



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:47 PM UTC

PDB ID : 2OUP / pdb_00002oup
Title : crystal structure of PDE10A
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Deposited on : 2007-02-12
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
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

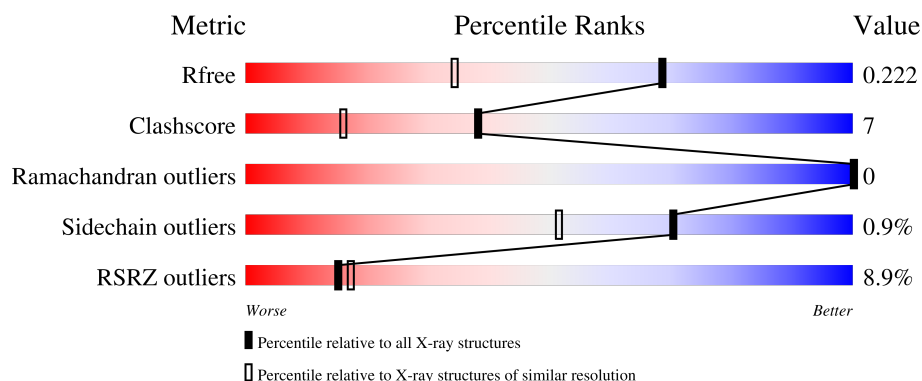
1 Overall quality at a glance

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	331	6% 86% 11% ..
1	B	331	12% 78% 20% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5693 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	324	Total	C	N	O	S	0	0	0
			2629	1678	447	479	25			
1	B	325	Total	C	N	O	S	0	0	0
			2635	1681	448	481	25			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	SER	-	cloning artifact	UNP Q9Y233
A	447	HIS	-	cloning artifact	UNP Q9Y233
A	448	MET	-	cloning artifact	UNP Q9Y233
B	446	SER	-	cloning artifact	UNP Q9Y233
B	447	HIS	-	cloning artifact	UNP Q9Y233
B	448	MET	-	cloning artifact	UNP Q9Y233

- 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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

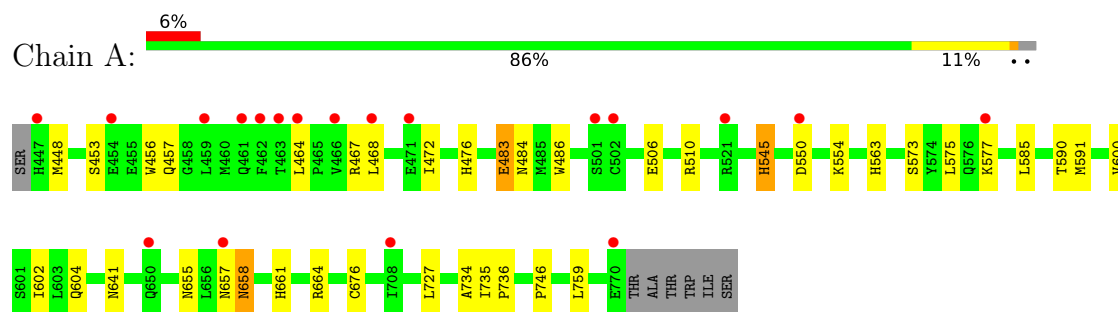
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	241	Total 241	O 241	0	0
4	B	184	Total 184	O 184	0	0

