



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:39 PM UTC

PDB ID : 8SCW / pdb_00008scw
Title : Crystal structure of IRAK4-HSA complexed with BMS-986147; 6-{5-CYANO-1H-PYRAZOLO[3,4-B]PYRIDIN-1-YL}-N-[(2R)-2-FLUOROROXY-3-METHYLBUTYL]-4-[(PROPAN-2-YL)AMINO]PYRIDINE-3-CARBOXAMIDE
Authors : Muckelbauer, J.K.; Ghosh, K.
Deposited on : 2023-04-05
Resolution : 2.76 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

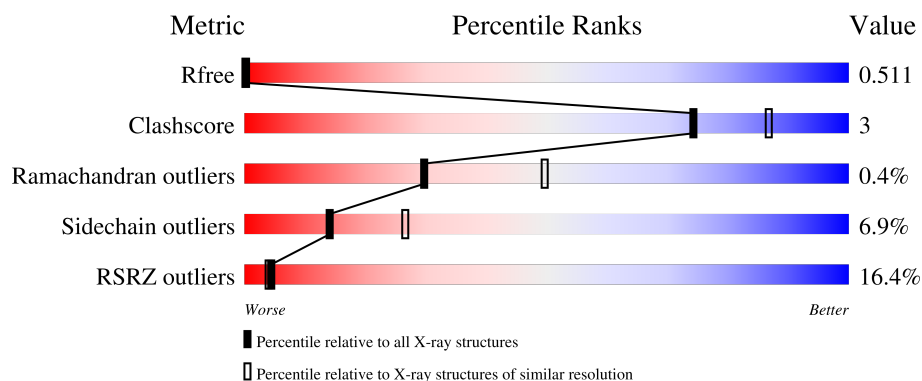
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	305	19% 79% 14% 6%
1	B	305	10% 78% 14% 6%
1	C	305	13% 78% 13% 7%
1	D	305	18% 79% 14% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8884 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.

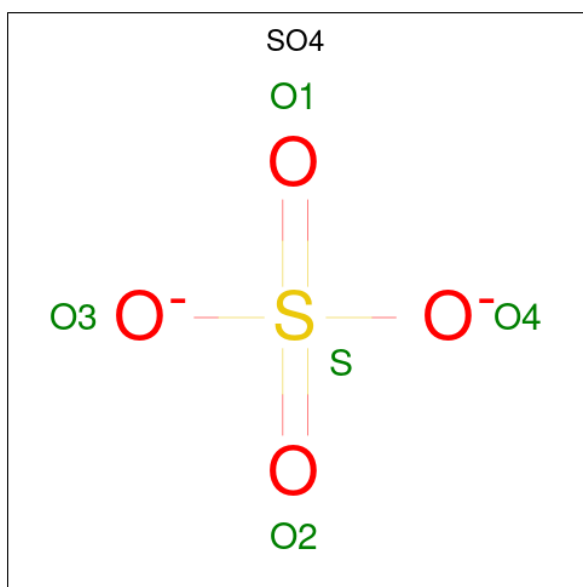
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	0	0
			2173	1360	367	429	3	14			
1	B	286	Total	C	N	O	P	S	0	0	0
			2166	1359	367	424	2	14			
1	C	284	Total	C	N	O	P	S	0	0	0
			2157	1352	367	422	2	14			
1	D	284	Total	C	N	O	P	S	0	0	0
			2165	1356	366	426	3	14			

There are 16 discrepancies between the modelled and reference sequences:

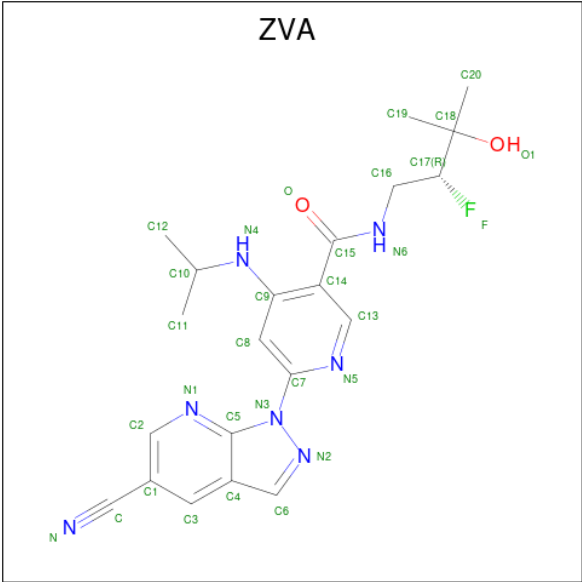
Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP Q9NWZ3
A	157	ALA	-	expression tag	UNP Q9NWZ3
A	158	MET	-	expression tag	UNP Q9NWZ3
A	159	GLY	-	expression tag	UNP Q9NWZ3
B	156	GLY	-	expression tag	UNP Q9NWZ3
B	157	ALA	-	expression tag	UNP Q9NWZ3
B	158	MET	-	expression tag	UNP Q9NWZ3
B	159	GLY	-	expression tag	UNP Q9NWZ3
C	156	GLY	-	expression tag	UNP Q9NWZ3
C	157	ALA	-	expression tag	UNP Q9NWZ3
C	158	MET	-	expression tag	UNP Q9NWZ3
C	159	GLY	-	expression tag	UNP Q9NWZ3
D	156	GLY	-	expression tag	UNP Q9NWZ3
D	157	ALA	-	expression tag	UNP Q9NWZ3
D	158	MET	-	expression tag	UNP Q9NWZ3
D	159	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is SULFATE ION (CCD ID: 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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (6M)-6-(5-cyano-1H-pyrazolo[3,4-b]pyridin-1-yl)-N-[(2R)-2-fluoro-3-hydroxy-3-methylbutyl]-4-[(propan-2-yl)amino]pyridine-3-carboxamide (CCD ID: ZVA) (formula: C₂₁H₂₄FN₇O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			31	21	1	7	2		
3	B	1	Total	C	F	N	O	0	0
			31	21	1	7	2		
3	C	1	Total	C	F	N	O	0	0
			31	21	1	7	2		
3	D	1	Total	C	F	N	O	0	0
			31	21	1	7	2		

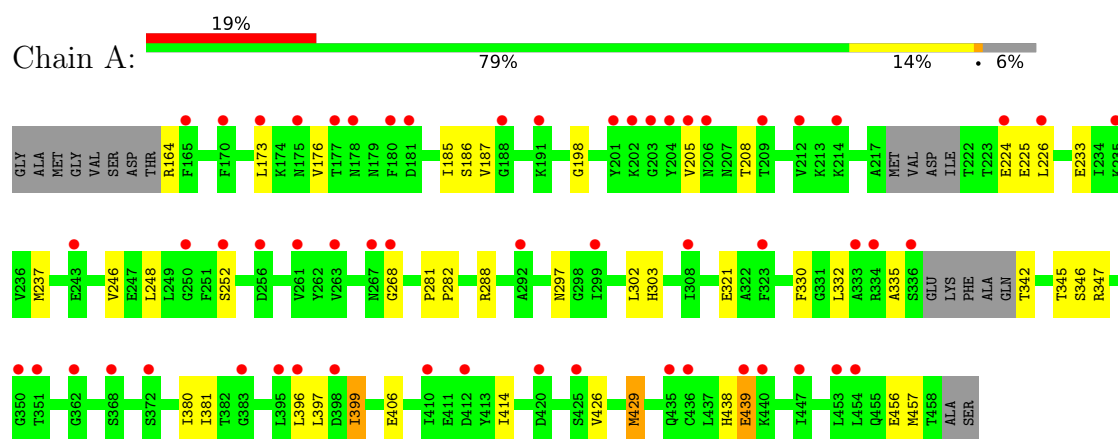
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	20	Total	O	0	0
			20	20		
4	C	10	Total	O	0	0
			10	10		
4	D	15	Total	O	0	0
			15	15		

