



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:48 am GMT

PDB ID : 1XM4
Title : Catalytic Domain Of Human Phosphodiesterase 4B In Complex With Piclami-
last
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 : 2004-10-01
Resolution : 2.31 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

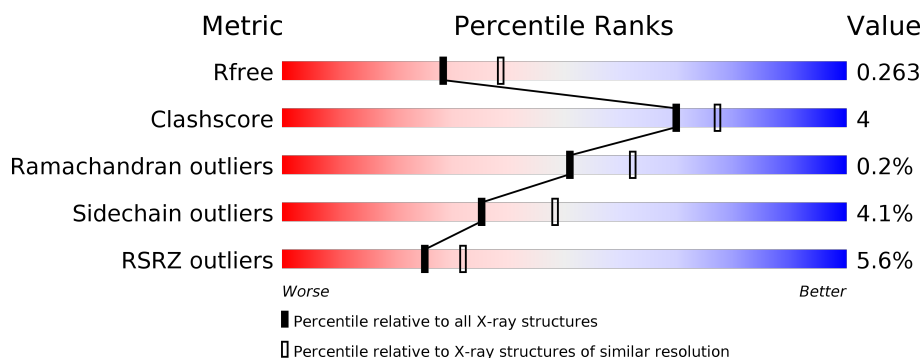
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	100719	4787 (2.34-2.30)
Clashscore	112137	5439 (2.34-2.30)
Ramachandran outliers	110173	5386 (2.34-2.30)
Sidechain outliers	110143	5385 (2.34-2.30)
RSRZ outliers	101464	4814 (2.34-2.30)

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. 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	398	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>13%</div> <div>•</div> <div>19%</div> </div> </div>
2	B	398	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>12%</div> <div>•</div> <div>19%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	B	1002	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5417 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-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2621	1655	441	504	21			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	MET	-	INITIATING METHIONINE	UNP Q07343
A	132	GLY	-	CLONING ARTIFACT	UNP Q07343
A	133	SER	-	CLONING ARTIFACT	UNP Q07343
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
A	432	CME	CYS	MODIFIED RESIDUE	UNP Q07343

- Molecule 2 is a protein called cAMP-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	323	Total	C	N	O	S	0	0	0
			2621	1655	441	504	21			

There are 23 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
B	320	CME	CYS	MODIFIED RESIDUE	UNP Q07343

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

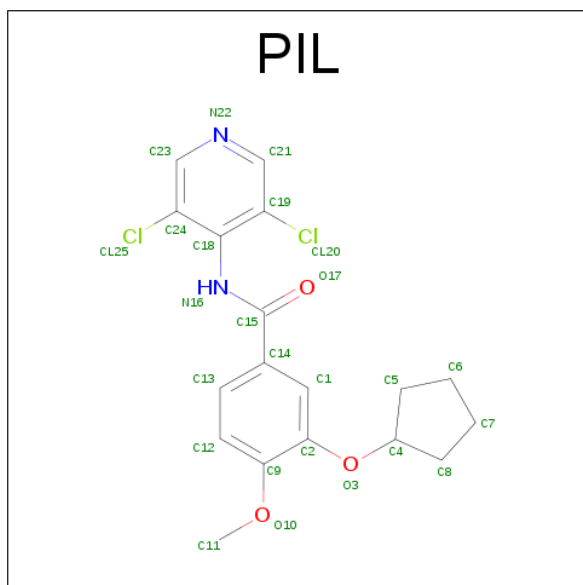
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 3-(CYCLOPENTYLOXY)-N-(3,5-DICHLOROPYRIDIN-4-YL)-4-METHOXYBENZAMIDE (three-letter code: PIL) (formula: $C_{18}H_{18}Cl_2N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	
			25	18	2	2	3	0
5	B	1	Total	C	Cl	N	O	
			25	18	2	2	3	0

