GLY:HA3	2.50	0.47
1:B:529:LEU:HD22	1:B:529:LEU:N	2.30	0.46
1:A:142:GLU:CD	1:A:142:GLU:N	2.61	0.46
1:A:233:SER:HB2	1:A:246:TYR:CZ	2.50	0.46
1:A:296:ASN:CG	1:A:299:LYS:NZ	2.74	0.46
1:A:459:MET:HG2	1:A:473:PRO:HA	1.98	0.45
1:B:106:LEU:HB3	1:B:108:LEU:HD23	1.97	0.45
1:B:216:LYS:O	1:B:220:LEU:HD13	2.17	0.45
1:A:238:VAL:CG2	1:A:239:SER:N	2.80	0.45
1:A:327:GLU:O	1:A:331:GLN:HG3	2.17	0.45
1:A:109:SER:OG	1:A:111:THR:HG23	2.16	0.44
1:A:86:PRO:O	1:A:133:ARG:NH2	2.50	0.44
1:B:93:ALA:HA	1:B:137:SER:HB3	1.99	0.44
1:B:6:VAL:HG22	1:B:94:LEU:HD23	1.99	0.44
1:B:51:LYS:N	1:B:52:GLU:CG	2.79	0.44
1:B:398:TRP:CE2	1:B:529:LEU:HB3	2.52	0.44
1:A:106:LEU:HA	1:A:106:LEU:HD12	1.84	0.43
1:B:434:LEU:HD23	1:B:509:ILE:HG12	1.99	0.43
1:B:456:LYS:NZ	3:B:2092:HOH:O	2.51	0.43
1:A:72:PRO:HB3	1:B:474:LYS:HB3	2.00	0.43
1:B:440:LYS:O	1:B:493:ARG:HG2	2.18	0.42
1:B:270:ASN:HA	1:B:271:PRO:HD3	1.90	0.42
1:B:284:ASN:OD1	1:B:307:LEU:HD22	2.20	0.42
1:B:460:ARG:NH2	1:B:474:LYS:NZ	2.67	0.42
1:A:314:MET:HA	1:A:368:PHE:CZ	2.55	0.42
1:B:240:GLU:HG3	1:B:244:LYS:NZ	2.35	0.42
1:B:327:GLU:HG3	1:B:331:GLN:NE2	2.34	0.42
1:A:23:THR:HG22	1:A:27:TYR:HB2	2.02	0.41
1:B:23:THR:HG22	1:B:27:TYR:HB2	2.02	0.41
1:A:70:GLU:C	1:A:72:PRO:HD3	2.46	0.41
1:A:103:LYS:HE2	1:A:114:LEU:N	2.35	0.41
1:A:85:TYR:HA	1:A:86:PRO:HD3	1.93	0.41
1:B:425:THR:HB	1:B:426:PRO:CD	2.51	0.41
1:A:355:PHE:CD1	1:A:355:PHE:C	2.98	0.41
1:B:501:SER:OG	1:B:502:ASN:N	2.53	0.41
1:B:54:TYR:CE2	1:B:150:ILE:HG12	2.56	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASN:ND2	1:B:36:GLN:OE1[1_454]	2.11	0.09

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	489/535 (91%)	468 (96%)	18 (4%)	3 (1%)	21	17
1	B	491/535 (92%)	473 (96%)	15 (3%)	3 (1%)	21	17
All	All	980/1070 (92%)	941 (96%)	33 (3%)	6 (1%)	21	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	SER
1	A	347	VAL
1	B	501	SER
1	B	235	ASN
1	A	78	GLY
1	B	464	ILE

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	384/453 (85%)	374 (97%)	10 (3%)	40	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	394/453 (87%)	389 (99%)	5 (1%)	61	68
All	All	778/906 (86%)	763 (98%)	15 (2%)	50	56