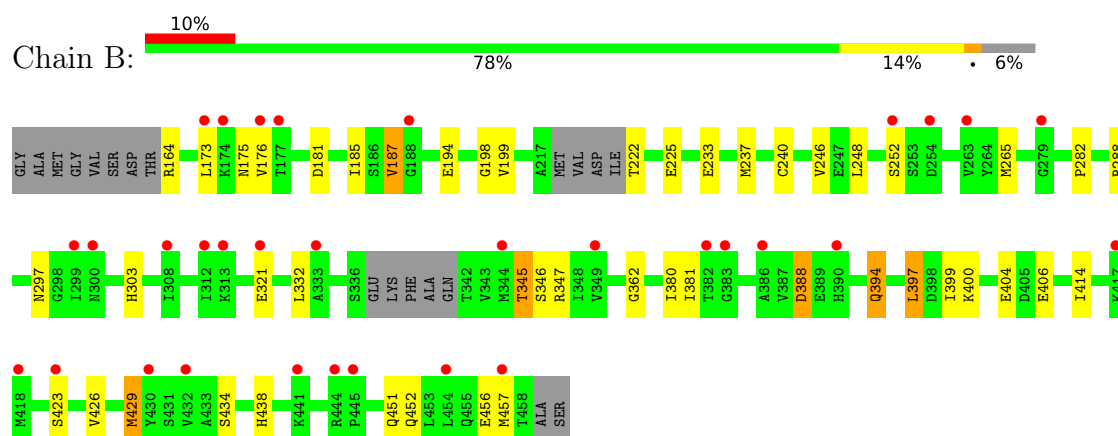
3 Residue-property plots [i](#)

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.

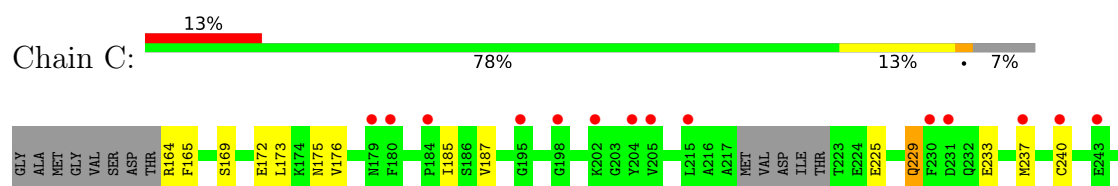
- Molecule 1: Interleukin-1 receptor-associated kinase 4

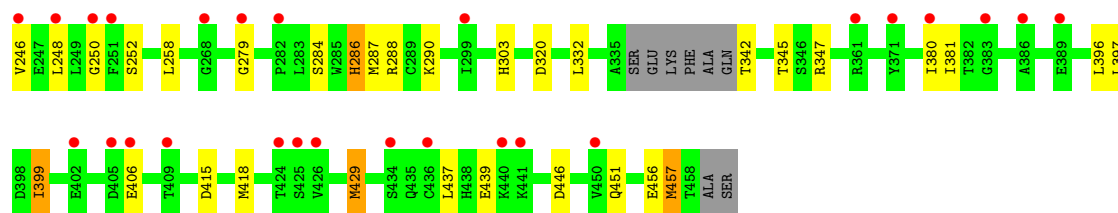


- Molecule 1: Interleukin-1 receptor-associated kinase 4

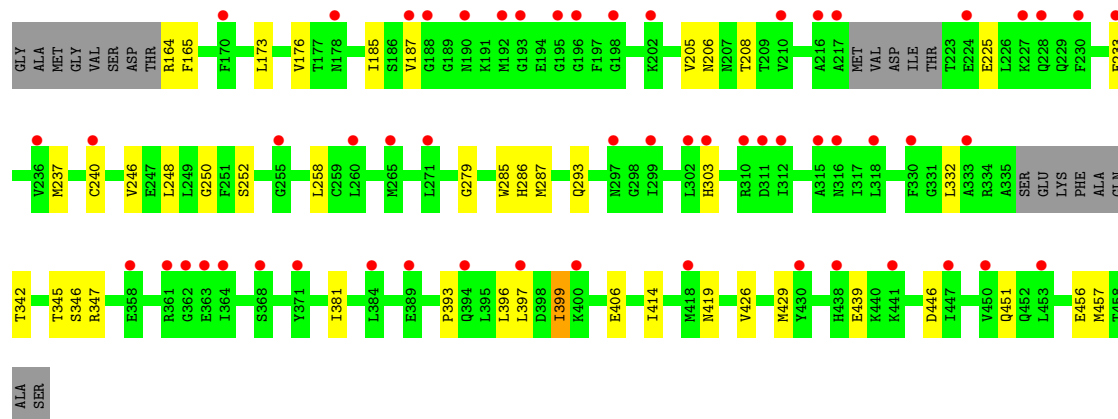
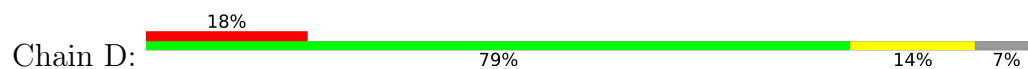


- Molecule 1: Interleukin-1 receptor-associated kinase 4





● Molecule 1: Interleukin-1 receptor-associated kinase 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.29Å 140.39Å 85.92Å 90.00° 126.60° 90.00°	Depositor
Resolution (Å)	36.68 – 2.76 36.68 – 2.76	Depositor EDS
% Data completeness (in resolution range)	98.9 (36.68-2.76) 86.5 (36.68-2.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.195 , 0.238 0.504 , 0.511	Depositor DCC
R_{free} test set	1599 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.850	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 544.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.048 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	8884	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.58 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5414e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TPO, SEP, SO4, ZVA

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	0.90	4/2176 (0.2%)	1.38	10/2948 (0.3%)
1	B	0.94	6/2174 (0.3%)	1.38	12/2944 (0.4%)
1	C	0.91	5/2164 (0.2%)	1.36	10/2929 (0.3%)
1	D	0.90	4/2168 (0.2%)	1.37	12/2935 (0.4%)
All	All	0.91	19/8682 (0.2%)	1.37	44/11756 (0.4%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	429	MET	SD-CE	-6.35	1.63	1.79
1	B	175	ASN	CG-OD1	6.00	1.34	1.23
1	B	303	HIS	ND1-CE1	5.80	1.38	1.32
1	D	303	HIS	ND1-CE1	5.62	1.38	1.32
1	C	175	ASN	CG-OD1	5.55	1.34	1.23
1	C	451	GLN	CD-OE1	5.51	1.34	1.23
1	A	303	HIS	ND1-CE1	5.49	1.38	1.32
1	B	429	MET	SD-CE	-5.49	1.65	1.79
1	B	438	HIS	ND1-CE1	5.43	1.38	1.32
1	B	451	GLN	CD-OE1	5.33	1.33	1.23
1	D	286	HIS	ND1-CE1	5.29	1.37	1.32
1	C	303	HIS	ND1-CE1	5.24	1.37	1.32
1	A	438	HIS	ND1-CE1	5.22	1.37	1.32
1	A	429	MET	SD-CE	-5.12	1.66	1.79
1	D	451	GLN	CD-OE1	5.11	1.33	1.23
1	D	303	HIS	CD2-NE2	-5.07	1.32	1.37
1	B	452	GLN	CD-OE1	5.07	1.33	1.23
1	C	286	HIS	ND1-CE1	5.07	1.37	1.32
1	A	303	HIS	CD2-NE2	-5.05	1.32	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	GLU	CB-CG-CD	7.65	125.60	112.60
1	D	286	HIS	CB-CG-CD2	-7.57	121.36	131.20
1	A	438	HIS	CA-C-N	7.54	130.71	120.38
1	A	438	HIS	C-N-CA	7.54	130.71	120.38
1	C	286	HIS	CB-CG-CD2	-7.54	121.40	131.20
1	B	303	HIS	CB-CG-CD2	-7.53	121.41	131.20
1	A	303	HIS	CB-CG-CD2	-7.40	121.58	131.20
1	B	438	HIS	CB-CG-CD2	-7.33	121.67	131.20
1	C	303	HIS	CB-CG-CD2	-7.25	121.77	131.20
1	A	438	HIS	CB-CG-CD2	-7.24	121.79	131.20
1	D	303	HIS	CB-CG-CD2	-7.14	121.91	131.20
1	C	229	GLN	CA-C-N	6.13	128.41	120.44
1	C	229	GLN	C-N-CA	6.13	128.41	120.44
1	B	456	GLU	CA-C-N	6.08	128.71	120.38
1	B	456	GLU	C-N-CA	6.08	128.71	120.38
1	D	393	PRO	CA-C-N	5.88	128.75	120.28
1	D	393	PRO	C-N-CA	5.88	128.75	120.28
1	A	456	GLU	CA-C-N	5.87	128.42	120.38
1	A	456	GLU	C-N-CA	5.87	128.42	120.38
1	A	335	ALA	CA-C-N	5.82	132.17	121.70
1	A	335	ALA	C-N-CA	5.82	132.17	121.70
1	D	456	GLU	CA-C-N	5.66	128.13	120.38
1	D	456	GLU	C-N-CA	5.66	128.13	120.38
1	C	437	LEU	N-CA-C	5.63	119.84	113.15
1	B	187	VAL	N-CA-CB	-5.60	106.05	112.21
1	C	240	CYS	N-CA-C	5.52	117.30	108.41
1	D	293	GLN	CA-C-N	5.43	126.00	119.98
1	D	293	GLN	C-N-CA	5.43	126.00	119.98
1	B	240	CYS	N-CA-C	5.38	117.40	108.20
1	B	404	GLU	CB-CG-CD	5.38	121.75	112.60
1	C	446	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	388	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	297	ASN	CA-C-N	5.24	125.75	119.94
1	B	297	ASN	C-N-CA	5.24	125.75	119.94
1	B	198	GLY	N-CA-C	5.14	118.48	110.88
1	D	446	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	285	TRP	CA-C-N	5.11	127.09	120.44
1	D	285	TRP	C-N-CA	5.11	127.09	120.44
1	A	198	GLY	N-CA-C	5.10	117.87	111.09
1	D	240	CYS	N-CA-C	5.08	116.89	108.20
1	B	181	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	320	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	456	GLU	CA-C-N	5.00	127.68	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	456	GLU	C-N-CA	5.00	127.68	120.38