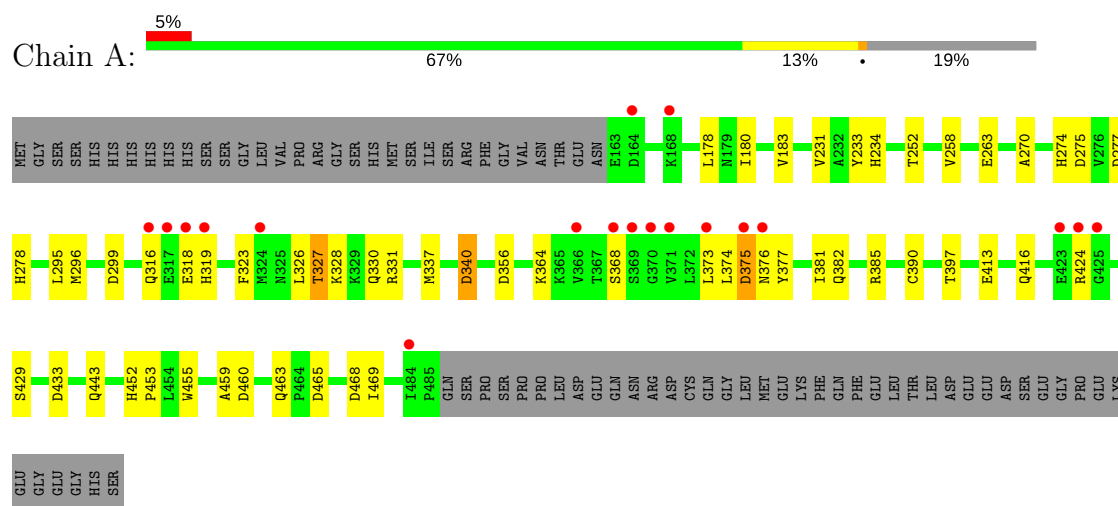
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	66	Total	O	0	0
			66	66		
6	B	55	Total	O	0	0
			55	55		

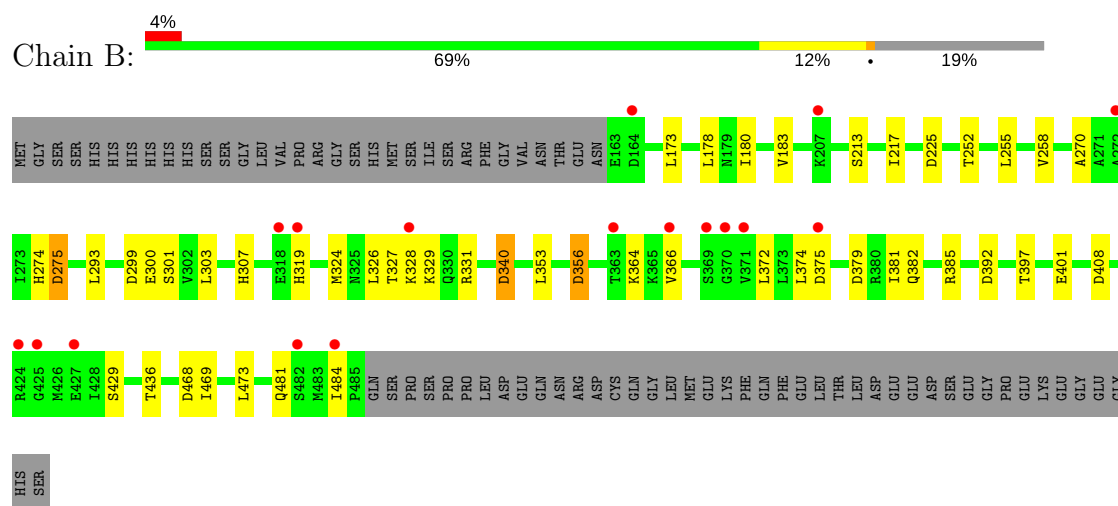
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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



