



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:08 PM UTC

PDB ID : 5MF6 / pdb_00005mf6
Title : Human Sirt6 in complex with activator UBCS039
Authors : Steegborn, C.; You, W.; Kambach, C.
Deposited on : 2016-11-17
Resolution : 1.87 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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

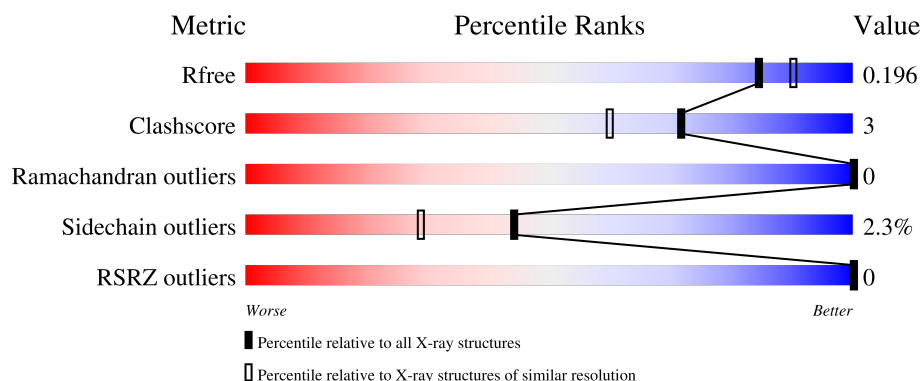
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 ≥ 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	302	
1	B	302	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4701 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 NAD-dependent protein deacetylase sirtuin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	1	0
			2202	1387	407	397	11			
1	B	275	Total	C	N	O	S	0	1	0
			2151	1353	400	387	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLY	-	expression tag	UNP Q8N6T7
A	8	ILE	GLY	expression tag	UNP Q8N6T7
A	9	ASP	LEU	expression tag	UNP Q8N6T7
A	10	PRO	SER	expression tag	UNP Q8N6T7
A	11	PHE	PRO	expression tag	UNP Q8N6T7
A	12	THR	TYR	expression tag	UNP Q8N6T7
B	7	GLY	-	expression tag	UNP Q8N6T7
B	8	ILE	GLY	expression tag	UNP Q8N6T7
B	9	ASP	LEU	expression tag	UNP Q8N6T7
B	10	PRO	SER	expression tag	UNP Q8N6T7
B	11	PHE	PRO	expression tag	UNP Q8N6T7
B	12	THR	TYR	expression tag	UNP Q8N6T7

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	B	1	Total 36	C 15	N 5	O 14	P 2	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



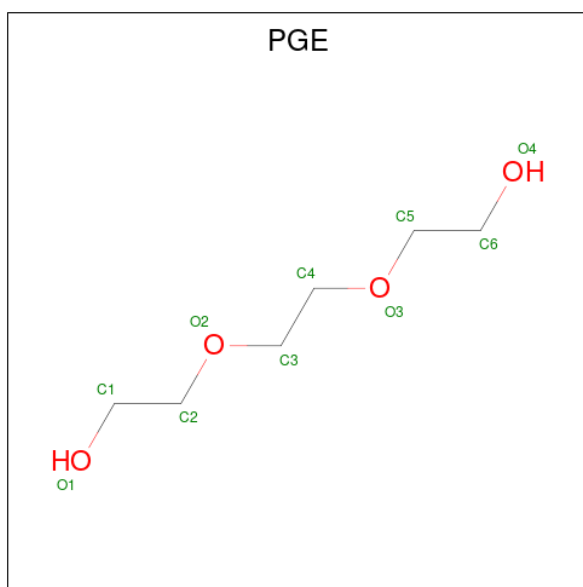
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



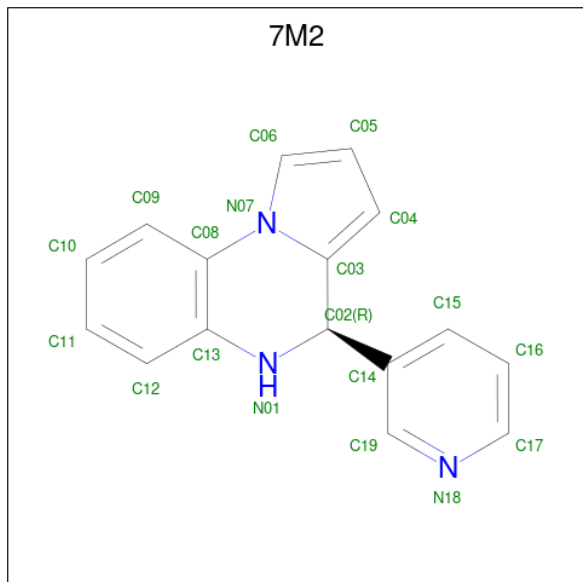
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is (4 {R})-4-pyridin-3-yl-4,5-dihydropyrrolo[1,2-a]quinoxaline (CCD ID: 7M2) (formula: C₁₆H₁₃N₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			19	16	3		
7	B	1	Total	C	N	0	0
			19	16	3		

