



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2017 – 02:42 PM EDT

PDB ID : 4X0F  
Title : Crystal structure of crosslink stabilized long-form PDE4B in complex with (R)-(-)-rolipram  
Authors : Cedervall, P.; Pandit, J.  
Deposited on : 2014-11-21  
Resolution : 3.22 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
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) : rb-20029077

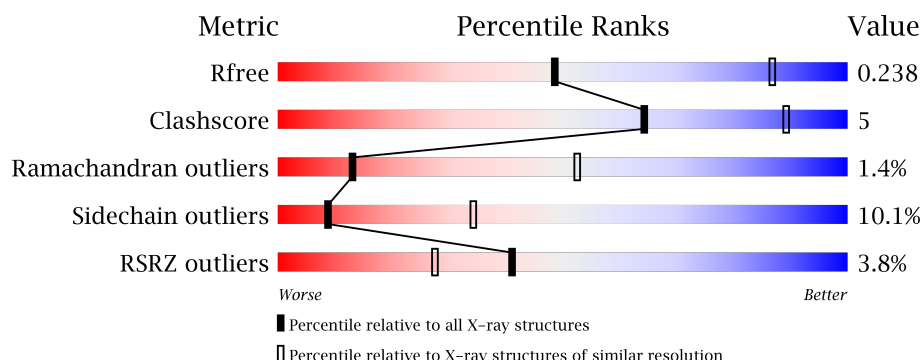
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.22 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	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (3.24-3.20)

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	655	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>11%</div> <div>•</div> <div>37%</div> </div> </div>
1	B	655	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>11%</div> <div>•</div> <div>37%</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	ROL	A	804	-	-	-	X
4	ROL	B	803	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6716 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	411	Total	C	N	O	S	0	0	0
			3319	2091	567	641	20			
1	B	414	Total	C	N	O	S	0	0	0
			3350	2111	568	650	21			

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	MET	-	initiating methionine	UNP Q07343
A	83	ALA	-	expression tag	UNP Q07343
A	84	GLY	-	expression tag	UNP Q07343
A	85	LEU	-	expression tag	UNP Q07343
A	86	ASN	-	expression tag	UNP Q07343
A	87	ASP	-	expression tag	UNP Q07343
A	88	ILE	-	expression tag	UNP Q07343
A	89	PHE	-	expression tag	UNP Q07343
A	90	GLU	-	expression tag	UNP Q07343
A	91	ALA	-	expression tag	UNP Q07343
A	92	GLN	-	expression tag	UNP Q07343
A	93	LYS	-	expression tag	UNP Q07343
A	94	ILE	-	expression tag	UNP Q07343
A	95	GLU	-	expression tag	UNP Q07343
A	96	TRP	-	expression tag	UNP Q07343
A	97	HIS	-	expression tag	UNP Q07343
A	98	GLU	-	expression tag	UNP Q07343
A	99	ASN	-	expression tag	UNP Q07343
A	100	LEU	-	expression tag	UNP Q07343
A	101	TYR	-	expression tag	UNP Q07343
A	102	PHE	-	expression tag	UNP Q07343
A	103	GLN	-	expression tag	UNP Q07343
A	104	GLY	-	expression tag	UNP Q07343
A	105	SER	-	expression tag	UNP Q07343
A	106	ASP	-	expression tag	UNP Q07343

