



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:18 PM UTC

PDB ID : 4LLJ / pdb_00004llj
Title : Crystal structure of PDE10A2 with fragment ZT214
Authors : Sridhar, V.; Badger, J.; Logan, C.; Chie-Leon, B.; Nienaber, V.
Deposited on : 2013-07-09
Resolution : 1.56 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

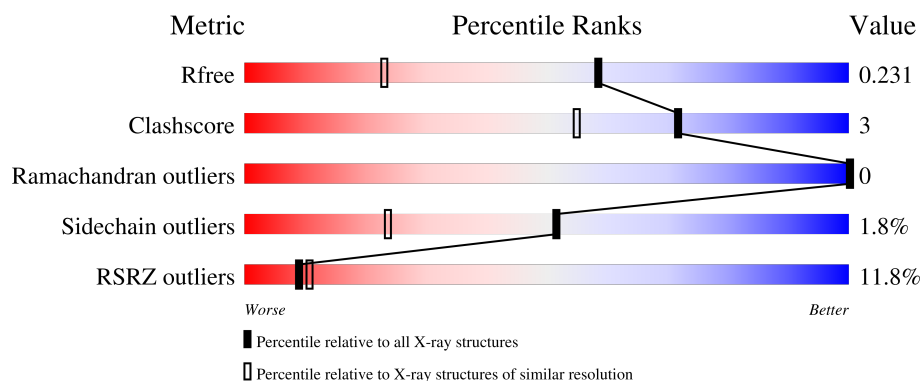
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.56 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	345	8% 87% 8% 5%
1	B	345	14% 84% 10% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5598 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.

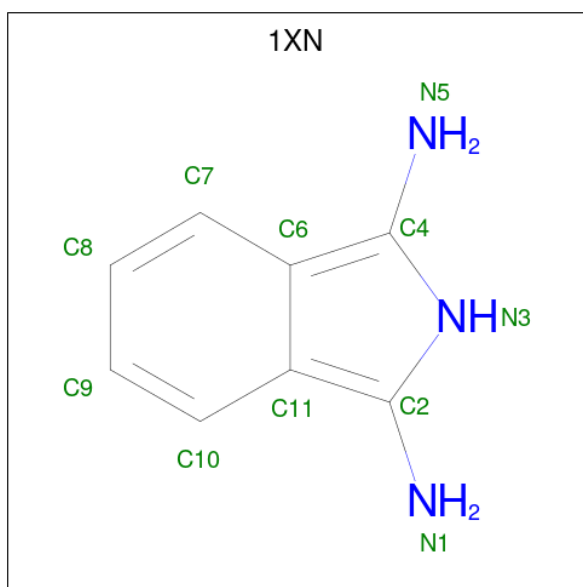
- Molecule 1 is a protein called cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	9	0
			2649	1694	447	484	24			
1	B	322	Total	C	N	O	S	0	8	0
			2576	1650	439	462	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	445	GLY	-	expression tag	UNP Q9Y233
A	446	ALA	-	expression tag	UNP Q9Y233
A	447	GLY	-	expression tag	UNP Q9Y233
A	448	THR	-	expression tag	UNP Q9Y233
B	445	GLY	-	expression tag	UNP Q9Y233
B	446	ALA	-	expression tag	UNP Q9Y233
B	447	GLY	-	expression tag	UNP Q9Y233
B	448	THR	-	expression tag	UNP Q9Y233

- Molecule 2 is 2H-isoindole-1,3-diamine (CCD ID: 1XN) (formula: C₈H₉N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			11	8	3		

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ni	0	0
			2	2		
3	B	2	Total	Ni	0	0
			2	2		

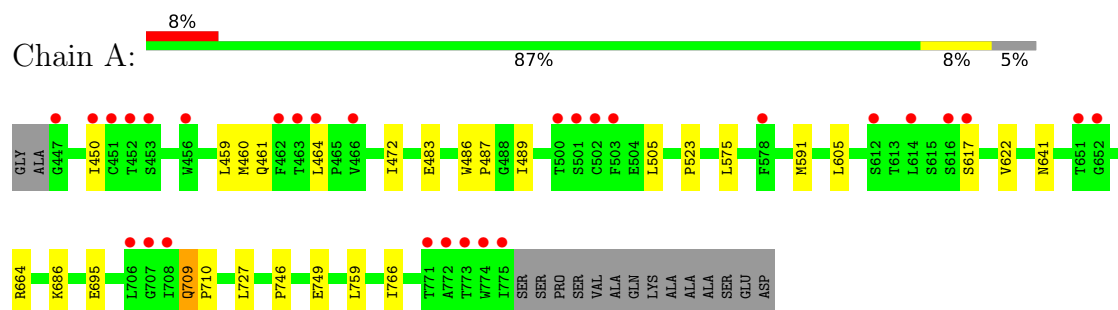
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	218	Total	O	0	0
			218	218		
4	B	140	Total	O	0	0
			140	140		

