



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:15 am BST

PDB ID : 4RWT  
Title : Structure of actin-Lmod complex  
Authors : Chen, X.; Ni, F.; Wang, Q.  
Deposited on : 2014-12-05  
Resolution : 2.98 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

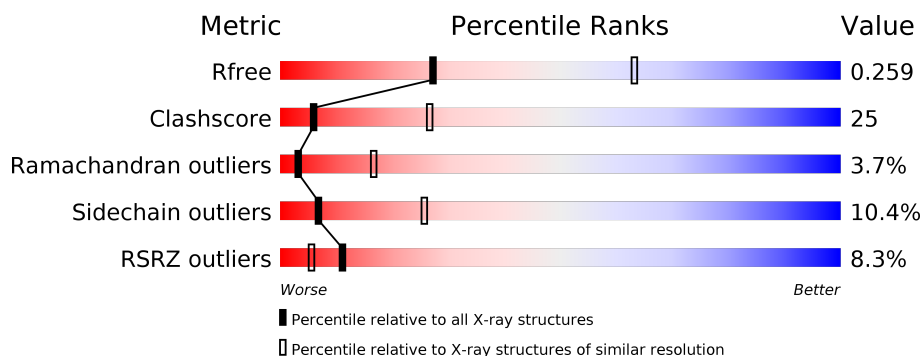
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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))
$R_{free}$	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 respectively. 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	384	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>33%</div> <div>.</div> <div>.</div> </div> </div>
1	B	384	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>33%</div> <div>.</div> <div>.</div> </div> </div>
2	C	506	<div> <div>2%</div> <div> <div>16%</div> <div>12%</div> <div>.</div> <div>67%</div> </div> </div>
2	D	506	<div> <div>13%</div> <div> <div>24%</div> <div>25%</div> <div>7%</div> <div>45%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9317 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 Actin-5C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2873	1817	485	550	21			
1	B	369	Total	C	N	O	S	0	0	0
			2871	1815	485	550	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	GLU	LYS	ENGINEERED MUTATION	UNP P10987
A	322	LYS	PRO	ENGINEERED MUTATION	UNP P10987
A	376	ALA	-	EXPRESSION TAG	UNP P10987
A	377	SER	-	EXPRESSION TAG	UNP P10987
A	378	HIS	-	EXPRESSION TAG	UNP P10987
A	379	HIS	-	EXPRESSION TAG	UNP P10987
A	380	HIS	-	EXPRESSION TAG	UNP P10987
A	381	HIS	-	EXPRESSION TAG	UNP P10987
A	382	HIS	-	EXPRESSION TAG	UNP P10987
A	383	HIS	-	EXPRESSION TAG	UNP P10987
B	291	GLU	LYS	ENGINEERED MUTATION	UNP P10987
B	322	LYS	PRO	ENGINEERED MUTATION	UNP P10987
B	376	ALA	-	EXPRESSION TAG	UNP P10987
B	377	SER	-	EXPRESSION TAG	UNP P10987
B	378	HIS	-	EXPRESSION TAG	UNP P10987
B	379	HIS	-	EXPRESSION TAG	UNP P10987
B	380	HIS	-	EXPRESSION TAG	UNP P10987
B	381	HIS	-	EXPRESSION TAG	UNP P10987
B	382	HIS	-	EXPRESSION TAG	UNP P10987
B	383	HIS	-	EXPRESSION TAG	UNP P10987

- Molecule 2 is a protein called Leiomodin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	168	Total 1338	C 829	N 242	O 259	S 8	0	0	0
2	D	280	Total 2171	C 1340	N 398	O 423	S 10	0	0	0

There are 142 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	EXPRESSION TAG	UNP Q6P5Q4
C	-9	ALA	-	EXPRESSION TAG	UNP Q6P5Q4
C	-8	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-7	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-6	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-5	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-4	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-3	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
C	-2	VAL	-	EXPRESSION TAG	UNP Q6P5Q4
C	-1	GLY	-	EXPRESSION TAG	UNP Q6P5Q4
C	0	THR	-	EXPRESSION TAG	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	LEU	DELETION	UNP Q6P5Q4
C	?	-	ILE	DELETION	UNP Q6P5Q4
C	?	-	PHE	DELETION	UNP Q6P5Q4
C	?	-	THR	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	ASN	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	VAL	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	VAL	DELETION	UNP Q6P5Q4
C	?	-	TYR	DELETION	UNP Q6P5Q4
C	?	-	THR	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	GLN	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	GLU	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	SER	DELETION	UNP Q6P5Q4
C	?	-	GLN	DELETION	UNP Q6P5Q4
C	?	-	ARG	DELETION	UNP Q6P5Q4
C	?	-	LEU	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	?	-	PRO	DELETION	UNP Q6P5Q4
C	426	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	427	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	428	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	429	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	431	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	432	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	434	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
C	435	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	-10	MET	-	EXPRESSION TAG	UNP Q6P5Q4
D	-9	ALA	-	EXPRESSION TAG	UNP Q6P5Q4
D	-8	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
D	-7	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
D	-6	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
D	-5	HIS	-	EXPRESSION TAG	UNP Q6P5Q4



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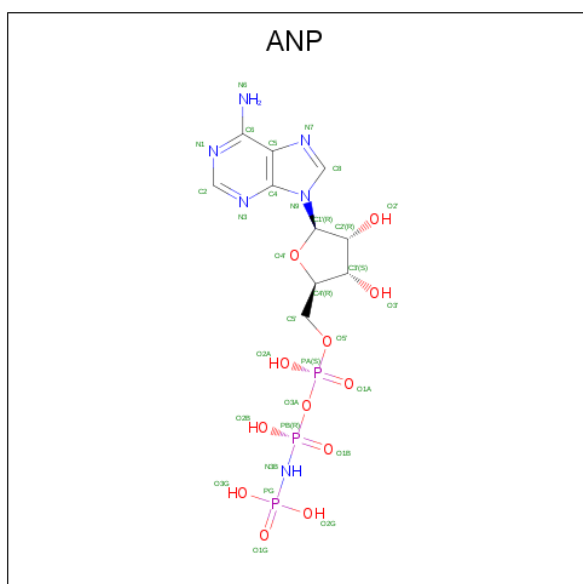
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
D	-3	HIS	-	EXPRESSION TAG	UNP Q6P5Q4
D	-2	VAL	-	EXPRESSION TAG	UNP Q6P5Q4
D	-1	GLY	-	EXPRESSION TAG	UNP Q6P5Q4
D	0	THR	-	EXPRESSION TAG	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	LEU	DELETION	UNP Q6P5Q4
D	?	-	ILE	DELETION	UNP Q6P5Q4
D	?	-	PHE	DELETION	UNP Q6P5Q4
D	?	-	THR	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	ASN	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	VAL	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	VAL	DELETION	UNP Q6P5Q4
D	?	-	TYR	DELETION	UNP Q6P5Q4
D	?	-	THR	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	GLN	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	GLU	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	SER	DELETION	UNP Q6P5Q4
D	?	-	GLN	DELETION	UNP Q6P5Q4
D	?	-	ARG	DELETION	UNP Q6P5Q4
D	?	-	LEU	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	?	-	PRO	DELETION	UNP Q6P5Q4
D	426	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	427	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	428	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	429	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	431	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	432	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	434	GLY	LYS	ENGINEERED MUTATION	UNP Q6P5Q4
D	435	SER	LYS	ENGINEERED MUTATION	UNP Q6P5Q4

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



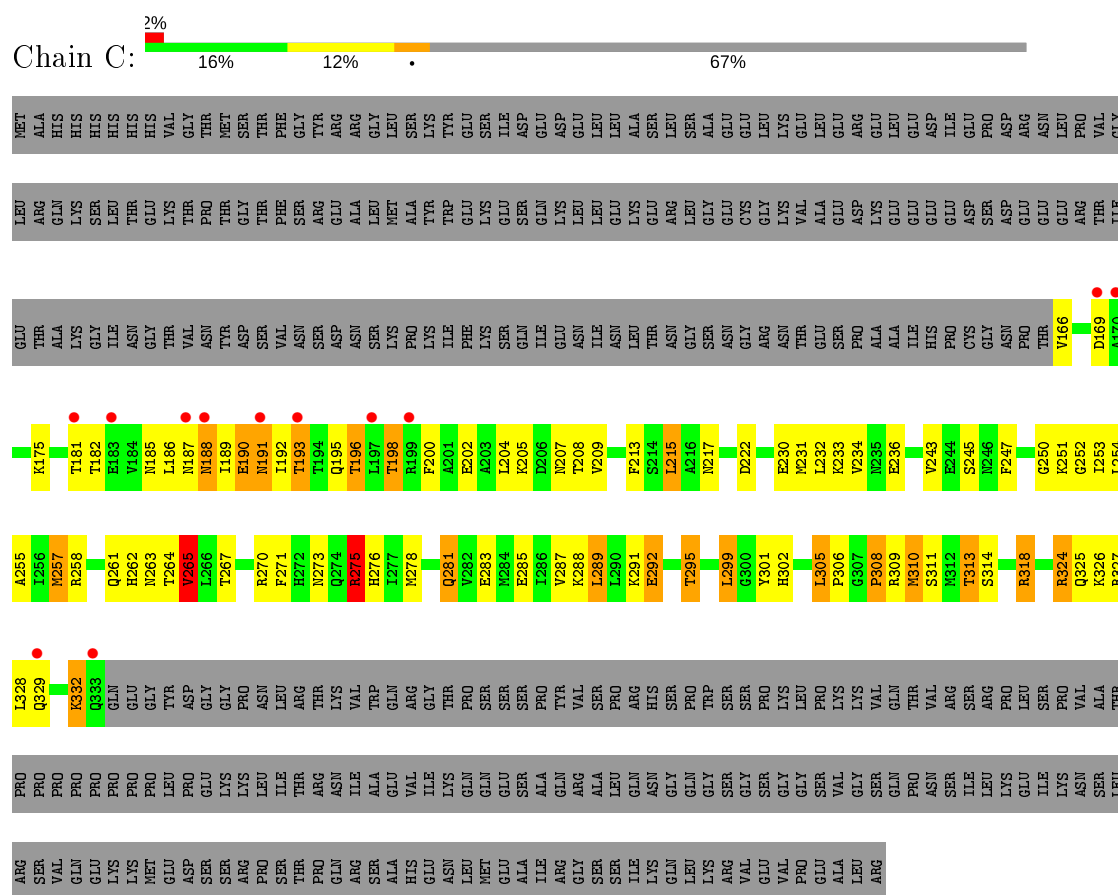
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

