



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 03:00 PM GMT

PDB ID : 1XOT
Title : Catalytic Domain Of Human Phosphodiesterase 4B In Complex With Vardenafil
Authors : Card, G.L.; England, B.P.; Suzuki, Y.; Fong, D.; Powell, B.; Lee, B.; Luu, C.; Tabrizizad, M.; Gillette, S.; Ibrahim, P.N.; Artis, D.R.; Bollag, G.; Milburn, M.V.; Kim, S.-H.; Schlessinger, J.; Zhang, K.Y.J.
Deposited on : 2004-10-06
Resolution : 2.34 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

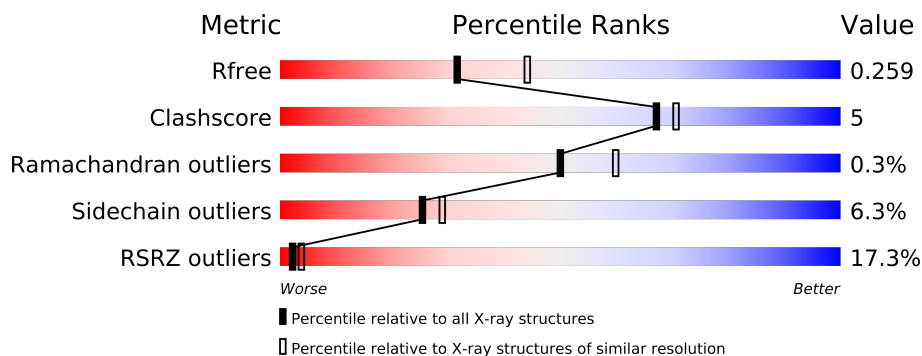
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.34 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}	66092	4049 (2.38-2.30)
Clashscore	79885	1094 (2.36-2.32)
Ramachandran outliers	78287	1080 (2.36-2.32)
Sidechain outliers	78261	1081 (2.36-2.32)
RSRZ outliers	66119	4050 (2.38-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	398	
1	B	398	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	VDN	B	102	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5352 atoms, of which 0 are hydrogen and 0 are deuterium.

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-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	323	Total	C	N	O	S	4	0	0
			2617	1653	441	503	20			
1	A	323	Total	C	N	O	S	4	0	0
			2617	1653	441	503	20			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	131	MET	-	INITIATING METHIONINE	UNP Q07343
B	132	GLY	-	CLONING ARTIFACT	UNP Q07343
B	133	SER	-	CLONING ARTIFACT	UNP Q07343
B	134	SER	-	CLONING ARTIFACT	UNP Q07343
B	135	HIS	-	EXPRESSION TAG	UNP Q07343
B	136	HIS	-	EXPRESSION TAG	UNP Q07343
B	137	HIS	-	EXPRESSION TAG	UNP Q07343
B	138	HIS	-	EXPRESSION TAG	UNP Q07343
B	139	HIS	-	EXPRESSION TAG	UNP Q07343
B	140	HIS	-	EXPRESSION TAG	UNP Q07343
B	141	SER	-	CLONING ARTIFACT	UNP Q07343
B	142	SER	-	CLONING ARTIFACT	UNP Q07343
B	143	GLY	-	CLONING ARTIFACT	UNP Q07343
B	144	LEU	-	CLONING ARTIFACT	UNP Q07343
B	145	VAL	-	CLONING ARTIFACT	UNP Q07343
B	146	PRO	-	CLONING ARTIFACT	UNP Q07343
B	147	ARG	-	CLONING ARTIFACT	UNP Q07343
B	148	GLY	-	CLONING ARTIFACT	UNP Q07343
B	149	SER	-	CLONING ARTIFACT	UNP Q07343
B	150	HIS	-	CLONING ARTIFACT	UNP Q07343
B	151	MET	-	CLONING ARTIFACT	UNP Q07343
B	194	CME	CYS	MODIFIED RESIDUE	UNP Q07343
A	131	MET	-	INITIATING METHIONINE	UNP Q07343
A	132	GLY	-	CLONING ARTIFACT	UNP Q07343
A	133	SER	-	CLONING ARTIFACT	UNP Q07343

