



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 06:33 AM EDT

PDB ID : 4ETW  
Title : Structure of the Enzyme-ACP Substrate Gatekeeper Complex Required for Biotin Synthesis  
Authors : Agarwal, V.; Nair, S.K.  
Deposited on : 2012-04-24  
Resolution : 2.05 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

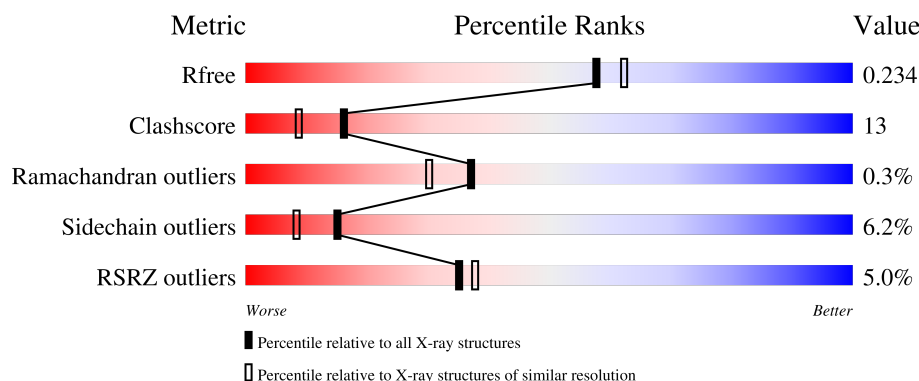
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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 of 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	264	<div> <div>4%</div> <div>77%</div> <div>17%</div> <div>• •</div> </div>
1	C	264	<div> <div>4%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
2	B	77	<div> <div>10%</div> <div>69%</div> <div>29%</div> <div>•</div> </div>
2	D	77	<div> <div>5%</div> <div>69%</div> <div>27%</div> <div>• •</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5439 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 Pimelyl-[acyl-carrier protein] methyl ester esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2002	1293	350	351	8			
1	C	255	Total	C	N	O	S	0	0	0
			2002	1293	350	351	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ALA	SER	engineered mutation	UNP Q83PW0
A	243	ALA	VAL	engineered mutation	UNP Q83PW0
A	258	GLU	-	expression tag	UNP Q83PW0
A	259	HIS	-	expression tag	UNP Q83PW0
A	260	HIS	-	expression tag	UNP Q83PW0
A	261	HIS	-	expression tag	UNP Q83PW0
A	262	HIS	-	expression tag	UNP Q83PW0
A	263	HIS	-	expression tag	UNP Q83PW0
A	264	HIS	-	expression tag	UNP Q83PW0
C	82	ALA	SER	engineered mutation	UNP Q83PW0
C	243	ALA	VAL	engineered mutation	UNP Q83PW0
C	258	GLU	-	expression tag	UNP Q83PW0
C	259	HIS	-	expression tag	UNP Q83PW0
C	260	HIS	-	expression tag	UNP Q83PW0
C	261	HIS	-	expression tag	UNP Q83PW0
C	262	HIS	-	expression tag	UNP Q83PW0
C	263	HIS	-	expression tag	UNP Q83PW0
C	264	HIS	-	expression tag	UNP Q83PW0

- Molecule 2 is a protein called Acyl carrier protein.

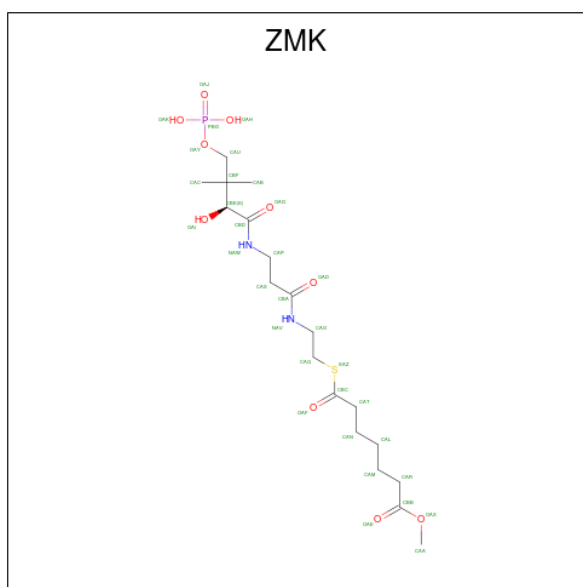
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	75	Total	C	N	O	S	0	0	0
			573	355	89	128	1			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	75	Total	C	N	O	S	0	0	0
			573	355	89	128	1			

