



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:28 AM UTC

PDB ID : 6XOG / pdb_00006xog
Title : Structure of SUMO1-ML786519 adduct bound to SAE
Authors : Sintchak, M.; Lane, W.; Bump, N.
Deposited on : 2020-07-07
Resolution : 1.98 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

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

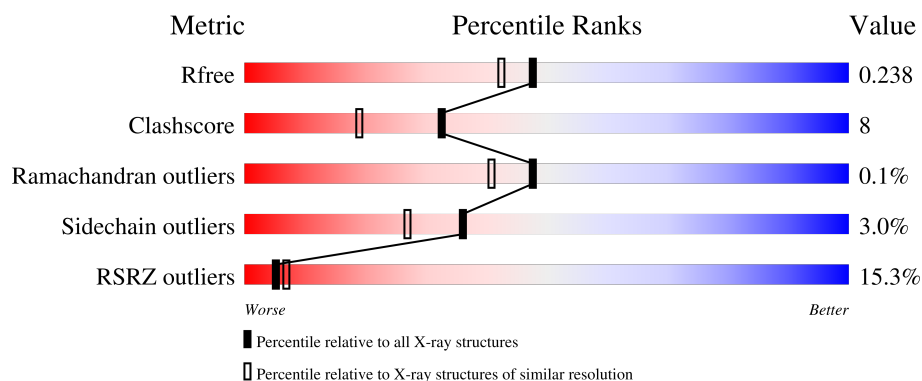
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	346	3% 81% 8% 10%
2	B	640	15% 65% 12% 22%
3	C	101	31% 43% 17% 39%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6931 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 SUMO-activating enzyme subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2387	1516	407	452	12			

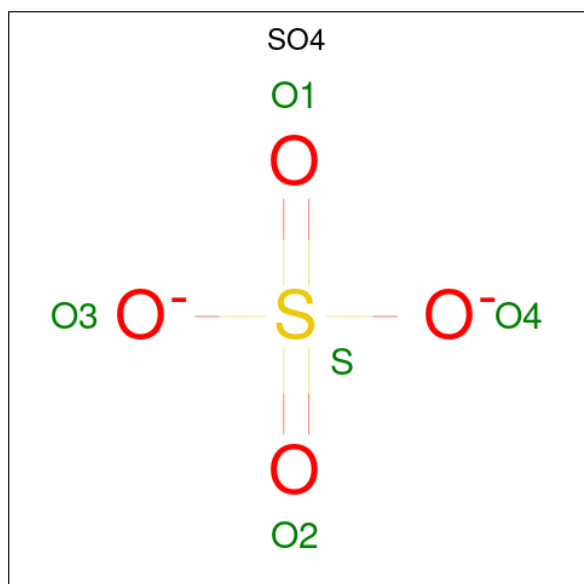
- Molecule 2 is a protein called SUMO-activating enzyme subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	500	Total	C	N	O	S	0	0	0
			3758	2405	632	702	19			

- Molecule 3 is a protein called Small ubiquitin-related modifier 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	62	Total	C	N	O	S	0	0	0
			489	310	83	94	2			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

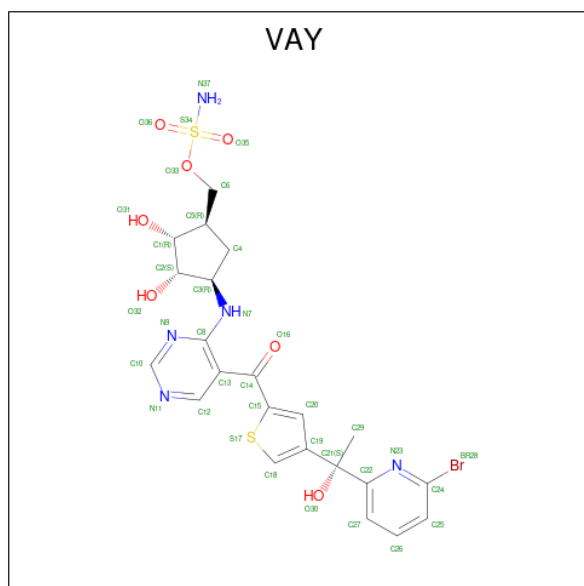


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 6 is {(1R,2R,3S,4R)-4-[(5-{4-[(1S)-1-(6-bromopyridin-2-yl)-1-hydroxyethyl]thiophene-2-carbonyl}pyrimidin-4-yl)amino]-2,3-dihydroxycyclopentyl}methyl sulfamate (CCD ID: VAY) (formula: C₂₂H₂₄BrN₅O₇S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	Br	C	N	O	S	
			37	1	22	5	7	2	0