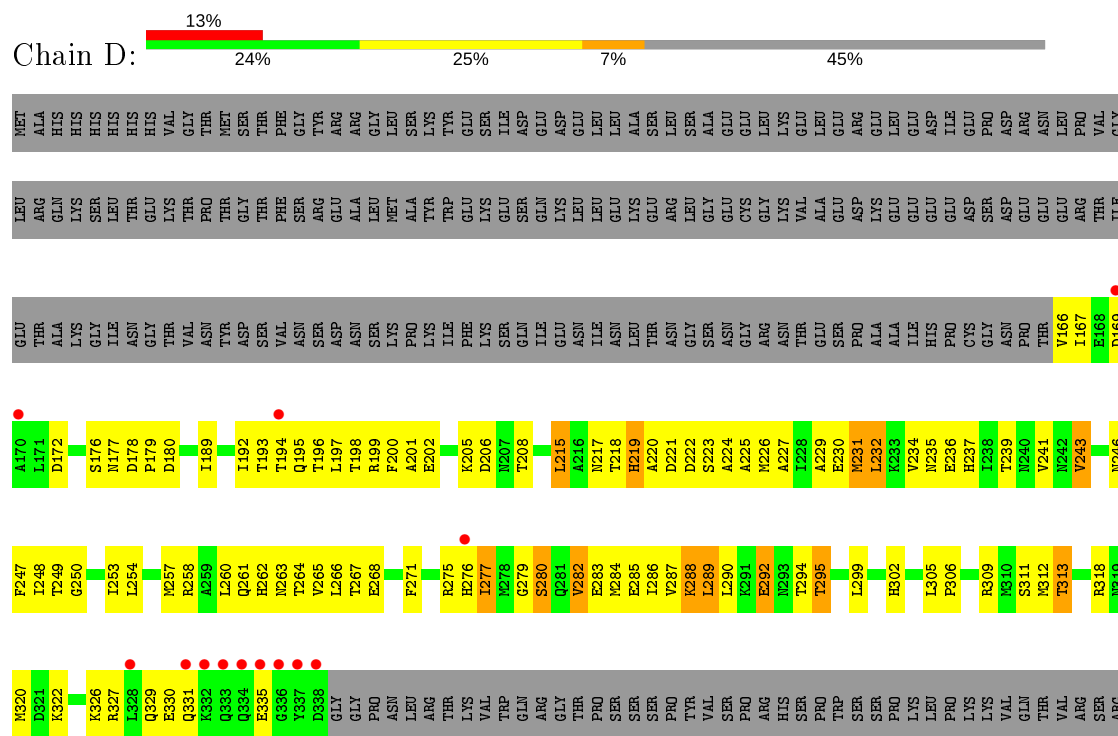
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

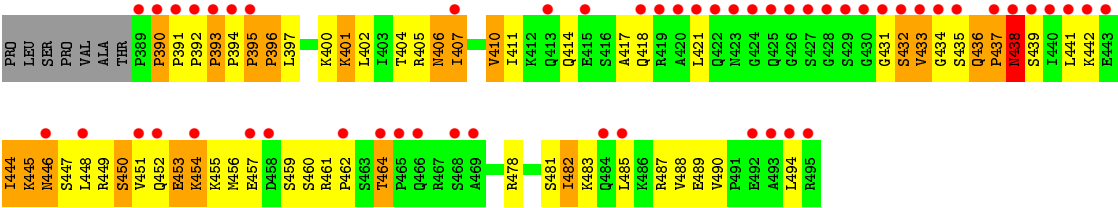






- Molecule 2: Leiomodlin-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.35Å 65.65Å 81.92Å 101.29° 90.94° 107.97°	Depositor
Resolution (Å)	51.07 – 2.98 47.15 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.5 (51.07-2.98) 97.5 (47.15-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.248 , 0.257 0.249 , 0.259	Depositor DCC
$R_{free}$ test set	1288 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	9317	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.29% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP

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	0.47	0/2934	0.63	1/3973 (0.0%)
1	B	0.49	0/2932	0.63	0/3970
2	C	0.46	1/1352 (0.1%)	0.57	0/1823
2	D	0.61	0/2199	0.64	0/2966
All	All	0.51	1/9417 (0.0%)	0.62	1/12732 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	332	LYS	CE-NZ	5.20	1.62	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	MET	N-CA-C	5.07	124.69	111.00

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	2873	0	2842	123	2
1	B	2871	0	2834	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1338	0	1364	89	0
2	D	2171	0	2190	204	2
3	A	31	0	13	2	0
3	B	31	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9317	0	9256	462	2

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 25.