- Molecule 3 is methyl 7-{[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl]sulfanyl}-7-oxoheptanoate (three-letter code: ZMK) (formula: C<sub>19</sub>H<sub>35</sub>N<sub>2</sub>O<sub>10</sub>PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total 33	C 19	N 2	O 10	P 1	S 1	0	0
3	B	1	Total 33	C 19	N 2	O 10	P 1	S 1	0	0

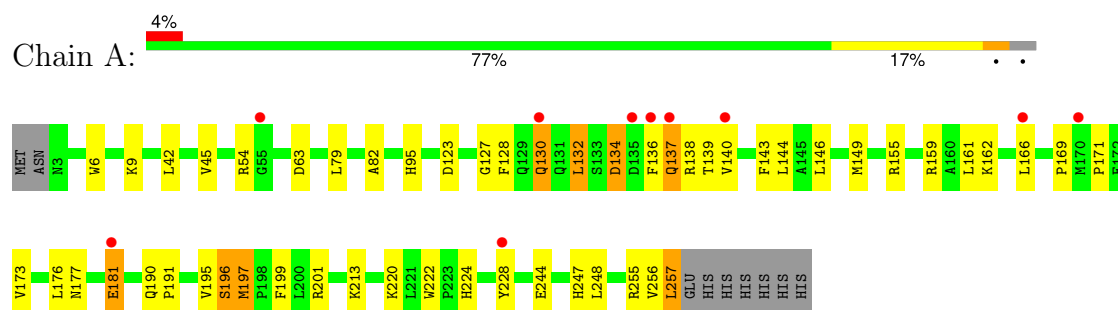
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	C	111	Total	O	0	0
			111	111		
4	D	5	Total	O	0	0
			5	5		
4	B	11	Total	O	0	0
			11	11		

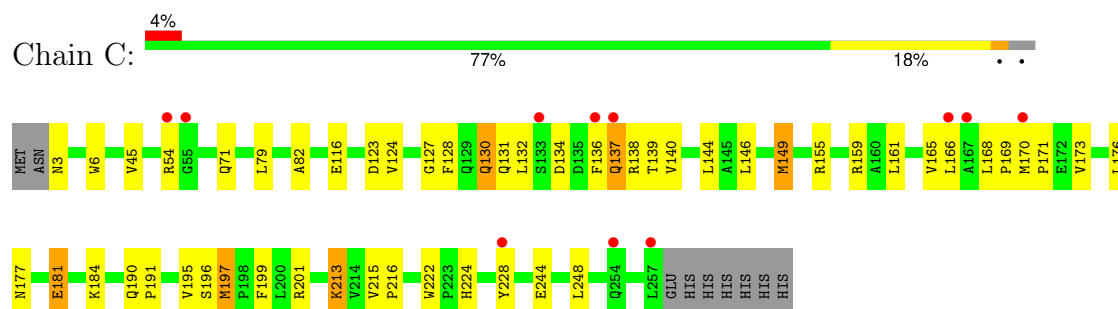
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

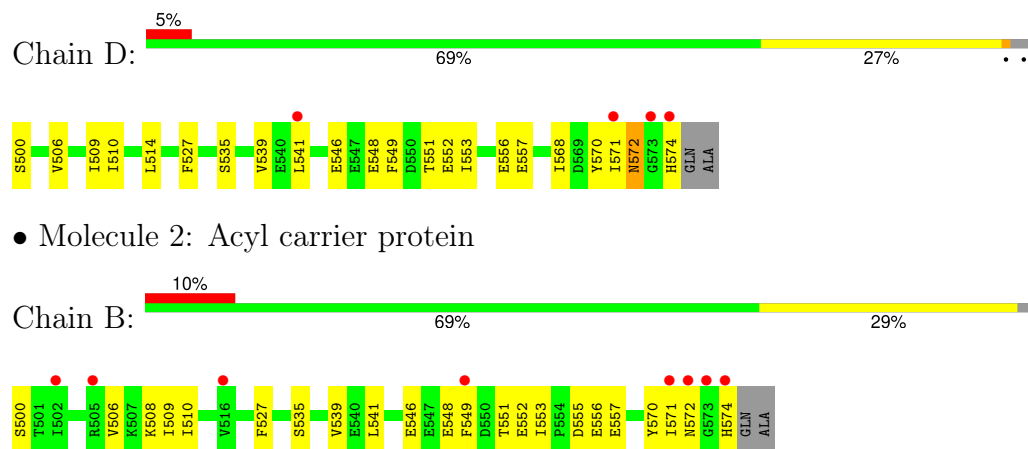
- Molecule 1: Pimelyl-[acyl-carrier protein] methyl ester esterase



