



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:29 PM UTC

PDB ID : 2H42 / pdb_00002h42
Title : Crystal structure of PDE5 in complex with sildenafil
Authors : Wang, H.; Ke, H.
Deposited on : 2006-05-23
Resolution : 2.30 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

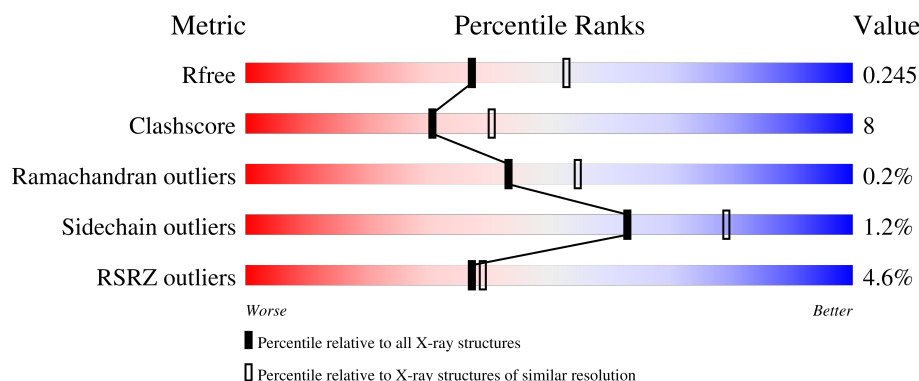
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	326	3% 81% 18%
1	B	326	6% 79% 17% • •
1	C	326	4% 77% 20% • •

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
2	ZN	B	503	-	-	-	X
2	ZN	C	505	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8218 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 cGMP-specific 3',5'-cyclic phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2650	1683	462	487	18			
1	B	317	Total	C	N	O	S	0	0	0
			2576	1635	450	473	18			
1	C	317	Total	C	N	O	S	0	0	0
			2576	1635	450	473	18			

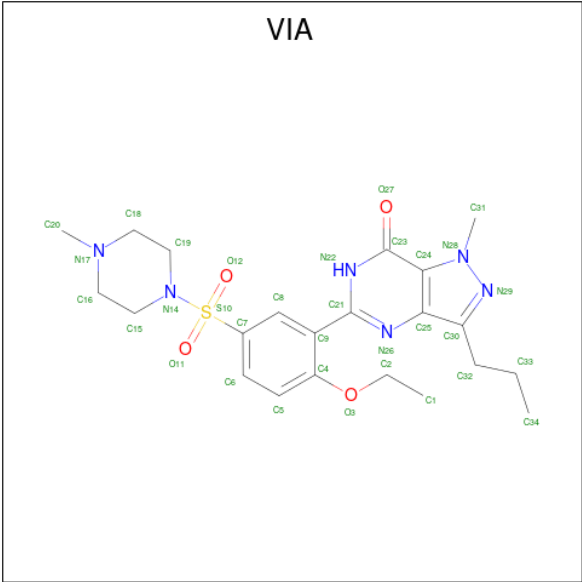
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 5-{2-ETHOXY-5-[(4-METHYLPIPERAZIN-1-YL)SULFONYL]PHENYL}-1-METHYL-3-PROPYL-1H,6H,7H-PYRAZOLO[4,3-D]PYRIMIDIN-7-ONE (CCD ID: VIA) (formula: C₂₂H₃₀N₆O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			33	22	6	4	1		
4	B	1	Total	C	N	O	S	0	0
			33	22	6	4	1		
4	C	1	Total	C	N	O	S	0	0
			33	22	6	4	1		

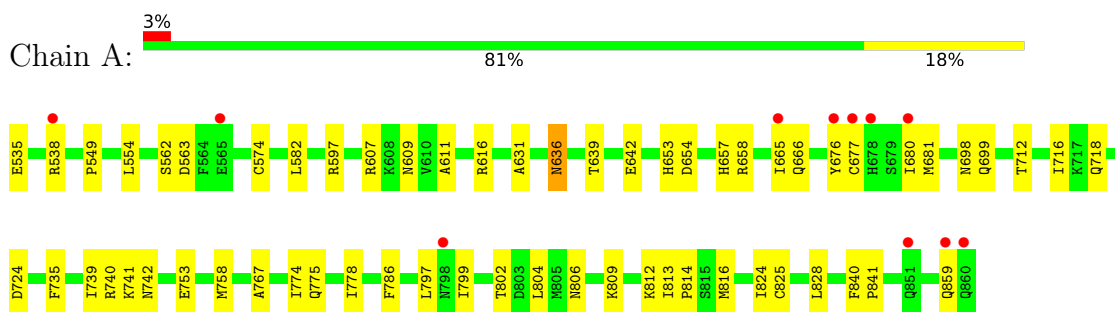
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total	O	0	0
			90	90		
5	B	103	Total	O	0	0
			103	103		
5	C	118	Total	O	0	0
			118	118		