All (462) 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:44:MET:O	1:A:46:GLY:N	1.76	1.19
1:A:121:GLN:NE2	2:D:320:MET:HB3	1.59	1.18
2:D:390:PRO:HB2	2:D:391:PRO:CD	1.77	1.14
2:C:187:ASN:HD22	1:B:49:GLN:HA	0.93	1.08
2:C:193:THR:HB	2:C:196:THR:HB	1.11	1.07
2:C:187:ASN:ND2	1:B:49:GLN:HA	1.70	1.06
1:A:125:GLU:OE2	2:D:327:ARG:NH2	1.91	1.01
2:C:310:MET:HB3	2:D:448:LEU:HB2	1.37	1.01
1:A:196:ARG:HH11	1:A:196:ARG:HG2	1.18	1.01
1:A:44:MET:O	1:A:45:VAL:C	2.00	0.99
1:A:351:THR:HB	2:D:411:ILE:CG2	1.93	0.99
2:D:448:LEU:HD21	2:D:452:GLN:HB2	1.43	0.99
2:C:187:ASN:HD22	1:B:49:GLN:CA	1.76	0.98
1:A:345:ILE:HG22	2:D:402:LEU:HD13	1.43	0.97
1:B:44:MET:HB3	1:B:64:ILE:HD12	1.46	0.96
2:D:390:PRO:HB2	2:D:391:PRO:HD3	1.46	0.96
1:A:60:SER:HB2	2:D:390:PRO:HD2	1.46	0.95
1:A:38:PRO:HB3	1:A:43:VAL:HG11	1.44	0.95
1:B:43:VAL:O	1:B:43:VAL:HG23	1.64	0.95
2:D:435:SER:HA	1:B:270:GLU:HG2	1.46	0.95
2:D:434:GLY:HA2	1:B:271:ALA:HB2	1.49	0.94
2:D:435:SER:C	2:D:437:PRO:HD3	1.90	0.92
1:B:39:ARG:O	1:B:40:HIS:HB2	1.70	0.91
1:A:121:GLN:HE22	2:D:320:MET:HB3	1.20	0.91
2:D:257:MET:HE1	2:D:290:LEU:HD11	1.54	0.90
2:C:311:SER:OG	2:D:452:GLN:HG3	1.74	0.87
2:C:193:THR:CB	2:C:196:THR:HB	2.02	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:218:THR:O	2:D:220:ALA:N	2.07	0.86
1:A:351:THR:HB	2:D:411:ILE:HG21	1.58	0.86
2:D:261:GLN:NE2	2:D:292:GLU:OE1	2.09	0.85
2:D:433:VAL:O	1:B:270:GLU:HG3	1.76	0.84
2:C:309:ARG:O	2:C:313:THR:HG22	1.77	0.84
2:C:310:MET:HG2	2:D:448:LEU:H	1.42	0.84
2:D:250:GLY:HA3	2:D:282:VAL:HG11	1.59	0.84
2:D:257:MET:HE1	2:D:290:LEU:CD1	2.11	0.80
2:C:202:GLU:HA	2:C:205:LYS:HB2	1.63	0.80
2:C:192:ILE:O	2:C:193:THR:OG1	1.99	0.80
2:D:243:VAL:CG1	2:D:243:VAL:O	2.31	0.79
2:D:264:THR:HA	2:D:295:THR:HG21	1.65	0.79
2:D:294:THR:CG2	2:D:322:LYS:HD2	2.14	0.78
1:B:191:LYS:O	1:B:195:GLU:HG2	1.84	0.78
2:D:457:GLU:HB2	1:B:371:HIS:CD2	2.18	0.78
1:A:196:ARG:CG	1:A:196:ARG:HH11	1.97	0.77
2:D:390:PRO:HB2	2:D:391:PRO:HD2	1.64	0.77
2:D:232:LEU:HD11	2:D:266:LEU:HD22	1.67	0.77
1:A:351:THR:HB	2:D:411:ILE:HG22	1.67	0.77
2:D:457:GLU:HB3	1:B:113:LYS:HD3	1.64	0.77
2:D:457:GLU:H	1:B:113:LYS:HZ2	1.34	0.76
2:C:189:ILE:HG13	2:C:191:ASN:HB2	1.68	0.75
2:D:435:SER:HA	1:B:270:GLU:CG	2.17	0.75
2:D:457:GLU:HG2	1:B:113:LYS:NZ	2.03	0.74
1:A:121:GLN:NE2	2:D:320:MET:CB	2.47	0.74
2:D:405:ARG:HG2	2:D:406:ASN:H	1.52	0.73
2:C:271:PHE:HE2	2:C:299:LEU:HD21	1.54	0.73
1:B:39:ARG:O	1:B:40:HIS:CB	2.37	0.73
2:D:451:VAL:HG12	2:D:452:GLN:H	1.55	0.72
1:B:248:ILE:HG12	1:B:249:THR:N	2.05	0.72
2:D:277:ILE:HG12	2:D:279:GLY:H	1.55	0.72
2:D:294:THR:HG23	2:D:322:LYS:HD2	1.72	0.72
2:D:167:ILE:HD11	2:D:189:ILE:HG21	1.72	0.72
2:C:328:LEU:O	2:C:332:LYS:HB2	1.90	0.71
2:D:166:VAL:HG12	2:D:167:ILE:H	1.55	0.71
2:D:485:LEU:HD11	1:B:345:ILE:HG13	1.71	0.71
1:A:60:SER:O	2:D:390:PRO:CG	2.38	0.71
1:A:64:ILE:O	1:A:64:ILE:HG22	1.91	0.71
1:A:39:ARG:HG3	1:A:64:ILE:C	2.11	0.70
2:D:459:SER:HB3	1:B:372:ARG:HE	1.56	0.70
1:B:39:ARG:N	1:B:64:ILE:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:326:LYS:O	2:C:329:GLN:HG2	1.90	0.70
2:D:435:SER:CA	1:B:270:GLU:HG2	2.19	0.70
1:A:351:THR:CG2	2:D:411:ILE:HG22	2.22	0.70
1:A:284:LYS:HB2	1:A:284:LYS:NZ	2.06	0.69
2:D:234:VAL:O	2:D:234:VAL:HG12	1.92	0.69
2:D:393:PRO:O	2:D:395:PRO:HD3	1.93	0.69
1:B:43:VAL:CG2	1:B:43:VAL:O	2.35	0.69
1:A:196:ARG:NH1	1:A:196:ARG:HG2	1.99	0.69
2:C:193:THR:HB	2:C:196:THR:CB	2.06	0.69
2:C:251:LYS:N	2:C:251:LYS:HD2	2.08	0.69
2:D:309:ARG:O	2:D:313:THR:HG22	1.92	0.69
1:A:221:LEU:HD21	1:A:311:ASP:HB2	1.73	0.69
1:A:349:LEU:HD11	2:D:407:ILE:HG23	1.75	0.68
1:A:148:THR:OG1	2:D:410:VAL:HG21	1.92	0.68
1:A:40:HIS:O	1:A:41:GLN:HB2	1.94	0.68
1:B:43:VAL:O	1:B:45:VAL:N	2.27	0.68
2:C:187:ASN:O	2:C:189:ILE:N	2.26	0.68
1:A:205:GLU:O	1:A:208:ILE:HG13	1.92	0.68
1:B:64:ILE:O	1:B:64:ILE:HG12	1.92	0.68
2:D:253:ILE:O	2:D:257:MET:HG2	1.94	0.68
2:D:236:GLU:HA	2:D:265:VAL:HG21	1.73	0.68
1:A:39:ARG:N	1:A:64:ILE:O	2.27	0.68
1:B:180:LEU:HD13	1:B:267:LEU:HD12	1.77	0.67
2:D:438:ASN:O	2:D:442:LYS:HG2	1.94	0.67
1:A:10:VAL:HB	1:A:105:LEU:CD2	2.25	0.67
2:D:390:PRO:CB	2:D:391:PRO:HD3	2.23	0.67
2:C:324:ARG:HA	2:C:327:ARG:NH1	2.10	0.67
1:B:370:VAL:O	1:B:374:CYS:HB2	1.94	0.67
2:C:275:ARG:HG3	2:C:276:HIS:H	1.60	0.67
1:A:180:LEU:HD21	1:A:261:LEU:HD23	1.77	0.66
2:C:230:GLU:HG3	2:C:233:LYS:HE3	1.78	0.66
2:D:390:PRO:CB	2:D:391:PRO:CD	2.63	0.66
1:A:163:VAL:HG13	1:A:175:ILE:CD1	2.26	0.65
2:D:267:THR:HG23	2:D:268:GLU:HG3	1.78	0.65
2:D:435:SER:CB	2:D:437:PRO:HD3	2.26	0.65
2:C:196:THR:O	2:C:200:PHE:HD1	1.77	0.65
2:D:215:LEU:HD11	2:D:243:VAL:HG22	1.78	0.65
1:A:121:GLN:HE21	2:D:320:MET:HB3	1.56	0.65
1:A:148:THR:HG21	1:A:167:GLU:OE2	1.97	0.65
1:B:171:LEU:HB3	1:B:173:HIS:CE1	2.31	0.65
2:D:257:MET:CE	2:D:290:LEU:HG	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:SER:HB2	2:D:390:PRO:CD	2.26	0.64
1:B:39:ARG:HB2	1:B:64:ILE:O	1.96	0.64
1:A:220:ALA:O	1:A:312:ARG:HD2	1.98	0.64
2:C:257:MET:HB3	2:C:289:LEU:HD13	1.77	0.64
1:A:306:TYR:CE2	3:A:401:ANP:H2	2.32	0.64
2:D:457:GLU:HG2	1:B:113:LYS:HZ2	1.62	0.64
1:A:219:VAL:HG11	1:A:262:PHE:CE1	2.32	0.64
2:D:431:GLY:HA3	1:B:176:LEU:HD22	1.80	0.64
1:A:276:GLU:HG2	1:A:320:LEU:HD11	1.79	0.64
1:B:250:ILE:HD12	1:B:254:ARG:HG2	1.80	0.64
2:D:241:VAL:HG23	2:D:266:LEU:HD11	1.79	0.63
2:D:459:SER:HB3	1:B:372:ARG:NE	2.12	0.63
2:D:437:PRO:O	2:D:441:LEU:HG	1.99	0.63
1:A:64:ILE:O	1:A:64:ILE:CG2	2.46	0.63
2:D:243:VAL:HG12	2:D:243:VAL:O	1.97	0.63
1:A:351:THR:CB	2:D:411:ILE:HG22	2.28	0.63
2:D:439:SER:O	2:D:445:LYS:NZ	2.31	0.63
1:A:25:ASP:HB2	2:D:401:LYS:H	1.64	0.63
1:B:220:ALA:O	1:B:312:ARG:HD3	1.98	0.63
2:D:432:SER:O	2:D:434:GLY:N	2.29	0.63
2:D:457:GLU:CB	1:B:371:HIS:CD2	2.82	0.63
1:A:218:TYR:OH	1:A:226:GLU:OE1	2.15	0.63
1:A:242:LEU:HB3	1:A:243:PRO:HD2	1.80	0.63
2:C:278:MET:CE	2:C:278:MET:HA	2.29	0.63
1:B:191:LYS:O	1:B:195:GLU:CG	2.46	0.62
1:B:219:VAL:HG11	1:B:262:PHE:CE1	2.33	0.62
2:C:302:HIS:HB2	1:B:78:ASN:HD22	1.63	0.62
2:C:327:ARG:NH2	1:B:363:ASP:OD1	2.33	0.62
2:C:291:LYS:O	2:C:318:ARG:NH2	2.28	0.62
1:B:44:MET:HE3	1:B:64:ILE:HB	1.82	0.61
2:C:258:ARG:HG3	2:C:289:LEU:HD21	1.83	0.61
2:C:243:VAL:O	2:C:271:PHE:HA	2.00	0.61
2:D:275:ARG:HG3	2:D:276:HIS:H	1.64	0.61
2:D:219:HIS:O	2:D:219:HIS:ND1	2.34	0.61
2:C:217:ASN:OD1	1:B:43:VAL:HG12	2.00	0.61
2:C:310:MET:CE	1:B:115:ASN:OD1	2.49	0.61
2:D:457:GLU:HB2	1:B:371:HIS:HD2	1.66	0.61
2:C:193:THR:CG2	2:C:196:THR:H	2.13	0.61
1:B:284:LYS:NZ	1:B:284:LYS:HB2	2.15	0.60
2:C:287:VAL:HG11	2:C:311:SER:HB2	1.84	0.60
1:A:162:THR:HG21	1:A:277:THR:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASP:HA	1:B:195:GLU:O	2.02	0.60
2:D:454:LYS:H	2:D:454:LYS:HD3	1.65	0.60
2:D:239:THR:HB	2:D:267:THR:HG22	1.83	0.60
2:C:236:GLU:HA	2:C:265:VAL:HG21	1.83	0.60