- Molecule 1: Pimelyl-[acyl-carrier protein] methyl ester esterase



- Molecule 2: Acyl carrier protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.08Å 57.21Å 60.95Å 101.99° 90.10° 112.74°	Depositor
Resolution (Å)	35.13 – 2.05 35.13 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.8 (35.13-2.05) 97.8 (35.13-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.15 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.7.1_743, REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.192 , 0.236 0.190 , 0.234	Depositor DCC
$R_{free}$ test set	2146 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.8	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	0.95	EDS
Total number of atoms	5439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.89% 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: ZMK

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	0.49	0/2055	0.61	0/2799
1	C	0.49	0/2055	0.62	0/2799
2	B	0.46	1/577 (0.2%)	0.56	0/783
2	D	0.51	2/577 (0.3%)	0.57	0/783
All	All	0.49	3/5264 (0.1%)	0.60	0/7164

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	572	ASN	CG-OD1	-6.96	1.08	1.24
2	B	572	ASN	CG-OD1	-6.88	1.08	1.24
2	D	572	ASN	CB-CG	-6.33	1.36	1.51

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	2002	0	2015	59	0
1	C	2002	0	2015	43	0
2	B	573	0	540	18	0
2	D	573	0	540	17	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	33	0	33	3	0
3	D	33	0	33	4	0
4	A	96	0	0	10	0
4	B	11	0	0	4	0
4	C	111	0	0	7	0
4	D	5	0	0	0	0
All	All	5439	0	5176	134	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 13.

All (134) 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:159:ARG:NH2	2:B:546:GLU:OE1	1.78	1.16
1:A:136:PHE:HE1	1:A:176:LEU:CD1	1.64	1.10
1:A:257:LEU:HD12	1:A:257:LEU:N	1.69	1.05
1:A:54:ARG:NH1	4:A:396:HOH:O	1.80	1.00
1:A:136:PHE:CE1	1:A:176:LEU:CD1	2.47	0.97
1:C:181:GLU:HA	1:C:181:GLU:OE1	1.70	0.91
1:A:136:PHE:HE1	1:A:176:LEU:HD13	1.37	0.90
1:A:181:GLU:OE1	1:A:181:GLU:HA	1.72	0.89
1:A:196:SER:OG	4:A:318:HOH:O	1.90	0.88
1:C:228:TYR:OH	1:C:244:GLU:OE1	1.91	0.87
1:A:228:TYR:OH	1:A:244:GLU:OE1	1.93	0.86
2:B:510:ILE:HD13	2:B:541:LEU:HD11	1.58	0.85
2:D:510:ILE:HD13	2:D:541:LEU:HD11	1.59	0.84
1:C:155:ARG:NH1	2:D:546:GLU:OE2	2.10	0.84
1:A:257:LEU:N	1:A:257:LEU:CD1	2.43	0.82
1:A:171:PRO:HG2	1:A:176:LEU:HD21	1.63	0.81
1:A:244:GLU:O	1:A:248:LEU:HD12	1.82	0.80
1:C:171:PRO:HG2	1:C:176:LEU:HD21	1.61	0.79
1:A:95:HIS:HD2	4:A:324:HOH:O	1.67	0.77
1:C:3:ASN:N	4:C:340:HOH:O	2.20	0.75
1:C:144:LEU:HD22	1:C:161:LEU:HB3	1.70	0.74
1:A:144:LEU:HD22	1:A:161:LEU:HB3	1.71	0.72
1:C:244:GLU:O	1:C:248:LEU:HD12	1.90	0.72
1:A:42:LEU:O	4:A:388:HOH:O	2.06	0.72
1:C:184:LYS:HE3	4:C:341:HOH:O	1.90	0.71
1:C:195:VAL:HG13	1:C:197:MET:SD	2.31	0.70
1:A:195:VAL:HG13	1:A:197:MET:SD	2.32	0.70