- Molecule 2: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.57Å 94.32Å 106.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.71 – 2.31 41.30 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.6 (70.71-2.31) 97.6 (41.30-2.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.212 , 0.263 0.217 , 0.263	Depositor DCC
R_{free} test set	1971 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5417	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 30.21 % 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 1.3587e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG, PIL, ZN, CME

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	0.82	1/2654 (0.0%)	0.94	6/3597 (0.2%)
2	B	0.81	0/2654	0.91	10/3597 (0.3%)
All	All	0.81	1/5308 (0.0%)	0.92	16/7194 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	TYR	CD2-CE2	6.20	1.48	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ASP	CB-CG-OD2	7.83	125.34	118.30
1	A	299	ASP	CB-CG-OD2	7.11	124.70	118.30
2	B	375	ASP	CB-CG-OD2	6.97	124.57	118.30
2	B	468	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	468	ASP	CB-CG-OD2	6.60	124.24	118.30
2	B	275	ASP	CB-CG-OD2	6.60	124.24	118.30
2	B	408	ASP	CB-CG-OD2	6.23	123.91	118.30
2	B	299	ASP	CB-CG-OD2	5.83	123.55	118.30
2	B	379	ASP	CB-CG-OD2	5.65	123.39	118.30
2	B	340	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	340	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	277	ASP	CB-CG-OD2	5.42	123.18	118.30
2	B	392	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	433	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	356	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	225	ASP	CB-CG-OD2	5.08	122.87	118.30

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	2621	0	2551	21	0
2	B	2621	0	2551	23	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	25	0	18	1	0
5	B	25	0	18	0	0
6	A	66	0	0	0	0
6	B	55	0	0	1	0
All	All	5417	0	5138	44	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 4.

All (44) 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)
2:B:328:LYS:HZ3	2:B:331:ARG:NH2	1.86	0.72
1:A:340:ASP:OD1	1:A:385:ARG:HD3	1.92	0.69
1:A:252:THR:HG22	1:A:465:ASP:OD2	1.93	0.69
2:B:255:LEU:HD23	2:B:372:LEU:HD12	1.81	0.62
1:A:327:THR:HG22	1:A:330:GLN:H	1.67	0.60
2:B:340:ASP:OD1	2:B:385:ARG:HD3	2.02	0.60
2:B:356:ASP:HB3	2:B:382:GLN:HE22	1.69	0.57
2:B:255:LEU:CD2	2:B:372:LEU:HD12	2.34	0.57
2:B:328:LYS:NZ	2:B:331:ARG:NH2	2.52	0.56
1:A:397:THR:HB	1:A:469:ILE:HG23	1.89	0.54
1:A:381:ILE:O	1:A:385:ARG:HG3	2.08	0.53
2:B:397:THR:HB	2:B:469:ILE:HG23	1.89	0.53
2:B:327:THR:HG22	2:B:328:LYS:N	2.23	0.53
1:A:356:ASP:HB3	1:A:382:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:ALA:O	2:B:274:HIS:HB3	2.12	0.49
1:A:180:ILE:HA	1:A:183:VAL:HG13	1.93	0.49
1:A:390:CYS:HB3	1:A:455:TRP:CZ2	2.47	0.49
1:A:270:ALA:O	1:A:274:HIS:HB3	2.13	0.49
2:B:328:LYS:HZ3	2:B:331:ARG:HH21	1.59	0.47
1:A:340:ASP:OD1	1:A:385:ARG:CD	2.63	0.46
2:B:173:LEU:HA	2:B:178:LEU:HD13	1.97	0.45
2:B:397:THR:HG22	2:B:473:LEU:HD13	1.99	0.45
2:B:303:LEU:HD12	6:B:119:HOH:O	2.17	0.45
1:A:443:GLN:NE2	5:A:1003:PIL:H81	2.32	0.44
1:A:275:ASP:O	1:A:278:HIS:HB2	2.18	0.44
2:B:300:GLU:O	2:B:301:SER:C	2.55	0.43
2:B:213:SER:O	2:B:217:ILE:HG12	2.19	0.43
2:B:258:VAL:HG11	2:B:374:LEU:HD12	2.00	0.43
2:B:481:GLN:HA	2:B:484:ILE:HD12	2.01	0.43
1:A:452:HIS:HB3	1:A:453:PRO:HD3	2.01	0.43
1:A:376:ASN:CG	1:A:377:TYR:H	2.22	0.42
2:B:180:ILE:HA	2:B:183:VAL:HG13	2.01	0.41
2:B:275:ASP:HA	2:B:307:HIS:CD2	2.55	0.41
1:A:258:VAL:HG11	1:A:374:LEU:HD12	2.01	0.41
1:A:234:HIS:ND1	1:A:413:GLU:OE2	2.38	0.41
1:A:459:ALA:O	1:A:463:GLN:HB3	2.20	0.41
2:B:252:THR:HG22	2:B:255:LEU:HD12	2.01	0.41
1:A:326:LEU:HD23	1:A:326:LEU:N	2.35	0.41
2:B:293:LEU:HD23	2:B:293:LEU:HA	1.92	0.41
1:A:364:LYS:NZ	1:A:460:ASP:O	2.52	0.41
2:B:381:ILE:O	2:B:385:ARG:HG3	2.21	0.41
1:A:323:PHE:HB3	1:A:326:LEU:HG	2.02	0.41
1:A:263:GLU:HG2	1:A:337:MET:SD	2.61	0.41
2:B:327:THR:HG22	2:B:329:LYS:H	1.86	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	319/398 (80%)	309 (97%)	9 (3%)	1 (0%)	44	54
2	B	319/398 (80%)	309 (97%)	10 (3%)	0	100	100
All	All	638/796 (80%)	618 (97%)	19 (3%)	1 (0%)	51	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	ASP

