



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:31 PM GMT

PDB ID : 1XMY  
Title : Catalytic Domain Of Human Phosphodiesterase 4B In Complex With (R)-Rolipram  
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 : 2004-10-04  
Resolution : 2.40 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](mailto: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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

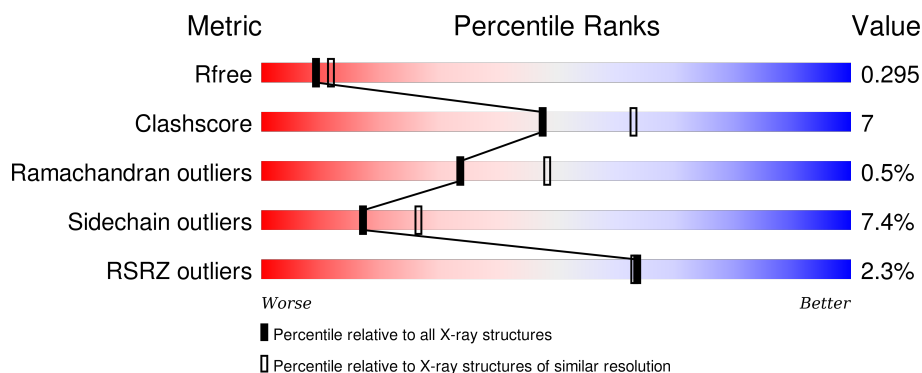
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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  $\geq 3$ , 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	
2	B	398	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5331 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
			2613	1651	441	502	19			

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	320	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
			2613	1651	441	502	19			

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	432	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).

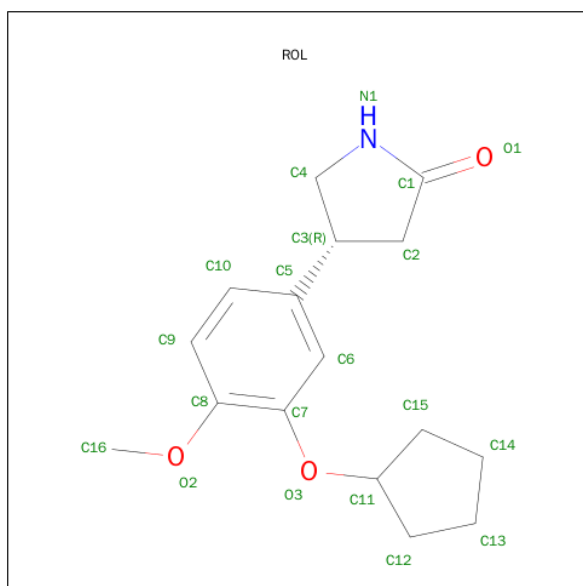
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

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

- Molecule 5 is ROLIPRAM (three-letter code: ROL) (formula:  $C_{16}H_{21}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	16	1	3		
5	B	1	Total	C	N	O	0	0
			20	16	1	3		

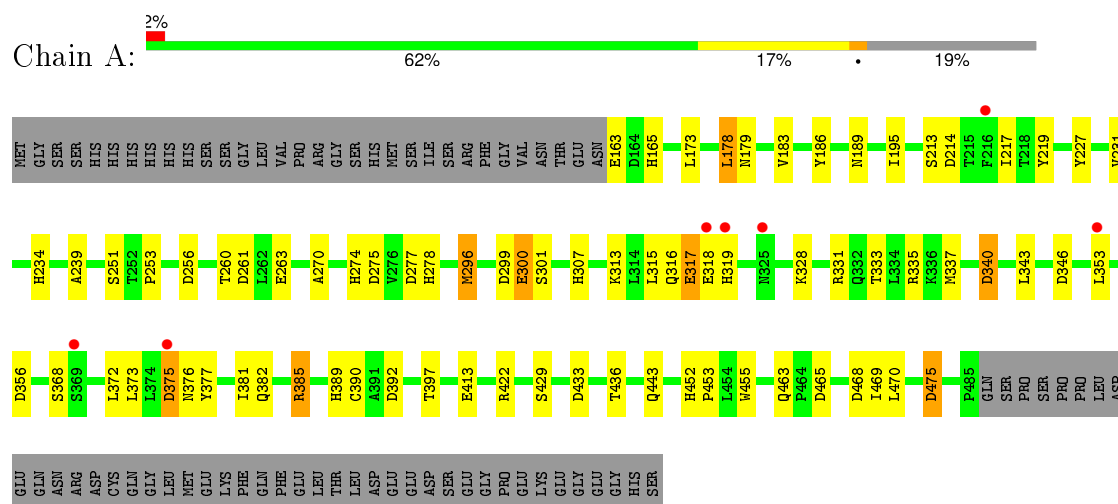
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	33	Total	O	0	0
			33	33		