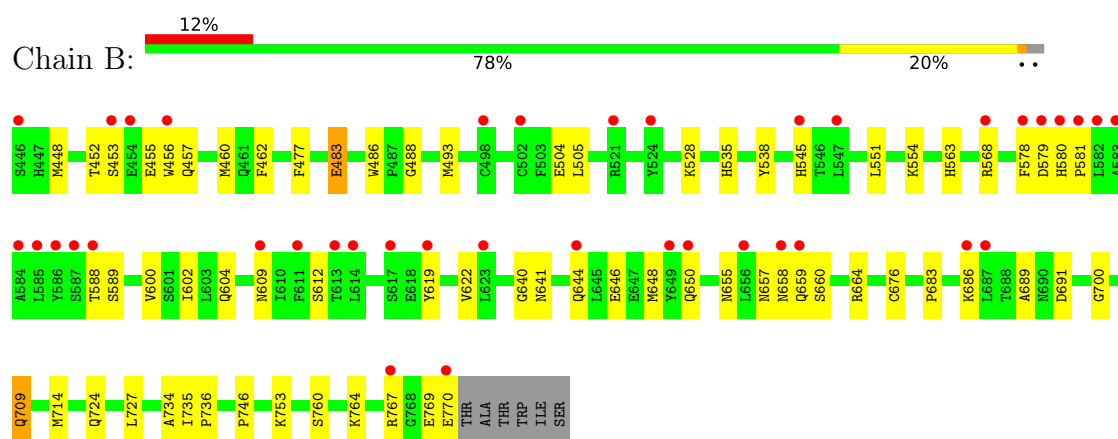
3 Residue-property plots

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: 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	51.08Å 82.04Å 155.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.56 30.00 – 1.56	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.56) 87.4 (30.00-1.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.56Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.223 0.198 , 0.222	Depositor DCC
R_{free} test set	8621 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5693	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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

5.1 Standard geometry

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

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	0.46	0/2694	0.86	7/3647 (0.2%)
1	B	0.44	0/2700	0.84	9/3655 (0.2%)
All	All	0.45	0/5394	0.85	16/7302 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	545	HIS	N-CA-C	7.39	120.20	111.71
1	B	563	HIS	N-CA-C	6.92	120.82	112.38
1	B	676	CYS	N-CA-C	6.90	121.16	112.87
1	A	563	HIS	N-CA-C	6.84	120.72	112.38
1	A	483	GLU	N-CA-C	6.01	118.33	111.11
1	A	734	ALA	N-CA-C	5.98	117.48	110.97
1	A	676	CYS	N-CA-C	5.91	119.97	112.87
1	B	734	ALA	N-CA-C	5.57	117.03	111.07
1	A	746	PRO	N-CA-C	5.45	117.34	110.70
1	B	504	GLU	N-CA-C	-5.43	101.61	109.59
1	B	746	PRO	N-CA-C	5.39	117.28	110.70
1	B	689	ALA	N-CA-C	5.32	117.77	111.33
1	A	545	HIS	N-CA-C	5.29	120.05	111.37
1	A	590	THR	N-CA-C	5.27	117.45	111.02
1	B	483	GLU	N-CA-C	5.12	117.25	111.11
1	B	691	ASP	N-CA-C	5.08	116.82	111.28

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	2629	0	2588	30	0
1	B	2635	0	2593	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	241	0	0	1	0
4	B	184	0	0	6	0
All	All	5693	0	5181	72	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 7.