2:C:287:VAL:HG11	2:C:311:SER:CB	2.31	0.60
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.84	0.60
1:A:363:ASP:OD1	2:D:327:ARG:NH1	2.20	0.59
1:A:156:GLY:HA2	3:A:401:ANP:O1A	2.02	0.59
2:C:325:GLN:O	2:C:328:LEU:HB3	2.01	0.59
1:A:43:VAL:HG13	1:A:64:ILE:HG21	1.85	0.59
2:D:434:GLY:CA	1:B:271:ALA:HB2	2.29	0.59
2:D:464:THR:O	2:D:464:THR:HG22	2.02	0.59
2:D:435:SER:HB3	2:D:437:PRO:HD3	1.85	0.59
2:D:451:VAL:HG12	2:D:452:GLN:N	2.17	0.59
1:B:230:ALA:HB2	1:B:236:LEU:HD23	1.85	0.59
2:C:310:MET:CB	2:D:448:LEU:HB2	2.25	0.58
2:D:222:ASP:OD1	2:D:249:THR:OG1	2.19	0.58
1:A:78:ASN:ND2	2:D:302:HIS:HB2	2.18	0.58
2:D:258:ARG:O	2:D:261:GLN:HB2	2.03	0.58
1:B:147:ARG:NH2	1:B:330:ILE:HG12	2.19	0.57
2:D:410:VAL:O	2:D:414:GLN:N	2.37	0.57
2:D:258:ARG:HG3	2:D:289:LEU:HD21	1.87	0.57
2:D:194:THR:CG2	2:D:223:SER:OG	2.53	0.57
2:C:193:THR:HG22	2:C:196:THR:H	1.70	0.57
2:C:285:GLU:O	2:C:289:LEU:HB2	2.05	0.57
1:B:104:LEU:HD12	1:B:133:TYR:HB3	1.87	0.56
1:A:284:LYS:HB2	1:A:284:LYS:HZ2	1.69	0.56
1:A:163:VAL:HG13	1:A:175:ILE:HD11	1.87	0.56
1:B:136:ILE:HB	1:B:139:VAL:HG13	1.86	0.56
2:D:405:ARG:HG2	2:D:406:ASN:N	2.18	0.56
1:A:151:ILE:HD11	1:A:162:THR:OG1	2.06	0.56
2:C:306:PRO:HB2	2:D:446:ASN:O	2.05	0.56
1:B:161:HIS:CE1	1:B:177:ARG:HG3	2.40	0.55
2:D:407:ILE:HD13	2:D:407:ILE:O	2.06	0.55
2:C:305:LEU:HB3	2:C:308:PRO:HG2	1.88	0.55
2:D:449:ARG:O	2:D:451:VAL:N	2.39	0.55
1:B:358:SER:HB2	1:B:361:GLU:HG3	1.88	0.55
1:A:125:GLU:CD	2:D:327:ARG:HH21	2.06	0.55
2:D:457:GLU:CG	1:B:113:LYS:NZ	2.70	0.55
2:D:294:THR:HG23	2:D:322:LYS:NZ	2.22	0.55
1:B:41:GLN:O	1:B:43:VAL:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:261:GLN:NE2	2:C:292:GLU:OE2	2.39	0.55
1:A:230:ALA:HB2	1:A:236:LEU:HD12	1.89	0.55
2:D:193:THR:HB	2:D:196:THR:H	1.71	0.55
1:B:136:ILE:HB	1:B:139:VAL:CG1	2.38	0.54
2:D:431:GLY:CA	1:B:176:LEU:HD22	2.37	0.54
1:B:296:ASN:O	1:B:298:VAL:HG23	2.07	0.54
1:B:186:THR:OG1	1:B:213:LYS:NZ	2.35	0.54
1:A:25:ASP:HB2	2:D:400:LYS:H	1.72	0.54
2:D:166:VAL:N	2:D:169:ASP:OD2	2.40	0.54
2:D:258:ARG:HG3	2:D:289:LEU:HD11	1.90	0.54
2:D:327:ARG:O	2:D:331:GLN:HB3	2.07	0.54
2:D:444:ILE:HG13	2:D:445:LYS:N	2.23	0.54
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.89	0.54
2:C:245:SER:HA	2:C:273:ASN:O	2.08	0.54
1:A:299:LEU:HD12	1:A:331:ALA:HB2	1.89	0.54
1:A:353:GLN:O	1:A:356:TRP:HD1	1.91	0.54
2:C:251:LYS:N	2:C:251:LYS:CD	2.71	0.54
2:D:431:GLY:O	2:D:432:SER:C	2.47	0.54
1:B:177:ARG:NH1	1:B:179:ASP:OD1	2.41	0.53
2:D:400:LYS:O	2:D:401:LYS:HB2	2.08	0.53
2:C:263:ASN:C	2:C:263:ASN:OD1	2.46	0.53
1:B:198:TYR:HB2	1:B:200:PHE:CE1	2.44	0.53
2:D:243:VAL:HG13	2:D:243:VAL:O	2.06	0.53
1:A:187:ASP:OD1	1:A:206:ARG:NH2	2.36	0.53
2:D:299:LEU:HD22	2:D:312:MET:CE	2.38	0.53
1:A:142:LEU:O	1:A:145:SER:OG	2.25	0.53
1:A:358:SER:HB2	1:A:361:GLU:HG3	1.91	0.53
1:A:163:VAL:HG13	1:A:175:ILE:HD13	1.90	0.53
1:B:227:MET:CE	1:B:256:ARG:HD2	2.38	0.53
1:A:60:SER:O	2:D:390:PRO:HG3	2.09	0.53
2:D:294:THR:HG23	2:D:322:LYS:HZ2	1.73	0.53
2:D:455:LYS:HE3	1:B:112:PRO:HB3	1.91	0.53
2:D:457:GLU:OE1	1:B:371:HIS:CG	2.62	0.53
1:A:10:VAL:HB	1:A:105:LEU:HD23	1.90	0.52
1:B:37:ARG:NH2	1:B:81:ASP:OD2	2.43	0.52
2:C:310:MET:HE1	1:B:115:ASN:OD1	2.08	0.52
2:D:239:THR:O	2:D:267:THR:HG22	2.09	0.52
1:A:335:ARG:HA	1:A:338:SER:HB3	1.92	0.52
1:A:190:MET:HG3	1:A:209:VAL:HG11	1.91	0.52
1:B:198:TYR:CD2	1:B:198:TYR:N	2.71	0.52
2:D:490:VAL:HG21	1:B:30:VAL:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:478:ARG:HG3	1:B:148:THR:HG22	1.91	0.52
1:A:47:MET:HE2	1:A:53:TYR:HE1	1.74	0.52
2:D:202:GLU:HA	2:D:205:LYS:HB2	1.91	0.52
2:D:294:THR:O	2:D:294:THR:HG22	2.10	0.52
1:B:131:ALA:HA	1:B:357:ILE:O	2.10	0.52
2:D:435:SER:C	2:D:437:PRO:CD	2.73	0.52
1:A:163:VAL:HG22	1:A:175:ILE:HD13	1.91	0.52
1:B:241:GLU:HG2	1:B:247:VAL:HG22	1.90	0.52
2:C:217:ASN:CG	1:B:43:VAL:HG12	2.30	0.52
1:A:221:LEU:HD21	1:A:311:ASP:CB	2.41	0.51
2:C:234:VAL:HG12	2:C:234:VAL:O	2.10	0.51
2:D:243:VAL:HG13	2:D:248:ILE:HD12	1.92	0.51
1:A:237:GLU:HG2	1:A:238:LYS:N	2.25	0.51
1:B:149:THR:OG1	1:B:167:GLU:OE2	2.23	0.51
2:C:188:ASN:HA	2:C:217:ASN:HB3	1.93	0.51
1:B:39:ARG:HB2	1:B:64:ILE:C	2.31	0.51
1:A:26:ALA:HB1	1:A:27:PRO:HD2	1.93	0.51
1:A:47:MET:CE	1:A:53:TYR:CE1	2.93	0.51
1:B:103:VAL:HG12	1:B:105:LEU:CD1	2.40	0.51
1:B:198:TYR:CE2	1:B:248:ILE:HD12	2.45	0.51
1:A:194:THR:HA	1:A:198:TYR:O	2.11	0.51
1:B:180:LEU:HD13	1:B:267:LEU:CD1	2.40	0.51
1:B:9:VAL:HG21	1:B:344:SER:HA	1.93	0.51
2:D:257:MET:CE	2:D:290:LEU:CG	2.89	0.51
1:A:106:THR:HB	1:A:137:GLN:HG3	1.92	0.51
2:D:455:LYS:HD2	1:B:113:LYS:HB2	1.91	0.51
1:A:43:VAL:HB	2:D:217:ASN:HD21	1.76	0.51
2:C:306:PRO:CB	2:D:446:ASN:O	2.59	0.50
2:D:299:LEU:HD22	2:D:312:MET:HE1	1.93	0.50
2:D:454:LYS:H	2:D:454:LYS:CD	2.24	0.50
1:B:194:THR:HA	1:B:198:TYR:O	2.12	0.50
2:D:435:SER:OG	1:B:269:MET:HA	2.10	0.50
2:D:331:GLN:HA	2:D:335:GLU:OE1	2.11	0.50
1:B:107:GLU:OE1	1:B:116:ARG:HG2	2.11	0.50
1:A:233:SER:OG	1:A:234:SER:N	2.45	0.50
1:B:131:ALA:HB1	1:B:356:TRP:HB3	1.94	0.50
2:D:435:SER:HA	1:B:270:GLU:CD	2.32	0.50
2:D:457:GLU:HG2	1:B:113:LYS:HZ3	1.75	0.50
1:A:317:ILE:O	1:A:317:ILE:HG22	2.12	0.50
1:A:372:ARG:HH12	1:A:373:LYS:HG2	1.77	0.50
2:C:243:VAL:O	2:C:243:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ARG:HA	1:B:338:SER:HB3	1.92	0.50
1:B:242:LEU:HB3	1:B:243:PRO:HD2	1.93	0.50
2:D:257:MET:HE3	2:D:290:LEU:HG	1.93	0.50
2:D:451:VAL:CG1	2:D:452:GLN:H	2.24	0.50
2:D:229:ALA:O	2:D:232:LEU:HB2	2.12	0.50
2:C:188:ASN:OD1	2:C:217:ASN:ND2	2.45	0.49
1:B:64:ILE:CG1	1:B:64:ILE:O	2.61	0.49
1:B:170:ALA:O	1:B:172:PRO:HD3	2.13	0.49
2:D:194:THR:HG23	2:D:223:SER:OG	2.10	0.49
1:A:60:SER:O	2:D:390:PRO:HG2	2.10	0.49
1:A:131:ALA:HA	1:A:357:ILE:O	2.11	0.49
2:D:258:ARG:CG	2:D:289:LEU:HD21	2.43	0.49
1:A:78:ASN:HD22	2:D:302:HIS:HB2	1.77	0.49
1:B:248:ILE:CG1	1:B:249:THR:N	2.74	0.49
2:C:258:ARG:CG	2:C:289:LEU:HD21	2.42	0.49
2:C:314:SER:HB3	2:D:453:GLU:OE1	2.13	0.49
2:D:447:SER:OG	1:B:112:PRO:HG3	2.13	0.49
1:A:41:GLN:O	1:A:43:VAL:N	2.45	0.48
1:A:43:VAL:O	1:A:44:MET:C	2.50	0.48
1:B:37:ARG:HB3	1:B:38:PRO:HD2	1.95	0.48
1:A:170:ALA:O	1:A:172:PRO:HD3	2.12	0.48
1:B:8:LEU:HD13	1:B:101:HIS:HB3	1.96	0.48
2:C:185:ASN:OD1	2:C:187:ASN:HB3	2.12	0.48
2:D:457:GLU:CD	1:B:113:LYS:HD3	2.34	0.48
2:D:485:LEU:HD13	1:B:24:ASP:O	2.14	0.48
2:D:201:ALA:O	2:D:231:MET:HG3	2.14	0.48
2:D:442:LYS:HE2	2:D:445:LYS:HD2	1.96	0.48
1:A:186:THR:OG1	1:A:213:LYS:NZ	2.43	0.48
2:D:457:GLU:CG	1:B:113:LYS:HZ2	2.25	0.48
1:B:282:ILE:O	1:B:285:CYS:HB2	2.13	0.48
2:C:207:ASN:OD1	2:C:208:THR:N	2.46	0.48
2:D:405:ARG:CG	2:D:406:ASN:H	2.25	0.48
2:D:196:THR:O	2:D:200:PHE:HD1	1.97	0.48
2:D:481:SER:C	2:D:483:LYS:H	2.16	0.48
2:D:435:SER:OG	1:B:270:GLU:N	2.45	0.48
1:A:295:ALA:HA	1:A:328:LYS:H	1.78	0.48
1:B:185:LEU:CD2	1:B:260:ALA:HB3	2.43	0.48