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:PHE:CE2	2:B:571:ILE:HG13	2.26	0.70
1:A:63:ASP:OD2	4:A:340:HOH:O	2.07	0.70
1:C:159:ARG:NH2	2:D:546:GLU:OE1	2.25	0.69
2:D:549:PHE:CE2	2:D:571:ILE:HG13	2.28	0.68
1:A:162:LYS:NZ	4:B:710:HOH:O	2.26	0.67
1:A:9:LYS:HG2	4:A:388:HOH:O	1.94	0.66
1:A:136:PHE:CE1	1:A:176:LEU:HD13	2.25	0.65
1:A:136:PHE:CE1	1:A:176:LEU:HD11	2.32	0.65
1:A:155:ARG:NH2	2:B:555:ASP:OD1	2.27	0.65
1:A:256:VAL:C	1:A:257:LEU:HD12	2.18	0.64
1:A:9:LYS:N	4:A:388:HOH:O	2.32	0.62
1:A:130:GLN:HA	1:A:130:GLN:OE1	2.00	0.60
2:D:568:ILE:O	2:D:572:ASN:HB2	2.01	0.60
1:A:257:LEU:HD12	1:A:257:LEU:H	1.66	0.60
1:C:168:LEU:HA	4:C:346:HOH:O	2.01	0.59
1:C:130:GLN:HA	1:C:130:GLN:OE1	2.03	0.59
1:A:136:PHE:O	1:A:140:VAL:HG23	2.03	0.57
1:A:137:GLN:C	1:A:139:THR:N	2.55	0.57
1:A:127:GLY:O	1:A:130:GLN:HB2	2.04	0.57
1:C:82:ALA:HB1	3:D:600:ZMK:CBB	2.35	0.57
2:B:509:ILE:HD11	2:B:548:GLU:CB	2.35	0.56
1:A:6:TRP:CZ3	1:A:45:VAL:HG22	2.40	0.56
1:A:134:ASP:HB3	4:A:377:HOH:O	2.03	0.56
2:D:509:ILE:HD11	2:D:548:GLU:CB	2.36	0.56
2:B:570:TYR:HD1	4:B:701:HOH:O	1.85	0.56
1:A:82:ALA:HB1	3:B:600:ZMK:CBB	2.36	0.56
1:A:137:GLN:O	1:A:139:THR:N	2.39	0.56
2:B:570:TYR:CD1	4:B:701:HOH:O	2.53	0.55
1:C:6:TRP:CZ3	1:C:45:VAL:HG22	2.41	0.55
1:A:137:GLN:O	1:A:138:ARG:C	2.45	0.55
1:C:224:HIS:O	1:C:224:HIS:ND1	2.40	0.55
1:A:256:VAL:C	1:A:257:LEU:CD1	2.75	0.54
2:B:506:VAL:O	2:B:510:ILE:HG12	2.08	0.54
2:D:509:ILE:HD11	2:D:548:GLU:HG2	1.89	0.54
1:C:244:GLU:O	1:C:248:LEU:CD1	2.56	0.54
1:C:124:VAL:CG1	3:D:600:ZMK:H16	2.38	0.54
2:B:509:ILE:HD11	2:B:548:GLU:HG2	1.89	0.54
1:A:143:PHE:HZ	3:B:600:ZMK:H2	1.74	0.52
1:C:137:GLN:C	1:C:139:THR:N	2.62	0.52
2:D:506:VAL:O	2:D:510:ILE:HG12	2.09	0.52
1:C:201:ARG:HD3	1:C:222:TRP:CZ3	2.45	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PHE:C	1:A:130:GLN:H	2.14	0.52
1:C:124:VAL:HG12	3:D:600:ZMK:H16	1.91	0.51
1:A:247:HIS:CD2	4:C:346:HOH:O	2.64	0.50
1:A:136:PHE:CZ	1:A:176:LEU:HD11	2.46	0.50
1:A:136:PHE:HE1	1:A:176:LEU:HD12	1.68	0.50
1:A:181:GLU:OE1	1:A:181:GLU:CA	2.52	0.49
1:C:155:ARG:NH1	2:D:546:GLU:CD	2.66	0.49
1:A:201:ARG:HD3	1:A:222:TRP:CZ3	2.47	0.49
1:A:224:HIS:O	1:A:224:HIS:ND1	2.45	0.49
1:A:136:PHE:CE1	1:A:176:LEU:HD12	2.43	0.49
1:A:95:HIS:CD2	4:A:324:HOH:O	2.52	0.48
1:C:136:PHE:CD2	1:C:137:GLN:N	2.82	0.48
1:A:132:LEU:HD22	1:A:136:PHE:CD1	2.48	0.48
1:C:173:VAL:O	1:C:177:ASN:HB2	2.13	0.48
2:D:510:ILE:HD12	2:D:527:PHE:CE1	2.48	0.48
2:D:549:PHE:CD2	2:D:571:ILE:HG13	2.48	0.48
2:B:510:ILE:HD12	2:B:527:PHE:CE1	2.49	0.48
2:B:549:PHE:CD2	2:B:571:ILE:HG13	2.48	0.48
3:B:600:ZMK:H28	3:B:600:ZMK:OAG	2.12	0.48
1:C:137:GLN:O	1:C:140:VAL:N	2.47	0.47
2:B:508:LYS:HE3	4:B:706:HOH:O	2.14	0.47
2:D:509:ILE:HD11	2:D:548:GLU:CG	2.44	0.47
1:C:128:PHE:C	1:C:130:GLN:H	2.17	0.47
1:C:137:GLN:O	1:C:138:ARG:C	2.51	0.47
2:B:509:ILE:HD11	2:B:548:GLU:CG	2.44	0.47
1:C:165:VAL:HG13	1:C:170:MET:SD	2.55	0.46
1:A:173:VAL:O	1:A:177:ASN:HB2	2.16	0.46
1:A:137:GLN:O	1:A:140:VAL:N	2.49	0.46
1:C:54:ARG:NH2	1:C:169:PRO:HB2	2.31	0.46
1:C:149:MET:HE3	1:C:149:MET:HB3	1.84	0.46
1:C:228:TYR:CD2	1:C:248:LEU:HD21	2.51	0.46
1:A:155:ARG:HB3	1:A:159:ARG:HH12	1.82	0.45
1:C:79:LEU:C	1:C:79:LEU:HD23	2.37	0.45
1:C:169:PRO:HD3	4:C:346:HOH:O	2.16	0.45
1:A:79:LEU:C	1:A:79:LEU:HD23	2.37	0.44
1:A:190:GLN:N	1:A:191:PRO:HD2	2.32	0.44
3:D:600:ZMK:NAW	3:D:600:ZMK:CAC	2.79	0.44
1:A:220:LYS:NZ	4:A:385:HOH:O	1.89	0.44
1:C:116:GLU:HG3	4:C:335:HOH:O	2.16	0.44
1:A:54:ARG:NH2	1:A:169:PRO:HB2	2.32	0.44
1:C:6:TRP:CE3	1:C:45:VAL:HG22	2.53	0.44