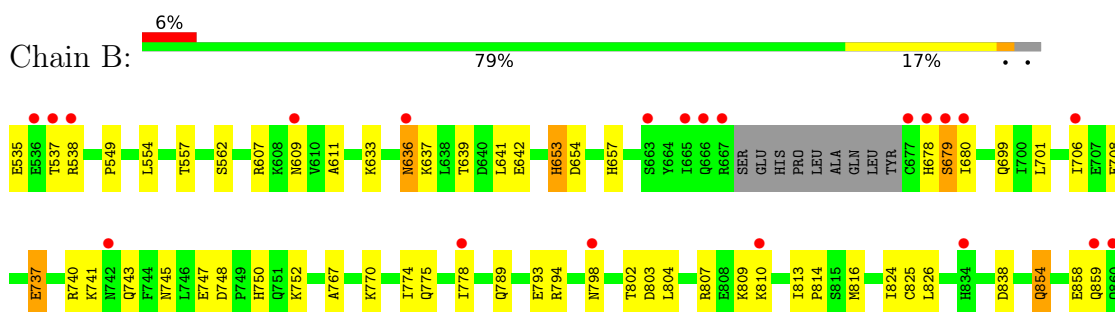
3 Residue-property plots [i](#)

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.

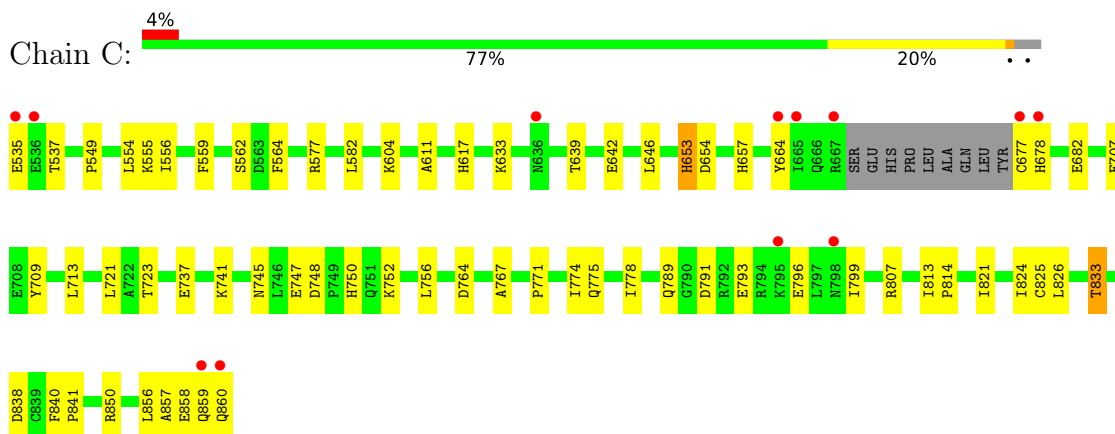
- Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	164.57Å 164.57Å 193.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.30) 96.4 (30.00-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.246 0.209 , 0.245	Depositor DCC
R_{free} test set	6946 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.8	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	0.93	EDS
Total number of atoms	8218	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: ZN, MG, VIA

