



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:11 PM GMT

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 wwPDB X-ray Structure 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/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

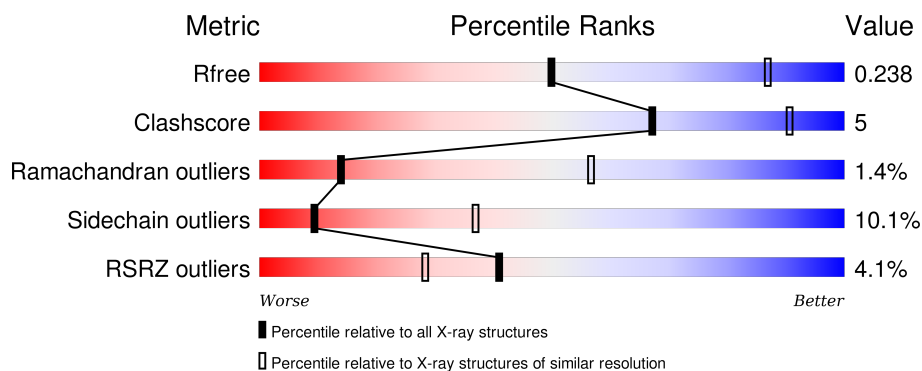
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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	655	 3% 50% 11% 37%
1	B	655	 2% 51% 11% 37%

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

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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

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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

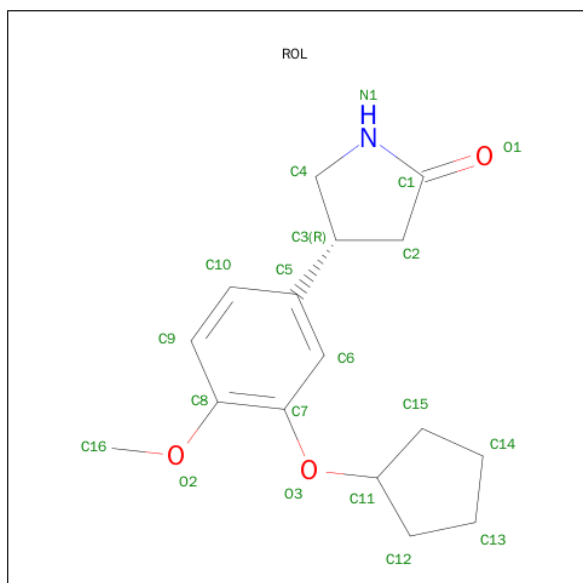
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is ROLIPRAM (three-letter code: ROL) (formula: C₁₆H₂₁NO₃).



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

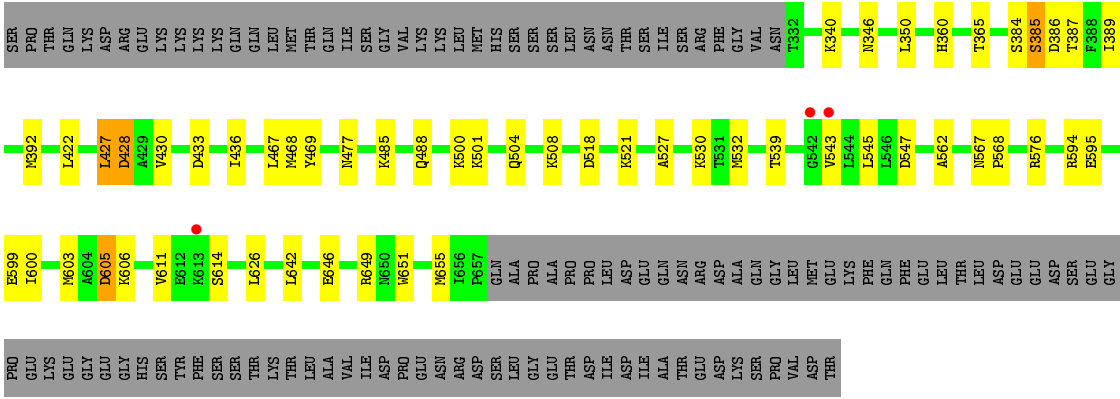
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	67.3	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 71.2	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 23620 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6716	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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 [i](#)

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.

The worst 5 of 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

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	405/655 (62%)	381 (94%)	18 (4%)	6 (2%)	13	55
1	B	408/655 (62%)	389 (95%)	14 (3%)	5 (1%)	16	60
All	All	813/1310 (62%)	770 (95%)	32 (4%)	11 (1%)	14	57

5 of 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

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	41
1	B	373/589 (63%)	332 (89%)	41 (11%)	8	33
All	All	742/1178 (63%)	667 (90%)	75 (10%)	9	37

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	649	ARG
1	B	236	ILE
1	B	605	ASP
1	B	173	LEU
1	B	218	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	615	GLN
1	B	567	ASN
1	B	270	GLN
1	A	456	GLN
1	B	269	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	27,30,30	0.71	1 (3%)
4	ROL	B	803	-	21,22,22	0.23	0	27,30,30	0.97	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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	ROL	C4-C3-C5	-4.38	108.04	115.88
4	A	804	ROL	C4-C3-C5	-2.59	111.24	115.88

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	411/655 (62%)	0.53	19 (4%)	36 24	23, 50, 138, 183	0
1	B	414/655 (63%)	0.50	15 (3%)	46 33	28, 78, 147, 177	0
All	All	825/1310 (62%)	0.51	34 (4%)	41 28	23, 64, 145, 183	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	GLN	4.8
1	A	177	ARG	3.9
1	B	235	THR	3.7
1	A	233	LEU	3.6
1	B	178	SER	3.5

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, 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	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.