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	TYR	-	expression tag	UNP Q07343
A	108	LYS	-	expression tag	UNP Q07343
A	109	ASP	-	expression tag	UNP Q07343
A	110	ASP	-	expression tag	UNP Q07343
A	111	ASP	-	expression tag	UNP Q07343
A	112	ASP	-	expression tag	UNP Q07343
A	113	LYS	-	expression tag	UNP Q07343
A	114	ASP	-	expression tag	UNP Q07343
A	115	LEU	-	expression tag	UNP Q07343
A	116	VAL	-	expression tag	UNP Q07343
A	117	PRO	-	expression tag	UNP Q07343
A	118	ARG	-	expression tag	UNP Q07343
A	119	GLY	-	expression tag	UNP Q07343
A	120	SER	-	expression tag	UNP Q07343
A	121	MET	-	expression tag	UNP Q07343
A	133	ALA	SER	engineered mutation	UNP Q07343
A	229	ALA	CYS	engineered mutation	UNP Q07343
A	267	CYS	SER	engineered mutation	UNP Q07343
A	366	ALA	CYS	engineered mutation	UNP Q07343
A	492	ALA	CYS	engineered mutation	UNP Q07343
A	562	ALA	CYS	engineered mutation	UNP Q07343
A	604	ALA	CYS	engineered mutation	UNP Q07343
A	610	CYS	SER	engineered mutation	UNP Q07343
A	654	ALA	SER	engineered mutation	UNP Q07343
A	659	ALA	SER	engineered mutation	UNP Q07343
A	661	ALA	SER	engineered mutation	UNP Q07343
A	671	ALA	CYS	engineered mutation	UNP Q07343
A	709	ALA	CYS	engineered mutation	UNP Q07343
B	82	MET	-	initiating methionine	UNP Q07343
B	83	ALA	-	expression tag	UNP Q07343
B	84	GLY	-	expression tag	UNP Q07343
B	85	LEU	-	expression tag	UNP Q07343
B	86	ASN	-	expression tag	UNP Q07343
B	87	ASP	-	expression tag	UNP Q07343
B	88	ILE	-	expression tag	UNP Q07343
B	89	PHE	-	expression tag	UNP Q07343
B	90	GLU	-	expression tag	UNP Q07343
B	91	ALA	-	expression tag	UNP Q07343
B	92	GLN	-	expression tag	UNP Q07343
B	93	LYS	-	expression tag	UNP Q07343
B	94	ILE	-	expression tag	UNP Q07343
B	95	GLU	-	expression tag	UNP Q07343

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	96	TRP	-	expression tag	UNP Q07343
B	97	HIS	-	expression tag	UNP Q07343
B	98	GLU	-	expression tag	UNP Q07343
B	99	ASN	-	expression tag	UNP Q07343
B	100	LEU	-	expression tag	UNP Q07343
B	101	TYR	-	expression tag	UNP Q07343
B	102	PHE	-	expression tag	UNP Q07343
B	103	GLN	-	expression tag	UNP Q07343
B	104	GLY	-	expression tag	UNP Q07343
B	105	SER	-	expression tag	UNP Q07343
B	106	ASP	-	expression tag	UNP Q07343
B	107	TYR	-	expression tag	UNP Q07343
B	108	LYS	-	expression tag	UNP Q07343
B	109	ASP	-	expression tag	UNP Q07343
B	110	ASP	-	expression tag	UNP Q07343
B	111	ASP	-	expression tag	UNP Q07343
B	112	ASP	-	expression tag	UNP Q07343
B	113	LYS	-	expression tag	UNP Q07343
B	114	ASP	-	expression tag	UNP Q07343
B	115	LEU	-	expression tag	UNP Q07343
B	116	VAL	-	expression tag	UNP Q07343
B	117	PRO	-	expression tag	UNP Q07343
B	118	ARG	-	expression tag	UNP Q07343
B	119	GLY	-	expression tag	UNP Q07343
B	120	SER	-	expression tag	UNP Q07343
B	121	MET	-	expression tag	UNP Q07343
B	133	ALA	SER	engineered mutation	UNP Q07343
B	229	ALA	CYS	engineered mutation	UNP Q07343
B	267	CYS	SER	engineered mutation	UNP Q07343
B	366	ALA	CYS	engineered mutation	UNP Q07343
B	492	ALA	CYS	engineered mutation	UNP Q07343
B	562	ALA	CYS	engineered mutation	UNP Q07343
B	604	ALA	CYS	engineered mutation	UNP Q07343
B	610	CYS	SER	engineered mutation	UNP Q07343
B	654	ALA	SER	engineered mutation	UNP Q07343
B	659	ALA	SER	engineered mutation	UNP Q07343
B	661	ALA	SER	engineered mutation	UNP Q07343
B	671	ALA	CYS	engineered mutation	UNP Q07343
B	709	ALA	CYS	engineered mutation	UNP Q07343

