



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:26 pm BST

PDB ID : 4ZBP
Title : Crystal structure of the AMPCPR-bound AtNUDT7
Authors : Tang, Q.; Liu, C.; Zhong, C.; Ding, J.
Deposited on : 2015-04-15
Resolution : 2.60 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 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

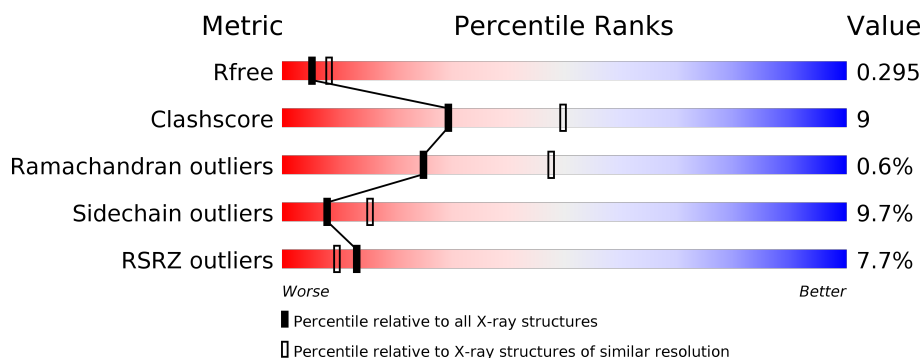
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	310	
1	B	310	
1	C	310	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADV	C	401	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6428 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 Nudix hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2050	1311	336	392	11			
1	B	270	Total	C	N	O	S	0	0	0
			2146	1369	354	412	11			
1	C	262	Total	C	N	O	S	0	0	0
			2086	1333	344	398	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	expression tag	UNP Q9SU14
A	-26	GLY	-	expression tag	UNP Q9SU14
A	-25	SER	-	expression tag	UNP Q9SU14
A	-24	HIS	-	expression tag	UNP Q9SU14
A	-23	HIS	-	expression tag	UNP Q9SU14
A	-22	HIS	-	expression tag	UNP Q9SU14
A	-21	HIS	-	expression tag	UNP Q9SU14
A	-20	HIS	-	expression tag	UNP Q9SU14
A	-19	HIS	-	expression tag	UNP Q9SU14
A	-18	HIS	-	expression tag	UNP Q9SU14
A	-17	HIS	-	expression tag	UNP Q9SU14
A	-16	GLY	-	expression tag	UNP Q9SU14
A	-15	SER	-	expression tag	UNP Q9SU14
A	-14	ASP	-	expression tag	UNP Q9SU14
A	-13	TYR	-	expression tag	UNP Q9SU14
A	-12	ASP	-	expression tag	UNP Q9SU14
A	-11	ILE	-	expression tag	UNP Q9SU14
A	-10	PRO	-	expression tag	UNP Q9SU14
A	-9	THR	-	expression tag	UNP Q9SU14
A	-8	THR	-	expression tag	UNP Q9SU14
A	-7	GLU	-	expression tag	UNP Q9SU14
A	-6	ASN	-	expression tag	UNP Q9SU14
A	-5	LEU	-	expression tag	UNP Q9SU14