All (72) 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:655:ASN:H	1:A:661:HIS:HD2	1.17	0.91
1:B:609:ASN:HD22	1:B:612:SER:HB3	1.40	0.87
1:B:646:GLU:HG2	1:B:650:GLN:HE21	1.46	0.81
1:B:658:ASN:OD1	1:B:660:SER:HB3	1.89	0.73
1:B:648:MET:HE1	1:B:664:ARG:HD2	1.71	0.73
1:B:683:PRO:HA	1:B:686:LYS:HE2	1.70	0.72
1:B:724:GLN:HG3	4:B:334:HOH:O	1.89	0.72
1:A:641:ASN:HD22	1:A:664:ARG:HH11	1.38	0.71
1:B:641:ASN:HD22	1:B:664:ARG:HH11	1.38	0.71
1:B:646:GLU:HG2	1:B:650:GLN:NE2	2.07	0.70
1:B:609:ASN:ND2	1:B:612:SER:HB3	2.09	0.67
1:A:573:SER:O	1:A:577:LYS:HG3	1.96	0.65
1:B:551:LEU:HD23	1:B:554:LYS:HE3	1.80	0.64
1:B:709:GLN:HE21	1:B:709:GLN:HA	1.63	0.63
1:A:448:MET:HE2	1:A:602:ILE:HG13	1.79	0.62
1:A:658:ASN:HD22	1:A:658:ASN:C	2.07	0.62
1:A:655:ASN:HD21	1:A:657:ASN:CG	2.09	0.61
1:A:550:ASP:O	1:A:554:LYS:HG3	2.02	0.60
1:B:460:MET:HE3	1:B:505:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:GLU:HA	1:B:486:TRP:CE2	2.40	0.56
1:A:655:ASN:H	1:A:661:HIS:CD2	2.09	0.56
1:B:648:MET:HE1	1:B:664:ARG:CD	2.35	0.56
1:A:464:LEU:HD21	1:A:472:ILE:HD12	1.87	0.55
1:A:456:TRP:CZ3	1:A:506:GLU:HG3	2.42	0.55
1:A:545:HIS:HD2	4:A:26:HOH:O	1.90	0.54
1:A:483:GLU:HA	1:A:486:TRP:CE2	2.43	0.54
1:A:727:LEU:HD12	1:A:759:LEU:HD11	1.89	0.54
1:A:655:ASN:N	1:A:661:HIS:HD2	1.96	0.53
1:B:600:VAL:O	1:B:604:GLN:HG3	2.06	0.53
1:A:506:GLU:OE1	1:A:510:ARG:NH2	2.35	0.51
1:B:655:ASN:C	1:B:655:ASN:HD22	2.17	0.51
1:B:655:ASN:ND2	1:B:657:ASN:H	2.08	0.51
1:B:640:GLY:O	1:B:644:GLN:HG3	2.13	0.49
1:B:644:GLN:NE2	1:B:664:ARG:NH2	2.60	0.49
1:A:453:SER:HA	1:A:456:TRP:NE1	2.27	0.49
1:A:476:HIS:CE1	1:B:767:ARG:HH11	2.31	0.49
1:B:619:TYR:O	1:B:622:VAL:HG12	2.13	0.48
1:A:573:SER:HB3	1:A:577:LYS:HE3	1.95	0.48
1:A:453:SER:O	1:A:457:GLN:HG3	2.14	0.47
1:B:769:GLU:C	1:B:770:GLU:HG2	2.38	0.47
1:B:453:SER:O	1:B:457:GLN:HG3	2.15	0.46
1:B:448:MET:HE2	1:B:602:ILE:HG13	1.97	0.46
1:B:580:HIS:HB3	1:B:581:PRO:HD2	1.98	0.46
1:B:456:TRP:HZ3	1:B:460:MET:SD	2.39	0.45
1:B:646:GLU:O	1:B:650:GLN:HG3	2.15	0.45
1:A:464:LEU:HD21	1:A:472:ILE:CD1	2.46	0.45
1:B:683:PRO:HA	1:B:686:LYS:CE	2.43	0.45
1:B:609:ASN:HD22	1:B:612:SER:CB	2.20	0.45
1:B:735:ILE:HB	1:B:736:PRO:HD3	1.99	0.45
1:B:764:LYS:HB3	1:B:770:GLU:H	1.82	0.45
1:B:528:LYS:HE2	4:B:299:HOH:O	2.15	0.45
1:A:727:LEU:CD1	1:A:759:LEU:HD11	2.47	0.45
1:B:568:ARG:NE	4:B:317:HOH:O	2.50	0.44
1:A:575:LEU:HD11	1:A:591:MET:SD	2.57	0.44
1:A:727:LEU:HD12	1:A:759:LEU:CD1	2.48	0.44
1:B:700:GLY:HA3	1:B:714:MET:O	2.18	0.43
1:A:735:ILE:HB	1:A:736:PRO:HD3	2.01	0.43
1:B:462:PHE:CD2	1:B:488:GLY:HA3	2.54	0.43
1:B:493:MET:HB3	1:B:538:TYR:CD1	2.54	0.43
1:A:468:LEU:O	1:A:472:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:753:LYS:HD3	4:B:331:HOH:O	2.19	0.42
1:B:578:PHE:O	1:B:579:ASP:C	2.62	0.42
1:B:588:THR:O	1:B:589:SER:C	2.62	0.42
1:A:658:ASN:C	1:A:658:ASN:ND2	2.77	0.41
1:A:600:VAL:O	1:A:604:GLN:HG3	2.20	0.41
1:A:476:HIS:CE1	1:B:767:ARG:NH1	2.88	0.41
1:A:467:ARG:NH2	1:B:760:SER:OG	2.49	0.41
1:B:477:PHE:HB3	1:B:535:HIS:CE1	2.56	0.41
1:A:641:ASN:ND2	1:A:664:ARG:HG2	2.35	0.41
1:B:659:GLN:HG3	4:B:261:HOH:O	2.21	0.41
1:B:568:ARG:CZ	4:B:317:HOH:O	2.69	0.40
1:B:452:THR:OG1	1:B:455:GLU: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	322/331 (97%)	316 (98%)	6 (2%)	0	100	100
1	B	323/331 (98%)	314 (97%)	9 (3%)	0	100	100
All	All	645/662 (97%)	630 (98%)	15 (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	293/299 (98%)	290 (99%)	3 (1%)	68	47
1	B	294/299 (98%)	292 (99%)	2 (1%)	76	59
All	All	587/598 (98%)	582 (99%)	5 (1%)	70	51