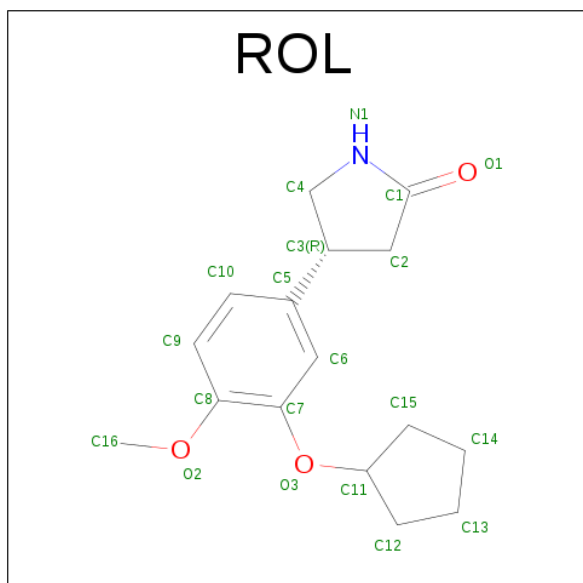
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

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

- Molecule 4 is ROLIPRAM (three-letter code: ROL) (formula: C<sub>16</sub>H<sub>21</sub>NO<sub>3</sub>).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

*Continued on next page...*

*Continued from previous page...*

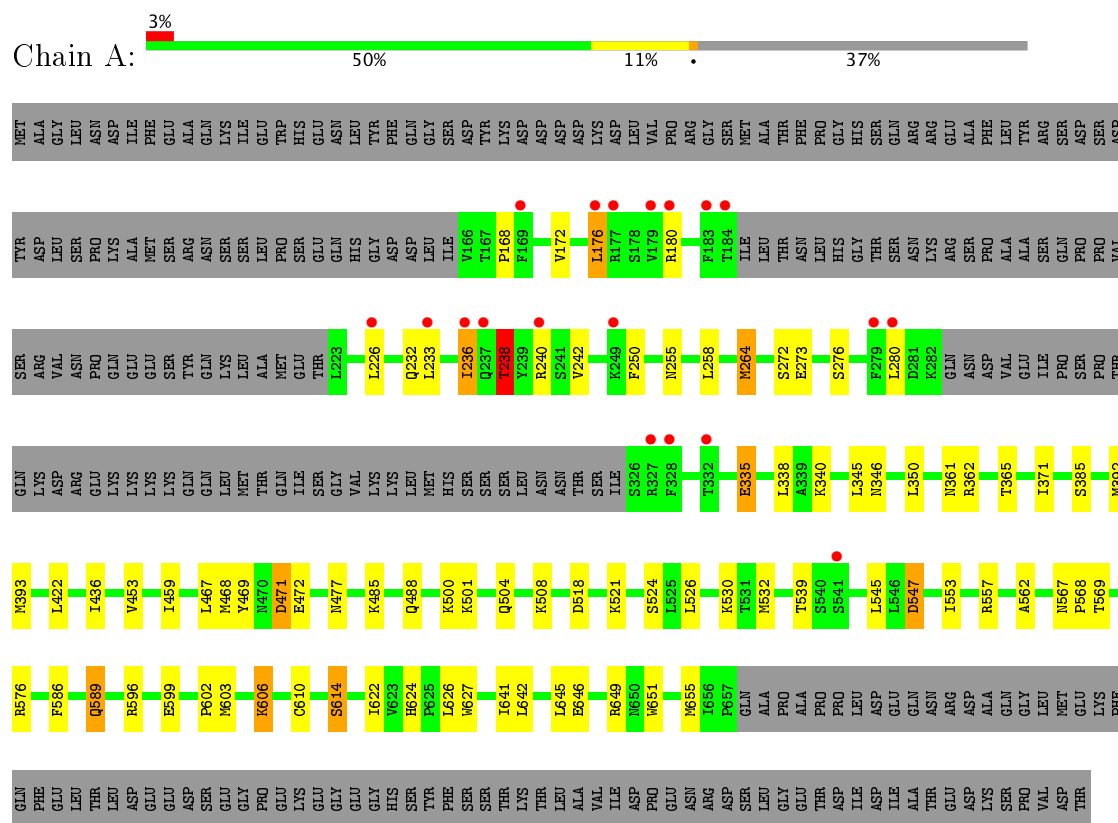
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		



