



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:09 PM UTC

PDB ID : 5C1W / pdb_00005c1w
Title : PDE10 complexed with 4,6-dichloro-2-cyclopropyl-5-methyl-pyrimidine
Authors : Yan, Y.
Deposited on : 2015-06-15
Resolution : 1.70 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

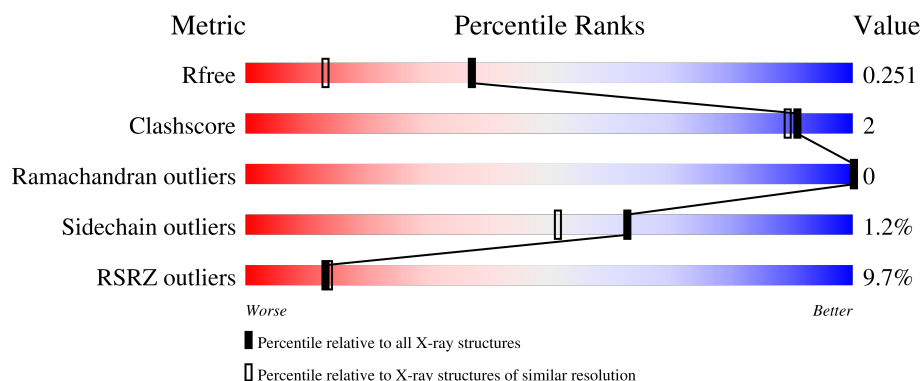
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	362	
1	B	362	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5636 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	325	Total	C	N	O	S	0	0	0
			2628	1677	446	480	25			
1	B	314	Total	C	N	O	S	0	0	0
			2534	1614	432	463	25			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	418	MET	-	initiating methionine	UNP Q9Y233
A	419	GLY	-	expression tag	UNP Q9Y233
A	420	SER	-	expression tag	UNP Q9Y233
A	421	SER	-	expression tag	UNP Q9Y233
A	422	HIS	-	expression tag	UNP Q9Y233
A	423	HIS	-	expression tag	UNP Q9Y233
A	424	HIS	-	expression tag	UNP Q9Y233
A	425	HIS	-	expression tag	UNP Q9Y233
A	426	HIS	-	expression tag	UNP Q9Y233
A	427	HIS	-	expression tag	UNP Q9Y233
A	428	SER	-	expression tag	UNP Q9Y233
A	429	SER	-	expression tag	UNP Q9Y233
A	430	GLY	-	expression tag	UNP Q9Y233
A	431	LEU	-	expression tag	UNP Q9Y233
A	432	VAL	-	expression tag	UNP Q9Y233
A	433	PRO	-	expression tag	UNP Q9Y233
A	434	ARG	-	expression tag	UNP Q9Y233
A	435	GLY	-	expression tag	UNP Q9Y233
A	436	SER	-	expression tag	UNP Q9Y233
A	437	HIS	-	expression tag	UNP Q9Y233
A	438	MET	-	expression tag	UNP Q9Y233
B	418	MET	-	initiating methionine	UNP Q9Y233
B	419	GLY	-	expression tag	UNP Q9Y233
B	420	SER	-	expression tag	UNP Q9Y233

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Chain	Residue	Modelled	Actual	Comment	Reference
B	421	SER	-	expression tag	UNP Q9Y233
B	422	HIS	-	expression tag	UNP Q9Y233
B	423	HIS	-	expression tag	UNP Q9Y233
B	424	HIS	-	expression tag	UNP Q9Y233
B	425	HIS	-	expression tag	UNP Q9Y233
B	426	HIS	-	expression tag	UNP Q9Y233
B	427	HIS	-	expression tag	UNP Q9Y233
B	428	SER	-	expression tag	UNP Q9Y233
B	429	SER	-	expression tag	UNP Q9Y233
B	430	GLY	-	expression tag	UNP Q9Y233
B	431	LEU	-	expression tag	UNP Q9Y233
B	432	VAL	-	expression tag	UNP Q9Y233
B	433	PRO	-	expression tag	UNP Q9Y233
B	434	ARG	-	expression tag	UNP Q9Y233
B	435	GLY	-	expression tag	UNP Q9Y233
B	436	SER	-	expression tag	UNP Q9Y233
B	437	HIS	-	expression tag	UNP Q9Y233
B	438	MET	-	expression tag	UNP Q9Y233

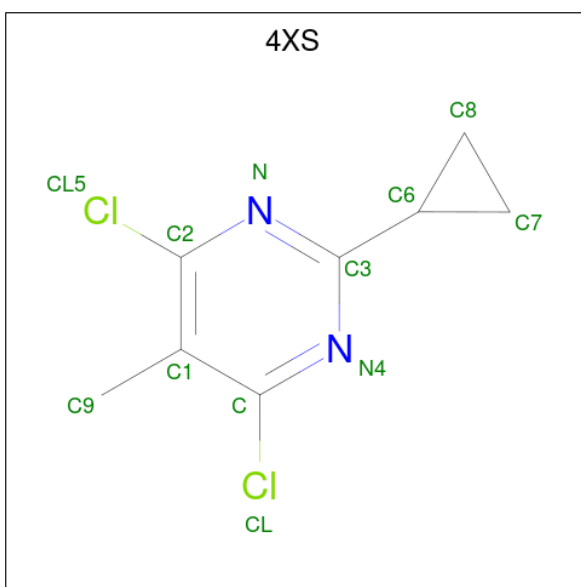
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 4,6-dichloro-2-cyclopropyl-5-methylpyrimidine (CCD ID: 4XS) (formula: C₈H₈Cl₂N₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			12	8	2	2		

- Molecule 5 is water.