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	0.38	0/2701	0.87	9/3645 (0.2%)
1	B	0.41	0/2623	0.87	8/3536 (0.2%)
1	C	0.42	0/2623	0.88	8/3536 (0.2%)
All	All	0.40	0/7947	0.87	25/10717 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	825	CYS	N-CA-C	8.95	122.79	111.24
1	B	824	ILE	N-CA-C	8.82	118.59	111.62
1	A	824	ILE	N-CA-C	8.72	118.51	111.62
1	A	825	CYS	N-CA-C	7.78	121.27	111.24
1	C	858	GLU	N-CA-C	-7.14	104.69	113.19
1	B	653	HIS	N-CA-C	7.10	121.05	112.38
1	C	825	CYS	N-CA-C	6.84	121.89	112.04
1	A	611	ALA	N-CA-C	6.75	119.21	111.11
1	B	679	SER	N-CA-C	-6.37	103.38	111.92
1	B	611	ALA	N-CA-C	6.37	119.04	111.33
1	C	653	HIS	N-CA-C	6.37	120.15	112.38
1	A	582	LEU	N-CA-C	-6.28	105.20	112.92
1	A	653	HIS	N-CA-C	6.22	119.97	112.38
1	C	611	ALA	N-CA-C	6.02	118.34	111.11
1	A	699	GLN	N-CA-C	5.93	118.81	109.39
1	A	802	THR	N-CA-C	-5.64	103.25	110.53
1	C	582	LEU	N-CA-C	-5.53	106.12	112.92
1	A	824	ILE	CB-CA-C	-5.51	106.14	111.05
1	B	802	THR	N-CA-C	-5.37	103.44	110.53
1	C	824	ILE	N-CA-C	5.35	116.61	112.12
1	B	770	LYS	N-CA-C	5.25	117.76	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	796	GLU	N-CA-C	5.16	118.03	111.69
1	B	826	LEU	N-CA-C	5.14	117.28	111.11
1	A	724	ASP	N-CA-C	-5.12	100.73	108.67
1	C	564	PHE	N-CA-C	5.09	117.22	111.11