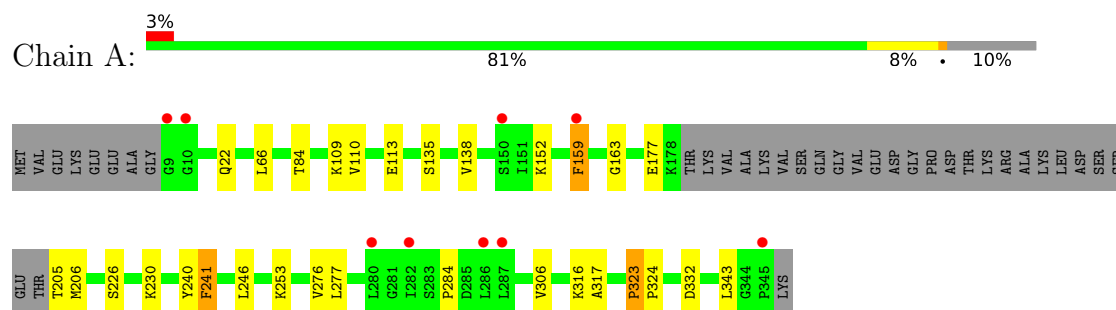
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	156	Total	O	0	0
			156	156		
7	B	86	Total	O	0	0
			86	86		
7	C	12	Total	O	0	0
			12	12		

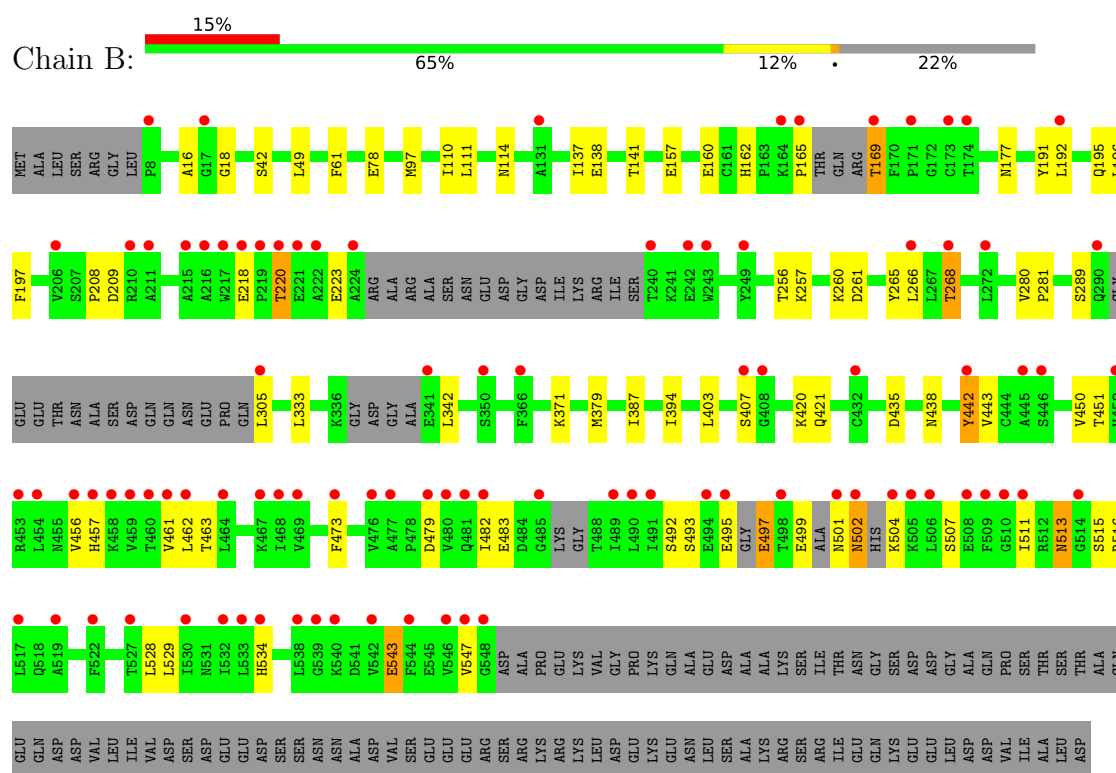
3 Residue-property plots [i](#)

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.

