



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4AJD / pdb_00004ajd
Title : Identification and structural characterization of PDE10 fragment inhibitors
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Deposited on : 2012-02-16
Resolution : 2.30 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

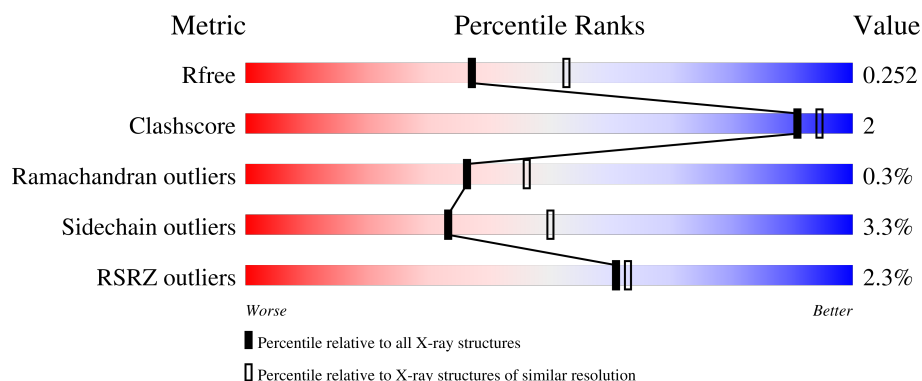
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	328	3% 91% 7% ..
1	D	328	2% 89% 9% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5619 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, PDE10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2622	1673	446	479	24			
1	D	323	Total	C	N	O	S	0	0	0
			2613	1668	445	476	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	447	ASN	-	expression tag	UNP Q9Y233
A	448	ALA	-	expression tag	UNP Q9Y233
D	447	ASN	-	expression tag	UNP Q9Y233
D	448	ALA	-	expression tag	UNP Q9Y233

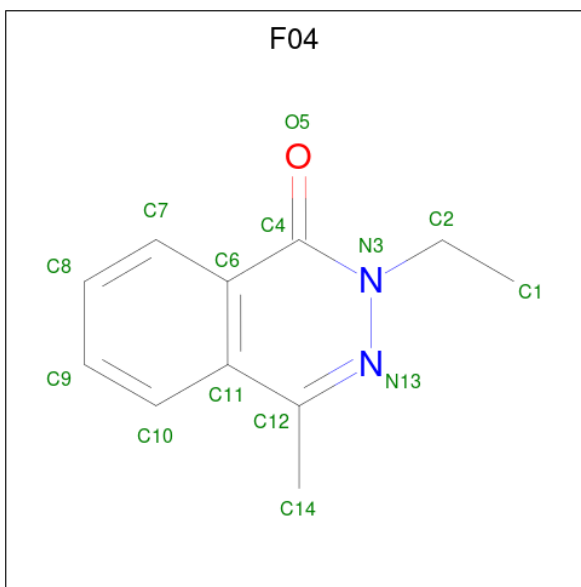
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is 2-ETHYL-4-METHYL-PHTHALAZIN-1-ONE (CCD ID: F04) (formula: C₁₁H₁₂N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	11	2	1		
4	D	1	Total	C	N	O	0	0
			14	11	2	1		

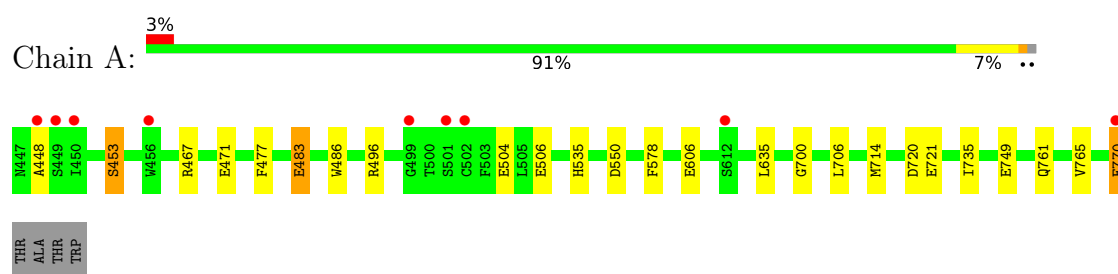
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	205	Total	O	0	0
			205	205		
5	D	147	Total	O	0	0
			147	147		