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	2650	0	2657	48	0
1	B	2576	0	2587	46	0
1	C	2576	0	2587	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	33	0	30	0	0
4	B	33	0	30	3	0
4	C	33	0	30	1	0
5	A	90	0	0	3	0
5	B	103	0	0	3	0
5	C	118	0	0	2	0
All	All	8218	0	7921	131	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 (131) 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:B:816:MET:HE2	4:B:902:VIA:H6	1.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:ARG:HH21	1:A:741:LYS:HE2	1.28	0.95
1:B:740:ARG:HH21	1:B:741:LYS:HE3	1.33	0.93
1:A:806:ASN:HD22	1:A:809:LYS:HG2	1.33	0.92
1:A:549:PRO:HG2	1:A:554:LEU:HD21	1.56	0.85
1:A:740:ARG:NH2	1:A:741:LYS:HE2	1.92	0.84
1:C:767:ALA:HB1	1:C:778:ILE:HG21	1.60	0.83
1:C:793:GLU:HB3	1:C:799:ILE:HD11	1.58	0.83
1:A:806:ASN:ND2	1:A:809:LYS:HG2	1.96	0.81
1:C:642:GLU:OE2	1:C:752:LYS:HD3	1.81	0.80
1:C:535:GLU:HG3	1:C:537:THR:H	1.47	0.79
1:B:642:GLU:OE2	1:B:752:LYS:HD3	1.84	0.78
1:A:742:ASN:HD21	1:B:804:LEU:H	1.30	0.78
1:A:767:ALA:HB1	1:A:778:ILE:HG21	1.65	0.77
1:B:699:GLN:HE21	1:B:701:LEU:H	1.29	0.77
1:A:740:ARG:HH21	1:A:741:LYS:CE	1.99	0.75
1:B:706:ILE:HG12	1:C:737:GLU:OE1	1.95	0.67
1:A:806:ASN:HD22	1:A:809:LYS:CG	2.04	0.67
1:A:814:PRO:HG2	5:A:115:HOH:O	1.94	0.67
1:B:562:SER:HB2	1:B:774:ILE:HD13	1.75	0.66
1:B:636:ASN:C	1:B:636:ASN:HD22	2.03	0.65
1:B:794:ARG:O	1:B:798:ASN:HA	1.97	0.65
1:B:767:ALA:HB1	1:B:778:ILE:HG21	1.79	0.64
1:A:804:LEU:HA	1:A:816:MET:HE1	1.81	0.63
1:B:641:LEU:HD11	1:B:708:GLU:HG2	1.80	0.63
1:B:636:ASN:HD22	1:B:637:LYS:N	1.97	0.63
1:A:639:THR:OG1	1:A:642:GLU:HG3	2.01	0.61
1:B:741:LYS:HB2	1:B:743:GLN:HE21	1.65	0.60
1:B:653:HIS:HD2	5:B:254:HOH:O	1.85	0.60
1:B:816:MET:CE	4:B:902:VIA:H6	2.23	0.60
1:B:854:GLN:O	1:B:858:GLU:HG3	2.02	0.59
1:B:741:LYS:CB	1:B:743:GLN:HE21	2.15	0.59
1:C:767:ALA:CB	1:C:778:ILE:HG21	2.32	0.59
1:A:742:ASN:ND2	1:B:804:LEU:H	1.99	0.59
1:A:562:SER:HB2	1:A:774:ILE:HD13	1.85	0.59
1:C:856:LEU:HG	1:C:860:GLN:HE21	1.69	0.58
1:A:735:PHE:CD2	1:A:758:MET:HE2	2.39	0.58
1:A:740:ARG:NH1	1:B:803:ASP:OD1	2.37	0.58
1:A:804:LEU:CA	1:A:816:MET:HE1	2.33	0.58
1:C:549:PRO:HG2	1:C:554:LEU:HD21	1.86	0.58
1:B:741:LYS:O	1:B:743:GLN:HG3	2.04	0.57
1:B:740:ARG:HH21	1:B:741:LYS:CE	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:GLN:HG2	5:A:62:HOH:O	2.04	0.56
1:A:680:ILE:HG23	1:A:681:MET:N	2.21	0.56
1:A:549:PRO:CG	1:A:554:LEU:HD21	2.34	0.55
1:B:813:ILE:HB	1:B:814:PRO:HD3	1.89	0.54
1:B:549:PRO:HG2	1:B:554:LEU:HD21	1.90	0.54
1:B:807:ARG:HG3	1:B:810:LYS:HE3	1.90	0.54
1:A:740:ARG:HH12	1:B:809:LYS:NZ	2.05	0.53
1:C:707:GLU:HG2	5:C:66:HOH:O	2.08	0.53
1:C:709:TYR:CZ	1:C:713:LEU:HD11	2.44	0.53
1:C:639:THR:OG1	1:C:642:GLU:HG3	2.09	0.52
1:A:718:GLN:NE2	1:A:753:GLU:OE2	2.42	0.52
1:C:789:GLN:O	1:C:793:GLU:HG3	2.09	0.52
1:A:666:GLN:HG2	5:A:310:HOH:O	2.09	0.52
1:A:735:PHE:HD2	1:A:758:MET:HE2	1.73	0.52
1:B:639:THR:OG1	1:B:642:GLU:HG3	2.09	0.52
1:A:597:ARG:HG2	1:A:698:ASN:OD1	2.11	0.51
1:B:535:GLU:HG3	1:B:538:ARG:H	1.75	0.51
1:C:535:GLU:HG3	1:C:537:THR:N	2.23	0.51
1:A:740:ARG:NH1	1:B:809:LYS:NZ	2.58	0.51
1:C:562:SER:HB2	1:C:774:ILE:HD13	1.92	0.51
1:B:549:PRO:CG	1:B:554:LEU:HD21	2.41	0.50
1:A:840:PHE:N	1:A:841:PRO:HD2	2.26	0.50