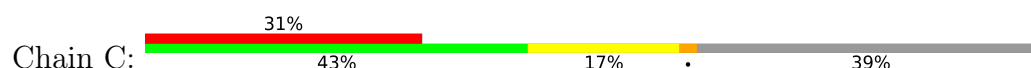
• Molecule 1: SUMO-activating enzyme subunit 1

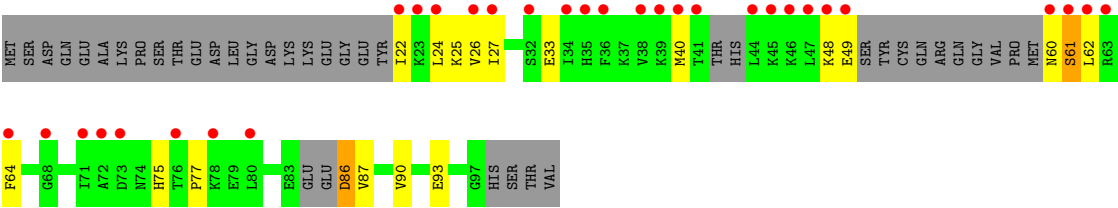


• Molecule 2: SUMO-activating enzyme subunit 2



• Molecule 3: Small ubiquitin-related modifier 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.90Å 72.42Å 126.87Å 90.00° 93.86° 90.00°	Depositor
Resolution (Å)	47.70 – 1.98 47.70 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.70-1.98) 98.5 (47.70-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.206 , 0.240 (Not available) , 0.238	Depositor DCC
R_{free} test set	3655 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6931	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% 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: SO4, ZN, VAY

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	0.77	3/2430 (0.1%)	1.15	3/3287 (0.1%)
2	B	0.61	0/3827	1.08	4/5209 (0.1%)
3	C	0.53	0/492	0.99	0/653
All	All	0.67	3/6749 (0.0%)	1.10	7/9149 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	MET	C-N	-8.37	1.21	1.33
1	A	323	PRO	C-O	-6.63	1.17	1.24
1	A	324	PRO	C-O	-5.33	1.17	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	GLU	CB-CA-C	6.93	121.25	109.53
2	B	420	LYS	N-CA-CB	-6.16	101.08	110.26
1	A	316	LYS	CB-CA-C	-6.00	101.46	110.88
2	B	218	GLU	CB-CA-C	5.72	116.64	108.68
1	A	241	PHE	CA-CB-CG	-5.31	108.49	113.80
2	B	78	GLU	CB-CG-CD	5.18	121.41	112.60
2	B	162	HIS	CB-CA-C	5.11	115.77	108.76

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	2387	0	2341	17	0
2	B	3758	0	3654	70	0
3	C	489	0	484	26	0
4	A	5	0	0	0	0
5	B	1	0	0	0	0
6	C	37	0	0	2	0
7	A	156	0	0	5	0
7	B	86	0	0	4	0
7	C	12	0	0	1	0
All	All	6931	0	6479	104	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 8.