2:D:436:GLN:N	2:D:437:PRO:CD	2.77	0.48
2:D:494:LEU:HB3	1:B:56:ASP:CG	2.34	0.47
1:A:282:ILE:O	1:A:285:CYS:HB2	2.14	0.47
1:B:140:LEU:O	1:B:342:GLY:HA3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:195:GLN:HA	2:D:198:THR:HB	1.95	0.47
2:D:257:MET:CE	2:D:290:LEU:CD1	2.89	0.47
1:A:148:THR:CG2	1:A:167:GLU:OE2	2.62	0.47
1:A:137:GLN:HG2	1:A:339:VAL:HG11	1.95	0.47
2:D:460:SER:HB2	1:B:372:ARG:HD3	1.96	0.47
2:D:280:SER:HA	2:D:283:GLU:HB2	1.96	0.47
2:D:254:LEU:HD22	2:D:285:GLU:HG2	1.97	0.47
2:C:231:MET:HE2	2:C:232:LEU:HD23	1.97	0.47
2:C:264:THR:HA	2:C:295:THR:HG21	1.97	0.47
2:D:294:THR:CG2	2:D:322:LYS:NZ	2.78	0.47
1:B:286:ASP:HB3	1:B:289:ILE:HG12	1.96	0.47
1:B:327:ILE:N	1:B:327:ILE:HD12	2.29	0.47
2:C:166:VAL:HB	2:C:169:ASP:HB3	1.96	0.47
2:D:166:VAL:HG12	2:D:167:ILE:N	2.25	0.47
2:C:230:GLU:HA	2:C:233:LYS:HE2	1.97	0.46
1:A:140:LEU:O	1:A:342:GLY:HA3	2.16	0.46
2:C:283:GLU:OE1	2:C:301:TYR:OH	2.32	0.46
1:B:284:LYS:HB2	1:B:284:LYS:HZ3	1.80	0.46
2:C:254:LEU:HB3	2:C:258:ARG:HH21	1.81	0.46
2:D:329:GLN:HG3	2:D:330:GLU:N	2.30	0.46
2:D:234:VAL:O	2:D:234:VAL:CG1	2.62	0.46
2:D:435:SER:CA	2:D:437:PRO:HD3	2.44	0.46
1:A:50:LYS:HD2	1:A:53:TYR:CE2	2.51	0.46
1:A:361:GLU:O	1:A:365:SER:OG	2.33	0.46
2:C:187:ASN:HD22	1:B:49:GLN:CB	2.27	0.46
2:C:278:MET:HA	2:C:278:MET:HE2	1.98	0.46
2:D:417:ALA:O	2:D:418:GLN:HG2	2.15	0.46
1:A:147:ARG:NH2	1:A:330:ILE:HG12	2.31	0.45
1:A:284:LYS:NZ	1:A:284:LYS:CB	2.76	0.45
1:A:286:ASP:HB3	1:A:289:ILE:HG12	1.96	0.45
2:C:187:ASN:C	2:C:189:ILE:H	2.18	0.45
2:D:178:ASP:C	2:D:180:ASP:H	2.20	0.45
1:A:185:LEU:CD2	1:A:260:ALA:HB3	2.47	0.45
1:B:21:PHE:O	1:B:24:ASP:HB2	2.16	0.45
2:D:208:THR:HA	2:D:237:HIS:CD2	2.51	0.45
1:B:213:LYS:HA	1:B:217:CYS:SG	2.56	0.45
2:C:187:ASN:OD1	2:C:187:ASN:O	2.35	0.45
2:D:172:ASP:O	2:D:176:SER:HB2	2.17	0.45
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.64	0.45
2:D:487:ARG:NH1	1:B:25:ASP:OD2	2.50	0.45
1:A:112:PRO:HB3	1:B:224:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:THR:HA	2:C:209:VAL:O	2.17	0.45
1:A:209:VAL:HA	1:A:212:ILE:HD12	1.97	0.45
1:A:279:TYR:HD1	1:A:294:TYR:HH	1.64	0.45
1:B:8:LEU:HD13	1:B:101:HIS:CB	2.47	0.45
2:D:396:PRO:HB2	2:D:397:LEU:H	1.63	0.45
1:B:49:GLN:HG2	1:B:49:GLN:H	1.68	0.45
2:C:253:ILE:HG13	2:C:278:MET:SD	2.57	0.45
1:A:34:ILE:HG22	1:A:69:TYR:CE2	2.52	0.45
1:B:66:THR:HG22	1:B:68:LYS:HE2	1.98	0.45
2:D:224:ALA:O	2:D:227:ALA:HB3	2.17	0.45
2:D:232:LEU:CD1	2:D:266:LEU:HD22	2.43	0.45
1:B:295:ALA:HA	1:B:328:LYS:H	1.82	0.45
1:B:42:GLY:O	1:B:43:VAL:C	2.54	0.45
2:C:189:ILE:O	2:C:190:GLU:C	2.54	0.45
1:B:180:LEU:CD1	1:B:267:LEU:CD1	2.94	0.44
2:D:194:THR:HG21	2:D:223:SER:OG	2.17	0.44
2:D:225:ALA:O	2:D:229:ALA:N	2.45	0.44
2:D:243:VAL:CG1	2:D:248:ILE:HD12	2.47	0.44
2:D:305:LEU:HA	2:D:306:PRO:HD3	1.86	0.44
2:D:436:GLN:N	2:D:437:PRO:HD3	2.32	0.44
2:D:461:ARG:O	2:D:461:ARG:HG3	2.16	0.44
1:A:43:VAL:HB	2:D:217:ASN:ND2	2.31	0.44
1:A:202:THR:O	1:A:205:GLU:HG2	2.17	0.44
1:A:64:ILE:HA	1:A:64:ILE:HD13	1.88	0.44
2:D:432:SER:C	2:D:434:GLY:N	2.71	0.44
2:C:281:GLN:O	2:C:285:GLU:HG2	2.16	0.44
2:D:457:GLU:CB	1:B:113:LYS:HD3	2.43	0.44
1:B:190:MET:HG3	1:B:209:VAL:HG21	1.98	0.44
2:D:260:LEU:HA	2:D:263:ASN:HB3	1.97	0.44
1:A:244:ASP:OD1	1:A:244:ASP:N	2.47	0.44
2:C:310:MET:HE2	1:B:115:ASN:OD1	2.17	0.44
2:C:186:LEU:HB3	2:C:191:ASN:HD22	1.83	0.43
1:A:47:MET:HE1	1:A:53:TYR:CD1	2.53	0.43
2:D:249:THR:CG2	2:D:275:ARG:HH21	2.30	0.43
1:A:200:PHE:HA	1:A:205:GLU:CD	2.39	0.43
1:A:47:MET:HE2	1:A:53:TYR:CE1	2.51	0.43
2:D:435:SER:N	1:B:270:GLU:HG2	2.33	0.43
2:C:195:GLN:HA	2:C:198:THR:HB	2.01	0.43
1:A:219:VAL:HG22	1:A:258:PRO:HB2	2.00	0.43
1:A:242:LEU:HB3	1:A:243:PRO:CD	2.46	0.43
2:C:204:LEU:HA	2:C:207:ASN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:213:PHE:CZ	2:C:215:LEU:HD22	2.53	0.43
2:D:288:LYS:HG3	2:D:289:LEU:N	2.33	0.43
2:D:490:VAL:HG21	1:B:30:VAL:HG21	2.00	0.43
1:A:221:LEU:CD2	1:A:311:ASP:HB2	2.46	0.43
2:C:254:LEU:HA	2:C:257:MET:HB2	2.00	0.43
2:C:271:PHE:CE2	2:C:299:LEU:HD21	2.44	0.43
2:D:294:THR:HG23	2:D:322:LYS:CD	2.46	0.43
1:B:332:PRO:O	1:B:335:ARG:NH1	2.49	0.43
2:C:175:LYS:H	2:C:175:LYS:HG2	1.60	0.43
2:C:247:PHE:CD2	2:C:275:ARG:HB3	2.54	0.43
1:A:70:PRO:HG3	1:A:81:ASP:HB3	2.00	0.42
2:D:442:LYS:NZ	1:B:73:HIS:CD2	2.88	0.42
2:D:226:MET:O	2:D:230:GLU:HG2	2.20	0.42
2:D:235:ASN:OD1	2:D:236:GLU:N	2.52	0.42
2:D:243:VAL:HG13	2:D:248:ILE:CD1	2.49	0.42
1:A:305:MET:HA	1:A:335:ARG:NH2	2.34	0.42
1:B:39:ARG:CB	1:B:64:ILE:O	2.65	0.42
2:D:221:ASP:C	2:D:221:ASP:OD1	2.56	0.42
2:D:178:ASP:HA	2:D:179:PRO:HD3	1.88	0.42
1:A:31:PHE:CD2	1:A:93:GLU:HG2	2.55	0.42
1:A:210:ARG:NH1	1:A:214:GLU:OE2	2.52	0.42
2:D:192:ILE:HG22	2:D:197:LEU:HG	2.02	0.42
1:B:291:GLU:HG3	1:B:325:MET:SD	2.60	0.42
2:D:236:GLU:O	2:D:265:VAL:HG11	2.18	0.42
1:A:41:GLN:HB3	1:A:42:GLY:H	1.68	0.42
2:D:282:VAL:O	2:D:286:ILE:HG13	2.20	0.42
1:B:38:PRO:HD3	1:B:47:MET:CE	2.50	0.42
1:A:351:THR:HG22	2:D:411:ILE:HG22	1.99	0.42
1:B:218:TYR:CE2	1:B:255:PHE:HB3	2.55	0.42
2:D:432:SER:CB	1:B:178:LEU:HD12	2.49	0.41
1:A:303:THR:O	1:A:303:THR:CG2	2.67	0.41
1:B:286:ASP:OD1	1:B:287:VAL:N	2.53	0.41
2:C:231:MET:CE	2:C:232:LEU:HD23	2.50	0.41
2:C:250:GLY:O	2:C:254:LEU:HG	2.19	0.41
2:D:193:THR:HG22	2:D:194:THR:N	2.34	0.41
2:D:199:ARG:HA	2:D:199:ARG:HD3	1.85	0.41
2:D:254:LEU:HD22	2:D:285:GLU:CG	2.50	0.41
1:B:134:VAL:HG13	1:B:134:VAL:O	2.20	0.41
2:C:252:GLY:O	2:C:255:ALA:HB3	2.21	0.41
2:D:442:LYS:CE	2:D:445:LYS:HB3	2.51	0.41
1:A:131:ALA:HB1	1:A:356:TRP:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:PHE:O	2:D:275:ARG:HD3	2.20	0.41
2:D:322:LYS:O	2:D:326:LYS:HB2	2.21	0.41
2:D:490:VAL:HG22	2:D:490:VAL:O	2.21	0.41
2:D:482:ILE:O	2:D:482:ILE:HG22	2.21	0.41
1:A:69:TYR:HA	1:A:70:PRO:HD3	1.95	0.41
2:C:251:LYS:H	2:C:251:LYS:CD	2.34	0.41
2:C:287:VAL:HG11	2:C:311:SER:HB3	1.99	0.41
2:D:243:VAL:HG13	2:D:246:ASN:HD22	1.85	0.41
1:A:202:THR:HG23	1:A:205:GLU:OE2	2.21	0.41
1:A:313:MET:HB3	1:A:329:ILE:CD1	2.51	0.41
1:B:162:THR:HG21	1:B:278:THR:HA	2.03	0.41
1:B:38:PRO:HG3	1:B:47:MET:SD	2.61	0.41
1:A:282:ILE:HG23	1:A:293:LEU:HD23	2.03	0.41
2:D:271:PHE:CD2	2:D:271:PHE:N	2.89	0.41
2:C:327:ARG:NH1	1:B:125:GLU:OE2	2.51	0.41
2:C:264:THR:C	2:C:265:VAL:HG22	2.41	0.40
2:D:444:ILE:HG21	1:B:72:GLU:OE1	2.21	0.40
2:D:481:SER:C	2:D:483:LYS:N	2.74	0.40
2:C:217:ASN:HD21	1:B:43:VAL:HA	1.86	0.40
1:A:284:LYS:HB2	1:A:284:LYS:HZ3	1.85	0.40
1:A:47:MET:HE1	1:A:65:LEU:HD21	2.04	0.40
1:B:213:LYS:O	1:B:217:CYS:HB2	2.20	0.40
1:B:34:ILE:HD13	1:B:67:LEU:HD13	2.03	0.40
2:C:306:PRO:O	2:C:310:MET:HB2	2.21	0.40
2:C:324:ARG:HA	2:C:327:ARG:HH12	1.84	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:GLN:OE1	2:D:447:SER:O[1_665]	2.15	0.05
1:A:232:SER:O	2:D:432:SER:O[1_665]	2.16	0.04