- Molecule 8 is water.

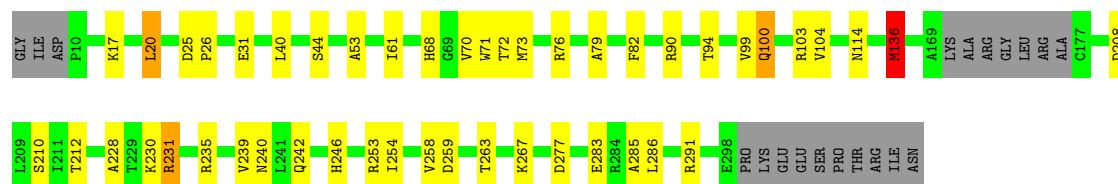
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	100	Total	O	0	0
			100	100		
8	B	74	Total	O	0	0
			74	74		

3 Residue-property plots

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.

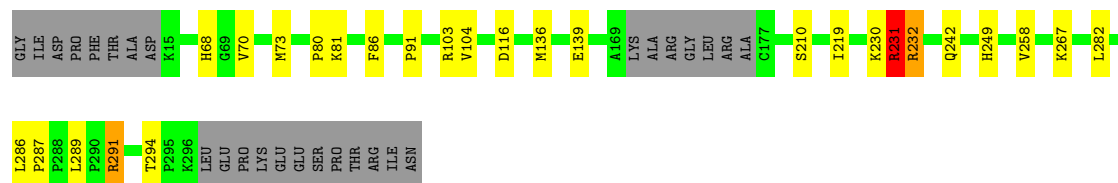
- Molecule 1: NAD-dependent protein deacetylase sirtuin-6

Chain A: 



- Molecule 1: NAD-dependent protein deacetylase sirtuin-6

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	91.30Å 91.30Å 144.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.65 – 1.87 45.65 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.65-1.87) 99.9 (45.65-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.190 , 0.220 0.164 , 0.196	Depositor DCC
R_{free} test set	2810 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.193 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.799 for H, K, L 0.201 for K, H, -L	Depositor
Outliers	0 of 56119 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4701	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, 0.333 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: PGE, AR6, 7M2, ZN, EDO, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.65	17/2254 (0.8%)	1.42	16/3057 (0.5%)
1	B	1.35	6/2201 (0.3%)	1.28	8/2984 (0.3%)
All	All	1.51	23/4455 (0.5%)	1.35	24/6041 (0.4%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	PRO	CA-C	11.84	1.58	1.51
1	A	254	ILE	N-CA	-7.96	1.36	1.46
1	A	61	ILE	CA-C	-6.58	1.47	1.53
1	A	285	ALA	CA-C	6.21	1.60	1.52
1	A	240	ASN	N-CA	6.18	1.53	1.46
1	B	291	ARG	N-CA	6.13	1.50	1.46
1	B	91	PRO	C-O	6.01	1.30	1.23
1	A	61	ILE	N-CA	-5.92	1.41	1.46
1	A	25	ASP	CA-C	-5.80	1.46	1.53
1	A	114	ASN	N-CA	-5.51	1.38	1.46
1	A	286	LEU	N-CA	5.50	1.53	1.45
1	A	82	PHE	N-CA	5.45	1.52	1.46
1	A	100	GLN	CA-C	-5.44	1.45	1.52
1	A	94	THR	C-O	5.36	1.30	1.24
1	A	246	HIS	CA-C	-5.28	1.46	1.53
1	A	277	ASP	N-CA	5.25	1.53	1.46
1	B	116	ASP	C-O	-5.22	1.17	1.24
1	B	139	GLU	C-O	5.21	1.30	1.23
1	A	20	LEU	C-O	5.18	1.30	1.23
1	A	212	THR	CA-C	-5.13	1.46	1.52
1	B	282	LEU	CA-C	-5.13	1.46	1.52
1	A	253	ARG	CA-CB	5.04	1.63	1.53
1	A	235	ARG	N-CA	-5.02	1.40	1.45

