



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:10 PM UTC

PDB ID : 3T66 / pdb_00003t66
Title : Crystal structure of Nickel ABC transporter from *Bacillus halodurans*
Authors : Agarwal, R.; Bonanno, J.B.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2011-07-28
Resolution : 2.80 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

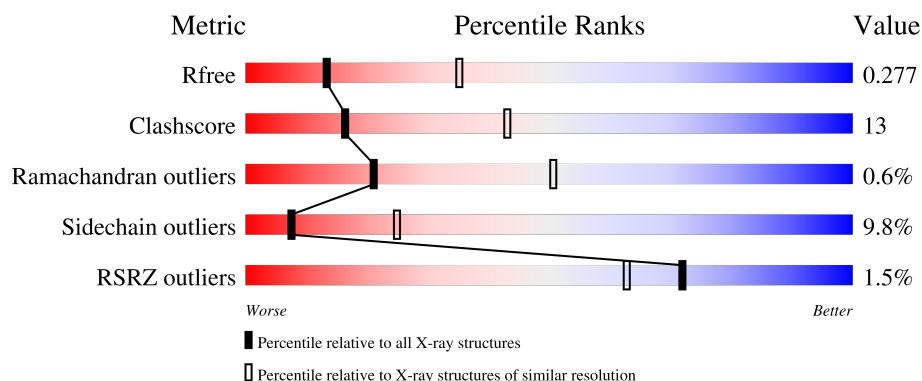
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	496	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3491 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 Nickel ABC transporter (Nickel-binding protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3481	2198	592	684	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9KBX8
A	2	VAL	-	expression tag	UNP Q9KBX8
A	489	ALA	-	expression tag	UNP Q9KBX8
A	490	GLU	-	expression tag	UNP Q9KBX8
A	491	ASN	-	expression tag	UNP Q9KBX8
A	492	LEU	-	expression tag	UNP Q9KBX8
A	493	TYR	-	expression tag	UNP Q9KBX8
A	494	PHE	-	expression tag	UNP Q9KBX8
A	495	GLN	-	expression tag	UNP Q9KBX8
A	496	SER	-	expression tag	UNP Q9KBX8

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

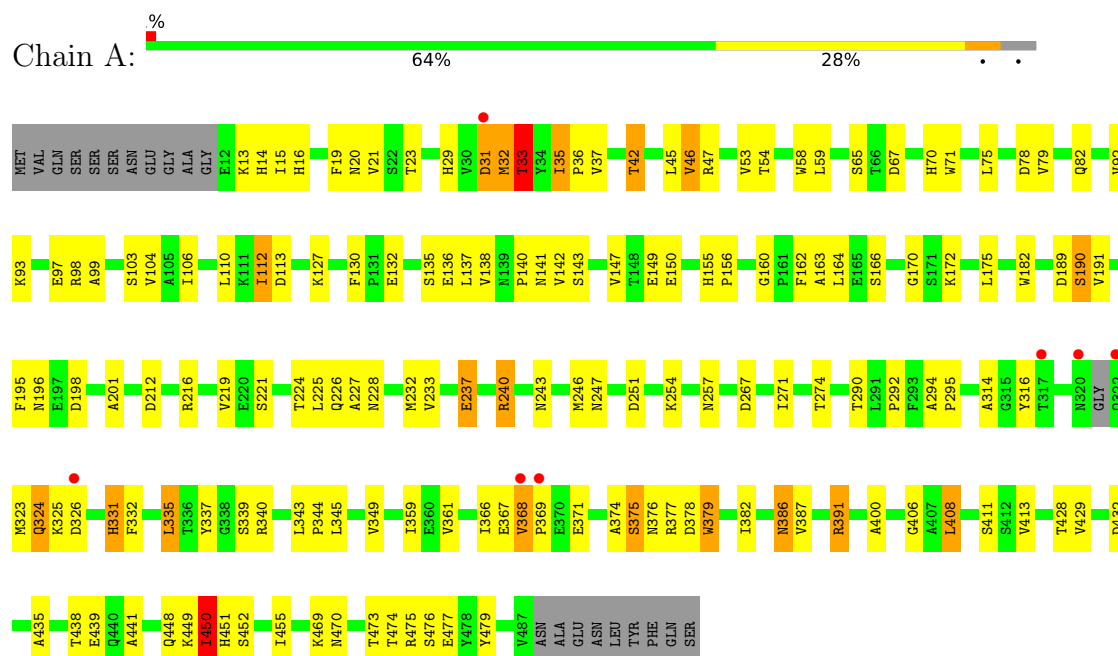
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		