## 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	367/384 (96%)	341 (93%)	18 (5%)	8 (2%)	6	29
1	B	367/384 (96%)	346 (94%)	14 (4%)	7 (2%)	8	33
2	C	166/506 (33%)	137 (82%)	23 (14%)	6 (4%)	3	17
2	D	276/506 (54%)	210 (76%)	43 (16%)	23 (8%)	1	3
All	All	1176/1780 (66%)	1034 (88%)	98 (8%)	44 (4%)	3	17

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	45	VAL
2	C	193	THR
2	C	265	VAL
2	D	219	HIS
2	D	390	PRO
2	D	393	PRO
2	D	406	ASN
2	D	436	GLN
2	D	450	SER
1	B	40	HIS
1	B	42	GLY
1	B	43	VAL
1	B	45	VAL
1	A	42	GLY
1	A	44	MET
1	A	182	GLY
2	D	392	PRO
2	D	396	PRO
2	D	401	LYS
2	D	432	SER
2	D	433	VAL
2	D	444	ILE
2	D	446	ASN
1	B	182	GLY
1	A	15	GLY
2	C	191	ASN
2	D	489	GLU
1	A	41	GLN
2	C	275	ARG

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Mol	Chain	Res	Type
2	D	394	PRO
2	D	395	PRO
2	D	421	LEU
2	D	437	PRO
2	D	488	VAL
1	B	15	GLY
1	B	356	TRP
1	A	356	TRP
2	C	188	ASN
2	D	464	THR
2	D	482	ILE
2	D	438	ASN
2	D	462	PRO
2	C	308	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/325 (96%)	282 (91%)	29 (9%)	9	31
1	B	310/325 (95%)	285 (92%)	25 (8%)	11	37
2	C	152/451 (34%)	129 (85%)	23 (15%)	3	12
2	D	241/451 (53%)	213 (88%)	28 (12%)	5	21
All	All	1014/1552 (65%)	909 (90%)	105 (10%)	7	26

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	CYS
1	A	18	LYS
1	A	40	HIS
1	A	44	MET
1	A	49	GLN
1	A	84	LYS
1	A	132	MET

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Mol	Chain	Res	Type
1	A	155	SER
1	A	162	THR
1	A	169	TYR
1	A	175	ILE
1	A	180	LEU
1	A	195	GLU
1	A	196	ARG
1	A	203	THR
1	A	225	GLN
1	A	232	SER
1	A	233	SER
1	A	237	GLU
1	A	281	SER
1	A	288	ASP
1	A	312	ARG
1	A	322	LYS
1	A	334	GLU
1	A	350	SER
1	A	351	THR
1	A	354	GLN
1	A	365	SER
1	A	368	SER
2	C	181	THR
2	C	190	GLU
2	C	196	THR
2	C	198	THR
2	C	215	LEU
2	C	222	ASP
2	C	257	MET
2	C	262	HIS
2	C	265	VAL
2	C	267	THR
2	C	270	ARG
2	C	275	ARG
2	C	281	GLN
2	C	288	LYS
2	C	289	LEU
2	C	292	GLU
2	C	295	THR
2	C	299	LEU
2	C	305	LEU
2	C	310	MET

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Mol	Chain	Res	Type
2	C	313	THR
2	C	318	ARG
2	C	324	ARG
2	D	177	ASN
2	D	206	ASP
2	D	215	LEU
2	D	231	MET
2	D	232	LEU
2	D	243	VAL
2	D	262	HIS
2	D	277	ILE
2	D	280	SER
2	D	282	VAL
2	D	284	MET
2	D	287	VAL
2	D	288	LYS
2	D	289	LEU
2	D	292	GLU
2	D	295	THR
2	D	311	SER
2	D	313	THR
2	D	318	ARG
2	D	404	THR
2	D	407	ILE
2	D	410	VAL
2	D	438	ASN
2	D	445	LYS
2	D	450	SER
2	D	453	GLU
2	D	454	LYS
2	D	456	MET
1	B	17	CYS
1	B	18	LYS
1	B	34	ILE
1	B	40	HIS
1	B	49	GLN
1	B	62	ARG
1	B	84	LYS
1	B	139	VAL
1	B	141	SER
1	B	148	THR
1	B	198	TYR

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Mol	Chain	Res	Type
1	B	201	THR
1	B	227	MET
1	B	232	SER
1	B	236	LEU
1	B	237	GLU
1	B	248	ILE
1	B	287	VAL
1	B	288	ASP
1	B	292	ASP
1	B	303	THR
1	B	336	LYS
1	B	351	THR
1	B	368	SER
1	B	372	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	78	ASN
2	C	187	ASN
2	C	191	ASN
2	C	261	GLN
2	C	302	HIS
2	D	185	ASN
2	D	207	ASN
2	D	217	ASN
2	D	237	HIS
2	D	246	ASN
2	D	261	GLN
2	D	406	ASN
1	B	73	HIS
1	B	161	HIS

### 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 4 ligands modelled in this entry, 2 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	$\# Z  > 2$
3	ANP	B	401	4	29,33,33	1.89	6 (20%)	31,52,52	1.67	6 (19%)
3	ANP	A	401	4	29,33,33	1.86	6 (20%)	31,52,52	1.65	5 (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
3	ANP	B	401	4	-	5/14/38/38	0/3/3/3
3	ANP	A	401	4	-	5/14/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ANP	PG-N3B	4.60	1.75	1.63
3	A	401	ANP	PB-N3B	4.46	1.75	1.63
3	B	401	ANP	PB-N3B	4.46	1.75	1.63
3	A	401	ANP	PG-N3B	4.41	1.74	1.63
3	B	401	ANP	PB-O1B	3.58	1.51	1.46
3	B	401	ANP	PG-O1G	3.50	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ANP	PB-O3A	3.42	1.63	1.59
3	A	401	ANP	PG-O1G	3.41	1.51	1.46
3	A	401	ANP	PB-O1B	3.25	1.51	1.46
3	A	401	ANP	PB-O3A	3.08	1.62	1.59
3	A	401	ANP	C5-C4	2.45	1.47	1.40
3	B	401	ANP	C5-C4	2.24	1.46	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ANP	O1G-PG-N3B	-5.17	104.16	111.77
3	A	401	ANP	O1G-PG-N3B	-4.98	104.43	111.77
3	B	401	ANP	N3-C2-N1	-3.66	122.95	128.68
3	B	401	ANP	O2B-PB-O1B	3.50	117.25	109.92
3	A	401	ANP	O2B-PB-O1B	3.31	116.86	109.92
3	A	401	ANP	O1B-PB-N3B	-3.25	106.99	111.77
3	A	401	ANP	N3-C2-N1	-3.23	123.63	128.68
3	B	401	ANP	O1B-PB-N3B	-2.42	108.21	111.77
3	B	401	ANP	O3G-PG-O2G	2.07	113.16	107.64
3	A	401	ANP	O3G-PG-O2G	2.07	113.15	107.64
3	B	401	ANP	C4-C5-N7	-2.02	107.29	109.40