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	MET	CA-CB-CG	10.29	134.68	114.10
1	A	61	ILE	CA-C-N	-6.70	113.40	120.03
1	A	61	ILE	C-N-CA	-6.70	113.40	120.03
1	B	294	THR	CA-C-N	-6.37	114.10	120.21
1	B	294	THR	C-N-CA	-6.37	114.10	120.21
1	B	231	ARG	N-CA-C	6.31	118.16	111.28
1	B	258	VAL	N-CA-CB	6.24	118.27	110.47
1	A	239	VAL	N-CA-C	-5.90	99.14	107.75
1	A	26	PRO	CA-C-N	5.77	125.45	119.05
1	A	26	PRO	C-N-CA	5.77	125.45	119.05
1	A	258	VAL	N-CA-CB	5.66	120.33	110.65
1	A	242	GLN	N-CA-C	-5.65	103.53	110.31
1	A	53	ALA	CA-C-O	5.53	126.19	119.38
1	A	79	ALA	CA-C-N	-5.53	114.90	120.21
1	A	79	ALA	C-N-CA	-5.53	114.90	120.21
1	A	25	ASP	CA-C-N	-5.53	114.68	120.38
1	A	25	ASP	C-N-CA	-5.53	114.68	120.38
1	A	283	GLU	N-CA-C	5.47	117.33	111.36
1	B	286	LEU	CA-C-N	-5.23	115.84	119.66
1	B	286	LEU	C-N-CA	-5.23	115.84	119.66
1	B	291	ARG	CA-C-N	-5.21	115.01	120.38
1	B	291	ARG	C-N-CA	-5.21	115.01	120.38
1	A	230	LYS	CA-C-N	5.17	129.41	121.19
1	A	230	LYS	C-N-CA	5.17	129.41	121.19

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	2202	0	2220	18	0
1	B	2151	0	2174	14	0
2	A	36	0	21	0	0
2	B	36	0	21	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	20	0	0	0	0
4	B	20	0	0	0	0
5	A	8	0	12	0	0
5	B	4	0	6	0	0
6	A	10	0	14	0	0
7	A	19	0	0	0	0
7	B	19	0	0	0	0
8	A	100	0	0	5	0
8	B	74	0	0	0	0
All	All	4701	0	4468	30	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 3.

All (30) 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:103[A]:ARG:HD3	8:A:590:HOH:O	1.71	0.89
1:B:86:PHE:CG	1:B:136:MET:HE1	2.08	0.89
1:A:103[A]:ARG:CD	8:A:590:HOH:O	2.35	0.71
1:B:86:PHE:CD2	1:B:136:MET:HE1	2.29	0.67
1:A:44:SER:HB3	1:A:208:ASP:OD1	1.99	0.63
1:A:68:HIS:CE1	1:B:73:MET:HE2	2.34	0.63
1:B:103[A]:ARG:CG	1:B:289:LEU:HG	2.30	0.62
1:A:20:LEU:HD13	8:A:570:HOH:O	2.01	0.59
1:B:231:ARG:HG2	1:B:232:ARG:N	2.18	0.57
1:A:20:LEU:HD12	8:A:545:HOH:O	2.06	0.56
1:B:103[A]:ARG:HG2	1:B:289:LEU:HG	1.89	0.54
1:A:228:ALA:O	1:A:231:ARG:HB2	2.07	0.54
1:A:259:ASP:O	1:A:263:THR:HG23	2.08	0.53
1:A:17:LYS:HB3	1:A:20:LEU:HD11	1.91	0.52
1:A:72:THR:O	1:A:76:ARG:HD3	2.11	0.51
1:A:73:MET:HE2	1:B:68:HIS:CE1	2.48	0.48
1:B:104:VAL:HB	1:B:291:ARG:HB3	1.96	0.47
1:B:230:LYS:HE2	1:B:249:HIS:O	2.16	0.46
1:A:100:GLN:HA	1:A:100:GLN:OE1	2.18	0.44
1:B:103[A]:ARG:HG3	1:B:289:LEU:HG	1.97	0.43
1:B:103[A]:ARG:NH1	1:B:289:LEU:HD21	2.34	0.42
1:A:136:MET:HB3	1:A:136:MET:HE3	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:VAL:HA	1:B:80:PRO:HB3	2.02	0.41
1:A:40:LEU:O	1:A:44:SER:OG	2.34	0.41
1:A:99:VAL:O	1:A:103[B]:ARG:HG3	2.20	0.41
1:A:90:ARG:HG3	8:A:516:HOH:O	2.21	0.41
1:A:70:VAL:HG12	1:A:71:TRP:CE3	2.56	0.40
1:B:242:GLN:HG3	2:B:401:AR6:O2'	2.22	0.40
1:A:104:VAL:HB	1:A:291:ARG:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	279/302 (92%)	274 (98%)	5 (2%)	0	100	100
1	B	272/302 (90%)	268 (98%)	4 (2%)	0	100	100
All	All	551/604 (91%)	542 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	238/256 (93%)	233 (98%)	5 (2%)	47	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	233/256 (91%)	227 (97%)	6 (3%)	40	24
All	All	471/512 (92%)	460 (98%)	11 (2%)	44	29