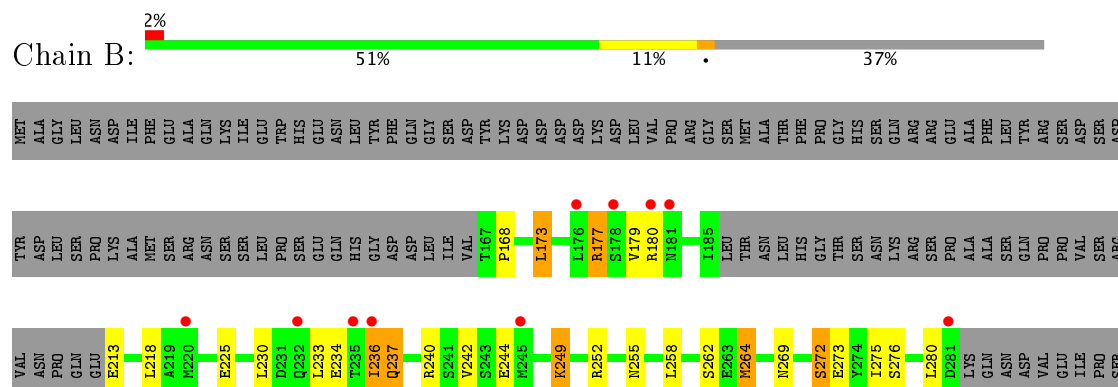
### 3 Residue-property plots

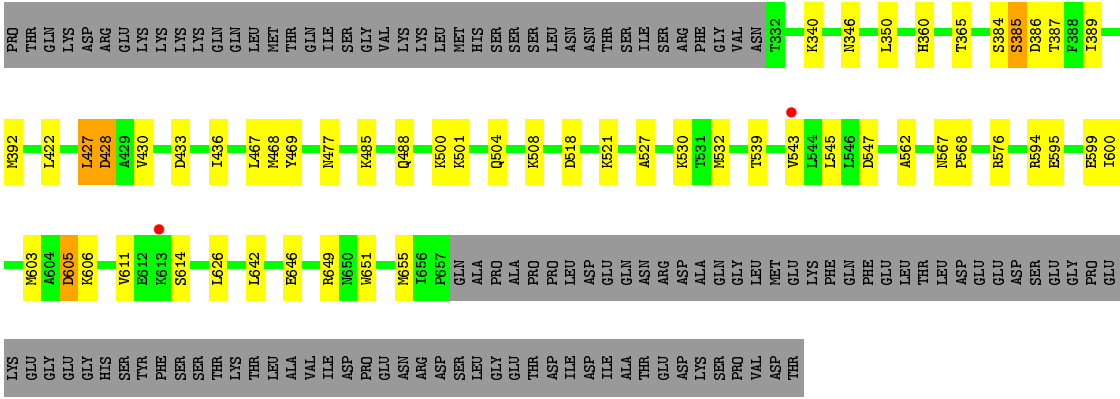
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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-specific 3',5'-cyclic phosphodiesterase 4B



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.40Å 137.40Å 142.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.00 – 3.22 118.99 – 3.22	Depositor EDS
% Data completeness (in resolution range)	91.8 (119.00-3.22) 91.8 (118.99-3.22)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.179 , 0.222 0.193 , 0.238	Depositor DCC
$R_{free}$ test set	1219 reflections (5.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.3	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 71.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 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: ZN, IOD, ROL, MG

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	0.53	0/3383	0.70	0/4584
1	B	0.49	0/3414	0.66	0/4625
All	All	0.51	0/6797	0.68	0/9209

There are no bond length outliers.