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Chain	Residue	Modelled	Actual	Comment	Reference
A	134	SER	-	CLONING ARTIFACT	UNP Q07343
A	135	HIS	-	EXPRESSION TAG	UNP Q07343
A	136	HIS	-	EXPRESSION TAG	UNP Q07343
A	137	HIS	-	EXPRESSION TAG	UNP Q07343
A	138	HIS	-	EXPRESSION TAG	UNP Q07343
A	139	HIS	-	EXPRESSION TAG	UNP Q07343
A	140	HIS	-	EXPRESSION TAG	UNP Q07343
A	141	SER	-	CLONING ARTIFACT	UNP Q07343
A	142	SER	-	CLONING ARTIFACT	UNP Q07343
A	143	GLY	-	CLONING ARTIFACT	UNP Q07343
A	144	LEU	-	CLONING ARTIFACT	UNP Q07343
A	145	VAL	-	CLONING ARTIFACT	UNP Q07343
A	146	PRO	-	CLONING ARTIFACT	UNP Q07343
A	147	ARG	-	CLONING ARTIFACT	UNP Q07343
A	148	GLY	-	CLONING ARTIFACT	UNP Q07343
A	149	SER	-	CLONING ARTIFACT	UNP Q07343
A	150	HIS	-	CLONING ARTIFACT	UNP Q07343
A	151	MET	-	CLONING ARTIFACT	UNP Q07343
A	194	CME	CYS	MODIFIED RESIDUE	UNP Q07343

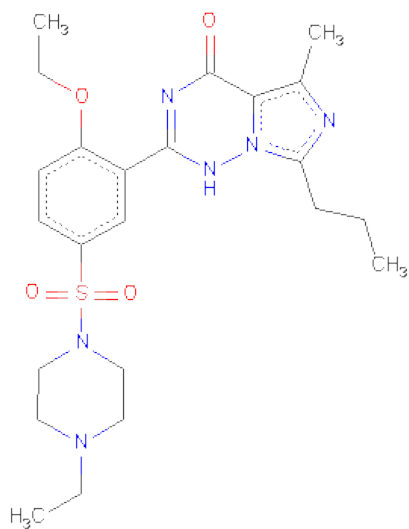
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 2-{2-ETHOXY-5-[(4-ETHYLPIPERAZIN-1-YL)SULFONYL]PHENYL}-5-METHYL-7-PROPYLIMIDAZO[5,1-F][1,2,4]TRIAZIN-4(1H)-ONE (three-letter code: VDN) (formula: C₂₃H₃₂N₆O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			34	23	6	4	1		
4	B	1	Total	C	N	O	S	0	0
			34	23	6	4	1		

- Molecule 5 is water.

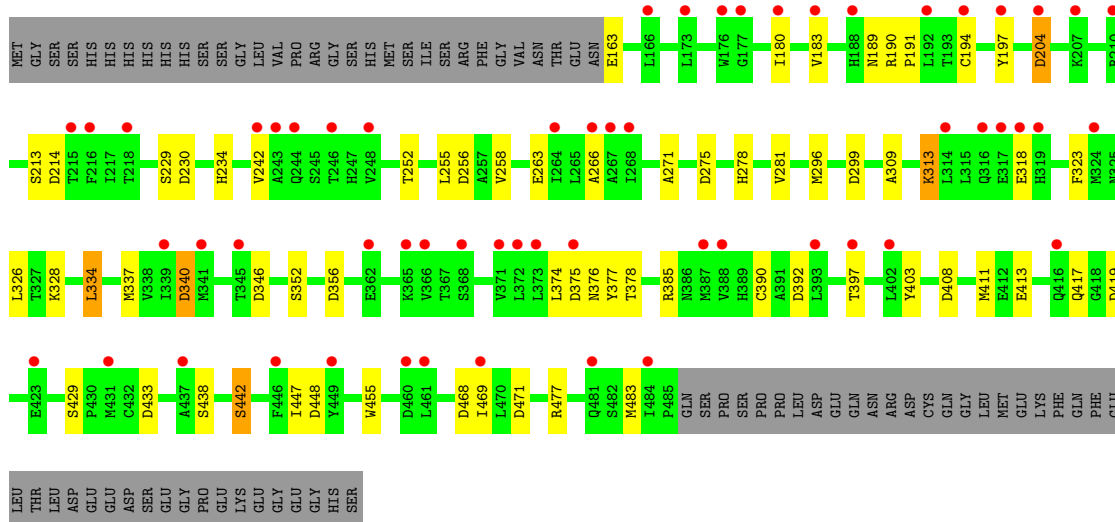
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	25	Total	O	0	0
			25	25		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