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	ANP	C5'-O5'-PA-O2A
3	A	401	ANP	PA-O3A-PB-O1B
3	A	401	ANP	PA-O3A-PB-O2B
3	A	401	ANP	O4'-C4'-C5'-O5'
3	A	401	ANP	C3'-C4'-C5'-O5'
3	B	401	ANP	C5'-O5'-PA-O3A
3	B	401	ANP	C5'-O5'-PA-O1A
3	B	401	ANP	PB-O3A-PA-O2A
3	A	401	ANP	C5'-O5'-PA-O1A
3	B	401	ANP	PG-N3B-PB-O3A

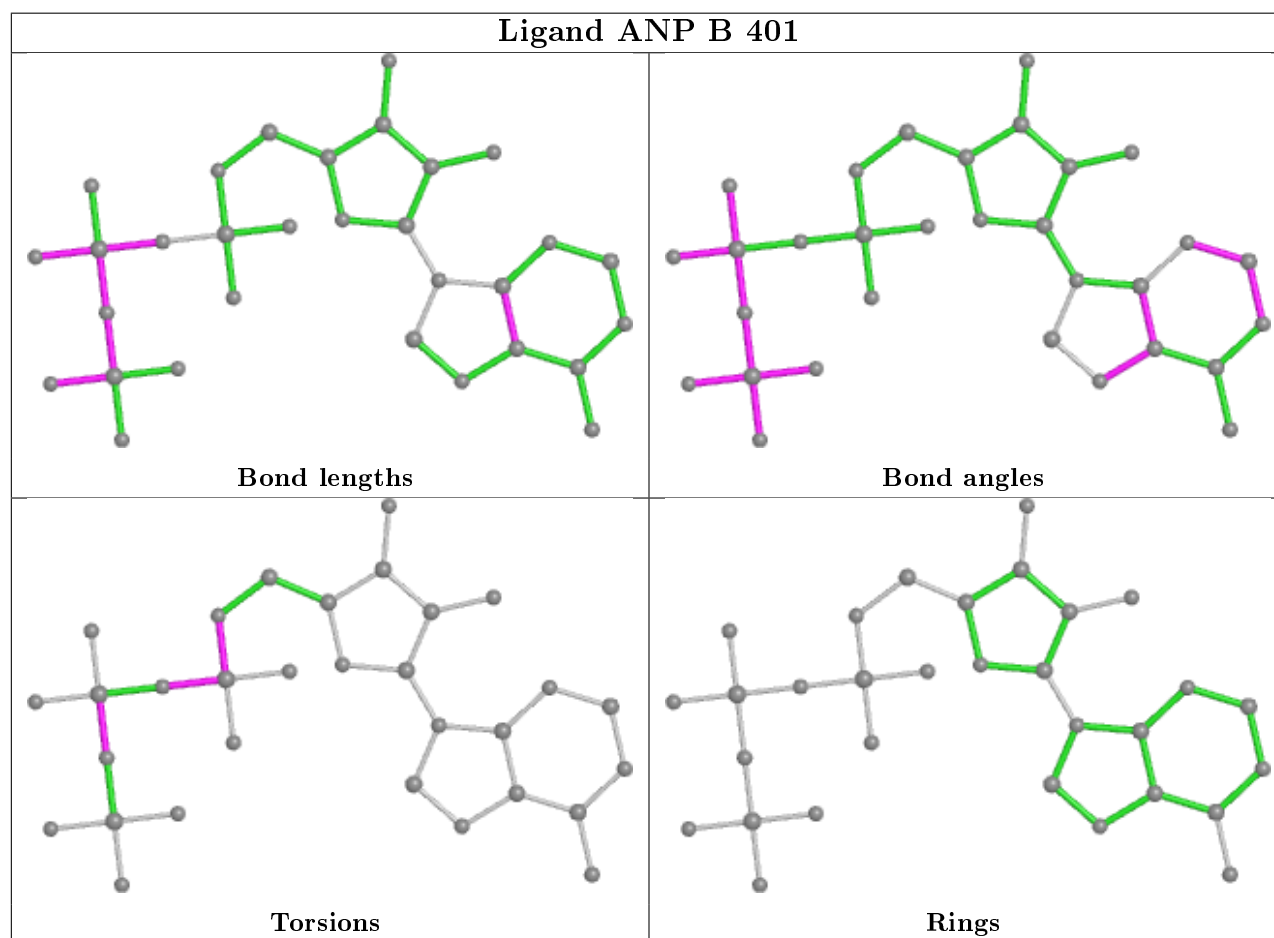
There are no ring outliers.

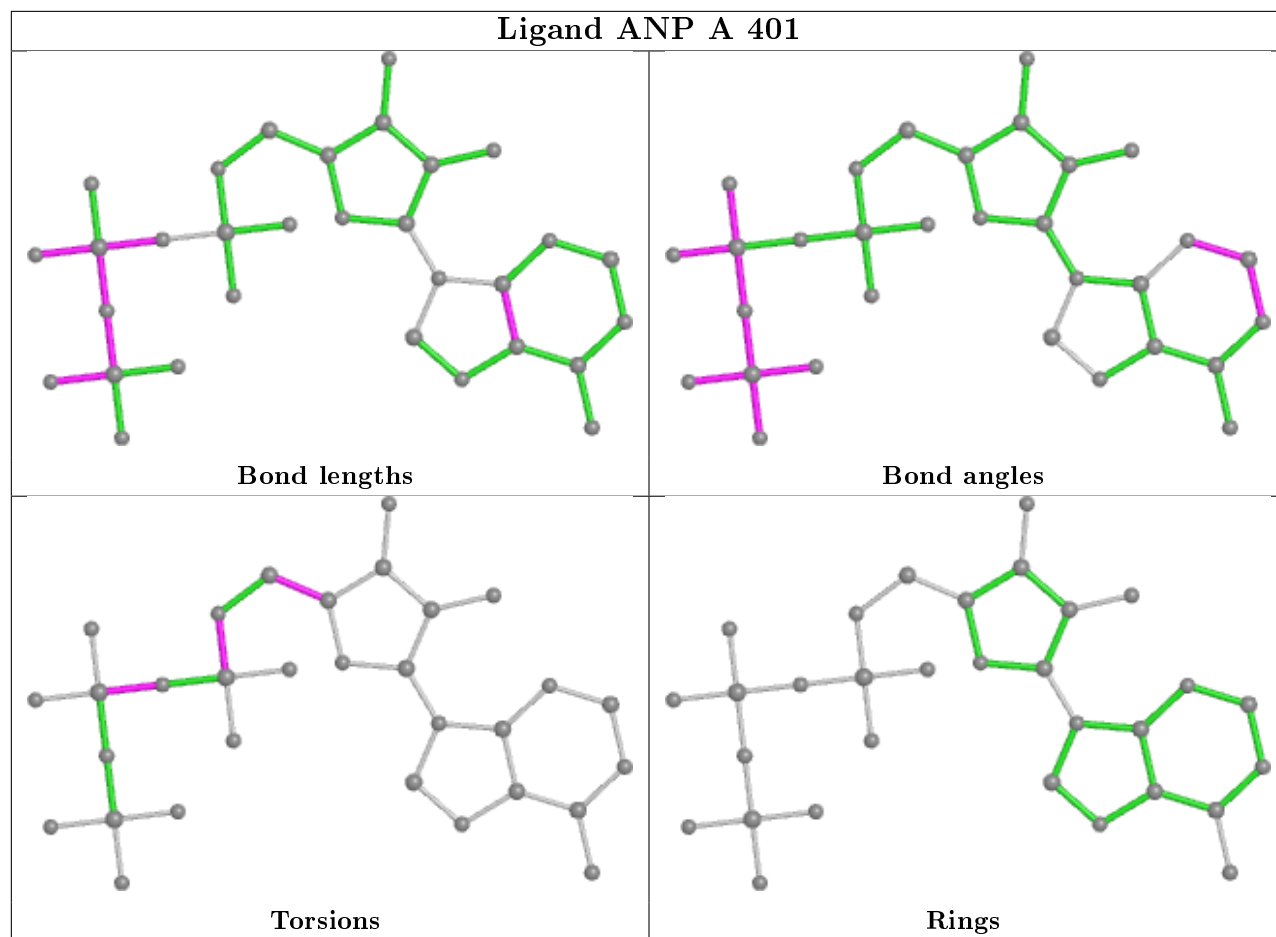
1 monomer is involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ANP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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	369/384 (96%)	0.09	13 (3%)	44 26	22, 39, 61, 94	0
1	B	369/384 (96%)	0.04	6 (1%)	72 52	22, 38, 63, 82	0
2	C	168/506 (33%)	0.36	12 (7%)	16 8	34, 54, 83, 150	0
2	D	280/506 (55%)	1.09	67 (23%)	0 0	34, 61, 184, 280	0
All	All	1186/1780 (66%)	0.35	98 (8%)	11 5	22, 46, 82, 280	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	389	PRO	8.2
2	D	440	ILE	8.0
2	D	494	LEU	7.2
2	D	431	GLY	6.9
2	D	391	PRO	6.2
2	D	338	ASP	6.0
2	C	197	LEU	5.8
2	D	335	GLU	5.5
2	D	332	LYS	5.3
2	D	423	ASN	5.3
2	D	420	ALA	5.3
2	C	170	ALA	4.8
1	A	42	GLY	4.8
2	D	425	GLN	4.8
2	D	433	VAL	4.7
2	D	439	SER	4.6
2	D	432	SER	4.6
2	D	390	PRO	4.6
2	D	393	PRO	4.5
2	D	426	GLY	4.3
2	D	468	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	464	THR	4.2
2	C	191	ASN	4.2
2	D	424	GLY	4.1
2	D	462	PRO	4.1
2	D	435	SER	4.0
2	D	421	LEU	4.0
2	D	429	SER	3.9
2	D	430	GLY	3.8
1	A	45	VAL	3.8
2	D	434	GLY	3.8
2	D	495	ARG	3.8
2	D	336	GLY	3.8
2	D	328	LEU	3.7
2	C	188	ASN	3.7
2	D	451	VAL	3.6
2	D	457	GLU	3.6
1	A	47	MET	3.6
2	D	334	GLN	3.6
2	D	441	LEU	3.5
2	D	392	PRO	3.4
2	D	418	GLN	3.4
1	A	41	GLN	3.4
2	D	458	ASP	3.3
1	B	41	GLN	3.3
2	D	437	PRO	3.2
2	D	395	PRO	3.2
2	D	427	SER	3.2
2	D	337	TYR	3.2
2	D	493	ALA	3.1
2	D	466	GLN	3.1
1	B	201	THR	3.1
2	D	465	PRO	3.0
2	D	331	GLN	3.0
2	D	485	LEU	2.9
2	D	448	LEU	2.9
2	D	446	ASN	2.9
2	C	169	ASP	2.9
1	A	245	GLY	2.9
2	D	428	GLY	2.9
2	C	333	GLN	2.8
2	D	469	ALA	2.8
2	D	484	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	193	THR	2.7
1	A	201	THR	2.7
1	A	46	GLY	2.7
1	A	44	MET	2.7
2	C	187	ASN	2.7
2	D	454	LYS	2.6
2	D	333	GLN	2.6
1	A	208	ILE	2.6
2	D	276	HIS	2.6
2	D	492	GLU	2.5
1	A	39	ARG	2.5
1	B	45	VAL	2.5
2	D	169	ASP	2.5
2	C	183	GLU	2.5
2	D	170	ALA	2.5
2	D	438	ASN	2.5
2	D	452	GLN	2.5
2	D	394	PRO	2.5
2	D	415	GLU	2.4
1	B	47	MET	2.4
2	D	194	THR	2.3
1	B	286	ASP	2.3
2	C	199	ARG	2.2
1	B	208	ILE	2.2
2	D	443	GLU	2.2
2	D	407	ILE	2.1
2	D	419	ARG	2.1
1	A	349	LEU	2.1
2	C	329	GLN	2.1
1	A	202	THR	2.1
2	D	413	GLN	2.1
2	C	181	THR	2.0
1	A	62	ARG	2.0
2	D	422	GLN	2.0
2	D	442	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