There are no bond angle outliers.

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	3319	0	3230	41	0
1	B	3350	0	3264	35	0
2	A	2	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	20	0	21	1	0
4	B	20	0	21	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	6716	0	6536	63	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 5.

All (63) 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:610:CYS:O	1:A:614:SER:HB2	1.87	0.74
1:B:594:ARG:HG3	1:B:600:ILE:HD11	1.73	0.69
1:A:485:LYS:HB2	1:B:467:LEU:HD21	1.79	0.64
1:B:262:SER:HB2	1:B:269:ASN:HD22	1.64	0.63
1:A:258:LEU:HD22	1:A:272:SER:HA	1.81	0.62
1:B:567:ASN:HD22	4:B:803:ROL:H91	1.67	0.60
1:A:467:LEU:HD21	1:B:485:LYS:HB2	1.83	0.60
1:A:518:ASP:HB3	1:A:521:LYS:HG2	1.84	0.60
1:B:173:LEU:HD11	1:B:234:GLU:HG2	1.84	0.58
1:A:606:LYS:HD2	1:A:606:LYS:H	1.68	0.57
1:B:518:ASP:HB3	1:B:521:LYS:HG2	1.86	0.57
1:A:586:PHE:CD2	1:A:603:MET:HB2	2.39	0.57
1:A:236:ILE:HG12	1:B:168:PRO:CB	2.35	0.56
1:A:362:ARG:HH12	1:A:393:MET:HA	1.70	0.56
1:A:459:ILE:HG12	1:A:471:ASP:HB3	1.89	0.55
1:B:385:SER:O	1:B:389:ILE:HD12	2.07	0.54
1:B:600:ILE:HG21	1:B:605:ASP:HB2	1.88	0.54
1:A:453:VAL:HG12	1:A:589:GLN:HG2	1.89	0.53
1:A:238:THR:HG21	1:B:244:GLU:OE2	2.09	0.53
1:A:236:ILE:HD11	1:B:249:LYS:HG2	1.91	0.51
1:A:500:LYS:HG2	1:A:504:GLN:HE21	1.74	0.51
1:A:606:LYS:CD	1:A:606:LYS:H	2.24	0.50
1:A:236:ILE:HG12	1:B:168:PRO:HB3	1.93	0.50
1:B:500:LYS:HG2	1:B:504:GLN:HE21	1.77	0.49
1:A:524:SER:HB3	1:B:240:ARG:HH12	1.77	0.49
1:A:569:THR:HB	1:A:641:ILE:HG23	1.95	0.49
1:B:562:ALA:HA	1:B:626:LEU:HD21	1.95	0.48
1:A:651:TRP:O	1:A:655:MET:HG2	2.14	0.48
1:B:469:TYR:CE1	1:B:477:ASN:HB3	2.48	0.48
1:B:365:THR:HG23	1:B:392:MET:HB3	1.96	0.48
1:A:624:HIS:HA	1:A:645:LEU:HD21	1.95	0.47
1:A:469:TYR:CE1	1:A:477:ASN:HB3	2.49	0.47
1:A:562:ALA:HA	1:A:626:LEU:HD21	1.95	0.47
1:B:258:LEU:HD22	1:B:272:SER:HA	1.97	0.47
1:A:627:TRP:CE3	1:A:641:ILE:HG21	2.49	0.47
1:B:651:TRP:O	1:B:655:MET:HG2	2.15	0.47
1:A:567:ASN:HD22	4:A:804:ROL:H91	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:PHE:CE2	1:A:603:MET:HB2	2.50	0.46
1:A:365:THR:HG23	1:A:392:MET:HB3	1.97	0.46
1:B:428:ASP:H	1:B:543:VAL:HG13	1.80	0.46
1:A:250:PHE:HE2	1:B:527:ALA:HA	1.81	0.45
1:A:226:LEU:HD13	1:B:179:VAL:HG11	1.99	0.45
1:B:576:ARG:HD3	1:B:651:TRP:CH2	2.52	0.45
1:B:427:LEU:HA	1:B:430:VAL:HG21	1.98	0.45
1:A:576:ARG:HD3	1:A:651:TRP:CH2	2.52	0.45
1:A:172:VAL:HG12	1:A:176:LEU:HD12	1.99	0.44
1:A:168:PRO:HG3	1:B:236:ILE:HG12	1.98	0.44
1:A:422:LEU:HD13	1:A:436:ILE:HG23	1.99	0.44
1:B:422:LEU:HD13	1:B:436:ILE:HG23	2.00	0.43
1:A:485:LYS:O	1:A:488:GLN:HB2	2.19	0.43
1:B:173:LEU:O	1:B:177:ARG:HB2	2.20	0.42
1:A:553:ILE:O	1:A:557:ARG:HG2	2.19	0.42
1:B:485:LYS:O	1:B:488:GLN:HB2	2.19	0.42
1:A:622:ILE:HD11	1:B:275:ILE:HG23	2.02	0.42
1:B:433:ASP:HA	1:B:436:ILE:HD12	2.02	0.41
1:A:168:PRO:HB2	1:B:236:ILE:HG21	2.02	0.41
1:A:345:LEU:HD11	1:A:371:ILE:HG13	2.02	0.41
1:A:642:LEU:HA	1:A:642:LEU:HD12	1.93	0.40
1:B:237:GLN:HG3	1:B:242:VAL:HG22	2.03	0.40
1:A:335:GLU:O	1:A:338:LEU:HB3	2.22	0.40
1:B:567:ASN:HB2	1:B:568:PRO:HD3	2.03	0.40
1:A:567:ASN:HB2	1:A:568:PRO:HD3	2.03	0.40
1:A:233:LEU:HD21	1:B:233:LEU:HD21	2.03	0.40