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ARG:HD3	1:C:222:TRP:HZ3	1.83	0.44
2:B:570:TYR:O	2:B:574:HIS:ND1	2.40	0.44
1:C:136:PHE:CD2	1:C:136:PHE:C	2.91	0.44
1:A:244:GLU:O	1:A:248:LEU:CD1	2.61	0.43
1:C:190:GLN:N	1:C:191:PRO:HD2	2.33	0.43
2:B:549:PHE:CE2	2:B:571:ILE:HG21	2.53	0.43
1:C:137:GLN:O	1:C:139:THR:N	2.51	0.43
2:D:553:ILE:HG23	2:D:557:GLU:HB2	2.00	0.43
2:D:535:SER:O	2:D:539:VAL:HG23	2.19	0.43
1:A:201:ARG:HD3	1:A:222:TRP:HZ3	1.84	0.43
1:C:213:LYS:HZ3	1:C:213:LYS:HG3	1.71	0.43
1:C:155:ARG:HB3	1:C:159:ARG:HH12	1.83	0.42
2:D:570:TYR:O	2:D:574:HIS:ND1	2.40	0.42
2:B:549:PHE:CD2	2:B:571:ILE:HD12	2.54	0.42
2:B:553:ILE:HG23	2:B:557:GLU:HB2	2.01	0.42
1:C:127:GLY:O	1:C:131:GLN:HG3	2.20	0.42
1:A:255:ARG:C	1:A:257:LEU:HD12	2.40	0.42
1:A:255:ARG:C	1:A:257:LEU:CD1	2.89	0.41
1:C:181:GLU:OE1	1:C:181:GLU:CA	2.51	0.41
2:B:535:SER:O	2:B:539:VAL:HG23	2.21	0.41
1:A:6:TRP:CE3	1:A:45:VAL:HG22	2.56	0.41
1:C:215:VAL:HB	1:C:216:PRO:HD3	2.02	0.41
1:A:228:TYR:HE1	4:C:314:HOH:O	2.02	0.41
2:D:571:ILE:HD13	2:D:571:ILE:HA	1.83	0.40
2:D:514:LEU:HD23	2:D:514:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	253/264 (96%)	246 (97%)	6 (2%)	1 (0%)	30 23