1:B:557:THR:HG22	1:B:557:THR:O	2.10	0.50
1:A:554:LEU:HD13	1:A:574:CYS:HA	1.92	0.50
1:B:678:HIS:O	1:B:679:SER:HB2	2.12	0.49
1:A:607:ARG:HB3	1:A:609:ASN:OD1	2.11	0.49
1:C:633:LYS:HD2	1:C:838:ASP:OD2	2.11	0.49
1:A:758:MET:HE3	1:A:828:LEU:HD13	1.94	0.49
1:B:654:ASP:O	1:B:657:HIS:HB2	2.13	0.48
1:A:712:THR:O	1:A:716:ILE:HG13	2.14	0.48
1:C:554:LEU:O	1:C:555:LYS:HB2	2.13	0.48
1:A:676:TYR:O	1:A:677:CYS:C	2.58	0.47
1:B:535:GLU:HG3	1:B:537:THR:H	1.78	0.47
1:A:607:ARG:HD2	1:A:657:HIS:O	2.13	0.47
1:B:807:ARG:O	1:B:810:LYS:HG3	2.14	0.47
1:A:631:ALA:HA	1:C:860:GLN:C	2.40	0.47
4:B:902:VIA:H202	5:B:246:HOH:O	2.14	0.47
1:A:665:ILE:O	1:A:665:ILE:HG13	2.15	0.46
1:B:748:ASP:OD1	1:B:750:HIS:HB3	2.15	0.46
1:C:793:GLU:HB3	1:C:799:ILE:CD1	2.38	0.46
1:C:791:ASP:CG	1:C:807:ARG:HH12	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:PHE:CE1	1:A:804:LEU:HD11	2.51	0.46
5:B:192:HOH:O	1:C:833:THR:HG21	2.15	0.46
1:B:636:ASN:C	1:B:636:ASN:ND2	2.71	0.45
1:A:813:ILE:N	1:A:814:PRO:HD2	2.31	0.45
1:A:658:ARG:N	1:A:658:ARG:HD2	2.31	0.45
1:C:677:CYS:SG	1:C:678:HIS:N	2.89	0.45
1:B:633:LYS:HD2	1:B:838:ASP:OD2	2.16	0.45
1:A:740:ARG:HH12	1:B:809:LYS:HZ3	1.65	0.45
1:A:636:ASN:C	1:A:636:ASN:HD22	2.25	0.45
1:C:857:ALA:C	1:C:859:GLN:H	2.23	0.45
1:A:797:LEU:O	1:A:799:ILE:HG23	2.17	0.44
1:C:840:PHE:N	1:C:841:PRO:CD	2.79	0.44
1:A:563:ASP:OD2	1:A:616:ARG:HD2	2.18	0.44
1:A:767:ALA:CB	1:A:778:ILE:HG21	2.44	0.44
1:B:807:ARG:HE	1:B:807:ARG:HB2	1.63	0.44
1:C:745:ASN:ND2	1:C:747:GLU:H	2.15	0.44
1:C:745:ASN:HD21	1:C:747:GLU:HG3	1.83	0.44
1:C:653:HIS:HD2	5:C:257:HOH:O	1.99	0.44
1:B:789:GLN:O	1:B:793:GLU:HG3	2.17	0.43
1:C:549:PRO:CG	1:C:554:LEU:HD21	2.47	0.43
1:B:535:GLU:HB3	1:B:538:ARG:HB3	2.01	0.43
1:C:646:LEU:HD11	1:C:756:LEU:HD22	2.00	0.43
1:C:654:ASP:O	1:C:657:HIS:HB2	2.19	0.43
1:C:737:GLU:OE1	1:C:741:LYS:HE3	2.18	0.42
1:C:813:ILE:N	1:C:814:PRO:HD2	2.34	0.42
1:C:617:HIS:HE1	1:C:764:ASP:O	2.02	0.42
1:B:745:ASN:ND2	1:B:747:GLU:H	2.17	0.42
1:C:771:PRO:HD2	1:C:774:ILE:HD12	2.01	0.42
1:C:856:LEU:O	1:C:859:GLN:HA	2.19	0.42
1:B:549:PRO:HG2	1:B:554:LEU:HD11	2.01	0.42
1:C:556:ILE:HD11	1:C:577:ARG:HG3	2.02	0.42
1:C:793:GLU:O	1:C:799:ILE:HG12	2.20	0.42
1:A:680:ILE:HG23	1:A:681:MET:H	1.85	0.41
1:A:812:LYS:O	1:A:816:MET:HG3	2.20	0.41
1:B:607:ARG:HB3	1:B:609:ASN:OD1	2.20	0.41
1:C:653:HIS:CG	1:C:723:THR:HG21	2.56	0.41
1:A:654:ASP:O	1:A:657:HIS:HB2	2.21	0.41
1:C:821:ILE:HG21	1:C:850:ARG:HB2	2.02	0.41
1:B:740:ARG:NH2	1:B:741:LYS:HE3	2.16	0.41
1:C:604:LYS:O	1:C:604:LYS:HG2	2.20	0.41
1:C:682:GLU:HB3	1:C:721:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:748:ASP:OD1	1:C:750:HIS:HB3	2.21	0.41
1:A:535:GLU:HG3	1:A:538:ARG:H	1.86	0.41
1:C:559:PHE:CD1	1:C:841:PRO:HB2	2.56	0.41
1:B:737:GLU:OE1	1:B:740:ARG:NH2	2.53	0.40
1:C:664:TYR:H	4:C:903:VIA:H151	1.86	0.40
1:A:735:PHE:CZ	1:A:739:ILE:HD11	2.57	0.40
1:C:857:ALA:C	1:C:859:GLN:N	2.77	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	324/326 (99%)	316 (98%)	7 (2%)	1 (0%)	36	46
1	B	313/326 (96%)	306 (98%)	6 (2%)	1 (0%)	36	46
1	C	313/326 (96%)	305 (97%)	8 (3%)	0	100	100
All	All	950/978 (97%)	927 (98%)	21 (2%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	859	GLN
1	B	859	GLN