All (104) 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)
2:B:165:PRO:HB3	3:C:61:SER:CB	1.72	1.18
3:C:93:GLU:HB2	7:C:310:HOH:O	1.49	1.11
2:B:165:PRO:HB3	3:C:61:SER:HB2	1.30	1.07
2:B:165:PRO:CB	3:C:61:SER:HB2	1.91	1.00
2:B:502:ASN:HD22	2:B:502:ASN:H	1.02	0.95
2:B:165:PRO:HB3	3:C:61:SER:HB3	1.48	0.95
2:B:499:GLU:HA	2:B:502:ASN:ND2	1.87	0.90
2:B:265:TYR:O	2:B:268:THR:HB	1.80	0.82
2:B:442:TYR:CE1	2:B:443:VAL:HG23	2.15	0.82
2:B:502:ASN:H	2:B:502:ASN:ND2	1.70	0.81
2:B:483:GLU:OE2	2:B:516:ARG:HD3	1.82	0.79
2:B:165:PRO:CG	3:C:61:SER:HB2	2.11	0.78
2:B:442:TYR:CD1	2:B:443:VAL:HG23	2.19	0.78
2:B:456:VAL:HG23	2:B:534:HIS:ND1	1.99	0.77
3:C:40:MET:HG3	3:C:77:PRO:HB2	1.69	0.75
2:B:502:ASN:HD22	2:B:502:ASN:N	1.83	0.74
2:B:165:PRO:HG3	3:C:61:SER:HB2	1.70	0.71
2:B:169:THR:HA	7:B:865:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:ASP:N	3:C:86:ASP:OD1	2.26	0.68
2:B:495:GLU:O	2:B:497:GLU:N	2.27	0.66
2:B:141:THR:HG22	2:B:394:ILE:HG13	1.79	0.64
2:B:499:GLU:CA	2:B:502:ASN:ND2	2.61	0.64
1:A:152:LYS:HE3	7:A:576:HOH:O	1.98	0.63
2:B:442:TYR:HE2	2:B:473:PHE:HD1	1.48	0.62
2:B:371:LYS:HD2	2:B:379:MET:HE1	1.81	0.62
3:C:24:LEU:CD2	3:C:86:ASP:N	2.63	0.61
2:B:403:LEU:O	2:B:407:SER:HB2	2.01	0.61
1:A:205:THR:N	7:A:501:HOH:O	2.35	0.60
2:B:61:PHE:HD1	7:B:804:HOH:O	1.84	0.60
2:B:479:ASP:OD1	2:B:493:SER:N	2.36	0.59
2:B:157:GLU:OE2	2:B:435:ASP:HB2	2.01	0.59
3:C:62:LEU:HD22	3:C:90:VAL:HG12	1.85	0.58
2:B:220:THR:O	2:B:223:GLU:HG3	2.03	0.57
1:A:323:PRO:HG2	2:B:421:GLN:NE2	2.20	0.57
2:B:114:ASN:ND2	2:B:138:GLU:OE1	2.29	0.57
2:B:442:TYR:CE1	2:B:443:VAL:CG2	2.85	0.57
2:B:450:VAL:HG13	2:B:528:LEU:HD11	1.85	0.57
2:B:501:ASN:O	2:B:504:LYS:N	2.38	0.56
3:C:24:LEU:HD23	3:C:86:ASP:N	2.21	0.56
1:A:113:GLU:CB	7:A:544:HOH:O	2.54	0.56
2:B:177:ASN:HD21	2:B:209:ASP:HB3	1.70	0.56
2:B:442:TYR:HE2	2:B:473:PHE:CD1	2.24	0.56
2:B:483:GLU:OE2	2:B:516:ARG:CB	2.55	0.55
3:C:48:LYS:HB2	3:C:64:PHE:CZ	2.42	0.55
2:B:483:GLU:OE2	2:B:516:ARG:HB2	2.07	0.54
1:A:159:PHE:CG	1:A:246:LEU:HD13	2.42	0.54
2:B:333:LEU:O	2:B:333:LEU:HG	2.08	0.53
3:C:27:ILE:HD12	3:C:87:VAL:HG11	1.92	0.52
2:B:16:ALA:O	2:B:42:SER:OG	2.28	0.52
2:B:463:THR:HG21	2:B:543:GLU:OE2	2.09	0.51
1:A:163:GLY:HA3	1:A:306:VAL:HG21	1.93	0.51
2:B:461:VAL:HG12	2:B:461:VAL:O	2.10	0.51
2:B:456:VAL:HG11	2:B:511:ILE:O	2.10	0.51
2:B:49:LEU:HD23	6:C:201:VAY:C13	2.41	0.51
2:B:18:GLY:HA3	2:B:110:ILE:HD13	1.93	0.51