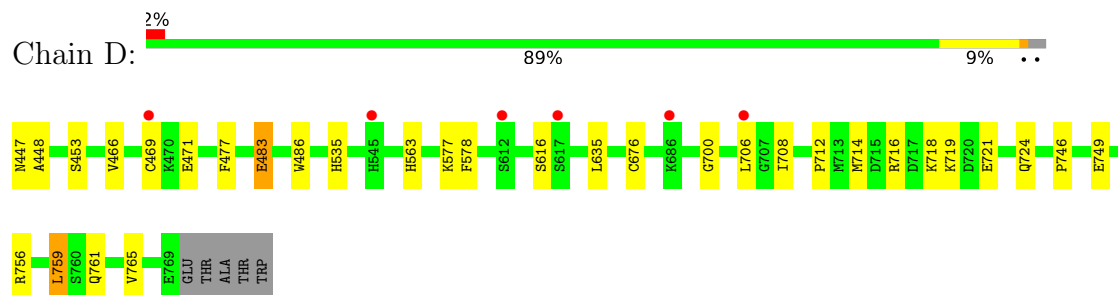
3 Residue-property plots [i](#)

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, PDE10



- Molecule 1: CAMP AND CAMP-INHIBITED CGMP 3', 5'-CYCLIC PHOSPHODIESTERASE 10A, PDE10



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.95Å 81.49Å 158.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.30 35.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.30) 99.9 (35.00-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.187 , 0.245 0.190 , 0.252	Depositor DCC
R_{free} test set	1486 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.799	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5619	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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, F04, ZN

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	0.87	0/2686	1.41	8/3637 (0.2%)
1	D	0.85	0/2677	1.42	4/3625 (0.1%)
All	All	0.86	0/5363	1.41	12/7262 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	676	CYS	N-CA-C	6.26	120.01	112.38
1	A	735	ILE	N-CA-CB	6.12	115.23	110.45
1	D	563	HIS	N-CA-C	5.56	118.87	111.75
1	D	483	GLU	N-CA-C	5.53	117.75	111.11
1	A	720	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	483	GLU	N-CA-C	5.33	117.50	111.11
1	A	550	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	721	GLU	CA-C-N	5.07	125.30	120.43
1	A	721	GLU	C-N-CA	5.07	125.30	120.43
1	D	746	PRO	N-CA-C	5.00	116.81	110.70
1	A	453	SER	CA-C-N	5.00	126.98	120.28
1	A	453	SER	C-N-CA	5.00	126.98	120.28

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	2622	0	2579	8	0
1	D	2613	0	2573	11	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	12	0	0
4	D	14	0	12	0	0
5	A	205	0	0	1	0
5	D	147	0	0	1	0
All	All	5619	0	5176	18	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 (18) 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:467:ARG:HH22	1:D:756:ARG:HB3	1.69	0.58
1:D:700:GLY:HA3	1:D:714:MET:O	2.07	0.55
1:D:477:PHE:HB3	1:D:535:HIS:CE1	2.45	0.51
1:A:477:PHE:HB3	1:A:535:HIS:CE1	2.46	0.51
1:D:469:CYS:HB2	5:D:2007:HOH:O	2.11	0.50
1:A:765:VAL:HA	1:A:770:GLU:HB3	1.94	0.49
1:D:578:PHE:CE1	1:D:706:LEU:HD13	2.49	0.48
1:A:606:GLU:HG3	5:A:2091:HOH:O	2.13	0.47
1:D:761:GLN:O	1:D:765:VAL:HG23	2.14	0.47
1:A:700:GLY:HA3	1:A:714:MET:O	2.16	0.45
1:D:759:LEU:C	1:D:759:LEU:HD12	2.43	0.43
1:D:712:PRO:HB3	1:D:718:LYS:HD3	2.01	0.42
1:A:578:PHE:CE1	1:A:706:LEU:HD13	2.54	0.42
1:A:483:GLU:HA	1:A:486:TRP:CE2	2.55	0.42
1:A:761:GLN:O	1:A:765:VAL:HG23	2.19	0.41
1:D:716:ARG:O	1:D:719:LYS:HG3	2.20	0.41
1:D:483:GLU:HA	1:D:486:TRP:CE2	2.57	0.40
1:D:578:PHE:CZ	1:D:708:ILE:HD12	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	322/328 (98%)	311 (97%)	10 (3%)	1 (0%)	36	46
1	D	321/328 (98%)	310 (97%)	10 (3%)	1 (0%)	36	46
All	All	643/656 (98%)	621 (97%)	20 (3%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	448	ALA
1	A	448	ALA