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	2173	0	2061	14	0
1	B	2166	0	2065	17	0
1	C	2157	0	2060	15	0
1	D	2165	0	2063	11	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	15	0	0	0	0
2	D	10	0	0	0	0
3	A	31	0	0	0	0
3	B	31	0	0	0	0
3	C	31	0	0	0	0
3	D	31	0	0	0	0
4	A	14	0	0	1	0
4	B	20	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	0	0
All	All	8884	0	8249	53	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 (53) 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:D:381:ILE:HG13	1:D:429:MET:HE2	1.62	0.81
1:C:284:SER:H	1:C:287:MET:HE3	1.47	0.79
1:C:381:ILE:HG13	1:C:429:MET:HE2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ILE:HG13	1:A:429:MET:HE2	1.65	0.78
1:B:381:ILE:HG13	1:B:429:MET:HE2	1.67	0.77
1:B:388:ASP:O	1:B:394:GLN:HG3	1.97	0.64
1:C:165:PHE:HB3	1:C:250:GLY:HA2	1.83	0.60
1:C:237:MET:HG2	1:C:248:LEU:HB2	1.84	0.59
1:A:237:MET:HG2	1:A:248:LEU:HB2	1.85	0.59
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.85	0.59
1:D:176:VAL:HG11	1:D:205:VAL:HG22	1.85	0.58
1:B:237:MET:HG2	1:B:248:LEU:HB2	1.86	0.58
1:D:237:MET:HG2	1:D:248:LEU:HB2	1.86	0.57
1:C:169:SER:HB3	1:C:172:GLU:HB2	1.87	0.55
1:A:176:VAL:HG11	1:A:205:VAL:HG22	1.88	0.54
1:A:281:PRO:HD3	1:B:321:GLU:HG3	1.89	0.54
1:D:173:LEU:HA	1:D:176:VAL:HG22	1.90	0.53
1:A:186:SER:HB2	1:D:419:ASN:HB2	1.92	0.52
1:B:265:MET:HA	1:B:265:MET:HE2	1.92	0.52
1:D:414:ILE:HG12	1:D:426:VAL:HG11	1.92	0.50
1:A:173:LEU:HA	1:A:176:VAL:HG22	1.93	0.50
1:A:414:ILE:HG12	1:A:426:VAL:HG11	1.94	0.50
1:A:288:ARG:HB3	1:A:380:ILE:HG23	1.94	0.49
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.93	0.49
1:B:173:LEU:HA	1:B:176:VAL:HG22	1.94	0.49
1:C:173:LEU:HA	1:C:176:VAL:HG22	1.95	0.48
1:A:205:VAL:O	1:A:208:THR:HB	2.16	0.46
1:D:165:PHE:HB3	1:D:250:GLY:HA2	1.96	0.46
1:D:396:LEU:HD12	1:D:399:ILE:HD13	1.98	0.46
1:C:396:LEU:HD12	1:C:399:ILE:HD13	1.98	0.46
1:C:288:ARG:HB3	1:C:380:ILE:HG23	1.97	0.45
1:D:381:ILE:CG1	1:D:429:MET:HE2	2.41	0.45
1:A:268:GLY:HA3	4:A:608:HOH:O	2.16	0.44
1:B:288:ARG:HB3	1:B:380:ILE:CG2	2.46	0.44
1:A:288:ARG:HB3	1:A:380:ILE:CG2	2.47	0.44
1:B:397:LEU:O	1:B:400:LYS:HB3	2.18	0.44
1:B:282:PRO:HG2	1:C:279:GLY:HA2	1.98	0.44
1:C:286:HIS:CE1	1:C:290:LYS:HE2	2.52	0.44
1:B:345:TPO:HG23	1:B:362:GLY:O	2.18	0.43
1:B:400:LYS:HE2	1:B:434:SER:HA	1.99	0.43
1:D:206:ASN:C	1:D:208:THR:H	2.26	0.43
1:B:288:ARG:HB3	1:B:380:ILE:HG23	2.01	0.43
1:B:380:ILE:CG2	1:B:429:MET:HE1	2.48	0.43
1:C:288:ARG:HB3	1:C:380:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PRO:HG2	1:D:279:GLY:HA2	2.01	0.42
1:C:380:ILE:CG2	1:C:429:MET:HE1	2.50	0.42
1:C:237:MET:HG2	1:C:248:LEU:CB	2.50	0.41
1:A:396:LEU:HD12	1:A:399:ILE:HD13	2.03	0.41
1:A:302:LEU:HD11	1:A:330:PHE:HE1	1.85	0.41
1:B:194:GLU:HB3	1:B:199:VAL:HG22	2.02	0.41
1:B:381:ILE:CG1	1:B:429:MET:HE2	2.46	0.40
1:C:429:MET:HB2	1:C:457:MET:HE2	2.01	0.40
1:B:237:MET:HG2	1:B:248:LEU:CB	2.50	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	278/305 (91%)	268 (96%)	9 (3%)	1 (0%)	30	50
1	B	278/305 (91%)	270 (97%)	7 (2%)	1 (0%)	30	50
1	C	276/305 (90%)	266 (96%)	9 (3%)	1 (0%)	30	50
1	D	276/305 (90%)	265 (96%)	10 (4%)	1 (0%)	30	50
All	All	1108/1220 (91%)	1069 (96%)	35 (3%)	4 (0%)	30	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	B	406	GLU
1	C	406	GLU
1	D	406	GLU

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	224/260 (86%)	207 (92%)	17 (8%)	12	23
1	B	224/260 (86%)	209 (93%)	15 (7%)	15	28
1	C	224/260 (86%)	209 (93%)	15 (7%)	15	28
1	D	224/260 (86%)	209 (93%)	15 (7%)	15	28
All	All	896/1040 (86%)	834 (93%)	62 (7%)	14	26

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	185	ILE
1	A	187	VAL
1	A	224	GLU
1	A	225	GLU
1	A	226	LEU
1	A	233	GLU
1	A	246	VAL
1	A	252	SER
1	A	297	ASN
1	A	321	GLU
1	A	332	LEU
1	A	347	ARG
1	A	397	LEU
1	A	399	ILE
1	A	439	GLU
1	A	457	MET
1	B	164	ARG
1	B	185	ILE
1	B	187	VAL
1	B	222	THR
1	B	225	GLU
1	B	233	GLU
1	B	246	VAL