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: Nickel ABC transporter (Nickel-binding protein)



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.05Å 147.13Å 75.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.98-2.80) 98.7 (19.98-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.25 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.219 , 0.274 0.223 , 0.277	Depositor DCC
R_{free} test set	864 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3491	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: 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	1.20	2/3556 (0.1%)	1.33	30/4873 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	LYS	C-O	6.87	1.32	1.24
1	A	33	THR	CA-CB	-5.39	1.46	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	GLU	N-CA-C	12.30	124.69	111.28
1	A	375	SER	N-CA-C	-12.07	98.20	111.36
1	A	31	ASP	N-CA-C	11.84	123.74	111.07
1	A	374	ALA	N-CA-C	8.78	120.62	111.14
1	A	369	PRO	N-CA-CB	8.06	110.02	101.88
1	A	141	ASN	CB-CA-C	-6.23	99.10	110.63
1	A	413	VAL	CB-CA-C	-6.03	103.25	111.33
1	A	326	ASP	CB-CA-C	-5.98	109.69	116.63
1	A	113	ASP	N-CA-C	5.97	117.87	111.36
1	A	112	ILE	N-CA-C	5.94	117.00	107.73
1	A	378	ASP	N-CA-C	5.85	117.33	111.07
1	A	274	THR	CA-C-N	-5.84	116.96	123.16
1	A	274	THR	C-N-CA	-5.84	116.96	123.16
1	A	428	THR	N-CA-C	5.70	117.70	108.41
1	A	190	SER	N-CA-C	5.64	117.42	108.79
1	A	455	ILE	N-CA-C	5.62	117.00	108.80
1	A	33	THR	N-CA-C	-5.53	106.89	113.97
1	A	160	GLY	CA-C-N	5.50	125.21	119.82
1	A	160	GLY	C-N-CA	5.50	125.21	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	TYR	N-CA-C	5.34	116.92	108.96
1	A	379	TRP	N-CA-C	5.33	118.17	110.28
1	A	406	GLY	N-CA-C	5.30	117.57	111.36
1	A	127	LYS	O-C-N	5.27	127.71	122.12
1	A	170	GLY	N-CA-C	-5.22	108.42	115.21
1	A	441	ALA	N-CA-C	-5.22	105.67	111.36
1	A	219	VAL	N-CA-C	5.21	115.43	110.53
1	A	450	ILE	CA-C-N	-5.13	113.98	122.39
1	A	450	ILE	C-N-CA	-5.13	113.98	122.39
1	A	191	VAL	CB-CA-C	-5.08	102.91	110.33
1	A	429	VAL	N-CA-C	5.06	116.52	111.00