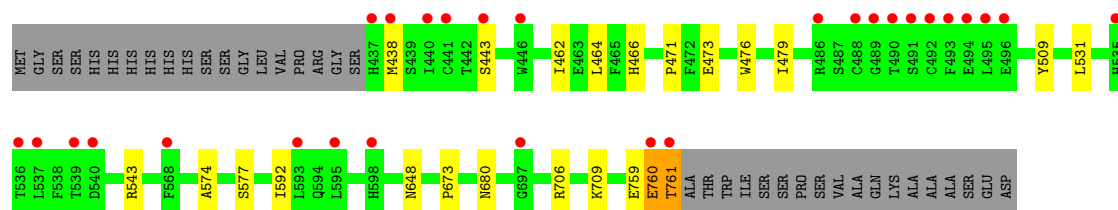
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	254	Total	O	0	0
			254	254		
5	B	204	Total	O	0	0
			204	204		

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.

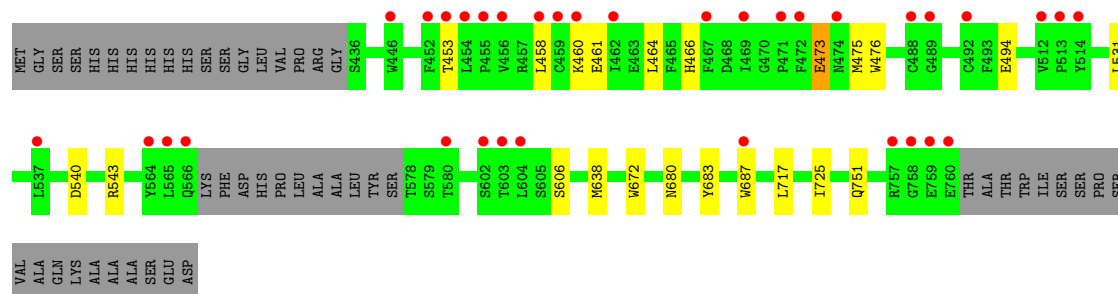
- Molecule 1: cAMP and cAMP-inhibited cGMP 3',5'-cyclic phosphodiesterase 10A

Chain A: 



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

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.43Å 81.85Å 153.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.06 – 1.70 47.06 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.06-1.70) 99.6 (47.06-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 1.70Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.203 , 0.229 (Not available) , 0.251	Depositor DCC
R_{free} test set	3500 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5636	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: MG, ZN, 4XS

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	0.85	0/2693	1.22	7/3648 (0.2%)
1	B	0.82	1/2594 (0.0%)	1.18	5/3511 (0.1%)
All	All	0.84	1/5287 (0.0%)	1.20	12/7159 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	638	MET	SD-CE	-5.44	1.66	1.79

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	648	ASN	CA-CB-CG	7.06	119.66	112.60
1	B	540	ASP	CA-CB-CG	5.91	118.50	112.60
1	B	460	LYS	CA-C-N	5.73	128.28	120.54
1	B	460	LYS	C-N-CA	5.73	128.28	120.54
1	B	473	GLU	N-CA-C	5.58	118.08	111.33
1	A	680	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	759	GLU	CA-C-N	5.41	131.88	121.54
1	A	759	GLU	C-N-CA	5.41	131.88	121.54
1	A	509	TYR	N-CA-C	-5.20	101.24	109.76
1	A	574	ALA	CA-C-N	5.12	127.09	120.44
1	A	574	ALA	C-N-CA	5.12	127.09	120.44
1	B	494	GLU	N-CA-C	-5.02	102.22	109.59

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	2628	0	2578	9	0
1	B	2534	0	2485	10	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	12	0	7	0	0
5	A	254	0	0	0	0
5	B	204	0	0	0	0
All	All	5636	0	5070	17	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 2.