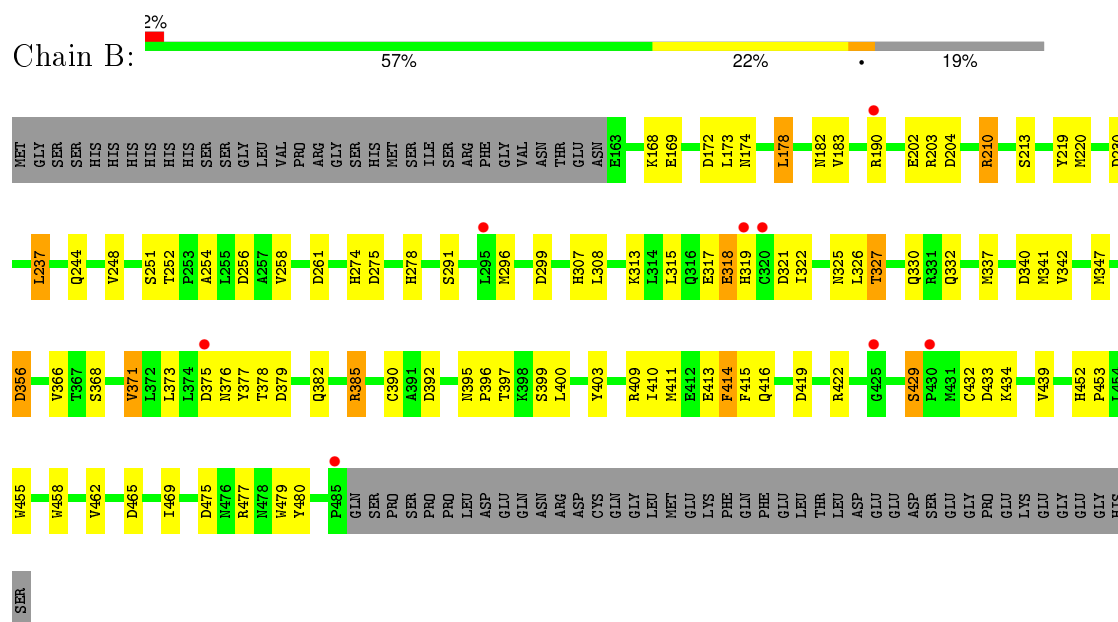
### 3 Residue-property plots [i](#)