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Mol	Chain	Res	Type
1	B	252	SER
1	B	332	LEU
1	B	347	ARG
1	B	394	GLN
1	B	397	LEU
1	B	399	ILE
1	B	423	SER
1	B	457	MET
1	C	164	ARG
1	C	185	ILE
1	C	187	VAL
1	C	225	GLU
1	C	229	GLN
1	C	233	GLU
1	C	246	VAL
1	C	252	SER
1	C	258	LEU
1	C	332	LEU
1	C	347	ARG
1	C	397	LEU
1	C	399	ILE
1	C	439	GLU
1	C	457	MET
1	D	164	ARG
1	D	185	ILE
1	D	187	VAL
1	D	225	GLU
1	D	233	GLU
1	D	246	VAL
1	D	252	SER
1	D	258	LEU
1	D	287	MET
1	D	332	LEU
1	D	347	ARG
1	D	397	LEU
1	D	399	ILE
1	D	439	GLU
1	D	457	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	GLN
1	B	394	GLN
1	B	435	GLN
1	B	451	GLN
1	C	229	GLN
1	C	297	ASN
1	C	435	GLN
1	C	451	GLN
1	D	297	ASN
1	D	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPO	D	345	1	8,10,11	1.08	0	10,14,16	1.13	1 (10%)
1	TPO	B	345	1	8,10,11	1.12	0	10,14,16	1.10	1 (10%)
1	SEP	B	346	1	8,9,10	0.70	0	7,12,14	1.93	2 (28%)
1	SEP	C	346	1	3,4,10	0.69	0	2,4,14	1.63	0
1	SEP	D	346	1	8,9,10	0.86	0	7,12,14	2.08	2 (28%)
1	TPO	A	342	1	8,10,11	0.89	0	10,14,16	1.51	1 (10%)
1	TPO	B	342	1	3,4,11	0.75	0	2,4,16	0.99	0
1	TPO	D	342	1	8,10,11	1.13	0	10,14,16	1.31	1 (10%)
1	TPO	A	345	1	8,10,11	1.13	1 (12%)	10,14,16	1.20	1 (10%)
1	TPO	C	345	1	8,10,11	1.08	0	10,14,16	1.05	1 (10%)
1	SEP	A	346	1	8,9,10	0.86	0	7,12,14	1.79	1 (14%)
1	TPO	C	342	1	8,10,11	1.44	1 (12%)	10,14,16	1.36	1 (10%)

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
1	TPO	D	345	1	-	2/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	SEP	C	346	1	-	1/1/2/10	-
1	SEP	D	346	1	-	0/6/8/10	-
1	TPO	A	342	1	-	1/9/11/13	-
1	TPO	B	342	1	-	1/1/2/13	-
1	TPO	D	342	1	-	1/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-
1	TPO	C	345	1	-	2/9/11/13	-
1	SEP	A	346	1	-	1/6/8/10	-
1	TPO	C	342	1	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	TPO	P-OG1	-2.79	1.54	1.59
1	A	345	TPO	CB-CA	2.07	1.58	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	SEP	OG-CB-CA	4.51	112.54	108.14
1	A	346	SEP	OG-CB-CA	3.93	111.97	108.14
1	B	346	SEP	OG-CB-CA	3.79	111.83	108.14
1	A	342	TPO	P-OG1-CB	-2.81	115.69	123.33
1	C	342	TPO	P-OG1-CB	-2.78	115.78	123.33
1	D	346	SEP	OG-P-O1P	2.68	113.69	106.44
1	D	342	TPO	P-OG1-CB	-2.58	116.31	123.33
1	B	346	SEP	O2P-P-OG	2.39	112.90	106.67
1	A	345	TPO	P-OG1-CB	-2.32	117.03	123.33
1	B	345	TPO	P-OG1-CB	-2.10	117.63	123.33
1	D	345	TPO	P-OG1-CB	-2.06	117.72	123.33
1	C	345	TPO	P-OG1-CB	-2.01	117.87	123.33

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	342	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	C	346	SEP	O-C-CA-CB
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	C	342	TPO	CB-OG1-P-O3P
1	A	342	TPO	CB-OG1-P-O1P
1	A	345	TPO	CB-OG1-P-O1P
1	B	345	TPO	CB-OG1-P-O1P
1	D	342	TPO	CB-OG1-P-O1P
1	A	346	SEP	CA-CB-OG-P
1	A	345	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	345	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	ZVA	C	504	-	31,33,33	1.85	9 (29%)	41,48,48	1.53	8 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	503	-	4,4,4	0.40	0	6,6,6	0.44	0
3	ZVA	B	503	-	31,33,33	2.07	12 (38%)	41,48,48	1.69	11 (26%)
2	SO4	C	501	-	4,4,4	0.44	0	6,6,6	0.30	0
2	SO4	B	502	-	4,4,4	0.46	0	6,6,6	0.15	0
2	SO4	D	502	-	4,4,4	0.68	0	6,6,6	0.17	0
3	ZVA	D	503	-	31,33,33	1.45	6 (19%)	41,48,48	1.52	9 (21%)
3	ZVA	A	502	-	31,33,33	1.66	8 (25%)	41,48,48	1.44	9 (21%)
2	SO4	B	501	-	4,4,4	0.28	0	6,6,6	0.16	0
2	SO4	D	501	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	501	-	4,4,4	0.74	0	6,6,6	0.22	0
2	SO4	C	502	-	4,4,4	0.28	0	6,6,6	0.16	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	ZVA	A	502	-	-	4/22/25/25	0/3/3/3
3	ZVA	C	504	-	-	5/22/25/25	0/3/3/3
3	ZVA	D	503	-	-	5/22/25/25	0/3/3/3
3	ZVA	B	503	-	-	4/22/25/25	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	ZVA	C8-C9	4.33	1.46	1.39
3	B	503	ZVA	N3-N2	4.32	1.42	1.38
3	C	504	ZVA	C2-C1	4.31	1.45	1.39
3	C	504	ZVA	C5-N3	4.14	1.41	1.37
3	B	503	ZVA	C5-N3	4.04	1.41	1.37
3	C	504	ZVA	C8-C9	3.89	1.45	1.39
3	A	502	ZVA	C8-C9	3.86	1.45	1.39
3	A	502	ZVA	C5-N3	3.64	1.41	1.37
3	D	503	ZVA	C15-N6	3.39	1.41	1.33
3	B	503	ZVA	C15-N6	3.34	1.41	1.33
3	D	503	ZVA	C8-C9	3.33	1.44	1.39
3	B	503	ZVA	C6-N2	3.13	1.35	1.32
3	D	503	ZVA	C1-C	-3.10	1.38	1.44
3	B	503	ZVA	C14-C9	3.01	1.45	1.41
3	C	504	ZVA	C5-N1	3.01	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ZVA	C7-N5	3.01	1.40	1.34
3	B	503	ZVA	C7-N5	2.94	1.40	1.34
3	D	503	ZVA	C7-N5	2.89	1.40	1.34
3	B	503	ZVA	C1-C	-2.86	1.38	1.44
3	C	504	ZVA	C7-N3	2.81	1.47	1.42
3	A	502	ZVA	C15-N6	2.80	1.39	1.33
3	C	504	ZVA	C15-N6	2.79	1.39	1.33
3	C	504	ZVA	C6-N2	2.52	1.34	1.32
3	B	503	ZVA	C5-N1	2.40	1.38	1.34
3	A	502	ZVA	C1-C	-2.36	1.39	1.44
3	D	503	ZVA	C5-N1	2.35	1.38	1.34
3	C	504	ZVA	C1-C	-2.33	1.39	1.44
3	A	502	ZVA	C6-N2	2.27	1.34	1.32
3	C	504	ZVA	C7-N5	2.25	1.39	1.34
3	A	502	ZVA	C5-N1	2.25	1.38	1.34
3	D	503	ZVA	C2-C1	2.24	1.42	1.39
3	A	502	ZVA	C8-C7	2.19	1.42	1.39
3	B	503	ZVA	C10-N4	2.16	1.50	1.46
3	B	503	ZVA	C8-C7	2.09	1.42	1.39
3	B	503	ZVA	C4-C6	2.04	1.44	1.42