All (17) 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:458:LEU:HD12	1:B:475:MET:HE1	1.65	0.78
1:B:458:LEU:CD1	1:B:475:MET:HE1	2.31	0.59
1:A:706:ARG:O	1:A:709:LYS:HG3	2.04	0.57
1:A:473:GLU:HA	1:A:476:TRP:CE2	2.43	0.54
1:A:760:GLU:HG3	1:A:761:THR:HG23	1.90	0.54
1:B:680:ASN:HB3	1:B:687:TRP:HZ3	1.76	0.51
1:B:672:TRP:CD1	1:B:751:GLN:HE21	2.30	0.50
1:B:473:GLU:HA	1:B:476:TRP:CE2	2.50	0.46
1:B:683:TYR:HB3	1:B:687:TRP:CE2	2.53	0.44
1:B:464:LEU:HD13	1:B:466:HIS:CE1	2.53	0.44
1:A:462:ILE:HD11	1:A:479:ILE:HG23	1.99	0.44
1:A:438:MET:HE2	1:A:592:ILE:HG13	2.00	0.43
1:A:673:PRO:HG2	1:B:717:LEU:HB3	2.00	0.43
1:B:531:LEU:HD22	1:B:543:ARG:HG2	2.00	0.43
1:A:531:LEU:HD22	1:A:543:ARG:HG2	2.01	0.41
1:A:464:LEU:HD13	1:A:466:HIS:CE1	2.55	0.41
1:A:471:PRO:HA	1:B:725:ILE:HG21	2.02	0.41

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	323/362 (89%)	317 (98%)	6 (2%)	0	100	100
1	B	310/362 (86%)	305 (98%)	5 (2%)	0	100	100
All	All	633/724 (87%)	622 (98%)	11 (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	292/323 (90%)	288 (99%)	4 (1%)	59	46
1	B	282/323 (87%)	279 (99%)	3 (1%)	65	54
All	All	574/646 (89%)	567 (99%)	7 (1%)	63	51

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	SER
1	A	577	SER
1	A	760	GLU
1	A	761	THR
1	B	453	THR

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Mol	Chain	Res	Type
1	B	461	GLU
1	B	606	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	B	447	GLN
1	B	466	HIS
1	B	583	GLN
1	B	649	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 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	$\# Z > 2$
4	4XS	A	803	-	10,13,13	1.22	1 (10%)	8,19,19	3.03	3 (37%)

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
4	4XS	A	803	-	-	0/4/6/6	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	4XS	C-N4	2.09	1.35	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	4XS	C1-C2-CL5	5.32	125.85	119.24
4	A	803	4XS	CL5-C2-N	-4.61	108.18	115.57
4	A	803	4XS	N-C3-N4	-4.33	120.08	126.15

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	325/362 (89%)	0.50	28 (8%) 16 17	17, 29, 54, 86	0
1	B	314/362 (86%)	0.69	34 (10%) 11 11	18, 32, 56, 109	0
All	All	639/724 (88%)	0.59	62 (9%) 13 14	17, 31, 55, 109	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	514	TYR	5.2
1	A	492	CYS	4.8
1	B	456	VAL	4.6
1	A	490	THR	4.5
1	B	467	PHE	4.2
1	B	459	CYS	4.2
1	B	603	THR	3.9
1	A	761	THR	3.9
1	B	458	LEU	3.8
1	B	566	GLN	3.7
1	B	460	LYS	3.7
1	B	452	PHE	3.7
1	B	512	VAL	3.7
1	B	462	ILE	3.6
1	A	536	THR	3.6
1	B	760	GLU	3.4
1	B	564	TYR	3.3
1	B	454	LEU	3.3
1	B	565	LEU	3.3
1	A	495	LEU	3.2
1	A	437	HIS	3.2
1	A	489	GLY	3.2
1	B	488	CYS	3.2
1	B	489	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	757	ARG	2.8
1	A	568	PHE	2.7
1	A	441	CYS	2.7
1	A	438	MET	2.7
1	B	455	PRO	2.6
1	B	471	PRO	2.6
1	B	474	ASN	2.6
1	B	537	LEU	2.6
1	B	604	LEU	2.6
1	B	469	ILE	2.6
1	B	513	PRO	2.5
1	B	687	TRP	2.4
1	B	758	GLY	2.4
1	A	598	HIS	2.4
1	A	488	CYS	2.3
1	A	494	GLU	2.3
1	B	492	CYS	2.3
1	A	493	PHE	2.3
1	A	595	LEU	2.3
1	A	486	ARG	2.3
1	B	446	TRP	2.2
1	B	602	SER	2.2
1	A	539	THR	2.2
1	B	453	THR	2.2
1	A	535	HIS	2.2
1	A	440	ILE	2.2
1	B	580	THR	2.1
1	A	697	GLY	2.1
1	A	446	TRP	2.1
1	A	491	SER	2.1
1	A	540	ASP	2.1
1	A	760	GLU	2.1
1	B	759	GLU	2.1
1	A	496	GLU	2.1
1	A	443	SER	2.1
1	A	537	LEU	2.1
1	A	593	LEU	2.1
1	B	472	PHE	2.1

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
4	4XS	A	803	12/12	0.90	0.10	24,28,35,55	0
2	ZN	B	801	1/1	0.99	0.10	31,31,31,31	0
3	MG	A	802	1/1	0.99	0.04	20,20,20,20	0
3	MG	B	802	1/1	0.99	0.04	21,21,21,21	0
2	ZN	A	801	1/1	0.99	0.06	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.