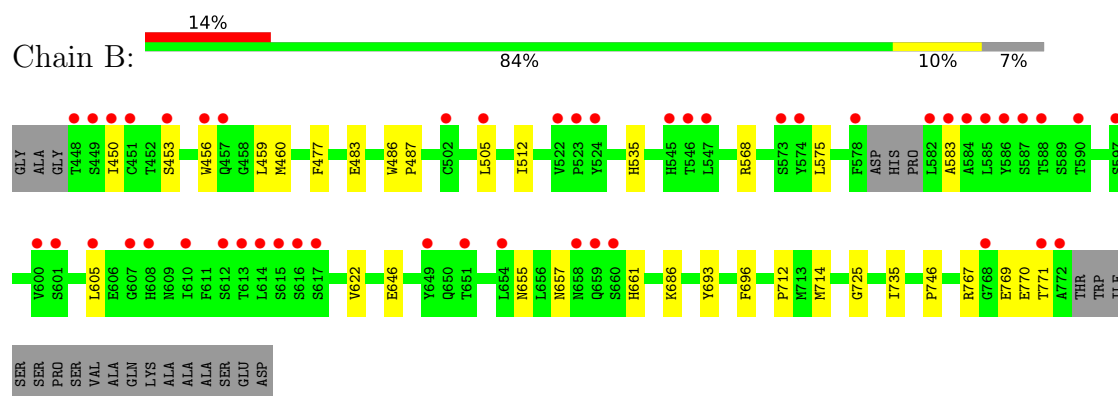
3 Residue-property plots [i](#)

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 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: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.76Å 82.06Å 155.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.59 – 1.56 41.59 – 1.56	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.59-1.56) 97.6 (41.59-1.56)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.209 , 0.241 0.202 , 0.231	Depositor DCC
R_{free} test set	4567 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.900	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5598	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: NI, 1XN

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	0.90	0/2760	0.95	3/3747 (0.1%)
1	B	0.83	0/2677	0.93	3/3630 (0.1%)
All	All	0.86	0/5437	0.94	6/7377 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	735	ILE	O-C-N	6.23	124.41	120.42
1	B	746	PRO	N-CA-C	6.17	118.23	110.70
1	A	749	GLU	CA-C-N	-5.58	113.92	119.56
1	A	749	GLU	C-N-CA	-5.58	113.92	119.56
1	B	512	ILE	N-CA-C	5.38	116.01	110.36
1	A	746	PRO	N-CA-C	5.24	117.09	110.70

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	2649	0	2573	17	0
1	B	2576	0	2513	16	0
2	A	11	0	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	218	0	0	1	0
4	B	140	0	0	1	0
All	All	5598	0	5095	34	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 3.

All (34) 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:655:ASN:H	1:B:661:HIS:HD2	1.12	0.93
1:B:450:ILE:HG22	1:B:605:LEU:HD13	1.64	0.79
1:B:655:ASN:H	1:B:661:HIS:CD2	2.03	0.73
1:A:641:ASN:HD22	1:A:664:ARG:HH11	1.40	0.70
1:A:727[B]:LEU:HG	1:A:766:ILE:CD1	2.22	0.70
1:A:464:LEU:HD21	1:A:472[B]:ILE:HD12	1.75	0.68
2:A:900:1XN:H6	4:A:1133:HOH:O	2.02	0.58
1:A:727[B]:LEU:HG	1:A:766:ILE:HD11	1.88	0.56
1:A:450:ILE:HG12	1:A:605:LEU:HD13	1.89	0.55
1:A:483:GLU:HA	1:A:486:TRP:CE2	2.44	0.53
1:A:460:MET:HE3	1:A:505:LEU:HD23	1.91	0.53
1:A:727[A]:LEU:HD12	1:A:759:LEU:HD11	1.92	0.52
1:A:472[A]:ILE:HD11	1:A:489:ILE:HG23	1.90	0.52
1:B:655:ASN:C	1:B:657:ASN:H	2.18	0.51
1:B:483:GLU:HA	1:B:486:TRP:CE2	2.45	0.51
1:B:696:PHE:O	1:B:714[B]:MET:HG3	2.11	0.51
1:A:523:PRO:HD2	1:A:695:GLU:HG3	1.93	0.50
1:A:727[A]:LEU:HD12	1:A:759:LEU:CD1	2.43	0.49
1:B:575:LEU:HB3	1:B:583:ALA:HB2	1.94	0.48
1:B:646:GLU:HG3	4:B:1075:HOH:O	2.13	0.48
1:A:709:GLN:HG2	1:A:710:PRO:HD2	1.96	0.46
1:B:767[B]:ARG:NH1	1:B:769:GLU:OE2	2.49	0.46
1:B:459[A]:LEU:HD13	1:B:487:PRO:HB2	1.99	0.45
1:A:472[A]:ILE:CD1	1:A:489:ILE:HG23	2.47	0.44
1:A:575:LEU:HD11	1:A:591:MET:SD	2.58	0.43
1:B:456:TRP:HZ3	1:B:460:MET:SD	2.41	0.43
1:B:456:TRP:CZ3	1:B:460:MET:SD	3.12	0.43
1:B:460:MET:HE3	1:B:505:LEU:HD23	2.01	0.42
1:A:727[B]:LEU:HG	1:A:766:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:PHE:HB3	1:B:535:HIS:CE1	2.54	0.42
1:B:686:LYS:NZ	1:B:771:THR:O	2.50	0.42
1:B:693:TYR:OH	1:B:725:GLY:HA3	2.20	0.41
1:A:459:LEU:HD13	1:A:487:PRO:HB2	2.02	0.41
1:A:727[A]:LEU:CD1	1:A:759:LEU:HD11	2.51	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	336/345 (97%)	332 (99%)	4 (1%)	0	100	100
1	B	326/345 (94%)	318 (98%)	8 (2%)	0	100	100
All	All	662/690 (96%)	650 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	292/306 (95%)	287 (98%)	5 (2%)	53	25
1	B	280/306 (92%)	275 (98%)	5 (2%)	51	24
All	All	572/612 (94%)	562 (98%)	10 (2%)	51	25