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



- 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, $\alpha$ , $\beta$ , $\gamma$	89.67Å 94.63Å 106.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.71 – 2.40 68.58 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (70.71-2.40) 99.1 (68.58-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, $R_{free}$	0.243 , 0.298 0.243 , 0.295	Depositor DCC
$R_{free}$ test set	1792 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.1	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	6 of 35799 reflections (0.017%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5331	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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 54.00 % 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 3.8896e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, ROL, 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	1.04	0/2654	1.12	16/3597 (0.4%)
2	B	1.13	1/2654 (0.0%)	1.13	16/3597 (0.4%)
All	All	1.09	1/5308 (0.0%)	1.12	32/7194 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	414	PHE	CE2-CZ	6.36	1.49	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	ASP	CB-CG-OD2	10.97	128.18	118.30
2	B	433	ASP	CB-CG-OD2	8.82	126.24	118.30
1	A	468	ASP	CB-CG-OD2	6.94	124.55	118.30
1	A	346	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	433	ASP	CB-CG-OD2	6.77	124.39	118.30
2	B	190	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	299	ASP	CB-CG-OD2	6.70	124.33	118.30
2	B	220	MET	CG-SD-CE	-6.58	89.68	100.20
2	B	379	ASP	CB-CG-OD2	6.56	124.20	118.30
2	B	203	ARG	NE-CZ-NH2	-6.54	117.03	120.30
2	B	261	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	214	ASP	CB-CG-OD2	6.45	124.11	118.30
1	A	277	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	261	ASP	CB-CG-OD2	6.34	124.00	118.30
2	B	210	ARG	NE-CZ-NH2	6.34	123.47	120.30
2	B	237	LEU	CB-CG-CD2	-6.31	100.27	111.00
1	A	385	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	340	ASP	CB-CG-OD2	5.95	123.65	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	392	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	256	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	422	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	475	ASP	CB-CG-OD1	5.69	123.42	118.30
2	B	256	ASP	CB-CG-OD2	5.63	123.37	118.30
2	B	465	ASP	CB-CG-OD1	5.57	123.31	118.30
2	B	299	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	346	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	385	ARG	NE-CZ-NH2	-5.35	117.63	120.30
2	B	385	ARG	NE-CZ-NH2	-5.31	117.64	120.30
2	B	475	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	375	ASP	CB-CG-OD2	5.24	123.01	118.30
2	B	385	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	B	230	ASP	CB-CG-OD2	5.04	122.84	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	2613	0	2541	36	0
2	B	2613	0	2541	45	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	20	0	21	0	0
5	B	20	0	21	1	0
6	A	28	0	0	0	0
6	B	33	0	0	2	0
All	All	5331	0	5124	77	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 (77) 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:397:THR:HB	2:B:469:ILE:HG23	1.54	0.88
2:B:356:ASP:HB3	2:B:382:GLN:NE2	2.04	0.72
2:B:340:ASP:OD1	2:B:385:ARG:HD3	1.92	0.69
1:A:234:HIS:ND1	1:A:413:GLU:OE2	2.26	0.69
5:B:102:ROL:H101	6:B:12:HOH:O	1.93	0.68
2:B:414:PHE:O	2:B:432:CME:HB2	1.93	0.68
1:A:270:ALA:O	1:A:274:HIS:HB3	1.95	0.67
2:B:219:TYR:CE1	2:B:315:LEU:HD23	2.30	0.67
2:B:356:ASP:HB3	2:B:382:GLN:HE22	1.61	0.65
2:B:327:THR:HG23	2:B:330:GLN:H	1.61	0.63
1:A:296:MET:SD	2:B:296:MET:SD	2.97	0.63
2:B:419:ASP:HA	2:B:422:ARG:NH1	2.14	0.63
1:A:397:THR:HB	1:A:469:ILE:HG23	1.79	0.63
1:A:317:GLU:OE2	1:A:319:HIS:HB2	2.00	0.62
1:A:356:ASP:HB3	1:A:382:GLN:NE2	2.15	0.62
2:B:337:MET:O	2:B:341:MET:HG3	2.03	0.58
1:A:165:HIS:HB3	1:A:186:TYR:CE2	2.40	0.56
1:A:213:SER:O	1:A:217:ILE:HG12	2.06	0.55
1:A:313:LYS:O	1:A:316:GLN:HG2	2.07	0.54
2:B:274:HIS:O	2:B:307:HIS:CD2	2.61	0.54
2:B:415:PHE:CG	2:B:434:LYS:HB3	2.43	0.53
1:A:340:ASP:OD1	1:A:385:ARG:HD3	2.10	0.52
2:B:400:LEU:HD11	2:B:479:TRP:CE3	2.45	0.51
1:A:381:ILE:O	1:A:385:ARG:HG3	2.12	0.50
1:A:296:MET:CE	2:B:313:LYS:NZ	2.74	0.50
2:B:248:VAL:O	2:B:251:SER:HB2	2.12	0.50
1:A:353:LEU:HD23	1:A:389:HIS:CD2	2.46	0.50
1:A:260:THR:OG1	1:A:263:GLU:HG3	2.12	0.50
1:A:234:HIS:HD1	1:A:413:GLU:CD	2.15	0.50
1:A:452:HIS:HB3	1:A:453:PRO:HD3	1.93	0.49
2:B:410:ILE:HD11	2:B:414:PHE:CE1	2.48	0.49
2:B:419:ASP:OD2	2:B:434:LYS:NZ	2.46	0.49
2:B:322:ILE:O	6:B:8:HOH:O	2.20	0.49
1:A:179:ASN:C	1:A:179:ASN:OD1	2.51	0.49
2:B:411:MET:HG3	2:B:439:VAL:HG22	1.95	0.49
2:B:210:ARG:HB2	2:B:325:ASN:HD22	1.78	0.49
2:B:395:ASN:N	2:B:396:PRO:CD	2.76	0.49
1:A:275:ASP:O	1:A:278:HIS:HB2	2.13	0.48
2:B:172:ASP:O	2:B:178:LEU:HB2	2.13	0.48
2:B:419:ASP:HA	2:B:422:ARG:HH12	1.79	0.48
1:A:381:ILE:HG13	1:A:381:ILE:O	2.12	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:GLU:OE2	2:B:319:HIS:N	2.46	0.48
2:B:254:ALA:O	2:B:371:VAL:HG22	2.14	0.47
2:B:376:ASN:CG	2:B:377:TYR:H	2.18	0.47
1:A:219:TYR:CE1	1:A:315:LEU:HD23	2.49	0.47
2:B:315:LEU:O	2:B:321:ASP:HB2	2.15	0.47
2:B:452:HIS:HB3	2:B:453:PRO:HD3	1.96	0.47
1:A:296:MET:CE	2:B:313:LYS:HZ1	2.28	0.47
2:B:413:GLU:O	2:B:416:GLN:HB2	2.15	0.46
1:A:227:TYR:CZ	1:A:239:ALA:HB2	2.50	0.46
1:A:253:PRO:HD2	1:A:465:ASP:CG	2.36	0.46
2:B:237:LEU:HD23	2:B:409:ARG:NH1	2.31	0.45
1:A:195:ILE:HD12	1:A:195:ILE:HA	1.81	0.45
2:B:390:CYS:HB3	2:B:455:TRP:CZ2	2.52	0.44
1:A:353:LEU:HD23	1:A:389:HIS:HD2	1.82	0.44
1:A:390:CYS:HB3	1:A:455:TRP:CZ2	2.53	0.44
1:A:296:MET:HE2	2:B:313:LYS:HZ1	1.82	0.44
1:A:333:THR:O	1:A:337:MET:HG3	2.18	0.44
1:A:376:ASN:O	1:A:377:TYR:C	2.56	0.43
2:B:429:SER:O	2:B:432:CME:N	2.51	0.43
1:A:300:GLU:O	1:A:301:SER:C	2.56	0.43
2:B:308:LEU:HG	2:B:342:VAL:HG11	2.01	0.43
2:B:399:SER:O	2:B:400:LEU:C	2.57	0.42
2:B:397:THR:CB	2:B:469:ILE:HG23	2.37	0.42
1:A:165:HIS:HB3	1:A:186:TYR:CZ	2.54	0.42
2:B:174:ASN:ND2	2:B:202:GLU:OE2	2.46	0.42
1:A:173:LEU:HA	1:A:178:LEU:HD13	2.01	0.42
2:B:403:TYR:CE2	2:B:480:TYR:CE2	3.08	0.42
2:B:173:LEU:O	2:B:244:GLN:NE2	2.53	0.42
2:B:275:ASP:O	2:B:278:HIS:HB2	2.19	0.41
1:A:165:HIS:CB	1:A:186:TYR:CZ	3.03	0.41
2:B:403:TYR:CE2	2:B:480:TYR:HE2	2.38	0.41
2:B:169:GLU:OE2	2:B:182:ASN:HB3	2.21	0.41
1:A:296:MET:HE3	2:B:313:LYS:HZ3	1.86	0.41
1:A:343:LEU:HD23	1:A:343:LEU:HA	1.96	0.40
1:A:275:ASP:HA	1:A:307:HIS:CD2	2.56	0.40
2:B:458:TRP:O	2:B:462:VAL:HG22	2.21	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%)	305 (96%)	13 (4%)	1 (0%)	46	63
2	B	319/398 (80%)	306 (96%)	11 (3%)	2 (1%)	30	43
All	All	638/796 (80%)	611 (96%)	24 (4%)	3 (0%)	34	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	ASP
2	B	291	SER
2	B	375	ASP