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	405/655 (62%)	381 (94%)	18 (4%)	6 (2%)	12	51
1	B	408/655 (62%)	389 (95%)	14 (3%)	5 (1%)	15	56
All	All	813/1310 (62%)	770 (95%)	32 (4%)	11 (1%)	13	52

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	MET
1	A	335	GLU
1	A	547	ASP
1	B	264	MET
1	B	547	ASP
1	B	611	VAL
1	A	238	THR
1	A	471	ASP
1	A	602	PRO
1	B	428	ASP
1	B	603	MET

### 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	369/589 (63%)	335 (91%)	34 (9%)	11	39
1	B	373/589 (63%)	332 (89%)	41 (11%)	7	31
All	All	742/1178 (63%)	667 (90%)	75 (10%)	9	34

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LEU
1	A	180	ARG
1	A	232	GLN
1	A	236	ILE
1	A	238	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	240	ARG
1	A	242	VAL
1	A	255	ASN
1	A	264	MET
1	A	273	GLU
1	A	276	SER
1	A	280	LEU
1	A	340	LYS
1	A	346	ASN
1	A	350	LEU
1	A	361	ASN
1	A	385	SER
1	A	468	MET
1	A	472	GLU
1	A	501	LYS
1	A	508	LYS
1	A	526	LEU
1	A	530	LYS
1	A	532	MET
1	A	539	THR
1	A	545	LEU
1	A	547	ASP
1	A	589	GLN
1	A	596	ARG
1	A	599	GLU
1	A	606	LYS
1	A	614	SER
1	A	646	GLU
1	A	649	ARG
1	B	173	LEU
1	B	177	ARG
1	B	180	ARG
1	B	213	GLU
1	B	218	LEU
1	B	225	GLU
1	B	230	LEU
1	B	236	ILE
1	B	237	GLN
1	B	249	LYS
1	B	252	ARG
1	B	255	ASN
1	B	264	MET