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	291/358 (81%)	276 (95%)	15 (5%)	27	36
2	B	291/358 (81%)	282 (97%)	9 (3%)	45	61
All	All	582/716 (81%)	558 (96%)	24 (4%)	35	48

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	LEU
1	A	231	VAL
1	A	295	LEU
1	A	296	MET
1	A	316	GLN
1	A	318	GLU
1	A	319	HIS
1	A	327	THR
1	A	328	LYS
1	A	331	ARG
1	A	368	SER
1	A	373	LEU

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Mol	Chain	Res	Type
1	A	416	GLN
1	A	424	ARG
1	A	429	SER
2	B	319	HIS
2	B	324	MET
2	B	326	LEU
2	B	353	LEU
2	B	364	LYS
2	B	366	VAL
2	B	401	GLU
2	B	429	SER
2	B	436	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	GLN
1	A	443	GLN
2	B	382	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	0.88	0	6,9,11	1.70	1 (16%)
1	CME	A	432	1	9,9,10	0.71	0	6,9,11	1.65	1 (16%)
2	CME	B	194	2	9,9,10	1.02	1 (11%)	6,9,11	1.64	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CME	B	320	2	9,9,10	1.27	1 (11%)	6,9,11	1.56	2 (33%)

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	-	0/5/8/10	0/0/0/0
1	CME	A	432	1	-	0/5/8/10	0/0/0/0
2	CME	B	194	2	-	0/5/8/10	0/0/0/0
2	CME	B	320	2	-	0/5/8/10	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	CME	CA-C	2.11	1.53	1.50
2	B	320	CME	CA-C	3.03	1.54	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	CME	O-C-CA	-2.96	116.85	125.02
2	B	194	CME	O-C-CA	-2.71	117.53	125.02
2	B	320	CME	O-C-CA	-2.71	117.53	125.02
2	B	320	CME	CB-SG-SD	2.03	107.78	103.83
2	B	194	CME	CE-SD-SG	2.29	114.91	103.40
1	A	194	CME	CE-SD-SG	2.71	117.02	103.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