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	136	MET
1	A	210	SER
1	A	231	ARG
1	A	267	LYS
1	B	81	LYS
1	B	210	SER
1	B	219	ILE
1	B	231	ARG
1	B	232	ARG
1	B	267	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	43	GLN
1	B	93	GLN

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

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	SO4	B	405	-	4,4,4	0.58	0	6,6,6	0.65	0
5	EDO	A	407	-	3,3,3	0.62	0	2,2,2	0.19	0
5	EDO	B	407	-	3,3,3	0.43	0	2,2,2	0.44	0
7	7M2	B	408	-	22,22,22	0.79	1 (4%)	28,31,31	0.73	2 (7%)
4	SO4	B	404	-	4,4,4	0.29	0	6,6,6	0.72	0
4	SO4	B	406	-	4,4,4	0.51	0	6,6,6	0.68	0
4	SO4	A	403	-	4,4,4	0.61	0	6,6,6	0.97	0
4	SO4	A	404	-	4,4,4	0.61	0	6,6,6	0.88	0
5	EDO	A	408	-	3,3,3	0.31	0	2,2,2	0.53	0
7	7M2	A	410	-	22,22,22	0.77	0	28,31,31	0.69	1 (3%)
4	SO4	A	406	-	4,4,4	0.50	0	6,6,6	0.42	0
6	PGE	A	409	-	9,9,9	0.63	0	8,8,8	0.41	0
4	SO4	B	403	-	4,4,4	0.49	0	6,6,6	0.77	0
2	AR6	B	401	-	39,39,39	1.54	7 (17%)	56,60,60	1.95	16 (28%)
4	SO4	A	405	-	4,4,4	0.41	0	6,6,6	0.67	0
2	AR6	A	401	-	39,39,39	1.80	5 (12%)	56,60,60	1.62	13 (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
5	EDO	A	407	-	-	1/1/1/1	-
2	AR6	A	401	-	-	0/22/54/54	0/4/4/4
5	EDO	B	407	-	-	1/1/1/1	-
7	7M2	B	408	-	-	2/4/16/16	0/4/4/4
7	7M2	A	410	-	-	2/4/16/16	0/4/4/4
6	PGE	A	409	-	-	3/7/7/7	-
2	AR6	B	401	-	-	1/22/54/54	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	408	-	-	1/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	AR6	PA-O3A	6.51	1.66	1.59
2	A	401	AR6	C1D-C2D	4.56	1.58	1.52
2	B	401	AR6	PA-O3A	3.85	1.63	1.59
2	B	401	AR6	C5-C4	3.73	1.45	1.39
2	B	401	AR6	C2-N1	3.70	1.40	1.33
2	B	401	AR6	C4-N3	3.29	1.40	1.34
2	A	401	AR6	C3'-C4'	3.14	1.61	1.53
7	B	408	7M2	C02-C03	2.92	1.53	1.50
2	A	401	AR6	C4-N3	2.82	1.39	1.34
2	B	401	AR6	C4-N9	-2.60	1.32	1.37
2	B	401	AR6	PB-O3A	-2.57	1.56	1.59
2	B	401	AR6	O4'-C4'	-2.17	1.40	1.45
2	A	401	AR6	O4'-C4'	-2.06	1.40	1.45