2:B:197:PHE:HB3	2:B:342:LEU:HD12	1.92	0.50
3:C:62:LEU:HD22	3:C:90:VAL:CG1	2.42	0.49
1:A:241:PHE:HB3	1:A:277:LEU:HD21	1.95	0.49
2:B:138:GLU:HG3	7:B:801:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:TYR:O	2:B:195:GLN:HG2	2.13	0.48
2:B:49:LEU:HD13	6:C:201:VAY:BR28	2.68	0.48
1:A:277:LEU:HD12	1:A:284:PRO:HA	1.95	0.47
3:C:48:LYS:HB2	3:C:64:PHE:CE1	2.49	0.46
2:B:457:HIS:ND1	2:B:507:SER:CB	2.79	0.46
2:B:499:GLU:HA	2:B:502:ASN:CG	2.39	0.46
2:B:499:GLU:H	2:B:502:ASN:HD21	1.64	0.46
3:C:25:LYS:HD2	3:C:33:GLU:OE2	2.16	0.46
1:A:253:LYS:HE2	7:A:563:HOH:O	2.16	0.46
2:B:457:HIS:CE1	2:B:507:SER:CB	2.99	0.46
2:B:513:ASN:HB2	2:B:534:HIS:HB3	1.98	0.46
2:B:208:PRO:HB3	2:B:266:LEU:HD13	1.97	0.45
1:A:66:LEU:C	1:A:66:LEU:HD23	2.41	0.45
3:C:26:VAL:HG13	3:C:90:VAL:CG2	2.47	0.45
3:C:62:LEU:HD13	3:C:90:VAL:HG11	1.99	0.45
2:B:438:ASN:OD1	2:B:438:ASN:C	2.60	0.45
2:B:256:THR:HG23	2:B:260:LYS:HD3	1.99	0.45
3:C:27:ILE:HD12	3:C:87:VAL:CG1	2.47	0.44
1:A:332:ASP:OD1	1:A:332:ASP:C	2.59	0.44
1:A:109:LYS:HD3	7:A:611:HOH:O	2.17	0.44
2:B:457:HIS:HD1	2:B:507:SER:CB	2.30	0.43
1:A:135:SER:OG	1:A:138:VAL:HG23	2.17	0.43
1:A:226:SER:O	1:A:230:LYS:HG3	2.18	0.43
2:B:456:VAL:H	2:B:534:HIS:CE1	2.36	0.43
2:B:483:GLU:HB2	2:B:516:ARG:O	2.19	0.43
1:A:22:GLN:HB3	2:B:387:ILE:HG22	2.01	0.42
1:A:240:TYR:CD1	1:A:343:LEU:HD13	2.54	0.42
2:B:492:SER:OG	2:B:497:GLU:HB3	2.20	0.42
2:B:305:LEU:HD22	7:B:874:HOH:O	2.19	0.42
2:B:257:LYS:HA	2:B:261:ASP:HB2	2.02	0.41
3:C:62:LEU:HB3	3:C:90:VAL:CG1	2.49	0.41
2:B:160:GLU:CD	2:B:443:VAL:HG21	2.44	0.41
1:A:152:LYS:HE2	1:A:317:ALA:O	2.20	0.41
3:C:26:VAL:CG1	3:C:90:VAL:CG2	2.98	0.41
2:B:165:PRO:CB	3:C:61:SER:CB	2.59	0.41
2:B:499:GLU:N	2:B:502:ASN:HD21	2.19	0.41
3:C:22:ILE:HD11	3:C:77:PRO:CG	2.51	0.41
3:C:49:GLU:OE1	3:C:49:GLU:HA	2.19	0.41
2:B:442:TYR:CD1	2:B:442:TYR:C	2.97	0.40
2:B:192:LEU:HD11	2:B:196:LEU:HD11	2.03	0.40
2:B:451:THR:HG22	2:B:547:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:LYS:HB2	3:C:25:LYS:HE3	1.88	0.40
2:B:111:LEU:HD11	2:B:137:ILE:HG13	2.04	0.40
2:B:461:VAL:O	2:B:461:VAL:CG1	2.70	0.40
2:B:280:VAL:HA	2:B:281:PRO:HD3	1.95	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	307/346 (89%)	298 (97%)	9 (3%)	0	100	100
2	B	482/640 (75%)	459 (95%)	22 (5%)	1 (0%)	43	35
3	C	54/101 (54%)	51 (94%)	3 (6%)	0	100	100
All	All	843/1087 (78%)	808 (96%)	34 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	513	ASN