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	3481	0	3070	85	0
2	A	1	0	0	0	0
3	A	9	0	0	0	0
All	All	3491	0	3070	85	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 (85) 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:316:TYR:HB3	1:A:323:MET:CE	1.90	1.01
1:A:42:THR:HG23	1:A:143:SER:HB2	1.39	0.99
1:A:324:GLN:HE21	1:A:324:GLN:C	1.72	0.98
1:A:20:ASN:HB3	1:A:21:VAL:HG23	1.62	0.80
1:A:42:THR:HG23	1:A:143:SER:CB	2.11	0.80
1:A:316:TYR:HB3	1:A:323:MET:HE1	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLN:C	1:A:324:GLN:NE2	2.42	0.78
1:A:225:LEU:O	1:A:226:GLN:C	2.26	0.76
1:A:31:ASP:O	1:A:32:MET:HB2	1.86	0.74
1:A:316:TYR:HB3	1:A:323:MET:HE3	1.71	0.72
1:A:316:TYR:CB	1:A:323:MET:HE1	2.19	0.72
1:A:324:GLN:HE21	1:A:325:LYS:N	1.88	0.70
1:A:474:THR:HG21	1:A:479:TYR:HB2	1.76	0.68
1:A:37:VAL:CG2	1:A:42:THR:HG22	2.26	0.65
1:A:343:LEU:HB2	1:A:344:PRO:HD3	1.79	0.64
1:A:45:LEU:HA	1:A:59:LEU:HB2	1.81	0.62
1:A:448:GLN:HB3	1:A:450:ILE:HD12	1.82	0.62
1:A:155:HIS:HA	1:A:164:LEU:HD23	1.80	0.61
1:A:316:TYR:CB	1:A:323:MET:CE	2.72	0.61
1:A:16:HIS:N	1:A:212:ASP:OD2	2.20	0.60
1:A:79:VAL:HG22	1:A:182:TRP:CG	2.36	0.60
1:A:335:LEU:HD12	1:A:382:ILE:HB	1.81	0.60
1:A:37:VAL:HG22	1:A:42:THR:HG22	1.84	0.59
1:A:476:SER:O	1:A:477:GLU:HB2	2.02	0.59
1:A:42:THR:CG2	1:A:143:SER:CB	2.79	0.59
1:A:54:THR:HG22	1:A:292:PRO:HG3	1.84	0.58
1:A:67:ASP:OD2	1:A:70:HIS:HD2	1.87	0.56
1:A:247:ASN:HB2	1:A:379:TRP:CZ3	2.40	0.56
1:A:82:GLN:HG2	1:A:163:ALA:HB2	1.87	0.56
1:A:345:LEU:O	1:A:349:VAL:HG23	2.04	0.56
1:A:31:ASP:O	1:A:32:MET:CB	2.49	0.55
1:A:103:SER:HB3	1:A:106:ILE:HD12	1.88	0.54
1:A:221:SER:O	1:A:224:THR:N	2.41	0.54
1:A:14:HIS:HD1	1:A:190:SER:HG	1.55	0.53
1:A:19:PHE:CG	1:A:20:ASN:N	2.77	0.52
1:A:196:ASN:ND2	1:A:198:ASP:H	2.07	0.52
1:A:156:PRO:HD2	1:A:164:LEU:CD2	2.39	0.52
1:A:37:VAL:HG23	1:A:42:THR:HG22	1.91	0.51
1:A:331:HIS:HA	1:A:359:ILE:HG23	1.92	0.51
1:A:162:PHE:HB3	1:A:175:LEU:HB3	1.92	0.51
1:A:267:ASP:C	1:A:267:ASP:OD2	2.54	0.51
1:A:130:PHE:CE2	1:A:132:GLU:HG2	2.46	0.50
1:A:367:GLU:O	1:A:368:VAL:CB	2.59	0.50
1:A:130:PHE:HE2	1:A:132:GLU:HG2	1.76	0.50
1:A:33:THR:HB	1:A:35:ILE:HG13	1.93	0.50
1:A:237:GLU:O	1:A:475:ARG:HG2	2.11	0.50
1:A:240:ARG:HA	1:A:387:VAL:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG12	1:A:138:VAL:HG22	1.94	0.49
1:A:243:ASN:HB2	1:A:452:SER:O	2.12	0.49
1:A:14:HIS:ND1	1:A:190:SER:OG	2.35	0.48
1:A:147:VAL:C	1:A:149:GLU:H	2.20	0.48
1:A:45:LEU:HD12	1:A:137:LEU:HD13	1.96	0.48
1:A:98:ARG:HD3	1:A:98:ARG:C	2.39	0.47
1:A:98:ARG:HD3	1:A:98:ARG:O	2.16	0.46
1:A:78:ASP:OD1	1:A:78:ASP:N	2.44	0.46
1:A:225:LEU:O	1:A:228:ASN:N	2.47	0.45
1:A:75:LEU:HD13	1:A:92:VAL:HG21	1.98	0.45
1:A:400:ALA:HB1	1:A:408:LEU:HD12	1.99	0.45
1:A:449:LYS:HA	1:A:449:LYS:HD3	1.88	0.44
1:A:243:ASN:HD21	1:A:386:ASN:HD21	1.66	0.43
1:A:47:ARG:HG2	1:A:58:TRP:HB2	1.99	0.43
1:A:65:SER:HB2	1:A:71:TRP:CE3	2.53	0.43
1:A:294:ALA:HA	1:A:295:PRO:HD3	1.80	0.43
1:A:450:ILE:O	1:A:451:HIS:CG	2.72	0.43
1:A:196:ASN:ND2	1:A:201:ALA:HB3	2.34	0.43
1:A:110:LEU:CD2	1:A:136:GLU:HB3	2.49	0.42
1:A:142:VAL:O	1:A:142:VAL:HG12	2.19	0.42
1:A:247:ASN:HB2	1:A:379:TRP:CH2	2.54	0.42
1:A:332:PHE:O	1:A:361:VAL:HA	2.18	0.42
1:A:375:SER:O	1:A:376:ASN:C	2.62	0.42
1:A:376:ASN:O	1:A:379:TRP:CD1	2.72	0.42
1:A:469:LYS:O	1:A:470:ASN:HB2	2.19	0.42
1:A:93:LYS:O	1:A:97:GLU:HG3	2.19	0.42
1:A:13:LYS:H	1:A:189:ASP:HB2	1.84	0.42
1:A:35:ILE:O	1:A:36:PRO:C	2.62	0.42
1:A:366:ILE:CB	1:A:371:GLU:OE1	2.68	0.42
1:A:257:ASN:HB2	1:A:314:ALA:HB2	2.01	0.41
1:A:29:HIS:CE1	1:A:99:ALA:HB2	2.56	0.41
1:A:225:LEU:O	1:A:227:ALA:N	2.54	0.40
1:A:251:ASP:HA	1:A:254:LYS:HG3	2.03	0.40
1:A:343:LEU:HB2	1:A:344:PRO:CD	2.49	0.40
1:A:246:MET:O	1:A:411:SER:OG	2.39	0.40
1:A:432:ASP:O	1:A:435:ALA:HB3	2.21	0.40
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.87	0.40
1:A:135:SER:O	1:A:391:ARG:HG3	2.21	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	471/496 (95%)	438 (93%)	30 (6%)	3 (1%)	21	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	ARG
1	A	339	SER
1	A	368	VAL