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	AR6	C4-N9-C8	6.10	112.15	105.74
2	B	401	AR6	N9-C8-N7	-4.19	107.99	113.94
2	B	401	AR6	C2-N1-C6	4.06	125.39	118.73
2	A	401	AR6	O1A-PA-O2A	3.98	130.94	112.44
2	B	401	AR6	C1D-C2D-C3D	3.83	107.00	102.29
2	B	401	AR6	N3-C2-N1	-3.65	123.06	128.58
2	A	401	AR6	C2-N1-C6	3.59	124.63	118.73
2	B	401	AR6	N3-C4-N9	3.45	133.03	127.17
2	B	401	AR6	O4'-C1'-N9	-3.23	101.89	108.09
2	B	401	AR6	C2'-C1'-N9	3.22	121.31	113.30
2	A	401	AR6	O3A-PB-O2B	3.09	120.01	110.70
2	B	401	AR6	C5-N7-C8	3.02	108.20	103.45
2	A	401	AR6	N3-C2-N1	-2.81	124.33	128.58
2	A	401	AR6	O3'-C3'-C2'	2.79	120.77	111.82
2	A	401	AR6	O1D-C1D-O4D	-2.71	107.67	111.12
2	B	401	AR6	C4-N9-C1'	-2.58	120.60	126.63
2	B	401	AR6	C5-C4-N3	-2.57	123.17	126.72
2	A	401	AR6	O4'-C1'-C2'	-2.50	101.27	106.62
2	A	401	AR6	C4-N9-C8	2.44	108.30	105.74
2	B	401	AR6	C2D-C3D-C4D	-2.43	97.91	102.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	AR6	N6-C6-N1	2.40	123.72	118.38
2	B	401	AR6	O2D-C2D-C3D	-2.36	104.25	111.82
2	B	401	AR6	C4-C5-N7	-2.29	107.96	110.58
7	A	410	7M2	C15-C14-C02	2.28	124.43	120.78
7	B	408	7M2	C04-C03-N07	-2.15	107.10	107.87
2	B	401	AR6	O5D-PB-O2B	2.12	117.34	108.94
7	B	408	7M2	C15-C14-C02	2.11	124.17	120.78
2	A	401	AR6	O2'-C2'-C3'	2.10	118.55	111.82
2	A	401	AR6	C4'-O4'-C1'	2.07	114.04	109.47
2	A	401	AR6	C4-C5-N7	-2.05	108.24	110.58
2	A	401	AR6	N6-C6-N1	2.04	122.92	118.38
2	A	401	AR6	O3'-C3'-C4'	-2.01	105.30	111.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	409	PGE	O3-C5-C6-O4
6	A	409	PGE	O1-C1-C2-O2
6	A	409	PGE	O2-C3-C4-O3
5	A	408	EDO	O1-C1-C2-O2
5	B	407	EDO	O1-C1-C2-O2
7	A	410	7M2	C03-C02-C14-C19
7	A	410	7M2	C03-C02-C14-C15
7	B	408	7M2	C03-C02-C14-C19
7	B	408	7M2	C03-C02-C14-C15
5	A	407	EDO	O1-C1-C2-O2
2	B	401	AR6	PA-O3A-PB-O1B