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	254/296 (86%)	250 (98%)	4 (2%)	55	50
2	B	394/552 (71%)	381 (97%)	13 (3%)	33	23
3	C	53/91 (58%)	49 (92%)	4 (8%)	12	4
All	All	701/939 (75%)	680 (97%)	21 (3%)	36	27

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	THR
1	A	110	VAL
1	A	159	PHE
1	A	276	VAL
2	B	97	MET
2	B	169	THR
2	B	220	THR
2	B	268	THR
2	B	289	SER
2	B	442	TYR
2	B	462	LEU
2	B	482	ILE
2	B	497	GLU
2	B	502	ASN
2	B	515	SER
2	B	529	LEU
2	B	543	GLU
3	C	60	ASN
3	C	61	SER
3	C	75	HIS
3	C	86	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	103	ASN
1	A	149	ASN
2	B	43	HIS
2	B	93	HIS
2	B	108	GLN
2	B	204	GLN
2	B	421	GLN

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Mol	Chain	Res	Type
2	B	502	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	401	-	4,4,4	0.30	0	6,6,6	0.13	0
6	VAY	C	201	3	39,40,40	3.39	10 (25%)	52,60,60	3.34	22 (42%)

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
6	VAY	C	201	3	-	6/29/46/46	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	201	VAY	C21-C19	14.45	1.64	1.51
6	C	201	VAY	S34-N37	8.77	1.69	1.58
6	C	201	VAY	O33-S34	-5.46	1.50	1.57
6	C	201	VAY	O35-S34	5.03	1.47	1.42
6	C	201	VAY	O36-S34	5.01	1.47	1.42
6	C	201	VAY	C3-N7	4.30	1.52	1.45
6	C	201	VAY	O30-C21	-3.95	1.38	1.43
6	C	201	VAY	C15-C14	3.31	1.54	1.47
6	C	201	VAY	C2-C3	2.27	1.56	1.53
6	C	201	VAY	C24-N23	2.18	1.34	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	201	VAY	O30-C21-C19	-13.43	88.19	109.96
6	C	201	VAY	C12-C13-C8	7.91	122.61	114.67
6	C	201	VAY	O30-C21-C22	7.06	122.08	108.58
6	C	201	VAY	O36-S34-O35	-5.63	114.21	119.94
6	C	201	VAY	O30-C21-C29	5.49	120.05	108.58
6	C	201	VAY	C25-C24-N23	-5.04	121.51	125.75
6	C	201	VAY	C13-C8-N9	-4.84	115.78	121.88
6	C	201	VAY	C24-N23-C22	4.83	119.97	116.91
6	C	201	VAY	C12-N11-C10	4.39	120.98	115.80
6	C	201	VAY	C13-C12-N11	-3.61	117.00	123.95
6	C	201	VAY	N7-C8-N9	3.56	123.05	118.00
6	C	201	VAY	O31-C1-C5	-3.35	103.81	112.56
6	C	201	VAY	C26-C25-C24	3.21	119.70	116.74
6	C	201	VAY	C4-C5-C6	-3.21	106.43	112.78
6	C	201	VAY	N11-C10-N9	-3.05	122.15	127.33
6	C	201	VAY	O33-C6-C5	2.45	113.30	108.24
6	C	201	VAY	C4-C3-C2	-2.35	99.46	103.17
6	C	201	VAY	C5-C1-C2	2.32	106.60	103.87
6	C	201	VAY	BR28-C24-C25	2.29	121.02	118.69
6	C	201	VAY	C21-C19-C18	-2.10	121.43	127.01
6	C	201	VAY	BR28-C24-N23	2.01	117.47	115.68
6	C	201	VAY	C25-C26-C27	-2.01	117.66	120.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	201	VAY	C29-C21-C22-N23

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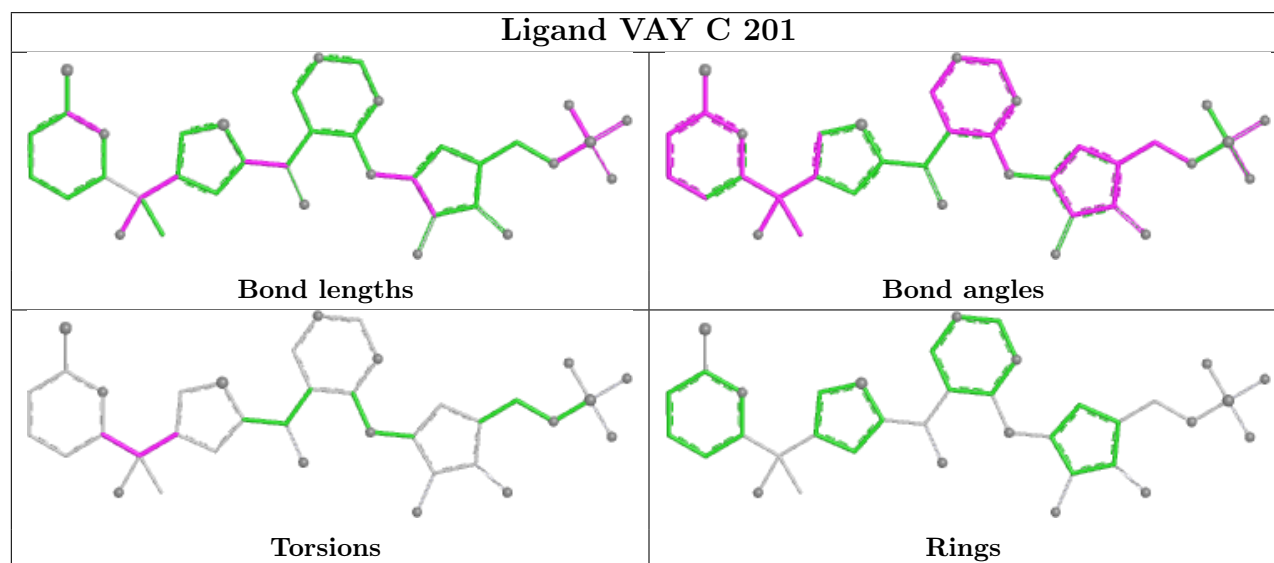
Mol	Chain	Res	Type	Atoms
6	C	201	VAY	C18-C19-C21-O30
6	C	201	VAY	C18-C19-C21-C29
6	C	201	VAY	C20-C19-C21-C22
6	C	201	VAY	C18-C19-C21-C22
6	C	201	VAY	C20-C19-C21-C29