### 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	291/358 (81%)	269 (92%)	22 (8%)	16	25
2	B	291/358 (81%)	270 (93%)	21 (7%)	18	28
All	All	582/716 (81%)	539 (93%)	43 (7%)	17	26

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	GLU
1	A	178	LEU
1	A	183	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	189	ASN
1	A	231	VAL
1	A	251	SER
1	A	296	MET
1	A	300	GLU
1	A	317	GLU
1	A	318	GLU
1	A	328	LYS
1	A	331	ARG
1	A	335	ARG
1	A	368	SER
1	A	372	LEU
1	A	373	LEU
1	A	429	SER
1	A	436	THR
1	A	443	GLN
1	A	463	GLN
1	A	470	LEU
1	A	475	ASP
2	B	168	LYS
2	B	178	LEU
2	B	183	VAL
2	B	204	ASP
2	B	213	SER
2	B	252	THR
2	B	258	VAL
2	B	317	GLU
2	B	318	GLU
2	B	326	LEU
2	B	327	THR
2	B	332	GLN
2	B	347	MET
2	B	356	ASP
2	B	366	VAL
2	B	368	SER
2	B	371	VAL
2	B	373	LEU
2	B	378	THR
2	B	429	SER
2	B	477	ARG

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	284	GLN
1	A	382	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	4,5,10	1.68	1 (25%)	3,5,11	3.80	3 (100%)
1	CME	A	320	1	4,5,10	1.41	0	3,5,11	1.78	1 (33%)
2	CME	B	194	2	4,5,10	1.50	1 (25%)	3,5,11	1.50	1 (33%)
2	CME	B	432	2	4,5,10	2.08	1 (25%)	3,5,11	2.46	2 (66%)