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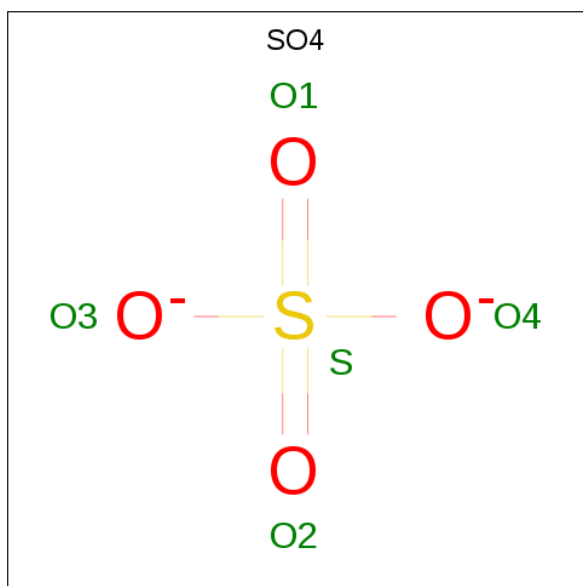
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	TYR	-	expression tag	UNP Q9SU14
A	-3	PHE	-	expression tag	UNP Q9SU14
A	-2	GLN	-	expression tag	UNP Q9SU14
A	-1	GLY	-	expression tag	UNP Q9SU14
A	0	SER	-	expression tag	UNP Q9SU14
B	-27	MET	-	expression tag	UNP Q9SU14
B	-26	GLY	-	expression tag	UNP Q9SU14
B	-25	SER	-	expression tag	UNP Q9SU14
B	-24	HIS	-	expression tag	UNP Q9SU14
B	-23	HIS	-	expression tag	UNP Q9SU14
B	-22	HIS	-	expression tag	UNP Q9SU14
B	-21	HIS	-	expression tag	UNP Q9SU14
B	-20	HIS	-	expression tag	UNP Q9SU14
B	-19	HIS	-	expression tag	UNP Q9SU14
B	-18	HIS	-	expression tag	UNP Q9SU14
B	-17	HIS	-	expression tag	UNP Q9SU14
B	-16	GLY	-	expression tag	UNP Q9SU14
B	-15	SER	-	expression tag	UNP Q9SU14
B	-14	ASP	-	expression tag	UNP Q9SU14
B	-13	TYR	-	expression tag	UNP Q9SU14
B	-12	ASP	-	expression tag	UNP Q9SU14
B	-11	ILE	-	expression tag	UNP Q9SU14
B	-10	PRO	-	expression tag	UNP Q9SU14
B	-9	THR	-	expression tag	UNP Q9SU14
B	-8	THR	-	expression tag	UNP Q9SU14
B	-7	GLU	-	expression tag	UNP Q9SU14
B	-6	ASN	-	expression tag	UNP Q9SU14
B	-5	LEU	-	expression tag	UNP Q9SU14
B	-4	TYR	-	expression tag	UNP Q9SU14
B	-3	PHE	-	expression tag	UNP Q9SU14
B	-2	GLN	-	expression tag	UNP Q9SU14
B	-1	GLY	-	expression tag	UNP Q9SU14
B	0	SER	-	expression tag	UNP Q9SU14
C	-27	MET	-	expression tag	UNP Q9SU14
C	-26	GLY	-	expression tag	UNP Q9SU14
C	-25	SER	-	expression tag	UNP Q9SU14
C	-24	HIS	-	expression tag	UNP Q9SU14
C	-23	HIS	-	expression tag	UNP Q9SU14
C	-22	HIS	-	expression tag	UNP Q9SU14
C	-21	HIS	-	expression tag	UNP Q9SU14
C	-20	HIS	-	expression tag	UNP Q9SU14
C	-19	HIS	-	expression tag	UNP Q9SU14

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	HIS	-	expression tag	UNP Q9SU14
C	-17	HIS	-	expression tag	UNP Q9SU14
C	-16	GLY	-	expression tag	UNP Q9SU14
C	-15	SER	-	expression tag	UNP Q9SU14
C	-14	ASP	-	expression tag	UNP Q9SU14
C	-13	TYR	-	expression tag	UNP Q9SU14
C	-12	ASP	-	expression tag	UNP Q9SU14
C	-11	ILE	-	expression tag	UNP Q9SU14
C	-10	PRO	-	expression tag	UNP Q9SU14
C	-9	THR	-	expression tag	UNP Q9SU14
C	-8	THR	-	expression tag	UNP Q9SU14
C	-7	GLU	-	expression tag	UNP Q9SU14
C	-6	ASN	-	expression tag	UNP Q9SU14
C	-5	LEU	-	expression tag	UNP Q9SU14
C	-4	TYR	-	expression tag	UNP Q9SU14
C	-3	PHE	-	expression tag	UNP Q9SU14
C	-2	GLN	-	expression tag	UNP Q9SU14
C	-1	GLY	-	expression tag	UNP Q9SU14
C	0	SER	-	expression tag	UNP Q9SU14

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



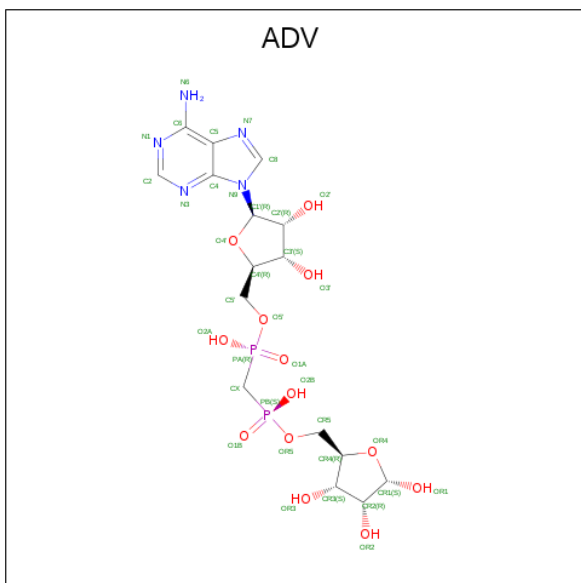
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is ALPHA-BETA METHYLENE ADP-RIBOSE (three-letter code: ADV) (formula: $C_{16}H_{25}N_5O_{13}P_2$).