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
5	PIL	A	1003	-	27,27,27	0.86	2 (7%)	37,37,37	1.75	6 (16%)
5	PIL	B	1003	-	27,27,27	0.81	1 (3%)	37,37,37	1.63	6 (16%)

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
5	PIL	A	1003	-	-	0/14/21/21	0/3/3/3
5	PIL	B	1003	-	-	0/14/21/21	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1003	PIL	C18-C19	-2.02	1.36	1.40
5	A	1003	PIL	O10-C9	2.03	1.40	1.37
5	B	1003	PIL	C19-CL20	2.24	1.79	1.73

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	PIL	C24-C23-N22	-4.99	117.69	122.86
5	B	1003	PIL	C24-C23-N22	-4.18	118.53	122.86
5	B	1003	PIL	C21-C19-C18	-2.92	118.56	120.16
5	A	1003	PIL	O17-C15-C14	-2.12	117.18	120.94
5	A	1003	PIL	C19-C21-N22	-2.12	120.67	122.86
5	B	1003	PIL	C18-C19-CL20	2.17	121.87	119.29
5	B	1003	PIL	C21-N22-C23	2.58	121.10	117.45
5	A	1003	PIL	C21-N22-C23	2.66	121.21	117.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1003	PIL	C11-O10-C9	3.11	122.02	117.54
5	B	1003	PIL	C23-C24-C18	3.90	122.30	120.16
5	B	1003	PIL	C11-O10-C9	4.57	124.11	117.54
5	A	1003	PIL	C23-C24-C18	6.67	123.82	120.16

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
5	A	1003	PIL	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	321/398 (80%)	0.34	19 (5%) 23 30	16, 22, 30, 39	0
2	B	321/398 (80%)	0.27	17 (5%) 27 34	16, 22, 30, 39	0
All	All	642/796 (80%)	0.30	36 (5%) 25 32	16, 22, 30, 39	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	369	SER	4.7
1	A	319	HIS	4.2
1	A	318	GLU	4.1
1	A	366	VAL	3.8
2	B	366	VAL	3.4
2	B	375	ASP	3.3
1	A	368	SER	3.3
2	B	319	HIS	3.1
1	A	425	GLY	3.1
1	A	317	GLU	2.8
2	B	484	ILE	2.8
1	A	324	MET	2.8
2	B	164	ASP	2.8
2	B	370	GLY	2.8
1	A	423	GLU	2.8
1	A	164	ASP	2.6
2	B	207	LYS	2.6
1	A	484	ILE	2.6
2	B	369	SER	2.6
2	B	482	SER	2.6
1	A	375	ASP	2.6
1	A	376	ASN	2.6
1	A	373	LEU	2.5
2	B	425	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	318	GLU	2.4
1	A	168	LYS	2.3
2	B	424	ARG	2.2
1	A	371	VAL	2.2
2	B	427	GLU	2.2
1	A	424	ARG	2.2
1	A	370	GLY	2.1
1	A	316	GLN	2.1
2	B	328	LYS	2.1
2	B	363	THR	2.1
2	B	272	ALA	2.1
2	B	371	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CME	B	194	10/11	0.95	0.10	-	29,31,54,54	0
1	CME	A	194	10/11	0.94	0.09	-	30,35,57,57	0
1	CME	A	432	10/11	0.92	0.12	-	38,43,62,63	0
2	CME	B	320	10/11	0.94	0.17	-	40,43,63,63	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	B	1002	1/1	0.97	0.21	2.33	30,30,30,30	0
4	MG	A	1002	1/1	0.99	0.19	1.14	26,26,26,26	0
5	PIL	A	1003	25/25	0.95	0.15	0.35	35,43,54,55	0
5	PIL	B	1003	25/25	0.95	0.14	-0.11	41,48,57,58	0
3	ZN	B	1001	1/1	1.00	0.15	-0.58	38,38,38,38	0
3	ZN	A	1001	1/1	0.99	0.14	-0.72	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.