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	201	VAY	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, 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	311/346 (89%)	0.10	9 (2%) 53 63	17, 32, 58, 80	0
2	B	500/640 (78%)	0.99	94 (18%) 3 4	18, 47, 93, 114	0
3	C	62/101 (61%)	2.16	31 (50%) 0 0	23, 77, 108, 115	0
All	All	873/1087 (80%)	0.76	134 (15%) 5 7	17, 41, 92, 115	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	61	SER	6.9
3	C	34	ILE	5.3
2	B	532	ILE	5.2
2	B	509	PHE	5.2
2	B	510	GLY	5.0
3	C	22	ILE	4.9
2	B	506	LEU	4.9
2	B	490	LEU	4.8
3	C	62	LEU	4.8
2	B	305	LEU	4.7
1	A	9	GLY	4.5
3	C	41	THR	4.5
3	C	36	PHE	4.4
3	C	48	LYS	4.2
2	B	480	VAL	4.2
2	B	215	ALA	4.1
3	C	44	LEU	3.9
2	B	459	VAL	3.9
2	B	173	CYS	3.9
2	B	517	LEU	3.8
2	B	243	TRP	3.8
2	B	240	THR	3.7
2	B	502	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	482	ILE	3.7
3	C	47	LEU	3.7
3	C	49	GLU	3.7
3	C	38	VAL	3.7
2	B	511	ILE	3.6
2	B	216	ALA	3.6
2	B	491	ILE	3.6
2	B	220	THR	3.5
2	B	522	PHE	3.5
2	B	538	LEU	3.5
2	B	219	PRO	3.5
2	B	533	LEU	3.5
3	C	35	HIS	3.4
2	B	461	VAL	3.4
2	B	544	PHE	3.4
2	B	249	TYR	3.3
3	C	27	ILE	3.3
3	C	60	ASN	3.3
1	A	286	LEU	3.1
3	C	26	VAL	3.1
2	B	222	ALA	3.1
2	B	224	ALA	3.1
2	B	548	GLY	3.1
3	C	24	LEU	3.0
2	B	481	GLN	3.0
2	B	165	PRO	3.0
2	B	505	LYS	3.0
2	B	268	THR	3.0
2	B	8	PRO	3.0
2	B	17	GLY	3.0
2	B	534	HIS	2.9
2	B	211	ALA	2.9
2	B	514	GLY	2.9
2	B	217	TRP	2.9
2	B	547	VAL	2.9
2	B	454	LEU	2.9
2	B	169	THR	2.8
2	B	174	THR	2.8
2	B	218	GLU	2.8
2	B	485	GLY	2.8
3	C	39	LYS	2.8
2	B	508	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	489	ILE	2.8
2	B	468	ILE	2.7
2	B	501	ASN	2.7
1	A	280	LEU	2.7
2	B	495	GLU	2.7
2	B	206	VAL	2.7
3	C	68	GLY	2.7
2	B	452	VAL	2.7
2	B	504	LYS	2.6
3	C	46	LYS	2.6
1	A	10	GLY	2.6
2	B	221	GLU	2.6
2	B	341	GLU	2.6
3	C	78	LYS	2.6
3	C	32	SER	2.6
3	C	45	LYS	2.6
2	B	462	LEU	2.5
2	B	498	THR	2.5
2	B	408	GLY	2.5
2	B	457	HIS	2.5
3	C	72	ALA	2.4
2	B	456	VAL	2.4
2	B	453	ARG	2.4
2	B	290	GLN	2.4
2	B	350	SER	2.4
3	C	76	THR	2.4
2	B	432	CYS	2.4
2	B	192	LEU	2.3
2	B	477	ALA	2.3
2	B	242	GLU	2.3
1	A	159	PHE	2.3
2	B	442	TYR	2.3
3	C	73	ASP	2.3
2	B	469	VAL	2.3
2	B	266	LEU	2.3
3	C	64	PHE	2.2
2	B	476	VAL	2.2
2	B	542	VAL	2.2
2	B	458	LYS	2.2
2	B	479	ASP	2.2
2	B	164	LYS	2.2
2	B	210	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	546	VAL	2.2
2	B	473	PHE	2.2
2	B	446	SER	2.2
2	B	171	PRO	2.2
2	B	467	LYS	2.2
1	A	150	SER	2.1
2	B	407	SER	2.1
1	A	345	PRO	2.1
2	B	272	LEU	2.1
2	B	464	LEU	2.1
3	C	80	LEU	2.1
2	B	540	LYS	2.1
3	C	23	LYS	2.1
3	C	63	ARG	2.1
2	B	494	GLU	2.1
1	A	287	LEU	2.1
2	B	445	ALA	2.1
2	B	366	PHE	2.1
2	B	460	THR	2.1
2	B	539	GLY	2.1
2	B	519	ALA	2.1
3	C	71	ILE	2.0
2	B	527	THR	2.0
3	C	40	MET	2.0
2	B	131	ALA	2.0
1	A	282	ILE	2.0
2	B	530	ILE	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 oligosaccharides in this entry.