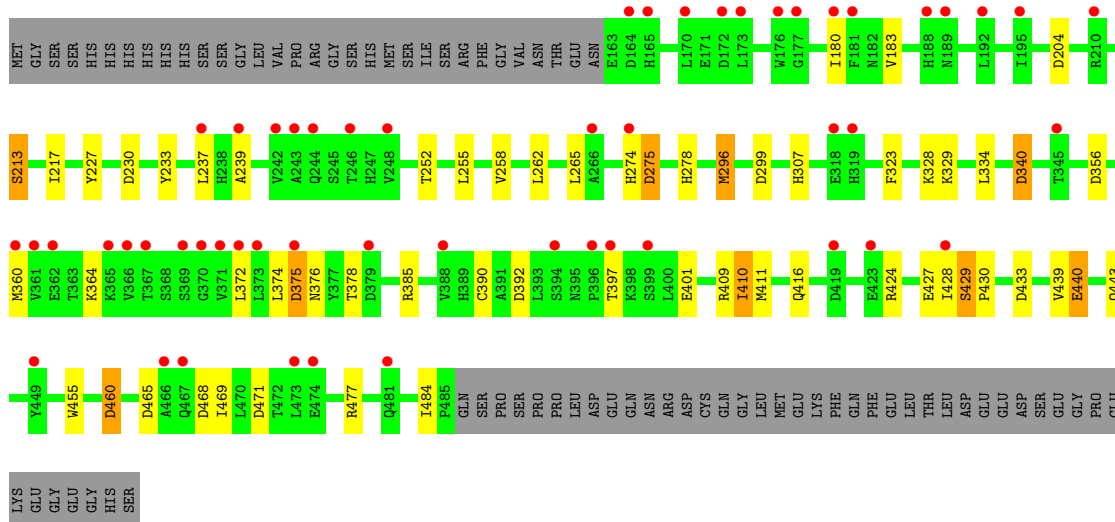
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B

Chain B: 



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.84Å 94.42Å 108.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.71 – 2.34 44.92 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (70.71-2.34) 99.4 (44.92-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.210 , 0.259 0.216 , 0.259	Depositor DCC
R_{free} test set	2101 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.6	EDS
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 41514 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5352	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.42 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3683e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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, CME, VDN

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	0.80	1/2661 (0.0%)	0.94	11/3608 (0.3%)
1	B	0.79	1/2661 (0.0%)	0.95	17/3608 (0.5%)
All	All	0.79	2/5322 (0.0%)	0.94	28/7216 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	GLU	CB-CG	15.93	1.82	1.52
1	A	440	GLU	CD-OE1	5.08	1.31	1.25

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	GLU	CA-CB-CG	-9.05	93.48	113.40
1	A	230	ASP	CB-CG-OD2	8.52	125.97	118.30
1	B	392	ASP	CB-CG-OD2	8.37	125.83	118.30
1	A	392	ASP	CB-CG-OD2	7.81	125.33	118.30
1	B	214	ASP	CB-CG-OD2	7.49	125.04	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2617	0	2546	25	0
1	B	2617	0	2546	26	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	34	0	32	4	0
4	B	34	0	32	5	0
5	A	21	0	0	0	0
5	B	25	0	0	2	0
All	All	5352	0	5156	52	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

The worst 5 of 52 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:102:VDN:H11	5:B:2008:HOH:O	1.83	0.77
1:B:266:ALA:HB2	1:B:334:LEU:HD12	1.69	0.73
4:B:102:VDN:C1	5:B:2008:HOH:O	2.37	0.69
1:A:411:MET:HG3	1:A:439:VAL:HG13	1.74	0.69
1:A:429:SER:HB3	4:A:101:VDN:H131	1.75	0.68