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	253/264 (96%)	246 (97%)	6 (2%)	1 (0%)	30	23
2	B	73/77 (95%)	70 (96%)	3 (4%)	0	100	100
2	D	73/77 (95%)	69 (94%)	4 (6%)	0	100	100
All	All	652/682 (96%)	631 (97%)	19 (3%)	2 (0%)	37	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	ASP
1	C	134	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	212/221 (96%)	199 (94%)	13 (6%)	15	9
1	C	212/221 (96%)	199 (94%)	13 (6%)	15	9
2	B	62/66 (94%)	58 (94%)	4 (6%)	14	7
2	D	62/66 (94%)	58 (94%)	4 (6%)	14	7
All	All	548/574 (96%)	514 (94%)	34 (6%)	15	8

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ASP
1	A	130	GLN
1	A	132	LEU
1	A	137	GLN
1	A	146	LEU
1	A	149	MET
1	A	166	LEU
1	A	181	GLU
1	A	196	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	197	MET
1	A	199	PHE
1	A	213	LYS
1	A	257	LEU
1	C	71	GLN
1	C	123	ASP
1	C	130	GLN
1	C	132	LEU
1	C	137	GLN
1	C	146	LEU
1	C	149	MET
1	C	166	LEU
1	C	181	GLU
1	C	196	SER
1	C	197	MET
1	C	199	PHE
1	C	213	LYS
2	D	500	SER
2	D	551	THR
2	D	552	GLU
2	D	556	GLU
2	B	500	SER
2	B	551	THR
2	B	552	GLU
2	B	556	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ZMK	D	600	2	30,32,32	1.16	2 (6%)	38,42,42	2.34	11 (28%)
3	ZMK	B	600	2	30,32,32	1.16	2 (6%)	38,42,42	2.14	9 (23%)

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	ZMK	D	600	2	-	21/40/40/40	-
3	ZMK	B	600	2	-	17/40/40/40	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	600	ZMK	CBC-SAZ	-4.15	1.66	1.76
3	D	600	ZMK	OAX-CBB	4.13	1.45	1.33
3	D	600	ZMK	CBC-SAZ	-3.97	1.66	1.76
3	B	600	ZMK	OAX-CBB	3.92	1.45	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600	ZMK	CAT-CBC-SAZ	7.71	122.59	113.40
3	B	600	ZMK	CAT-CBC-SAZ	7.14	121.91	113.40
3	B	600	ZMK	CAS-CAP-NAW	-5.35	100.62	112.00
3	D	600	ZMK	CAS-CAP-NAW	-4.94	101.49	112.00
3	B	600	ZMK	OAF-CBC-SAZ	-4.91	116.43	122.68
3	D	600	ZMK	OAF-CBC-SAZ	-4.43	117.04	122.68
3	D	600	ZMK	CAQ-CAO-NAV	-4.38	103.28	112.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	600	ZMK	CAP-NAW-CBD	3.60	129.02	122.55
3	B	600	ZMK	CAQ-CAO-NAV	-3.50	105.11	112.41
3	D	600	ZMK	OAF-CBC-CAT	-3.13	120.37	123.98
3	D	600	ZMK	CAO-NAV-CBA	2.93	128.28	122.82
3	D	600	ZMK	OAY-CAU-CBF	-2.87	105.93	110.55
3	D	600	ZMK	CAP-CAS-CBA	-2.75	107.80	112.39
3	B	600	ZMK	OAY-CAU-CBF	-2.54	106.47	110.55
3	D	600	ZMK	OAX-CBB-CAR	2.38	121.13	112.14
3	B	600	ZMK	CAP-NAW-CBD	2.23	126.55	122.55
3	B	600	ZMK	CAP-CAS-CBA	-2.21	108.70	112.39
3	D	600	ZMK	OAH-PBG-OAY	-2.07	101.27	106.67
3	B	600	ZMK	CAA-OAX-CBB	2.06	122.67	116.07
3	B	600	ZMK	OAF-CBC-CAT	-2.01	121.66	123.98