5.3.2 Protein sidechains

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	291/295 (99%)	283 (97%)	8 (3%)	39	58
1	D	290/295 (98%)	279 (96%)	11 (4%)	29	44
All	All	581/590 (98%)	562 (97%)	19 (3%)	33	50

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	453	SER
1	A	471	GLU
1	A	496	ARG
1	A	504	GLU

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Mol	Chain	Res	Type
1	A	506	GLU
1	A	635	LEU
1	A	749	GLU
1	A	770	GLU
1	D	447	ASN
1	D	453	SER
1	D	466	VAL
1	D	471	GLU
1	D	577	LYS
1	D	616	SER
1	D	635	LEU
1	D	721	GLU
1	D	724	GLN
1	D	749	GLU
1	D	759	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	GLN
1	A	476	HIS
1	A	659	GLN
1	D	447	ASN
1	D	457	GLN
1	D	650	GLN
1	D	761	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	F04	A	1773	-	14,15,15	2.94	8 (57%)	17,21,21	2.05	6 (35%)
4	F04	D	1772	-	14,15,15	2.39	7 (50%)	17,21,21	1.89	4 (23%)

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	F04	A	1773	-	-	1/2/2/2	0/2/2/2
4	F04	D	1772	-	-	2/2/2/2	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1773	F04	C7-C6	6.01	1.49	1.39
4	D	1772	F04	C7-C6	4.40	1.46	1.39
4	A	1773	F04	C9-C8	4.27	1.47	1.38
4	A	1773	F04	C8-C7	3.67	1.45	1.38
4	D	1772	F04	C9-C8	3.65	1.46	1.38
4	A	1773	F04	C6-C4	3.62	1.54	1.47
4	D	1772	F04	N3-N13	3.13	1.44	1.37
4	A	1773	F04	C10-C11	3.11	1.44	1.39
4	A	1773	F04	N3-N13	2.99	1.44	1.37
4	D	1772	F04	C10-C11	2.81	1.44	1.39
4	D	1772	F04	C6-C4	2.68	1.52	1.47
4	A	1773	F04	C9-C10	2.67	1.43	1.38
4	D	1772	F04	C12-N13	2.62	1.35	1.30
4	D	1772	F04	C4-N3	2.25	1.42	1.38
4	A	1773	F04	O5-C4	-2.16	1.18	1.22

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1773	F04	C6-C4-N3	4.28	120.50	114.42
4	A	1773	F04	C6-C11-C12	-3.90	115.25	118.12
4	D	1772	F04	O5-C4-N3	3.56	123.54	120.55
4	D	1772	F04	C2-N3-N13	3.50	118.02	113.46
4	D	1772	F04	C6-C4-N3	3.30	119.11	114.42
4	A	1773	F04	C2-N3-N13	2.87	117.20	113.46
4	A	1773	F04	C2-N3-C4	2.35	124.79	119.61
4	D	1772	F04	O5-C4-C6	-2.24	117.34	123.11
4	A	1773	F04	C10-C11-C6	2.21	121.74	119.26
4	A	1773	F04	C9-C8-C7	-2.18	117.55	120.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1772	F04	C1-C2-N3-C4
4	A	1773	F04	C1-C2-N3-C4
4	D	1772	F04	C1-C2-N3-N13

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	324/328 (98%)	-0.06	9 (2%) 55 57	16, 30, 60, 116	3 (0%)
1	D	323/328 (98%)	0.01	6 (1%) 66 68	20, 34, 58, 74	3 (0%)
All	All	647/656 (98%)	-0.02	15 (2%) 61 63	16, 32, 60, 116	6 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	612	SER	2.9
1	D	612	SER	2.7
1	D	469	CYS	2.7
1	A	456	TRP	2.7
1	A	448	ALA	2.6
1	A	502	CYS	2.6
1	A	449	SER	2.5
1	D	617	SER	2.4
1	D	545	HIS	2.3
1	A	770	GLU	2.2
1	D	686	LYS	2.2
1	D	706	LEU	2.2
1	A	501	SER	2.2
1	A	450	ILE	2.1
1	A	499	GLY	2.1

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
4	F04	D	1772	14/14	0.95	0.07	23,29,34,35	0
4	F04	A	1773	14/14	0.96	0.05	20,23,25,25	0
3	MG	D	1771	1/1	0.99	0.01	21,21,21,21	0
2	ZN	D	1770	1/1	0.99	0.03	31,31,31,31	0
3	MG	A	1772	1/1	0.99	0.04	17,17,17,17	0
2	ZN	A	1771	1/1	1.00	0.02	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.