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	-	0/1/4/10	0/0/0/0
1	CME	A	320	1	-	0/1/4/10	0/0/0/0
2	CME	B	194	2	-	0/1/4/10	0/0/0/0
2	CME	B	432	2	-	0/1/4/10	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	CME	CB-SG	-2.58	1.75	1.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	CME	CB-CA	-2.20	1.50	1.53
2	B	432	CME	CB-CA	3.70	1.57	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	CME	CA-CB-SG	-5.07	102.86	114.48
1	A	194	CME	O-C-CA	-3.41	116.59	125.49
2	B	194	CME	O-C-CA	-2.53	118.89	125.49
2	B	432	CME	O-C-CA	-2.44	119.14	125.49
1	A	320	CME	CA-CB-SG	-2.12	109.63	114.48
1	A	194	CME	CB-CA-C	2.44	117.44	111.47
2	B	432	CME	CA-CB-SG	2.94	121.21	114.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	432	CME	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	ROL	A	101	-	21,22,22	1.30	3 (14%)	27,30,30	2.42	10 (37%)
5	ROL	B	102	-	21,22,22	1.17	2 (9%)	27,30,30	2.30	5 (18%)

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	ROL	A	101	-	-	0/10/26/26	0/3/3/3
5	ROL	B	102	-	-	0/10/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	102	ROL	C5-C3	2.55	1.56	1.52
5	A	101	ROL	O2-C8	2.61	1.41	1.37
5	A	101	ROL	O3-C7	2.63	1.42	1.37
5	A	101	ROL	C5-C3	2.82	1.57	1.52
5	B	102	ROL	O3-C7	2.93	1.42	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	102	ROL	C4-C3-C5	-6.30	104.60	115.88
5	B	102	ROL	O3-C11-C12	-5.04	91.97	109.14
5	A	101	ROL	O3-C11-C12	-4.89	92.48	109.14
5	A	101	ROL	C2-C3-C5	-4.62	104.70	114.95
5	B	102	ROL	O1-C1-C2	-3.82	121.06	126.43
5	A	101	ROL	C10-C5-C3	-3.12	114.42	121.13
5	A	101	ROL	O1-C1-C2	-3.01	122.20	126.43
5	A	101	ROL	O2-C8-C9	-3.00	119.30	124.35
5	B	102	ROL	C4-N1-C1	-2.42	112.06	114.35
5	A	101	ROL	C14-C13-C12	-2.25	98.96	106.09
5	A	101	ROL	C2-C1-N1	2.25	110.97	108.67
5	A	101	ROL	C16-O2-C8	3.61	123.02	117.54
5	A	101	ROL	O2-C8-C7	4.59	121.95	115.40
5	A	101	ROL	C6-C5-C3	5.12	128.41	120.89
5	B	102	ROL	C16-O2-C8	6.37	127.20	117.54

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	B	102	ROL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	321/398 (80%)	0.20	7 (2%) 65 64	14, 23, 29, 42	0
2	B	321/398 (80%)	0.22	8 (2%) 61 60	15, 23, 29, 33	0
All	All	642/796 (80%)	0.21	15 (2%) 64 63	14, 23, 29, 42	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	GLU	4.2
1	A	319	HIS	3.9
2	B	319	HIS	3.2
2	B	430	PRO	3.2
1	A	369	SER	2.6
2	B	320	CYS	2.5
2	B	425	GLY	2.5
2	B	375	ASP	2.2
2	B	190	ARG	2.1
2	B	295	LEU	2.1
1	A	325	ASN	2.1
2	B	485	PRO	2.1
1	A	353	LEU	2.0
1	A	375	ASP	2.0
1	A	216	PHE	2.0

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	CME	A	194	6/11	0.94	0.14	-	31,32,35,44	0
1	CME	A	320	6/11	0.86	0.13	-	44,46,46,55	0
2	CME	B	432	6/11	0.88	0.11	-	33,36,38,48	0
2	CME	B	194	6/11	0.95	0.11	-	30,32,34,44	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	1001	1/1	0.99	0.16	0.94	39,39,39,39	0
4	MG	A	1002	1/1	0.97	0.16	0.62	30,30,30,30	0
5	ROL	A	101	20/20	0.92	0.16	0.32	40,44,46,53	0
5	ROL	B	102	20/20	0.95	0.16	0.19	38,43,48,49	0
3	ZN	B	1001	1/1	0.99	0.13	-1.76	41,41,41,41	0
4	MG	B	1002	1/1	0.92	0.13	-1.81	26,26,26,26	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.