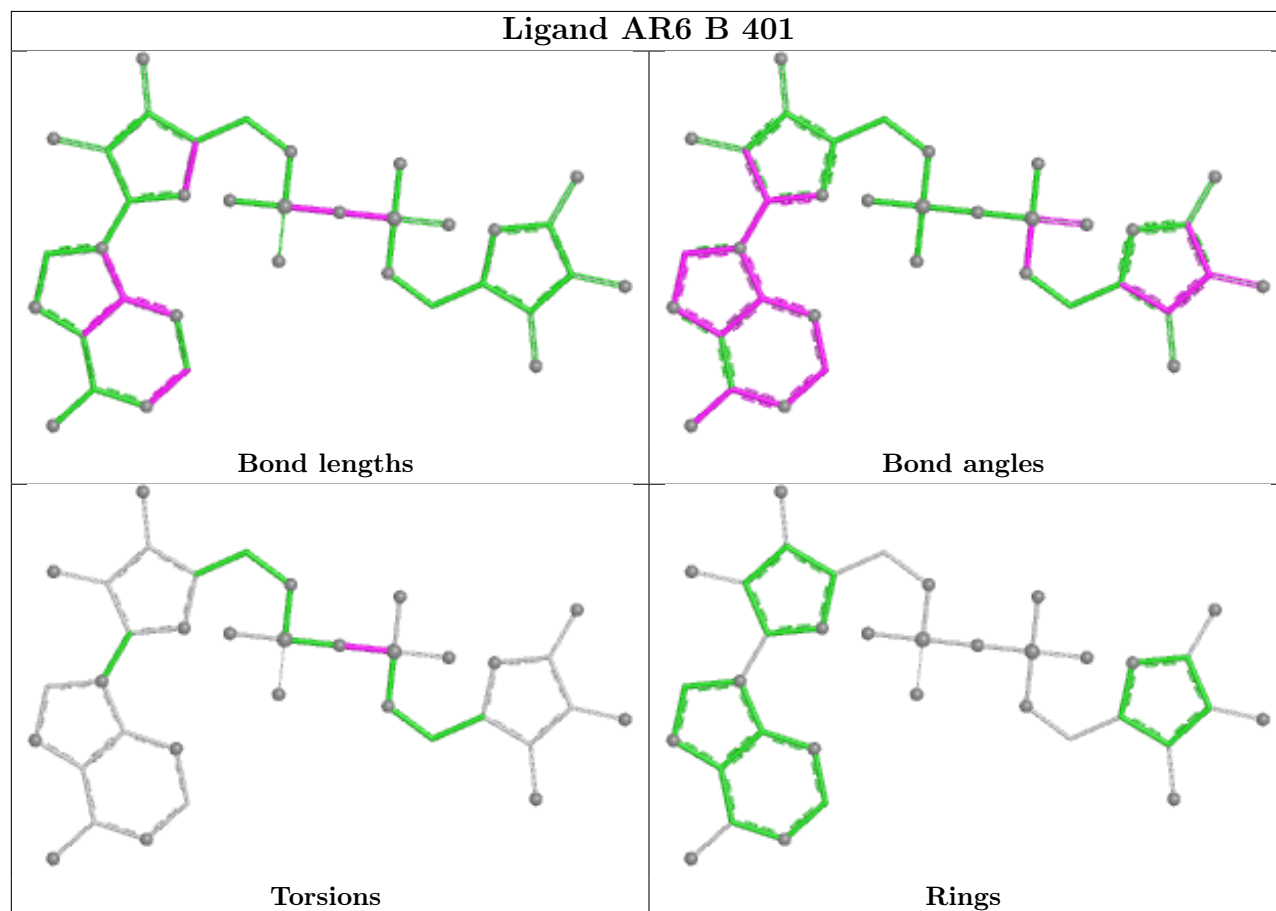
There are no ring outliers.