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	ZVA	N1-C5-N3	4.14	130.53	125.88
3	B	503	ZVA	C3-C1-C2	3.71	121.84	118.28
3	B	503	ZVA	C9-N4-C10	3.57	129.75	124.66
3	B	503	ZVA	C14-C9-N4	-3.57	117.93	121.08
3	C	504	ZVA	C4-C3-C1	-3.51	115.88	120.66
3	D	503	ZVA	C4-C3-C1	-3.49	115.91	120.66
3	D	503	ZVA	C3-C1-C2	3.44	121.58	118.28
3	C	504	ZVA	C3-C1-C2	3.32	121.46	118.28
3	C	504	ZVA	F-C17-C16	-3.27	105.03	108.06
3	A	502	ZVA	C6-N2-N3	3.19	108.16	106.14
3	B	503	ZVA	C5-N3-N2	-3.18	109.13	110.41
3	B	503	ZVA	C4-C6-N2	-3.00	109.78	112.05
3	B	503	ZVA	C6-N2-N3	2.91	107.99	106.14
3	D	503	ZVA	N1-C5-N3	2.90	129.14	125.88
3	D	503	ZVA	C9-C14-C15	2.86	124.63	120.96
3	D	503	ZVA	C8-C7-N3	2.86	121.49	119.62
3	C	504	ZVA	C6-N2-N3	2.85	107.95	106.14
3	C	504	ZVA	C8-C7-N3	2.82	121.47	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	504	ZVA	C5-N3-N2	-2.81	109.28	110.41
3	A	502	ZVA	C4-C5-N1	-2.73	123.20	126.88
3	B	503	ZVA	C8-C7-N3	2.66	121.36	119.62
3	B	503	ZVA	C4-C3-C1	-2.64	117.06	120.66
3	B	503	ZVA	C2-C1-C	-2.64	117.24	120.05
3	D	503	ZVA	C6-N2-N3	2.62	107.81	106.14
3	A	502	ZVA	C4-C6-N2	-2.61	110.08	112.05
3	B	503	ZVA	C5-C4-C6	2.57	106.45	104.40
3	C	504	ZVA	N1-C5-N3	2.49	128.68	125.88
3	A	502	ZVA	C14-C9-N4	-2.43	118.94	121.08
3	A	502	ZVA	C3-C1-C2	2.41	120.59	118.28
3	C	504	ZVA	C14-C9-N4	-2.40	118.96	121.08
3	B	503	ZVA	N1-C5-N3	2.37	128.54	125.88
3	A	502	ZVA	C5-N3-N2	-2.37	109.46	110.41
3	A	502	ZVA	F-C17-C16	-2.31	105.92	108.06
3	D	503	ZVA	C2-C1-C	-2.27	117.63	120.05
3	D	503	ZVA	F-C17-C16	2.15	110.06	108.06
3	D	503	ZVA	C16-N6-C15	-2.14	118.60	122.54
3	A	502	ZVA	C5-C4-C6	2.02	106.01	104.40

There are no chirality outliers.

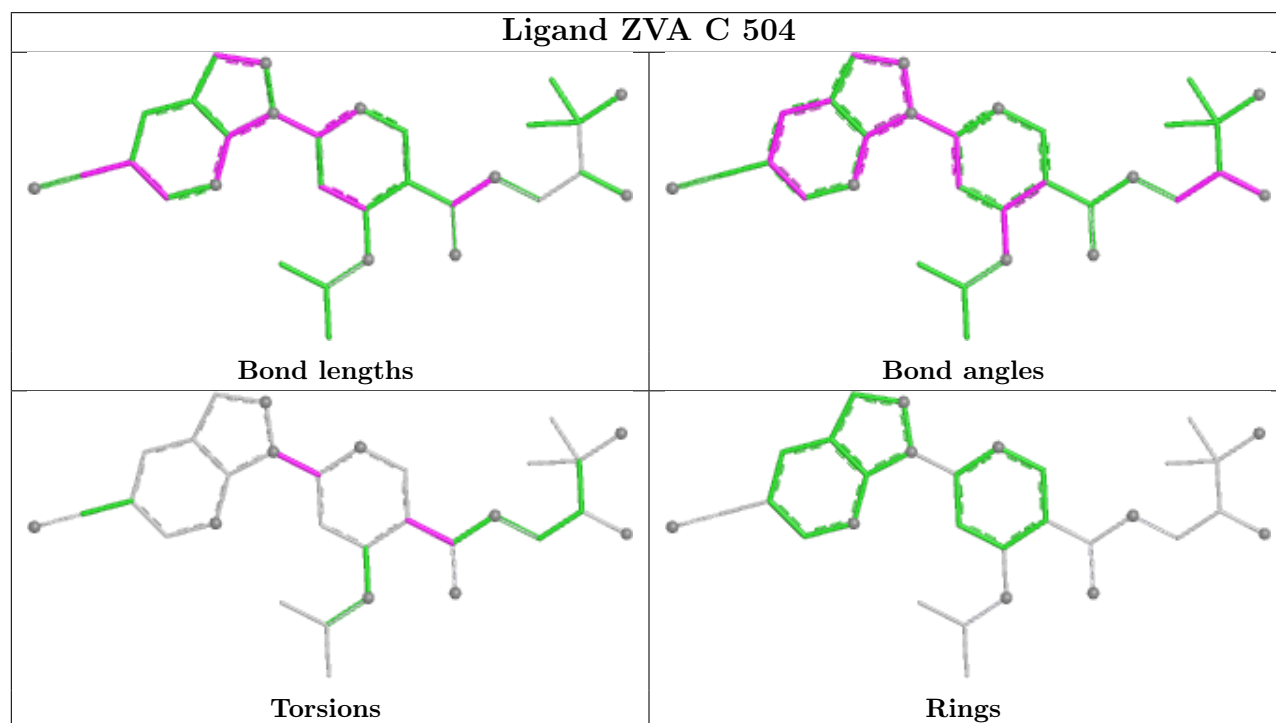
All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	503	ZVA	N5-C7-N3-C5
3	A	502	ZVA	C13-C14-C15-O
3	C	504	ZVA	C13-C14-C15-O
3	D	503	ZVA	C13-C14-C15-O
3	A	502	ZVA	C13-C14-C15-N6
3	C	504	ZVA	C13-C14-C15-N6
3	D	503	ZVA	C13-C14-C15-N6
3	D	503	ZVA	C8-C7-N3-N2
3	B	503	ZVA	C13-C14-C15-O
3	B	503	ZVA	C13-C14-C15-N6
3	B	503	ZVA	C8-C7-N3-N2
3	C	504	ZVA	C8-C7-N3-N2
3	C	504	ZVA	N5-C7-N3-C5
3	A	502	ZVA	C8-C7-N3-N2
3	A	502	ZVA	N5-C7-N3-N2
3	D	503	ZVA	N5-C7-N3-N2
3	B	503	ZVA	N5-C7-N3-N2
3	C	504	ZVA	N5-C7-N3-N2