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	272	SER
1	B	273	GLU
1	B	276	SER
1	B	280	LEU
1	B	340	LYS
1	B	346	ASN
1	B	350	LEU
1	B	360	HIS
1	B	384	SER
1	B	385	SER
1	B	386	ASP
1	B	387	THR
1	B	427	LEU
1	B	468	MET
1	B	501	LYS
1	B	508	LYS
1	B	530	LYS
1	B	532	MET
1	B	539	THR
1	B	545	LEU
1	B	595	GLU
1	B	599	GLU
1	B	605	ASP
1	B	606	LYS
1	B	614	SER
1	B	642	LEU
1	B	646	GLU
1	B	649	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	GLN
1	A	269	ASN
1	A	456	GLN
1	A	567	ASN
1	A	615	GLN
1	B	269	ASN
1	B	270	GLN
1	B	456	GLN
1	B	567	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 7 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	ROL	A	804	-	21,22,22	0.27	0	26,30,30	0.62	0
4	ROL	B	803	-	21,22,22	0.24	0	26,30,30	0.80	1 (3%)

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	ROL	A	804	-	-	0/10/26/26	0/3/3/3
4	ROL	B	803	-	-	0/10/26/26	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	B	803	ROL	C4-C3-C5	-3.15	108.04	114.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	ROL	1	0
4	B	803	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	411/655 (62%)	0.49	19 (4%) 33 21	23, 50, 138, 183	0
1	B	414/655 (63%)	0.46	12 (2%) 52 38	28, 78, 147, 177	0
All	All	825/1310 (62%)	0.48	31 (3%) 41 27	23, 64, 145, 183	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	GLN	4.6
1	A	177	ARG	3.8
1	B	235	THR	3.6
1	A	233	LEU	3.5
1	B	178	SER	3.4
1	B	236	ILE	3.4
1	B	543	VAL	3.2
1	A	328	PHE	3.1
1	A	176	LEU	3.0
1	B	281	ASP	3.0
1	A	327	ARG	3.0
1	B	180	ARG	3.0
1	A	237	GLN	2.8
1	A	183	PHE	2.7
1	A	226	LEU	2.7
1	A	249	LYS	2.7
1	A	236	ILE	2.7
1	A	169	PHE	2.6
1	A	184	THR	2.6
1	B	181	ASN	2.5
1	A	179	VAL	2.5
1	A	240	ARG	2.5
1	A	332	THR	2.4
1	B	220	MET	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	541	SER	2.4
1	B	245	MET	2.2
1	B	176	LEU	2.2
1	A	280	LEU	2.2
1	A	279	PHE	2.1
1	B	613	LYS	2.1
1	A	180	ARG	2.0

## 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 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(Å <sup>2</sup> )	Q<0.9
4	ROL	A	804	20/20	0.98	0.39	2.52	39,40,51,51	0
4	ROL	B	803	20/20	0.93	0.44	1.78	60,76,82,82	0
2	ZN	A	801	1/1	0.98	0.26	1.48	47,47,47,47	0
2	ZN	A	802	1/1	0.99	0.22	-0.18	48,48,48,48	0
5	MG	B	804	1/1	0.62	0.23	-0.51	39,39,39,39	0
2	ZN	B	801	1/1	0.99	0.22	-0.54	50,50,50,50	0
5	MG	A	805	1/1	0.80	0.14	-4.28	34,34,34,34	0
3	IOD	B	802	1/1	0.98	0.17	-	80,80,80,80	0
3	IOD	A	803	1/1	0.99	0.18	-	91,91,91,91	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.