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	325/433 (75%)	293 (90%)	32 (10%)	7	25

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	23	THR
1	A	32	MET
1	A	33	THR
1	A	35	ILE
1	A	42	THR
1	A	46	VAL
1	A	53	VAL

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Mol	Chain	Res	Type
1	A	104	VAL
1	A	112	ILE
1	A	140	PRO
1	A	166	SER
1	A	172	LYS
1	A	195	PHE
1	A	216	ARG
1	A	232	MET
1	A	233	VAL
1	A	237	GLU
1	A	240	ARG
1	A	271	ILE
1	A	290	THR
1	A	324	GLN
1	A	331	HIS
1	A	335	LEU
1	A	340	ARG
1	A	386	ASN
1	A	391	ARG
1	A	408	LEU
1	A	438	THR
1	A	439	GLU
1	A	450	ILE
1	A	473	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	70	HIS
1	A	139	ASN
1	A	196	ASN
1	A	324	GLN
1	A	386	ASN
1	A	414	ASN
1	A	440	GLN
1	A	466	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is 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 [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	475/496 (95%)	-0.23	7 (1%) 72 63	33, 55, 80, 96	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	369	PRO	3.1
1	A	322	GLN	2.7
1	A	326	ASP	2.6
1	A	320	ASN	2.4
1	A	317	THR	2.4
1	A	368	VAL	2.3
1	A	31	ASP	2.2

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	CA	A	497	1/1	0.91	0.10	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.