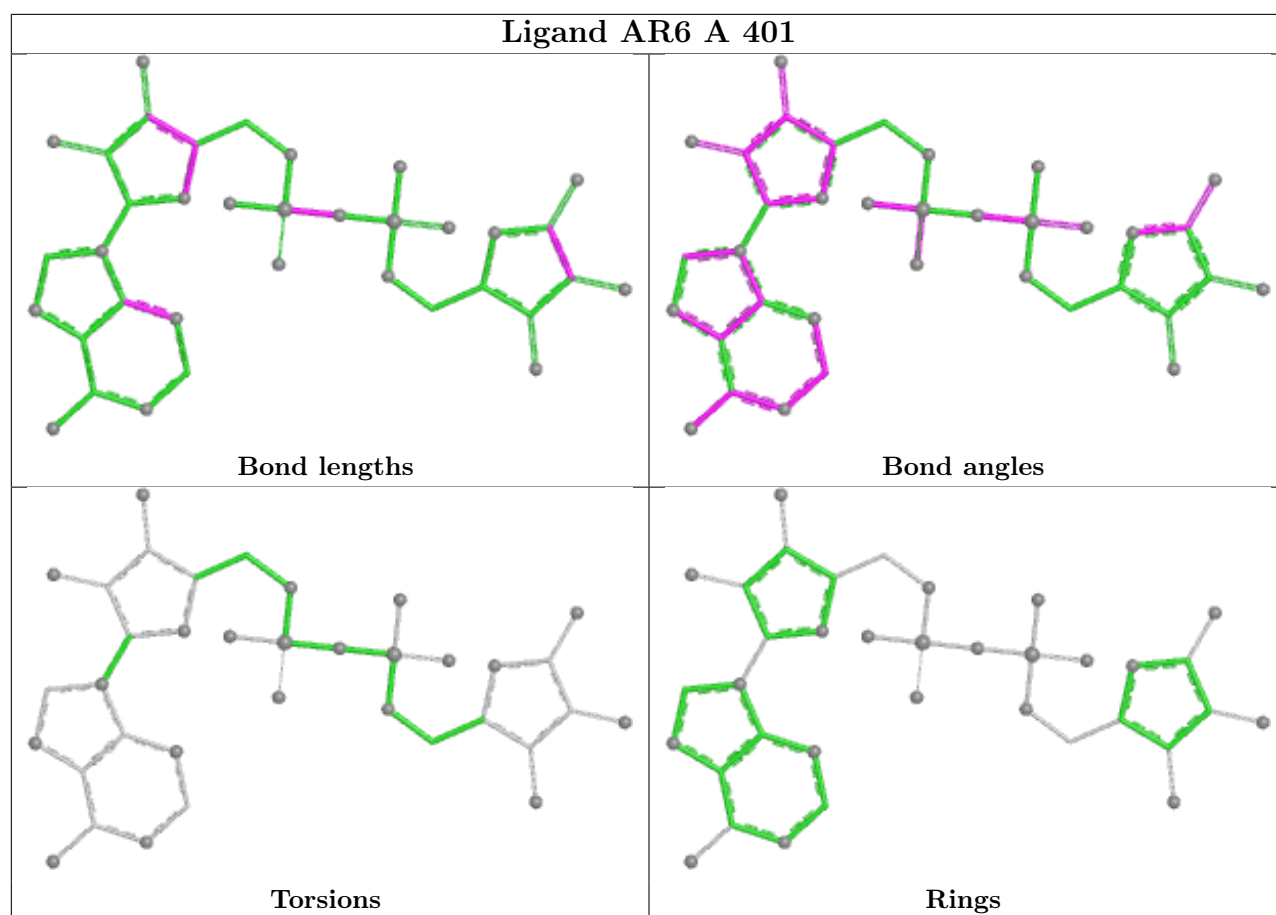
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	AR6	1	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 [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	282/302 (93%)	-1.15	0 100 100	12, 25, 48, 65	1 (0%)
1	B	275/302 (91%)	-1.00	0 100 100	14, 33, 60, 78	1 (0%)
All	All	557/604 (92%)	-1.07	0 100 100	12, 29, 55, 78	2 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
6	PGE	A	409	10/10	0.97	0.08	52,62,71,71	0
5	EDO	A	408	4/4	0.98	0.07	44,47,48,57	0
5	EDO	B	407	4/4	0.98	0.07	52,53,53,58	0
5	EDO	A	407	4/4	0.98	0.09	46,49,50,51	0
7	7M2	B	408	19/19	0.98	0.06	32,49,54,55	0
4	SO4	A	406	5/5	0.99	0.03	46,55,59,61	0
4	SO4	B	403	5/5	0.99	0.06	34,35,43,58	0

Continued on next page...

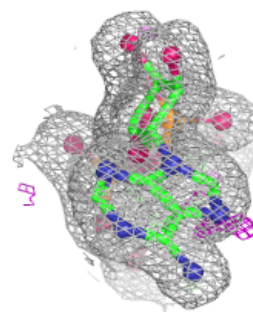
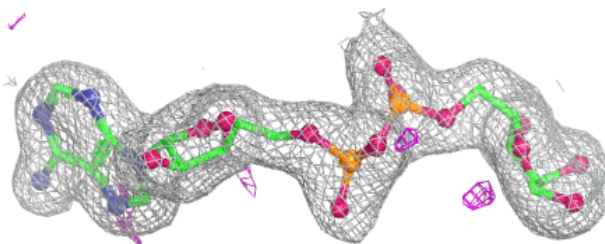
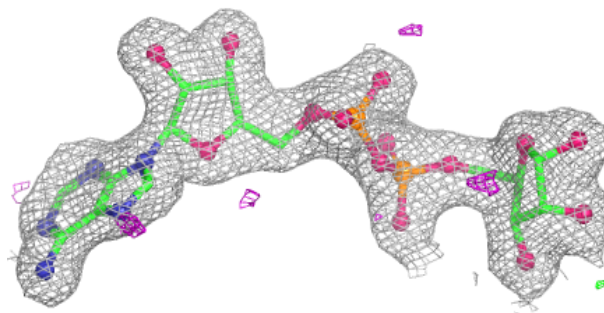
Continued from previous page...