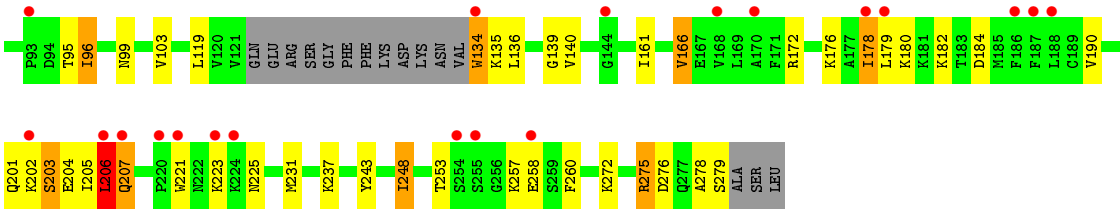
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			36	16	5	13	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	32	Total	O	0	0
			32	32		
4	C	29	Total	O	0	0
			29	29		

- Molecule 1: Nudix hydrolase 7





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	48.20Å 258.72Å 157.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 30.29 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.60) 96.0 (30.29-2.59)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.238 , 0.290 0.245 , 0.295	Depositor DCC
R_{free} test set	1525 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6428	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: ADV, 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	0.61	2/2095 (0.1%)	0.69	1/2840 (0.0%)
1	B	0.63	2/2192 (0.1%)	0.67	0/2969
1	C	0.62	3/2132 (0.1%)	0.70	1/2888 (0.0%)
All	All	0.62	7/6419 (0.1%)	0.68	2/8697 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	TRP	CD2-CE2	5.52	1.48	1.41
1	C	134	TRP	CD2-CE2	5.50	1.48	1.41
1	C	54	TRP	CD2-CE2	5.31	1.47	1.41
1	A	45	TRP	CD2-CE2	5.31	1.47	1.41
1	A	210	TRP	CD2-CE2	5.30	1.47	1.41
1	C	221	TRP	CD2-CE2	5.23	1.47	1.41
1	B	134	TRP	CD2-CE2	5.12	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	53	ILE	CG1-CB-CG2	-5.34	99.66	111.40
1	A	179	LEU	CA-CB-CG	5.13	127.11	115.30

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	2050	0	2017	49	0
1	B	2146	0	2122	30	0
1	C	2086	0	2063	46	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
3	C	36	0	23	3	0
4	A	29	0	0	4	0
4	B	32	0	0	1	0
4	C	29	0	0	0	0
All	All	6428	0	6225	119	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 9.