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	320/398 (80%)	310 (97%)	9 (3%)	1 (0%)	50	60
1	B	320/398 (80%)	308 (96%)	11 (3%)	1 (0%)	50	60
All	All	640/796 (80%)	618 (97%)	20 (3%)	2 (0%)	50	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	375	ASP
1	A	430	PRO

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	292/359 (81%)	271 (93%)	21 (7%)	21	22
1	B	292/359 (81%)	276 (94%)	16 (6%)	30	36
All	All	584/718 (81%)	547 (94%)	37 (6%)	25	29

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	ASP
1	A	329	LYS
1	A	460	ASP
1	A	213	SER
1	A	296	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	443	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	CME	A	194	1	9,9,10	4.81	3 (33%)	7,9,11	2.85	5 (71%)
1	CME	B	194	1	9,9,10	7.16	3 (33%)	7,9,11	3.13	3 (42%)

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
1	CME	A	194	1	-	0/6/8/10	0/0/0/0
1	CME	B	194	1	-	0/6/8/10	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	CME	O-C	20.97	1.25	1.11
1	A	194	CME	O-C	13.56	1.20	1.11
1	A	194	CME	OH-CZ	-3.51	1.23	1.42
1	B	194	CME	OH-CZ	-3.44	1.23	1.42
1	A	194	CME	CA-C	2.90	1.53	1.48

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	CME	CB-CA-N	5.15	119.00	110.27
1	B	194	CME	CB-SG-SD	5.11	114.07	103.87
1	B	194	CME	CB-CA-N	4.38	117.70	110.27
1	B	194	CME	CA-CB-SG	-3.41	102.67	113.36
1	A	194	CME	CE-SD-SG	3.12	119.65	103.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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	VDN	A	101	-	36,37,37	3.17	8 (22%)	46,54,54	3.53	26 (56%)
4	VDN	B	102	-	36,37,37	3.17	9 (25%)	46,54,54	2.86	20 (43%)

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	VDN	A	101	-	-	0/24/34/34	0/2/4/4
4	VDN	B	102	-	-	0/24/34/34	0/2/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	101	VDN	C7-S10	-10.02	1.61	1.76
4	B	102	VDN	C7-S10	-9.85	1.61	1.76
4	A	101	VDN	C21-N22	9.58	1.48	1.32
4	B	102	VDN	C21-N22	9.37	1.48	1.32
4	B	102	VDN	C24-N25	-6.89	1.31	1.40

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	101	VDN	C28-C24-N25	14.68	105.82	103.62
4	B	102	VDN	C9-C21-N26	-7.51	110.01	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	102	VDN	O11-S10-N14	7.11	113.95	106.71
4	B	102	VDN	C30-N25-C24	7.06	115.98	108.44
4	A	101	VDN	O11-S10-N14	7.01	113.85	106.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	323/398 (81%)	1.15	53 (16%) 2 4	14, 26, 32, 53	1 (0%)
1	B	323/398 (81%)	1.15	58 (17%) 2 3	18, 26, 32, 53	1 (0%)
All	All	646/796 (81%)	1.15	111 (17%) 2 4	14, 26, 32, 53	2 (0%)

The worst 5 of 111 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	GLU	6.2
1	A	370	GLY	5.4
1	B	373	LEU	5.2
1	A	366	VAL	4.7
1	A	369	SER	4.5

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CME	B	194	10/11	0.28	0.92	38,42,67,71	0
1	CME	A	194	10/11	0.21	-0.01	37,40,70,72	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	VDN	B	102	34/34	0.28	2.42	59,64,67,68	34
4	VDN	A	101	34/34	0.18	-0.35	63,66,68,71	34
3	MG	B	1002	1/1	0.10	-2.21	30,30,30,30	0
3	MG	A	1002	1/1	0.07	-3.55	35,35,35,35	0
2	ZN	B	1001	1/1	0.04	-3.59	44,44,44,44	0
2	ZN	A	1001	1/1	0.04	-5.81	46,46,46,46	0

6.5 Other polymers

There are no such residues in this entry.