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	ASN
1	A	585	LEU
1	A	658	ASN
1	B	709	GLN
1	B	727	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	484	ASN
1	A	545	HIS
1	A	604	GLN
1	A	621	GLN
1	A	641	ASN
1	A	650	GLN
1	A	655	ASN
1	A	657	ASN
1	A	658	ASN
1	A	661	HIS
1	A	690	ASN
1	A	726	GLN
1	A	761	GLN
1	B	457	GLN
1	B	461	GLN
1	B	593	GLN
1	B	609	ASN
1	B	641	ASN
1	B	644	GLN
1	B	650	GLN
1	B	655	ASN
1	B	709	GLN
1	B	724	GLN

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Mol	Chain	Res	Type
1	B	731	ASN
1	B	761	GLN

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 4 ligands modelled in this entry, 4 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 [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	324/331 (97%)	0.35	19 (5%) 28 34	12, 20, 34, 42	0
1	B	325/331 (98%)	0.71	39 (12%) 9 10	13, 22, 40, 50	0
All	All	649/662 (98%)	0.53	58 (8%) 15 17	12, 21, 38, 50	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	580	HIS	6.3
1	B	770	GLU	4.1
1	A	521	ARG	3.8
1	A	447	HIS	3.8
1	B	585	LEU	3.8
1	B	609	ASN	3.8
1	A	657	ASN	3.7
1	B	582	LEU	3.7
1	B	446	SER	3.7
1	B	586	TYR	3.6
1	A	471	GLU	3.6
1	B	584	ALA	3.5
1	B	644	GLN	3.4
1	B	650	GLN	3.3
1	B	588	THR	3.3
1	B	578	PHE	3.3
1	B	583	ALA	3.3
1	A	462	PHE	3.2
1	A	463	THR	3.2
1	B	659	GLN	3.1
1	B	568	ARG	3.1
1	A	650	GLN	3.0
1	A	708	ILE	2.9
1	B	658	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	617	SER	2.9
1	B	619	TYR	2.8
1	B	502	CYS	2.8
1	B	656	LEU	2.8
1	A	501	SER	2.8
1	B	614	LEU	2.8
1	A	577	LYS	2.7
1	B	524	TYR	2.7
1	A	459	LEU	2.7
1	A	461	GLN	2.7
1	A	466	VAL	2.6
1	B	613	THR	2.6
1	B	521	ARG	2.5
1	A	464	LEU	2.4
1	A	454	GLU	2.4
1	B	579	ASP	2.4
1	A	550	ASP	2.3
1	B	581	PRO	2.3
1	B	547	LEU	2.3
1	B	545	HIS	2.3
1	B	456	TRP	2.2
1	A	502	CYS	2.2
1	B	611	PHE	2.2
1	A	770	GLU	2.2
1	B	623	LEU	2.1
1	B	687	LEU	2.1
1	B	767	ARG	2.1
1	B	686	LYS	2.1
1	A	468	LEU	2.1
1	B	649	TYR	2.1
1	B	454	GLU	2.1
1	B	587	SER	2.0
1	B	498	CYS	2.0
1	B	453	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
3	MG	B	778	1/1	0.96	0.05	17,17,17,17	0
3	MG	A	778	1/1	0.99	0.03	13,13,13,13	0
2	ZN	B	777	1/1	0.99	0.21	26,26,26,26	0
2	ZN	A	777	1/1	1.00	0.03	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.