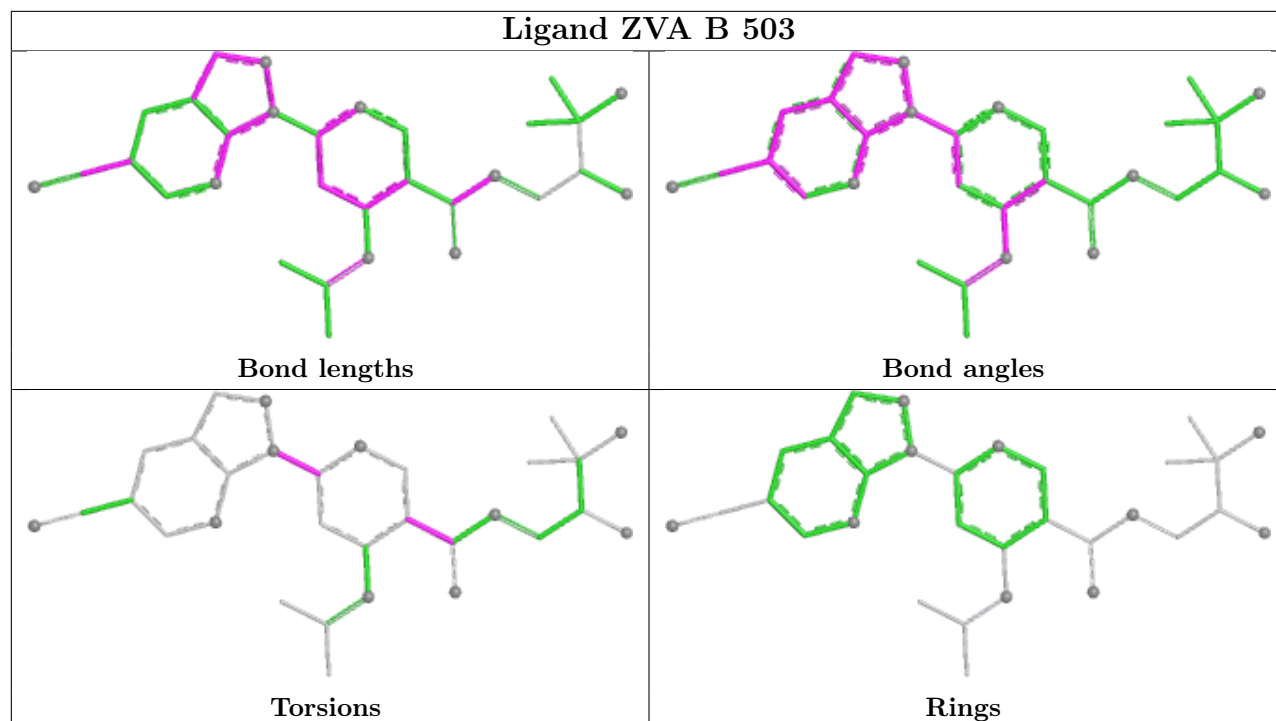
There are no ring outliers.

No monomer is involved in short contacts.

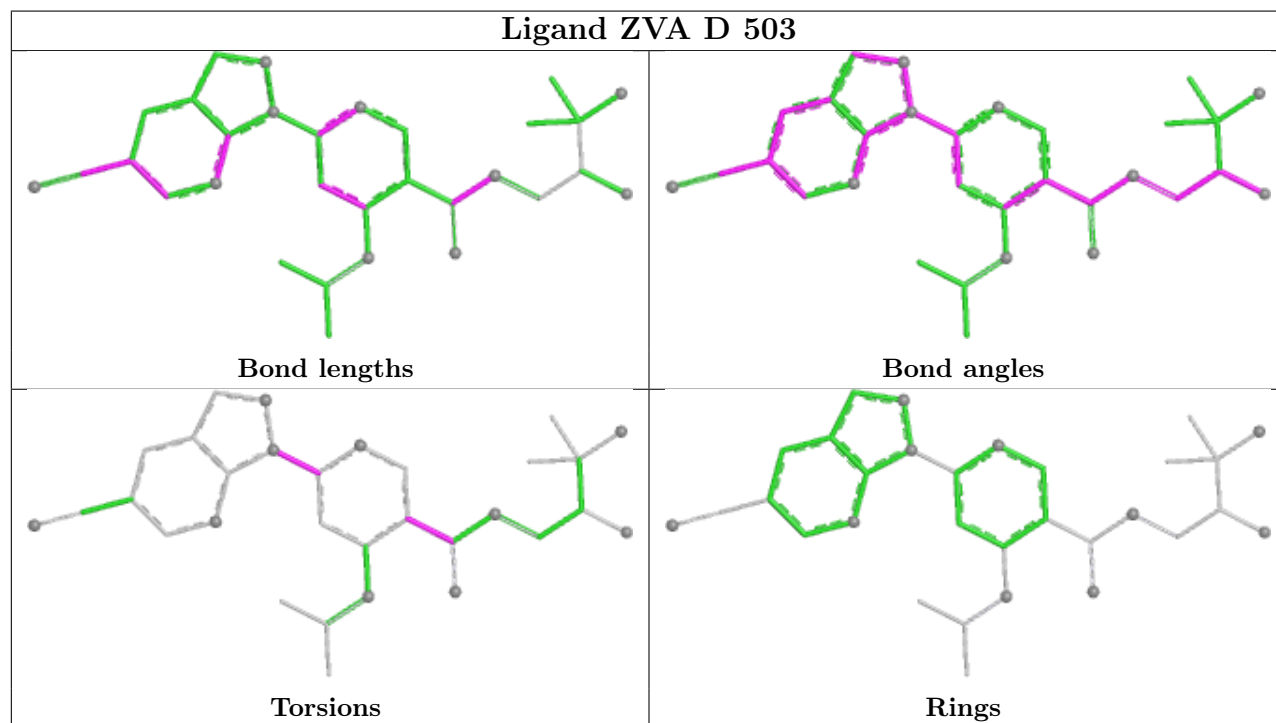
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