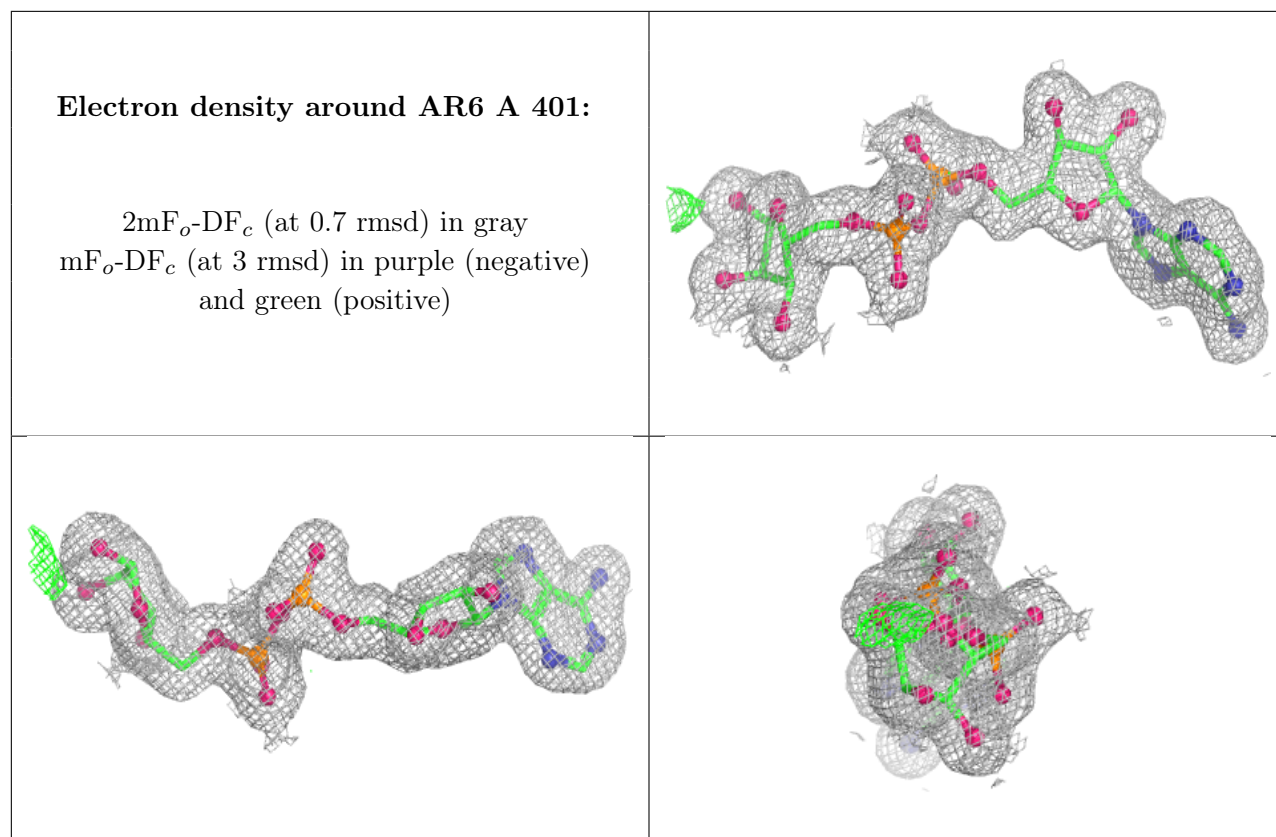
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	404	5/5	0.99	0.04	52,54,60,60	0
4	SO4	B	405	5/5	0.99	0.04	49,53,59,61	0
4	SO4	B	406	5/5	0.99	0.04	49,57,64,66	0
2	AR6	B	401	36/36	0.99	0.03	20,25,31,34	0
3	ZN	A	402	1/1	0.99	0.02	38,38,38,38	0
3	ZN	B	402	1/1	0.99	0.02	51,51,51,51	0
4	SO4	A	404	5/5	0.99	0.09	38,40,46,47	0
7	7M2	A	410	19/19	0.99	0.05	24,46,56,58	0
4	SO4	A	405	5/5	0.99	0.04	45,48,58,58	0
4	SO4	A	403	5/5	1.00	0.04	37,48,53,54	0
2	AR6	A	401	36/36	1.00	0.02	15,18,23,24	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 AR6 B 401:

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.