All (119) 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:C:205:ILE:HA	1:C:206:LEU:HB2	1.20	1.16
1:A:59:LEU:HB2	1:A:81:GLU:HA	1.47	0.93
1:A:206:LEU:HD22	4:A:401:HOH:O	1.70	0.92
1:B:180:LYS:HA	1:B:180:LYS:HE3	1.53	0.88
1:A:45:TRP:O	1:A:50:LYS:HA	1.81	0.80
1:A:35:THR:HG22	1:A:67:ALA:HB1	1.64	0.79
1:C:205:ILE:CA	1:C:206:LEU:HB2	2.09	0.79
1:A:58:PRO:HG2	1:A:61:LEU:HD13	1.67	0.76
1:C:103:VAL:HB	1:C:178:ILE:HG21	1.70	0.74
1:A:50:LYS:O	1:A:89:ILE:HG22	1.88	0.74
1:C:25:MET:HE1	1:C:34:PHE:HE1	1.53	0.74
1:A:199:THR:O	1:A:202:LYS:HG3	1.88	0.73
1:A:175:HIS:HB2	1:A:177:ALA:N	2.06	0.71
1:C:25:MET:CE	1:C:34:PHE:HE1	2.04	0.70
1:C:103:VAL:HB	1:C:178:ILE:HG13	1.71	0.70
1:A:50:LYS:O	1:A:89:ILE:CG2	2.40	0.69
1:C:16:ASP:HB3	1:C:18:TYR:H	1.57	0.69
1:C:248:ILE:HD12	1:C:260:PHE:HB3	1.75	0.68
1:C:23:VAL:HG11	1:C:25:MET:HE2	1.75	0.68
1:C:103:VAL:HB	1:C:178:ILE:CG2	2.25	0.67
1:C:134:TRP:N	1:C:135:LYS:HA	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:GLN:O	1:C:207:GLN:HG2	1.95	0.65
1:C:275:ARG:HG3	1:C:276:ASP:N	2.13	0.63
1:A:203:SER:N	4:A:401:HOH:O	2.31	0.62
1:C:88:TRP:CH2	1:C:95:THR:HG22	2.34	0.62
1:C:275:ARG:HG3	1:C:276:ASP:H	1.65	0.61
1:A:174:SER:O	1:A:175:HIS:HB3	2.01	0.59
1:C:16:ASP:HB2	1:C:20:GLY:H	1.69	0.58
1:B:104:VAL:HG22	1:B:185:MET:HB3	1.86	0.58
1:A:205:ILE:HG22	1:A:205:ILE:O	2.04	0.57
1:C:166:VAL:HG13	1:C:190:VAL:HG13	1.84	0.57
1:C:25:MET:HE1	1:C:34:PHE:CE1	2.38	0.57
1:B:179:LEU:O	1:B:180:LYS:HG2	2.04	0.57
1:A:51:LYS:HB3	1:A:90:SER:HB2	1.86	0.57
1:B:180:LYS:HA	1:B:180:LYS:CE	2.29	0.56
1:C:74:ARG:HH22	1:C:96:ILE:HD11	1.70	0.55
1:B:39:ARG:NH1	4:B:401:HOH:O	2.39	0.55
1:C:278:ALA:N	1:C:279:SER:HA	2.21	0.55
1:B:21:VAL:HG12	1:B:53:ILE:HD12	1.90	0.54
1:A:46:ARG:O	1:A:50:LYS:HG2	2.07	0.54
1:A:75:TYR:O	1:B:80:PRO:HA	2.06	0.54
1:B:248:ILE:HD11	1:B:262:TYR:CZ	2.43	0.54
1:A:31:SER:O	1:A:35:THR:HG23	2.07	0.54
1:B:162:ILE:HG23	1:B:194:ARG:HB2	1.90	0.53
1:A:219:GLN:HG2	1:A:220:PRO:CD	2.38	0.53
1:C:207:GLN:O	1:C:207:GLN:CG	2.56	0.53
1:A:219:GLN:HG2	1:A:220:PRO:HD2	1.89	0.53
1:A:101:SER:HB2	1:B:101:SER:HB3	1.91	0.53
1:A:221:TRP:O	1:A:224:LYS:HB2	2.09	0.52
1:A:108:ALA:HB3	1:A:137:PRO:HG2	1.92	0.52
1:B:173:GLN:HA	1:B:184:ASP:O	2.10	0.52
1:C:74:ARG:HH12	1:C:96:ILE:HD11	1.75	0.52
1:A:58:PRO:HA	1:A:82:TYR:HA	1.91	0.51
1:C:74:ARG:HH12	1:C:96:ILE:CD1	2.24	0.51
1:A:221:TRP:CD1	1:A:221:TRP:C	2.84	0.51
1:A:219:GLN:CG	1:A:220:PRO:HD2	2.40	0.51
1:C:202:LYS:O	1:C:203:SER:CB	2.57	0.51
1:C:23:VAL:CG1	1:C:25:MET:HE2	2.39	0.51
1:C:205:ILE:HA	1:C:206:LEU:CB	2.11	0.50
1:B:94:ASP:OD1	1:B:96:ILE:HG13	2.10	0.50
1:B:21:VAL:HG12	1:B:53:ILE:CD1	2.41	0.49
1:A:103:VAL:O	1:A:184:ASP:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LYS:HB3	1:A:90:SER:CB	2.41	0.49