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	600	ZMK	CAT-CBC-SAZ-CAQ
3	D	600	ZMK	OAF-CBC-SAZ-CAQ
3	D	600	ZMK	CAO-CAQ-SAZ-CBC
3	D	600	ZMK	CAQ-CAO-NAV-CBA
3	D	600	ZMK	NAW-CAP-CAS-CBA
3	D	600	ZMK	OAY-CAU-CBF-CBE
3	D	600	ZMK	OAY-CAU-CBF-CAC
3	D	600	ZMK	OAY-CAU-CBF-CAB
3	B	600	ZMK	NAW-CAP-CAS-CBA
3	B	600	ZMK	OAY-CAU-CBF-CBE
3	B	600	ZMK	CAU-OAY-PBG-OAK
3	B	600	ZMK	CAU-OAY-PBG-OAH
3	B	600	ZMK	CAR-CBB-OAX-CAA
3	B	600	ZMK	OAE-CBB-OAX-CAA
3	D	600	ZMK	CAR-CBB-OAX-CAA
3	B	600	ZMK	CAL-CAM-CAR-CBB
3	B	600	ZMK	CAN-CAL-CAM-CAR
3	D	600	ZMK	CAL-CAM-CAR-CBB
3	B	600	ZMK	CAM-CAL-CAN-CAT
3	D	600	ZMK	OAE-CBB-OAX-CAA
3	D	600	ZMK	OAI-CBE-CBF-CAC
3	D	600	ZMK	OAI-CBE-CBF-CAB
3	D	600	ZMK	NAW-CBD-CBE-OAI
3	B	600	ZMK	CAN-CAT-CBC-OAF

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	600	ZMK	CAN-CAT-CBC-SAZ
3	D	600	ZMK	CBD-CBE-CBF-CAC
3	D	600	ZMK	CBD-CBE-CBF-CAU
3	B	600	ZMK	OAY-CAU-CBF-CAC
3	B	600	ZMK	OAY-CAU-CBF-CAB
3	B	600	ZMK	CAQ-CAO-NAV-CBA
3	D	600	ZMK	OAI-CBE-CBF-CAU
3	B	600	ZMK	OAG-CBD-CBE-CBF
3	B	600	ZMK	NAW-CBD-CBE-CBF
3	D	600	ZMK	CAN-CAL-CAM-CAR
3	D	600	ZMK	CAM-CAR-CBB-OAX
3	B	600	ZMK	CAU-OAY-PBG-OAJ
3	D	600	ZMK	CBD-CBE-CBF-CAB
3	D	600	ZMK	OAG-CBD-CBE-CBF

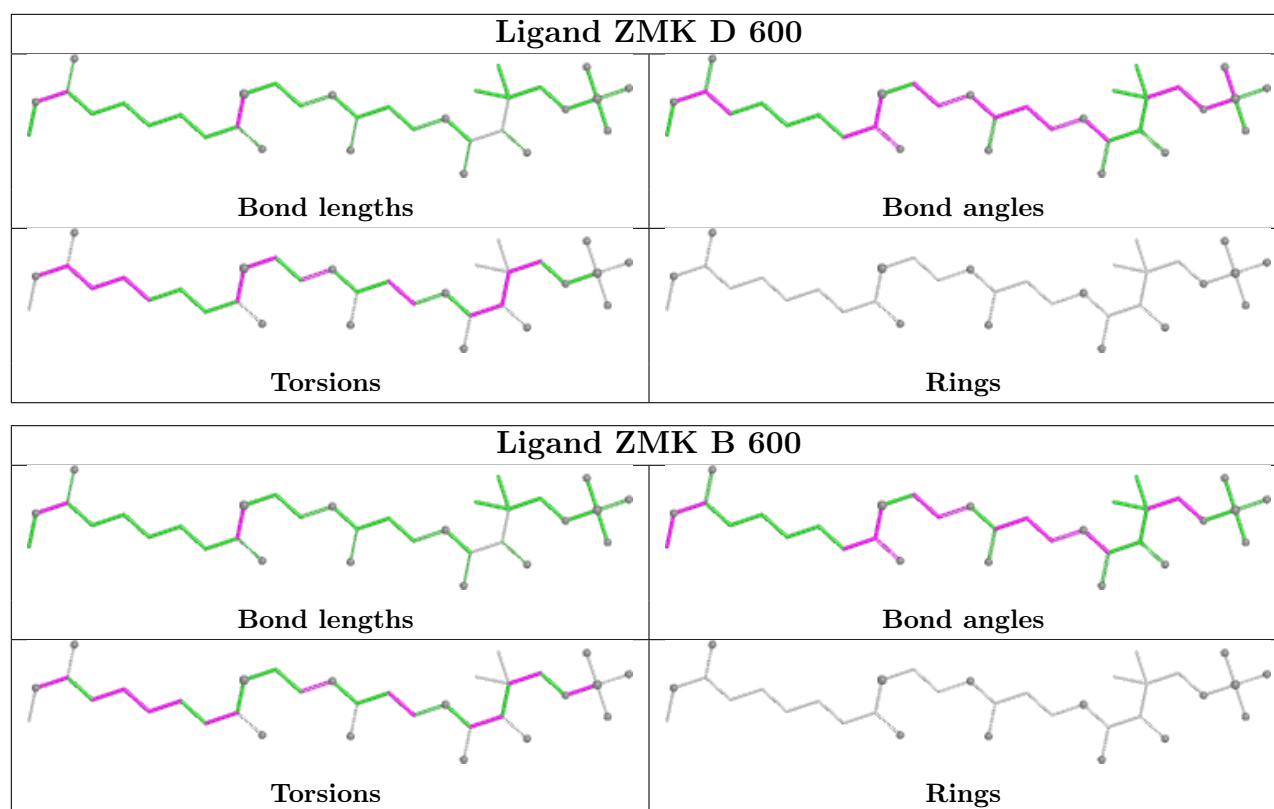
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	600	ZMK	4	0
3	B	600	ZMK	3	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	255/264 (96%)	0.07	10 (3%) 44 46	17, 37, 71, 119	0
1	C	255/264 (96%)	0.02	11 (4%) 40 43	18, 38, 70, 119	0
2	B	75/77 (97%)	0.82	8 (10%) 12 12	40, 62, 98, 112	0
2	D	75/77 (97%)	0.65	4 (5%) 33 35	40, 63, 98, 113	0
All	All	660/682 (96%)	0.20	33 (5%) 35 38	17, 42, 84, 119	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	PHE	6.7
1	C	228	TYR	4.7
1	A	228	TYR	4.0
2	B	572	ASN	3.6
1	C	55	GLY	3.1
1	A	137	GLN	3.0
1	A	135	ASP	2.9
1	A	55	GLY	2.8
1	C	136	PHE	2.7
1	A	170	MET	2.7
2	B	574	HIS	2.7
2	B	502	ILE	2.7
2	D	573	GLY	2.5
1	C	254	GLN	2.5
2	B	505	ARG	2.5
2	B	516	VAL	2.4
1	C	54	ARG	2.4
1	C	166	LEU	2.3
2	B	549	PHE	2.3
1	C	257	LEU	2.3
1	C	170	MET	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	137	GLN	2.3
2	B	571	ILE	2.3
1	A	166	LEU	2.3
2	B	573	GLY	2.2
2	D	541	LEU	2.2
1	A	130	GLN	2.2
1	A	181	GLU	2.1
1	C	133	SER	2.1
2	D	571	ILE	2.1
1	C	167	ALA	2.1
2	D	574	HIS	2.1
1	A	140	VAL	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