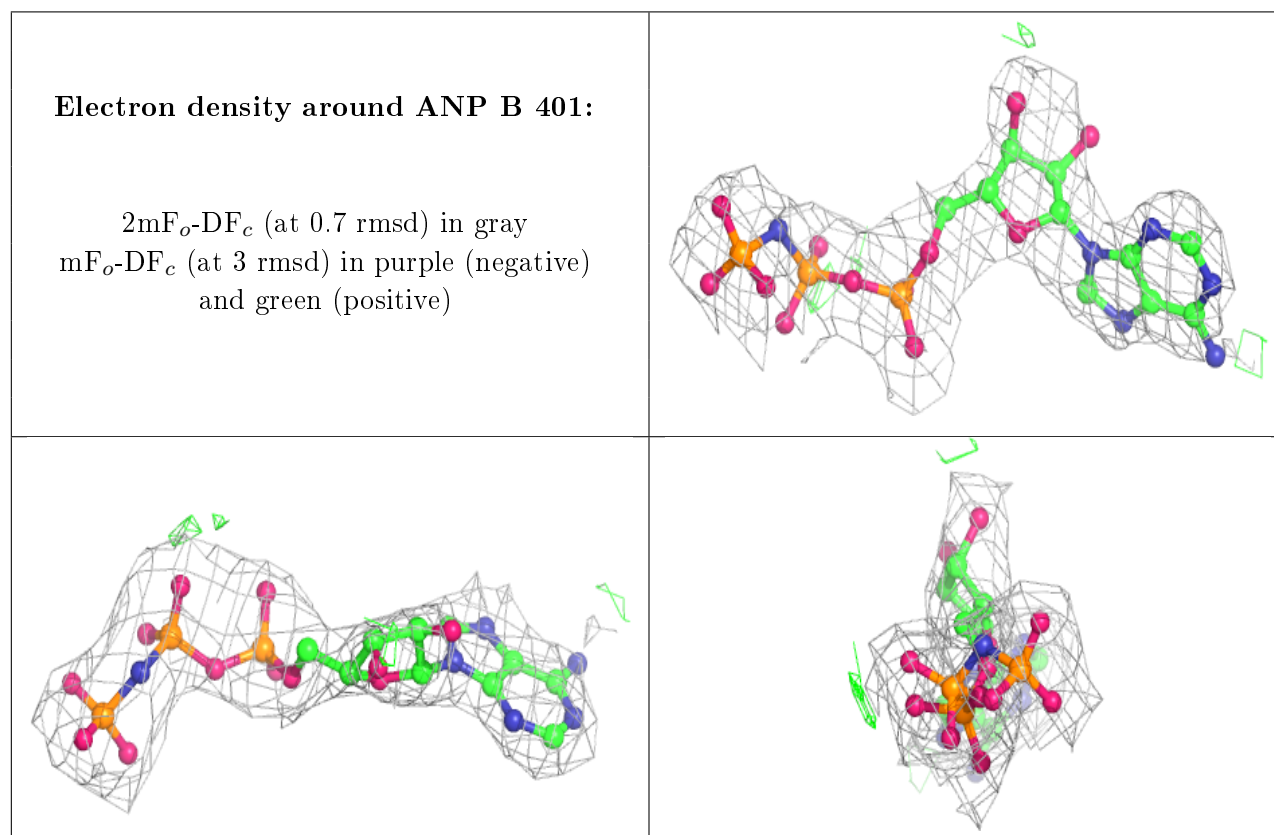
There are no carbohydrates in this entry.

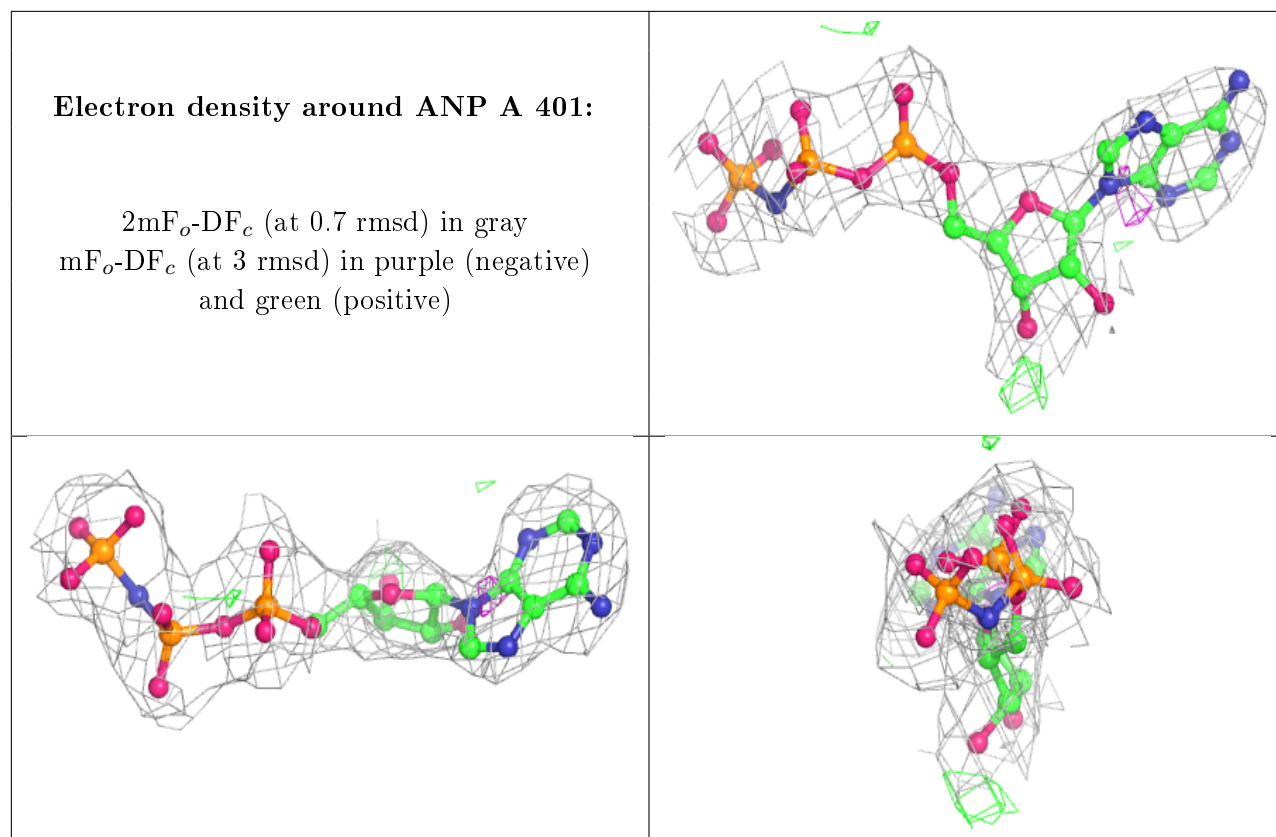
## 6.4 Ligands [i](#)

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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	402	1/1	0.88	0.25	44,44,44,44	0
3	ANP	B	401	31/31	0.90	0.18	40,50,60,64	0
4	MG	B	402	1/1	0.90	0.23	39,39,39,39	0
3	ANP	A	401	31/31	0.91	0.17	34,43,55,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.