1:A:80:PRO:HB3	1:B:74:ARG:HD2	1.95	0.49
1:C:178:ILE:HG12	1:C:184:ASP:HB2	1.94	0.49
1:A:222:ASN:O	1:A:223:LYS:HG2	2.13	0.48
1:C:180:LYS:HD3	1:C:180:LYS:N	2.27	0.48
1:C:179:LEU:H	1:C:182:LYS:HB2	1.79	0.48
1:A:206:LEU:HB3	4:A:401:HOH:O	2.13	0.47
1:C:134:TRP:N	1:C:135:LYS:CA	2.77	0.47
1:C:178:ILE:HG12	1:C:184:ASP:CA	2.44	0.47
1:C:204:GLU:O	1:C:206:LEU:HD23	2.14	0.47
1:A:200:GLU:HA	1:A:201:GLN:HA	1.66	0.47
1:A:134:TRP:H	1:A:219:GLN:HE22	1.62	0.47
1:C:257:LYS:HD2	1:C:258:GLU:H	1.79	0.47
1:B:74:ARG:HH21	1:B:96:ILE:HD11	1.80	0.46
1:B:162:ILE:HG12	1:B:194:ARG:HD2	1.97	0.46
1:B:174:SER:O	1:B:183:THR:HA	2.16	0.46
1:C:103:VAL:CB	1:C:178:ILE:HG21	2.44	0.46
1:A:175:HIS:HA	1:A:176:LYS:C	2.35	0.46
1:A:221:TRP:O	1:A:224:LYS:N	2.48	0.46
1:C:25:MET:CE	1:C:34:PHE:CE1	2.93	0.46
1:A:46:ARG:HA	1:A:50:LYS:HB3	1.98	0.45
1:A:136:LEU:HD13	1:A:216:TYR:CZ	2.52	0.45
1:A:27:GLU:HG2	1:C:36:GLU:OE2	2.16	0.45
1:B:46:ARG:NH2	1:B:91:GLU:HG2	2.30	0.45
1:C:202:LYS:O	1:C:203:SER:HB2	2.17	0.45
1:A:100:ALA:HB1	1:B:140:VAL:HB	1.99	0.44
1:A:122:GLN:HE21	1:A:122:GLN:C	2.21	0.44
1:C:178:ILE:HD13	1:C:178:ILE:HA	1.69	0.44
1:B:179:LEU:HD12	1:B:180:LYS:H	1.81	0.44
1:B:178:ILE:HG22	1:B:178:ILE:O	2.17	0.44
1:B:102:HIS:ND1	1:B:183:THR:HG23	2.32	0.43
1:C:179:LEU:O	1:C:180:LYS:HB2	2.18	0.43
1:A:134:TRP:H	1:A:219:GLN:NE2	2.16	0.43
3:C:401:ADV:O5'	3:C:401:ADV:H8	2.19	0.43
1:B:21:VAL:CG1	1:B:53:ILE:HD12	2.49	0.43
1:A:176:LYS:H	1:A:176:LYS:HE3	1.84	0.42
1:A:221:TRP:O	1:A:222:ASN:C	2.57	0.42
1:A:221:TRP:CZ2	1:A:232:ALA:HB2	2.54	0.42
1:C:119:LEU:HD22	1:C:161:ILE:HD11	2.01	0.42
1:C:25:MET:HE3	1:C:34:PHE:HE1	1.82	0.42
1:B:92:THR:HB	1:B:93:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:CD	4:A:401:HOH:O	2.67	0.41
1:C:206:LEU:HD13	1:C:207:GLN:H	1.85	0.41
1:A:251:THR:HG23	1:B:226:GLU:OE2	2.20	0.41
1:C:140:VAL:HG23	3:C:401:ADV:H5R2	2.03	0.41
1:A:134:TRP:N	1:A:219:GLN:HE22	2.18	0.41
1:A:146:ASP:HA	1:B:173:GLN:OE1	2.20	0.41
1:B:188:LEU:HD11	1:B:235:CYS:SG	2.60	0.41
1:B:177:ALA:O	1:B:179:LEU:N	2.54	0.41
1:B:249:VAL:HA	1:B:250:PRO:HD3	1.83	0.41
1:C:139:GLY:HA2	3:C:401:ADV:H5R1	2.03	0.41
1:A:50:LYS:O	1:A:89:ILE:HG23	2.17	0.41
1:A:203:SER:HB2	1:A:206:LEU:HB3	2.02	0.40
1:C:237:LYS:HB3	1:C:243:TYR:HB2	2.03	0.40
1:A:203:SER:HB2	1:A:206:LEU:CB	2.51	0.40
1:B:233:ASN:C	1:B:237:LYS:HZ3	2.25	0.40
1:C:272:LYS:HA	1:C:275:ARG:HG2	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	252/310 (81%)	242 (96%)	8 (3%)	2 (1%)	19	39
1	B	266/310 (86%)	258 (97%)	7 (3%)	1 (0%)	34	57
1	C	258/310 (83%)	251 (97%)	5 (2%)	2 (1%)	19	39
All	All	776/930 (83%)	751 (97%)	20 (3%)	5 (1%)	25	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	206	LEU