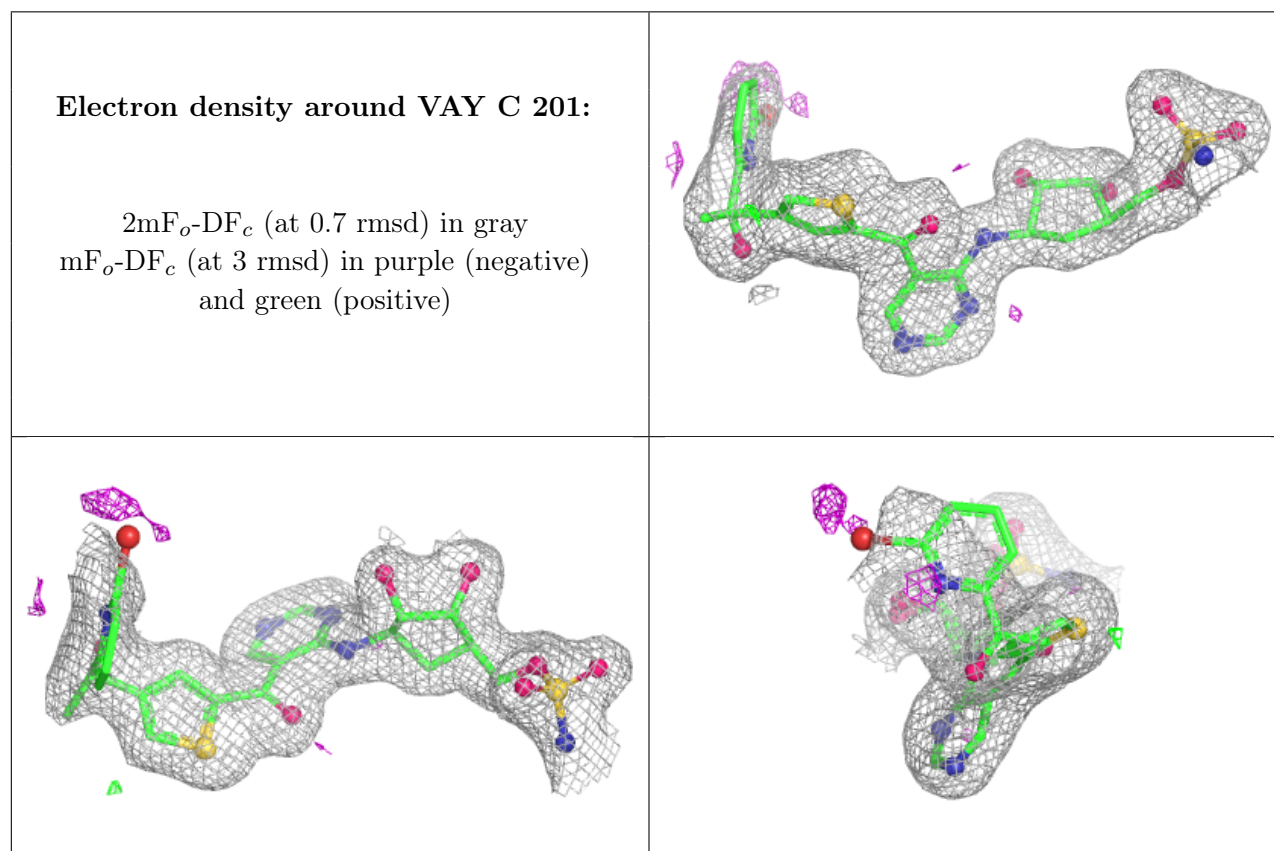
6.4 Ligands [i](#)

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
4	SO4	A	401	5/5	0.93	0.08	45,51,58,60	0
6	VAY	C	201	37/37	0.96	0.10	21,32,119,210	0
5	ZN	B	700	1/1	0.97	0.04	41,41,41,41	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.