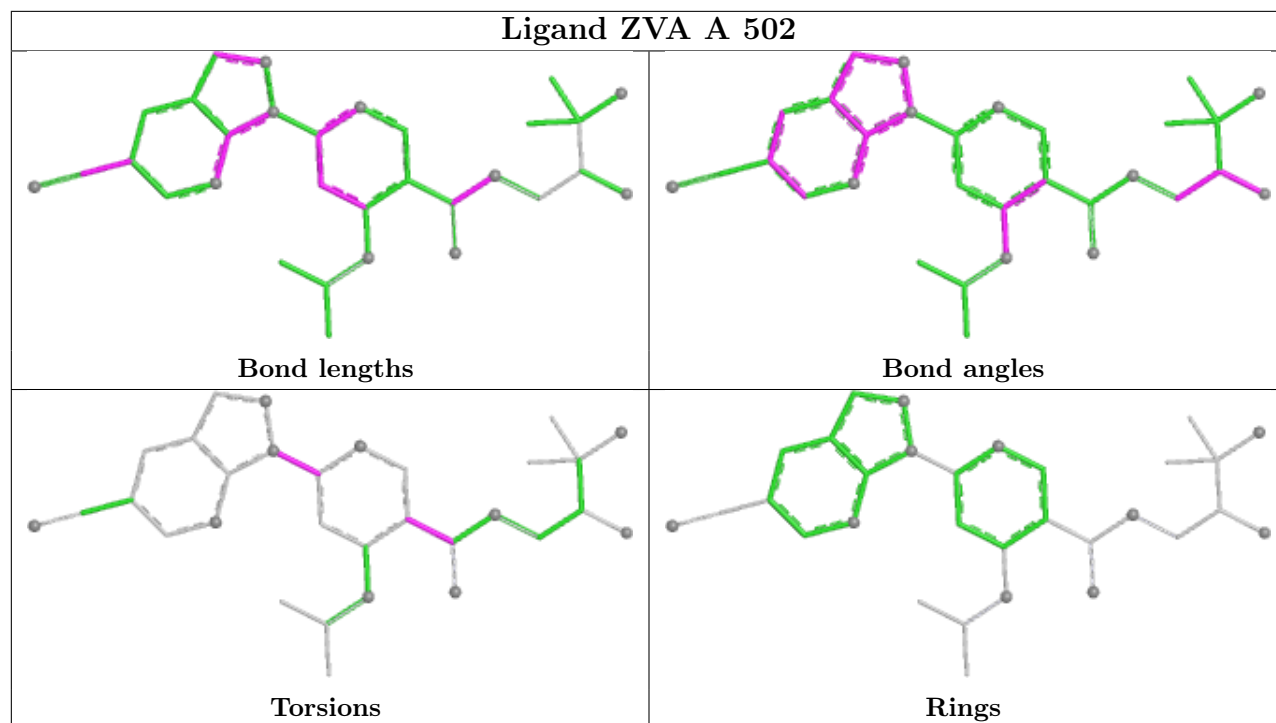


Ligand ZVA B 503



Ligand ZVA D 503





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	283/305 (92%)	1.07	57 (20%) 3 2	29, 54, 85, 123	0
1	B	283/305 (92%)	0.76	32 (11%) 10 8	29, 54, 83, 113	0
1	C	281/305 (92%)	1.08	40 (14%) 6 5	30, 56, 100, 116	0
1	D	281/305 (92%)	1.20	56 (19%) 3 2	33, 59, 94, 115	0
All	All	1128/1220 (92%)	1.03	185 (16%) 4 4	29, 55, 92, 123	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	434	SER	13.4
1	C	426	VAL	7.5
1	D	193	GLY	7.2
1	C	231	ASP	6.3
1	D	255	GLY	6.1
1	C	282	PRO	5.9
1	B	252	SER	5.8
1	A	177	THR	5.8
1	C	251	PHE	5.7
1	D	333	ALA	5.7
1	A	351	THR	5.5
1	A	368	SER	5.5
1	C	361	ARG	5.0
1	A	362	GLY	5.0
1	C	243	GLU	5.0
1	A	243	GLU	5.0
1	D	362	GLY	5.0
1	D	361	ARG	4.9
1	D	310	ARG	4.9
1	B	188	GLY	4.8
1	C	383	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	330	PHE	4.6
1	D	368	SER	4.6
1	B	349	VAL	4.5
1	A	268	GLY	4.5
1	D	196	GLY	4.4
1	D	260	LEU	4.4
1	D	438	HIS	4.4
1	C	179	ASN	4.4
1	D	299	ILE	4.4
1	D	230	PHE	4.3
1	D	195	GLY	4.3
1	C	406	GLU	4.3
1	D	178	ASN	4.2
1	A	206	ASN	4.1
1	B	300	ASN	4.1
1	A	395	LEU	4.1
1	D	187	VAL	4.0
1	D	190	ASN	4.0
1	B	321	GLU	3.9
1	D	297	ASN	3.9
1	A	453	LEU	3.8
1	B	254	ASP	3.8
1	A	372	SER	3.8
1	A	263	VAL	3.8
1	A	170	PHE	3.8
1	D	316	ASN	3.7
1	D	418	MET	3.7
1	A	323	PHE	3.7
1	D	384	LEU	3.7
1	A	439	GLU	3.7
1	D	227	LYS	3.6
1	B	444	ARG	3.6
1	C	250	GLY	3.6
1	D	228	GLN	3.6
1	A	454	LEU	3.5
1	A	256	ASP	3.5
1	C	402	GLU	3.5
1	B	417	LYS	3.4
1	A	410	ILE	3.4
1	D	363	GLU	3.4
1	D	371	TYR	3.4
1	A	420	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	389	GLU	3.3
1	C	202	LYS	3.3
1	B	445	PRO	3.3
1	D	233	GLU	3.3
1	B	386	ALA	3.3
1	D	453	LEU	3.2
1	D	315	ALA	3.2
1	A	202	LYS	3.2
1	C	389	GLU	3.2
1	D	271	LEU	3.2
1	A	204	TYR	3.2
1	C	436	CYS	3.2
1	D	312	ILE	3.2
1	A	333	ALA	3.2
1	B	441	LYS	3.1
1	C	386	ALA	3.1
1	A	440	LYS	3.1
1	D	302	LEU	3.1
1	A	261	VAL	3.1
1	D	441	LYS	3.0
1	B	454	LEU	3.0
1	B	177	THR	3.0
1	B	423	SER	3.0
1	A	336	SER	2.9
1	A	201	TYR	2.9
1	A	412	ASP	2.9
1	C	440	LYS	2.9
1	B	299	ILE	2.9
1	D	358	GLU	2.9
1	D	364	ILE	2.8
1	D	216	ALA	2.8
1	C	215	LEU	2.7
1	B	432	VAL	2.7
1	C	248	LEU	2.7
1	A	383	GLY	2.7
1	B	308	ILE	2.7
1	D	192	MET	2.7
1	B	312	ILE	2.7
1	B	418	MET	2.7
1	B	390	HIS	2.7
1	C	204	TYR	2.6
1	D	240	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	224	GLU	2.6
1	C	198	GLY	2.6
1	D	210	VAL	2.6
1	A	435	GLN	2.6
1	C	299	ILE	2.6
1	A	396	LEU	2.6
1	A	188	GLY	2.6
1	B	176	VAL	2.6
1	C	371	TYR	2.6
1	D	303	HIS	2.6
1	D	311	ASP	2.5
1	D	318	LEU	2.5
1	A	165	PHE	2.5
1	D	394	GLN	2.5
1	A	235	LYS	2.5
1	B	333	ALA	2.5
1	A	191	LYS	2.5
1	C	441	LYS	2.5
1	B	430	TYR	2.5
1	C	240	CYS	2.5
1	A	214	LYS	2.4
1	A	267	ASN	2.4
1	D	198	GLY	2.4
1	C	380	ILE	2.4
1	A	181	ASP	2.4
1	A	250	GLY	2.4
1	C	405	ASP	2.4
1	A	350	GLY	2.4
1	C	184	PRO	2.4
1	C	268	GLY	2.4
1	A	178	ASN	2.4
1	A	252	SER	2.4
1	A	203	GLY	2.4
1	A	334	ARG	2.4
1	D	450	VAL	2.3
1	D	170	PHE	2.3
1	B	174	LYS	2.3
1	B	383	GLY	2.3
1	C	246	VAL	2.3
1	D	447	ILE	2.2
1	D	236	VAL	2.2
1	D	397	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	308	ILE	2.2
1	B	313	LYS	2.2
1	D	224	GLU	2.2
1	B	457	MET	2.2
1	C	230	PHE	2.2
1	C	195	GLY	2.2
1	D	400	LYS	2.2
1	A	205	VAL	2.2
1	A	299	ILE	2.2
1	A	173	LEU	2.2
1	C	180	PHE	2.2
1	B	382	THR	2.1
1	A	180	PHE	2.1
1	C	409	THR	2.1
1	C	237	MET	2.1
1	A	175	ASN	2.1
1	A	447	ILE	2.1
1	A	209	THR	2.1
1	C	279	GLY	2.1
1	D	430	TYR	2.1
1	B	263	VAL	2.1
1	C	205	VAL	2.1
1	C	450	VAL	2.1
1	C	425	SER	2.0
1	D	202	LYS	2.0
1	A	226	LEU	2.0
1	B	173	LEU	2.0
1	B	279	GLY	2.0
1	A	436	CYS	2.0
1	A	292	ALA	2.0
1	A	398	ASP	2.0
1	D	217	ALA	2.0
1	A	425	SER	2.0
1	B	344	MET	2.0
1	C	424	THR	2.0
1	D	265	MET	2.0
1	D	188	GLY	2.0
1	A	212	VAL	2.0

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

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
1	SEP	C	346	5/11	0.91	0.14	96,96,99,99	0
1	TPO	D	342	11/12	0.91	0.14	80,83,88,88	0
1	TPO	D	345	11/12	0.94	0.13	72,73,76,78	0
1	TPO	C	342	11/12	0.96	0.14	116,118,120,120	0
1	TPO	A	342	11/12	0.96	0.15	119,122,127,127	0
1	SEP	A	346	10/11	0.96	0.11	112,115,120,120	0
1	TPO	B	342	5/12	0.96	0.18	89,90,93,94	0
1	SEP	D	346	10/11	0.96	0.09	77,84,94,95	0
1	TPO	B	345	11/12	0.97	0.15	93,100,102,103	0
1	TPO	A	345	11/12	0.97	0.14	109,111,112,113	0
1	SEP	B	346	10/11	0.98	0.19	98,102,110,110	0
1	TPO	C	345	11/12	0.98	0.17	98,100,101,101	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	SO4	D	502	5/5	0.94	0.25	74,77,79,81	0
3	ZVA	A	502	31/31	0.94	0.13	26,33,40,50	0
3	ZVA	D	503	31/31	0.95	0.11	22,37,43,47	0
2	SO4	C	502	5/5	0.96	0.10	142,147,147,148	0
3	ZVA	B	503	31/31	0.96	0.10	27,35,41,42	0
2	SO4	B	502	5/5	0.96	0.15	120,124,125,125	0
2	SO4	C	501	5/5	0.97	0.12	84,89,89,90	0
2	SO4	B	501	5/5	0.97	0.12	108,113,113,113	0
2	SO4	C	503	5/5	0.97	0.08	66,69,71,72	0
3	ZVA	C	504	31/31	0.97	0.12	34,40,50,51	0