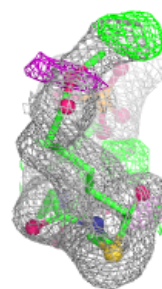
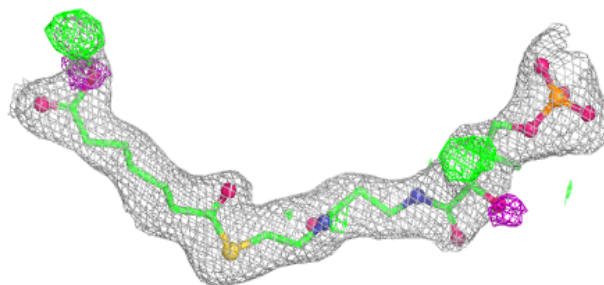
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	ZMK	D	600	33/33	0.89	0.14	23,46,98,99	0
3	ZMK	B	600	33/33	0.91	0.12	22,49,79,94	0

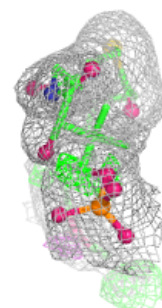
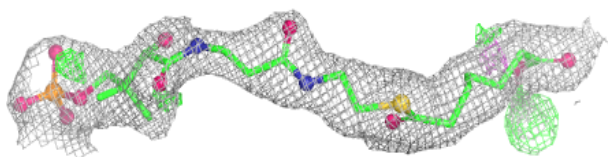
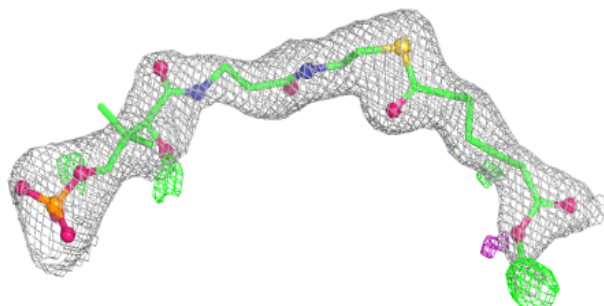
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ZMK D 600:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ZMK B 600:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.