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	617	SER
1	A	622	VAL
1	A	686	LYS
1	A	709	GLN
1	B	453	SER
1	B	568	ARG
1	B	622	VAL
1	B	712	PRO
1	B	770	GLU

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	461	GLN
1	A	641	ASN
1	A	709	GLN
1	A	724	GLN
1	B	655	ASN
1	B	661	HIS

5.3.3 RNA [i](#)

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 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	1XN	A	900	-	5,12,12	1.61	2 (40%)	9,17,17	3.13	4 (44%)

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	1XN	A	900	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	1XN	C2-N1	-2.57	1.28	1.34
2	A	900	1XN	C4-N5	-2.17	1.29	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	1XN	C8-C7-C6	-5.49	116.39	121.80
2	A	900	1XN	C9-C10-C11	-5.46	116.42	121.80
2	A	900	1XN	C6-C4-N5	-3.19	127.41	130.21
2	A	900	1XN	C11-C2-N1	-2.54	127.98	130.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	1XN	1	0

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

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	329/345 (95%)	0.40	29 (8%) 15 17	17, 27, 50, 66	9 (2%)
1	B	322/345 (93%)	0.88	48 (14%) 5 6	19, 32, 61, 75	8 (2%)
All	All	651/690 (94%)	0.64	77 (11%) 9 11	17, 29, 54, 75	17 (2%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	585	LEU	6.5
1	B	584	ALA	6.0
1	A	775	ILE	5.2
1	B	772	ALA	5.1
1	B	450	ILE	5.0
1	B	586	TYR	4.5
1	B	578	PHE	4.4
1	B	582	LEU	4.3
1	B	456	TRP	4.3
1	A	707	GLY	4.2
1	A	773	THR	3.8
1	B	605	LEU	3.8
1	B	607	GLY	3.7
1	A	706	LEU	3.6
1	A	708	ILE	3.5
1	A	774	TRP	3.5
1	B	583	ALA	3.4
1	B	523	PRO	3.3
1	B	505	LEU	3.3
1	A	616	SER	3.2
1	A	462	PHE	3.1
1	A	771	THR	3.0
1	A	463	THR	3.0
1	B	448	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	449	SER	3.0
1	B	617	SER	3.0
1	A	617	SER	2.9
1	B	522	VAL	2.9
1	A	502	CYS	2.9
1	B	573	SER	2.9
1	B	574	TYR	2.9
1	B	660	SER	2.9
1	B	588	THR	2.8
1	B	600	VAL	2.7
1	A	578	PHE	2.7
1	B	502	CYS	2.7
1	B	547[A]	LEU	2.7
1	B	590	THR	2.7
1	A	503	PHE	2.7
1	A	452	THR	2.7
1	B	608	HIS	2.7
1	A	501	SER	2.7
1	B	597[A]	SER	2.7
1	A	451	CYS	2.7
1	B	658	ASN	2.6
1	A	456	TRP	2.6
1	A	464	LEU	2.6
1	A	772	ALA	2.6
1	A	500	THR	2.6
1	B	771	THR	2.6
1	A	466	VAL	2.6
1	A	612	SER	2.6
1	B	451	CYS	2.5
1	B	613	THR	2.5
1	A	447	GLY	2.5
1	B	546	THR	2.5
1	B	649	TYR	2.5
1	A	453	SER	2.5
1	A	450	ILE	2.5
1	B	453	SER	2.5
1	B	610	ILE	2.4
1	B	612	SER	2.3
1	B	524	TYR	2.3
1	B	768	GLY	2.3
1	B	616	SER	2.3
1	B	651	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	587	SER	2.3
1	A	651	THR	2.2
1	A	652	GLY	2.2
1	B	601	SER	2.1
1	B	615	SER	2.1
1	B	545	HIS	2.1
1	A	614	LEU	2.0
1	B	659	GLN	2.0
1	B	457	GLN	2.0
1	B	614	LEU	2.0
1	B	654	LEU	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	1XN	A	900	11/11	0.77	0.13	54,55,55,56	0
3	NI	A	901	1/1	0.99	0.03	22,22,22,22	0
3	NI	A	902	1/1	0.99	0.14	31,31,31,31	0
3	NI	B	901	1/1	0.99	0.11	33,33,33,33	0
3	NI	B	902	1/1	0.99	0.21	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.