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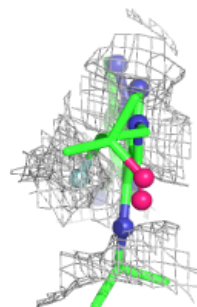
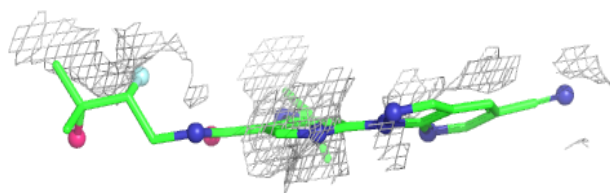
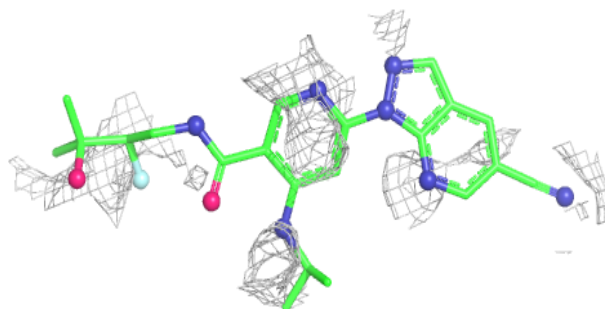
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	501	5/5	0.97	0.13	159,163,164,164	0
2	SO4	A	501	5/5	0.98	0.12	85,89,90,91	0

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.

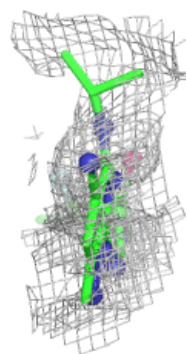
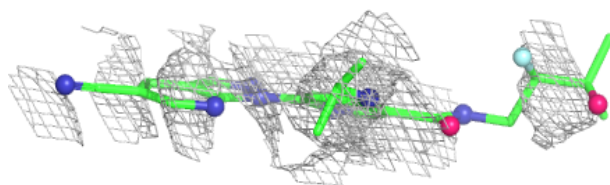
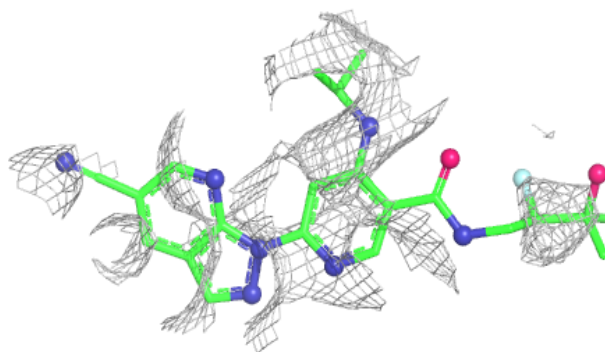
Electron density around ZVA A 502:

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

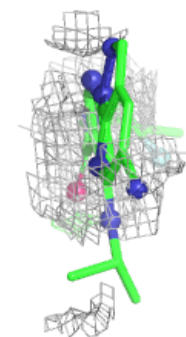
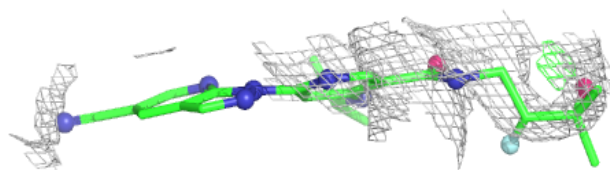
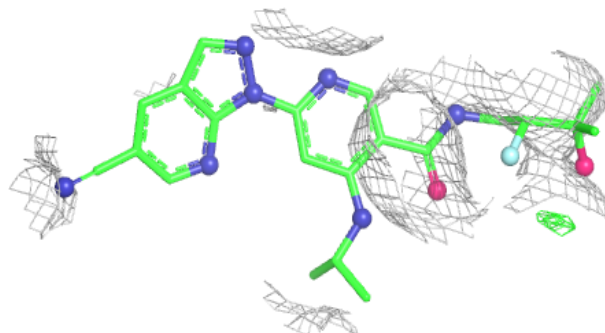


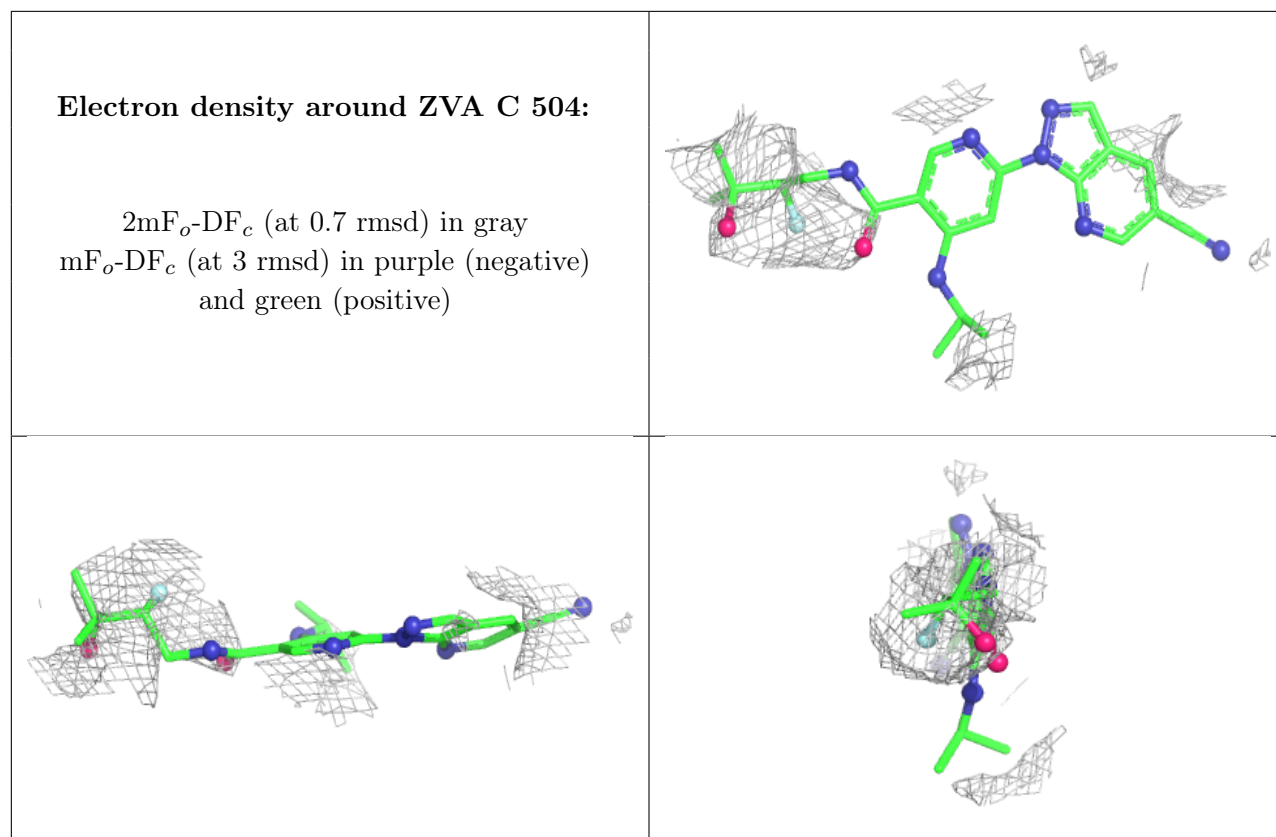
Electron density around ZVA D 503:

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

**Electron density around ZVA B 503:**

$2mF_o-DF_c$ (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.