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	8	SER
1	A	106	LEU
1	A	111	THR
1	A	116	GLU
1	A	133	ARG
1	A	142	GLU
1	A	288	VAL
1	A	336	SER
1	A	355	PHE
1	B	118	VAL
1	B	133	ARG
1	B	170	ARG
1	B	220	LEU
1	B	521	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	HIS
1	A	251	HIS
1	B	151	ASN
1	B	342	GLN
1	B	366	ASN
1	B	391	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 [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	NCA	B	1536	-	9,9,9	2.82	4 (44%)	11,11,11	1.87	5 (45%)
2	NCA	A	1536	-	9,9,9	2.82	4 (44%)	11,11,11	2.01	6 (54%)

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	NCA	B	1536	-	-	0/4/4/4	0/1/1/1
2	NCA	A	1536	-	-	0/4/4/4	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1536	NCA	C7-N7	6.58	1.45	1.33
2	A	1536	NCA	C7-N7	6.55	1.45	1.33
2	A	1536	NCA	C2-C3	-3.42	1.33	1.39
2	B	1536	NCA	C2-C3	-3.32	1.33	1.39
2	B	1536	NCA	C4-C3	3.19	1.44	1.39
2	A	1536	NCA	C4-C3	3.04	1.44	1.39
2	A	1536	NCA	C3-C7	-2.44	1.47	1.50
2	B	1536	NCA	C3-C7	-2.07	1.47	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1536	NCA	C3-C7-N7	3.24	121.73	117.74
2	A	1536	NCA	C5-C4-C3	-3.19	117.23	120.36
2	A	1536	NCA	C4-C3-C2	2.92	120.86	117.61
2	A	1536	NCA	C3-C7-N7	2.90	121.31	117.74
2	B	1536	NCA	C5-C4-C3	-2.54	117.87	120.36
2	B	1536	NCA	C6-N1-C2	2.46	121.16	116.85
2	B	1536	NCA	O7-C7-N7	-2.43	119.10	122.62
2	A	1536	NCA	O7-C7-N7	-2.30	119.29	122.62
2	B	1536	NCA	C4-C3-C2	2.22	120.08	117.61
2	A	1536	NCA	C6-N1-C2	2.19	120.69	116.85
2	A	1536	NCA	C3-C2-N1	-2.04	120.46	123.50

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	51:LYS	C	52:GLU	N	2.04

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	501/535 (93%)	0.24	23 (4%) 37 39	15, 41, 76, 87	0
1	B	501/535 (93%)	0.20	23 (4%) 37 39	14, 37, 70, 101	1 (0%)
All	All	1002/1070 (93%)	0.22	46 (4%) 37 39	14, 39, 72, 101	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	LYS	7.6
1	B	3	ASP	7.1
1	B	351	VAL	5.6
1	A	520	HIS	5.5
1	A	349	GLU	5.1
1	B	187	ALA	4.9
1	B	36	GLN	4.9
1	B	501	SER	4.8
1	A	354	GLY	4.5
1	A	36	GLN	4.4
1	A	187	ALA	4.3
1	A	51	LYS	4.3
1	A	504	ILE	4.2
1	A	200	SER	3.9
1	A	521	THR	3.8
1	B	4	ASP	3.7
1	B	521	THR	3.6
1	B	238	VAL	3.4
1	A	347	VAL	3.3
1	B	502	ASN	3.2
1	A	170	ARG	3.1
1	B	535	SER	3.0
1	A	535	SER	3.0
1	B	504	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	235	ASN	2.9
1	B	237	THR	2.9
1	A	171	GLY	2.8
1	A	439	GLY	2.8
1	B	466	GLY	2.7
1	B	465	ASP	2.6
1	A	269	THR	2.6
1	B	113	PRO	2.4
1	B	350	LEU	2.4
1	A	239	SER	2.4
1	B	37	LYS	2.3
1	A	110	LEU	2.3
1	A	238	VAL	2.2
1	A	496	SER	2.2
1	A	501	SER	2.2
1	B	169	THR	2.2
1	B	347	VAL	2.2
1	B	26	GLY	2.2
1	A	111	THR	2.2
1	B	126	ARG	2.1
1	B	108	LEU	2.1
1	A	27	TYR	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($\text{\AA}^2$)	Q<0.9
2	NCA	A	1536	9/9	0.96	0.06	30,35,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NCA	B	1536	9/9	0.96	0.07	34,41,48,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.