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Mol	Chain	Res	Type
1	B	178	ILE
1	A	48	GLU
1	C	203	SER
1	A	222	ASN

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	225/270 (83%)	198 (88%)	27 (12%)	5	9
1	B	236/270 (87%)	216 (92%)	20 (8%)	10	21
1	C	229/270 (85%)	209 (91%)	20 (9%)	10	20
All	All	690/810 (85%)	623 (90%)	67 (10%)	8	15

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	14	GLU
1	A	17	ASN
1	A	35	THR
1	A	50	LYS
1	A	53	ILE
1	A	59	LEU
1	A	64	LEU
1	A	82	TYR
1	A	83	LEU
1	A	122	GLN
1	A	161	ILE
1	A	162	ILE
1	A	172	ARG
1	A	175	HIS
1	A	179	LEU
1	A	191	LEU
1	A	200	GLU

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Mol	Chain	Res	Type
1	A	201	GLN
1	A	202	LYS
1	A	219	GLN
1	A	221	TRP
1	A	222	ASN
1	A	225	ASN
1	A	251	THR
1	A	252	THR
1	A	277	GLN
1	B	10	LEU
1	B	46	ARG
1	B	79	GLU
1	B	81	GLU
1	B	83	LEU
1	B	88	TRP
1	B	115	THR
1	B	123	GLU
1	B	135	LYS
1	B	149	THR
1	B	179	LEU
1	B	180	LYS
1	B	181	LYS
1	B	188	LEU
1	B	206	LEU
1	B	225	ASN
1	B	240	GLU
1	B	248	ILE
1	B	253	THR
1	B	258	GLU
1	C	10	LEU
1	C	21	VAL
1	C	74	ARG
1	C	83	LEU
1	C	96	ILE
1	C	99	ASN
1	C	136	LEU
1	C	166	VAL
1	C	172	ARG
1	C	176	LYS
1	C	178	ILE
1	C	201	GLN
1	C	206	LEU

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Mol	Chain	Res	Type
1	C	207	GLN
1	C	223	LYS
1	C	225	ASN
1	C	231	MET
1	C	248	ILE
1	C	253	THR
1	C	275	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	122	GLN
1	A	201	GLN
1	A	219	GLN
1	B	7	GLN
1	B	44	HIS
1	B	112	ASN
1	B	132	ASN
1	B	201	GLN
1	B	219	GLN
1	C	99	ASN
1	C	219	GLN
1	C	267	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

5 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	ADV	C	401	-	34,39,39	1.09	4 (11%)	37,60,60	1.83	9 (24%)
2	SO4	B	301	-	4,4,4	0.29	0	6,6,6	0.07	0
2	SO4	C	402	-	4,4,4	0.32	0	6,6,6	0.12	0
2	SO4	B	302	-	4,4,4	0.33	0	6,6,6	0.17	0
2	SO4	A	301	-	4,4,4	0.32	0	6,6,6	0.05	0

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	ADV	C	401	-	-	10/18/54/54	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	ADV	PB-OR5	2.50	1.61	1.57
3	C	401	ADV	PB-O2B	2.34	1.61	1.56
3	C	401	ADV	PA-O2A	2.26	1.61	1.56
3	C	401	ADV	O4'-C1'	2.19	1.44	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ADV	N3-C2-N1	-5.08	120.74	128.68
3	C	401	ADV	O1A-PA-CX	3.61	118.62	109.07
3	C	401	ADV	O2A-PA-CX	3.46	120.73	106.58
3	C	401	ADV	O2A-PA-O1A	3.07	120.32	110.07
3	C	401	ADV	C5-C6-N6	-2.90	115.94	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	ADV	N6-C6-N1	2.80	124.38	118.57
3	C	401	ADV	OR1-CR1-OR4	-2.73	107.63	111.13
3	C	401	ADV	C3'-C2'-C1'	2.52	104.78	100.98
3	C	401	ADV	CR1-CR2-CR3	2.49	105.42	102.30

There are no chirality outliers.

All (10) torsion outliers are listed below:

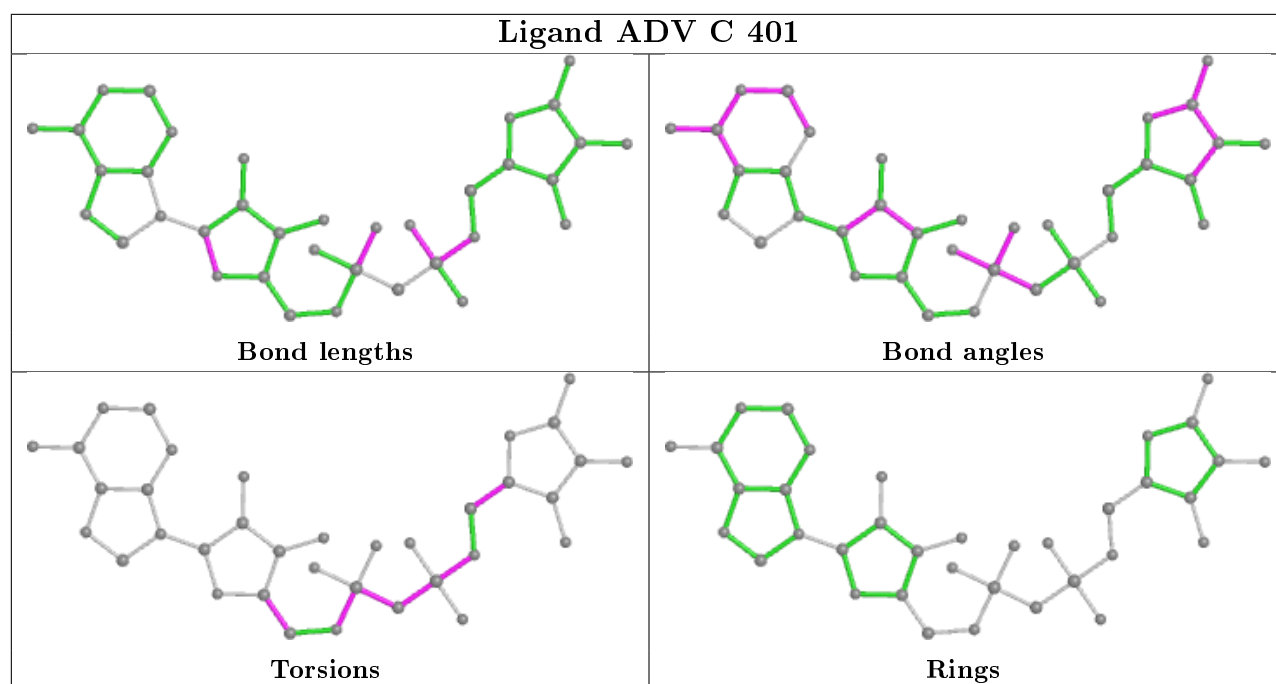
Mol	Chain	Res	Type	Atoms
3	C	401	ADV	PB-CX-PA-O1A
3	C	401	ADV	O4'-C4'-C5'-O5'
3	C	401	ADV	C3'-C4'-C5'-O5'
3	C	401	ADV	PA-CX-PB-O1B
3	C	401	ADV	CR5-OR5-PB-O1B
3	C	401	ADV	OR4-CR4-CR5-OR5
3	C	401	ADV	C5'-O5'-PA-CX
3	C	401	ADV	CR3-CR4-CR5-OR5
3	C	401	ADV	PA-CX-PB-OR5
3	C	401	ADV	CR5-OR5-PB-O2B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	ADV	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, 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	258/310 (83%)	0.62	26 (10%) 7 4	38, 60, 102, 123	0
1	B	270/310 (87%)	0.22	14 (5%) 27 21	35, 51, 90, 120	0
1	C	262/310 (84%)	0.34	21 (8%) 12 9	32, 58, 95, 122	0
All	All	790/930 (84%)	0.39	61 (7%) 13 10	32, 56, 97, 123	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	222	ASN	10.0
1	A	279	SER	8.2
1	C	179	LEU	7.8
1	B	256	GLY	7.0
1	A	205	ILE	5.9
1	A	220	PRO	5.9
1	A	201	GLN	5.2
1	A	200	GLU	5.1
1	B	178	ILE	5.1
1	C	207	GLN	5.1
1	A	224	LYS	4.5
1	B	179	LEU	4.2
1	A	206	LEU	4.2
1	B	254	SER	4.1
1	A	278	ALA	4.0
1	C	220	PRO	3.9
1	C	223	LYS	3.9
1	A	277	GLN	3.8
1	A	51	LYS	3.8
1	C	202	LYS	3.8
1	B	93	PRO	3.7
1	C	206	LEU	3.3
1	A	223	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	LYS	3.1
1	C	187	PHE	3.0
1	C	255	SER	3.0
1	A	49	GLY	3.0
1	C	134	TRP	3.0
1	A	168	VAL	2.9
1	B	277	GLN	2.9
1	B	242	GLU	2.9
1	A	209	LYS	2.9
1	C	18	TYR	2.8
1	B	258	GLU	2.7
1	A	18	TYR	2.7
1	C	178	ILE	2.7
1	A	160	GLY	2.7
1	B	281	SER	2.7
1	C	93	PRO	2.6
1	A	203	SER	2.6
1	C	188	LEU	2.6
1	C	221	TRP	2.6
1	A	17	ASN	2.6
1	C	168	VAL	2.5
1	B	282	LEU	2.4
1	C	170	ALA	2.4
1	C	258	GLU	2.4
1	B	255	SER	2.3
1	C	254	SER	2.2
1	A	50	LYS	2.2
1	A	95	THR	2.2
1	A	189	CYS	2.2
1	A	176	LYS	2.2
1	B	170	ALA	2.2
1	B	188	LEU	2.2
1	A	256	GLY	2.1
1	C	186	PHE	2.1
1	C	144	GLY	2.1
1	B	92	THR	2.0
1	A	81	GLU	2.0
1	C	224	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](#)