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	291/291 (100%)	289 (99%)	2 (1%)	76	87
1	B	283/291 (97%)	278 (98%)	5 (2%)	51	70
1	C	283/291 (97%)	280 (99%)	3 (1%)	65	81
All	All	857/873 (98%)	847 (99%)	10 (1%)	63	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	636	ASN
1	A	775	GLN
1	B	636	ASN
1	B	680	ILE
1	B	737	GLU
1	B	775	GLN
1	B	854	GLN
1	C	775	GLN
1	C	826	LEU
1	C	833	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	589	GLN
1	A	635	GLN
1	A	636	ASN
1	A	683	HIS
1	A	742	ASN
1	A	745	ASN
1	A	806	ASN
1	B	583	ASN
1	B	635	GLN
1	B	636	ASN
1	B	666	GLN
1	B	699	GLN
1	B	718	GLN
1	B	743	GLN
1	B	745	ASN
1	B	798	ASN
1	C	586	GLN

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Mol	Chain	Res	Type
1	C	589	GLN
1	C	718	GLN
1	C	745	ASN
1	C	776	GLN
1	C	798	ASN
1	C	859	GLN
1	C	860	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	VIA	C	903	-	36,36,36	2.18	4 (11%)	53,53,53	2.41	23 (43%)
4	VIA	B	902	-	36,36,36	2.16	4 (11%)	53,53,53	2.46	21 (39%)
4	VIA	A	901	-	36,36,36	2.19	4 (11%)	53,53,53	2.56	23 (43%)

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
4	VIA	C	903	-	-	6/22/32/32	0/4/4/4
4	VIA	B	902	-	-	5/22/32/32	0/4/4/4
4	VIA	A	901	-	-	3/22/32/32	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	VIA	N28-N29	-6.82	1.23	1.36
4	B	902	VIA	N28-N29	-6.78	1.23	1.36
4	C	903	VIA	N28-N29	-6.75	1.23	1.36
4	A	901	VIA	O11-S10	6.50	1.50	1.43
4	A	901	VIA	O12-S10	6.46	1.50	1.43
4	C	903	VIA	O12-S10	6.45	1.50	1.43
4	C	903	VIA	O11-S10	6.44	1.50	1.43
4	B	902	VIA	O12-S10	6.41	1.50	1.43
4	B	902	VIA	O11-S10	6.34	1.50	1.43
4	C	903	VIA	C9-C21	-4.55	1.39	1.47
4	A	901	VIA	C9-C21	-4.54	1.39	1.47
4	B	902	VIA	C9-C21	-4.44	1.39	1.47