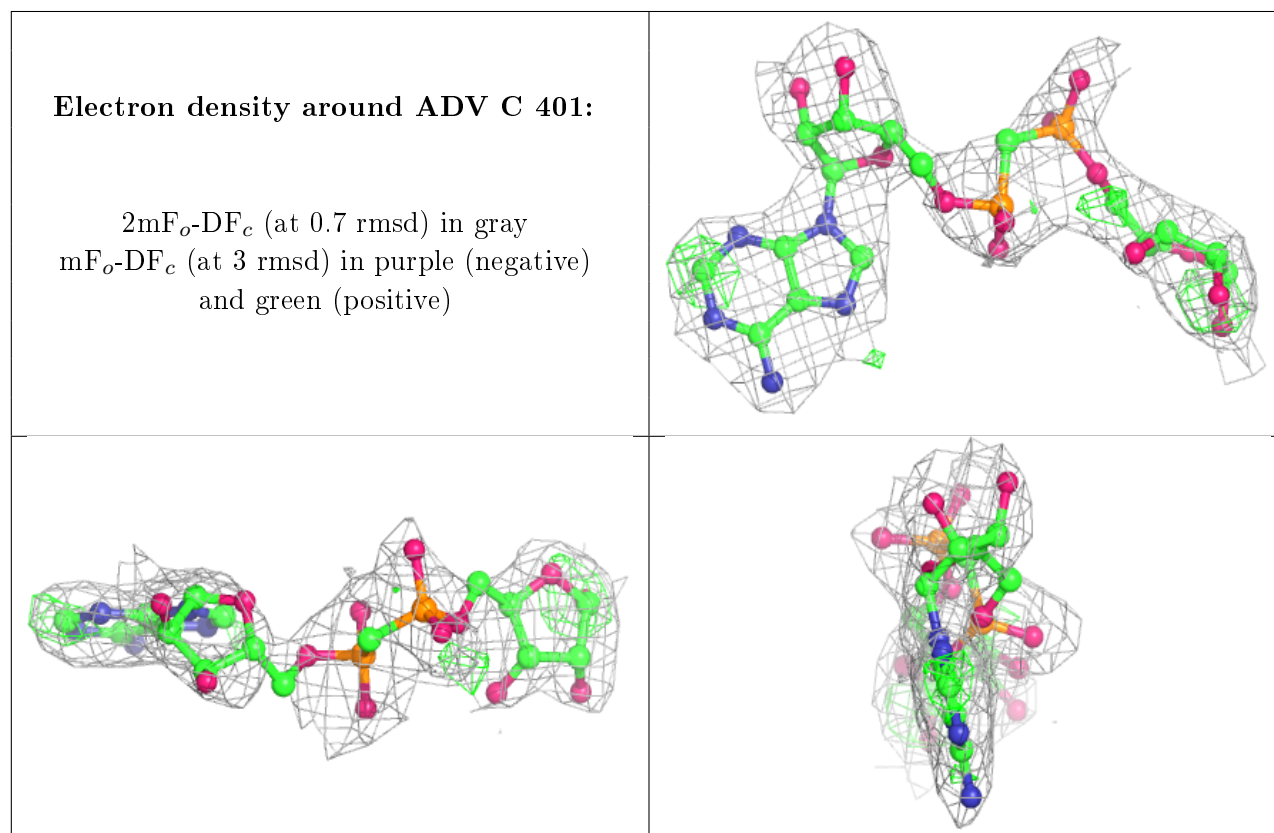
There are no carbohydrates in this entry.

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, 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(\AA^2)	Q<0.9
3	ADV	C	401	36/36	0.72	0.40	49,68,75,76	36
2	SO4	A	301	5/5	0.87	0.17	69,70,70,71	5
2	SO4	B	302	5/5	0.88	0.31	65,65,67,67	5
2	SO4	C	402	5/5	0.93	0.14	57,59,60,60	5
2	SO4	B	301	5/5	0.96	0.16	65,65,66,66	5

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

There are no such residues in this entry.