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	903	VIA	O12-S10-O11	-6.70	109.13	119.59
4	B	902	VIA	O12-S10-O11	-6.67	109.18	119.59
4	A	901	VIA	O12-S10-O11	-6.65	109.21	119.59
4	B	902	VIA	C25-N26-C21	5.90	120.92	114.57
4	C	903	VIA	C25-N26-C21	5.70	120.70	114.57
4	A	901	VIA	C25-N26-C21	5.58	120.58	114.57
4	A	901	VIA	C15-N14-C19	4.66	117.47	112.12
4	B	902	VIA	C19-N14-S10	-4.42	108.83	117.06
4	A	901	VIA	C16-C15-N14	4.33	113.56	108.97
4	A	901	VIA	C24-C23-N22	4.28	118.48	110.94
4	B	902	VIA	C24-C23-N22	4.26	118.43	110.94
4	A	901	VIA	C18-C19-N14	4.26	113.49	108.97
4	C	903	VIA	C24-C23-N22	4.25	118.42	110.94
4	C	903	VIA	C23-C24-N28	4.24	135.01	131.24
4	A	901	VIA	C23-N22-C21	-4.22	119.49	125.86
4	C	903	VIA	C23-N22-C21	-4.12	119.65	125.86
4	B	902	VIA	C23-N22-C21	-4.11	119.66	125.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	902	VIA	C23-C24-N28	4.10	134.88	131.24
4	A	901	VIA	C7-S10-N14	3.98	112.08	107.28
4	A	901	VIA	C31-N28-C24	-3.92	123.94	129.21
4	A	901	VIA	C23-C24-N28	3.91	134.72	131.24
4	C	903	VIA	C31-N28-C24	-3.87	124.01	129.21
4	B	902	VIA	C31-N28-C24	-3.77	124.14	129.21
4	B	902	VIA	C15-N14-S10	-3.73	110.11	117.06
4	C	903	VIA	C18-C19-N14	3.59	112.78	108.97
4	B	902	VIA	C24-C25-N26	-3.58	121.56	124.87
4	C	903	VIA	C7-S10-N14	3.51	111.52	107.28
4	A	901	VIA	C24-C25-N26	-3.49	121.65	124.87
4	C	903	VIA	C24-C25-N26	-3.47	121.67	124.87
4	A	901	VIA	C2-O3-C4	-3.39	111.16	118.08
4	A	901	VIA	C30-C25-N26	3.36	133.95	129.76
4	B	902	VIA	C2-O3-C4	-3.34	111.26	118.08
4	B	902	VIA	C30-C25-N26	3.30	133.87	129.76
4	C	903	VIA	C30-C25-N26	3.21	133.76	129.76
4	B	902	VIA	C7-S10-N14	3.15	111.08	107.28
4	C	903	VIA	C32-C30-N29	3.01	127.07	121.89
4	C	903	VIA	C2-O3-C4	-3.01	111.93	118.08
4	A	901	VIA	C31-N28-N29	2.99	123.76	119.29
4	B	902	VIA	O12-S10-N14	2.97	109.49	106.69
4	B	902	VIA	C4-C9-C21	-2.88	119.35	124.48
4	A	901	VIA	C32-C30-N29	2.87	126.83	121.89
4	B	902	VIA	C31-N28-N29	2.84	123.54	119.29
4	C	903	VIA	C31-N28-N29	2.82	123.50	119.29
4	B	902	VIA	C32-C30-N29	2.77	126.67	121.89
4	A	901	VIA	C4-C9-C21	-2.77	119.55	124.48
4	C	903	VIA	C25-C24-C23	-2.70	119.19	121.36
4	B	902	VIA	C25-C24-C23	-2.67	119.21	121.36
4	A	901	VIA	O27-C23-C24	-2.64	121.13	127.62
4	C	903	VIA	C15-N14-S10	-2.64	112.15	117.06
4	B	902	VIA	O27-C23-C24	-2.64	121.15	127.62
4	C	903	VIA	O12-S10-N14	2.61	109.14	106.69
4	C	903	VIA	O27-C23-C24	-2.61	121.22	127.62
4	A	901	VIA	C25-C24-C23	-2.59	119.27	121.36
4	B	902	VIA	N22-C21-N26	-2.54	120.20	122.85
4	B	902	VIA	C30-N29-N28	2.53	110.15	106.63
4	A	901	VIA	C30-N29-N28	2.50	110.11	106.63
4	C	903	VIA	C16-C15-N14	2.49	111.61	108.97
4	B	902	VIA	O11-S10-N14	2.48	109.02	106.69
4	C	903	VIA	C4-C9-C21	-2.46	120.09	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	903	VIA	C30-N29-N28	2.45	110.05	106.63
4	C	903	VIA	N22-C21-N26	-2.38	120.37	122.85
4	A	901	VIA	O12-S10-N14	2.35	108.90	106.69
4	A	901	VIA	C16-N17-C18	-2.27	105.93	109.54
4	A	901	VIA	N22-C21-N26	-2.22	120.53	122.85
4	C	903	VIA	C25-C24-N28	-2.14	105.81	107.25
4	C	903	VIA	O11-S10-N14	2.14	108.70	106.69
4	A	901	VIA	O11-S10-N14	2.10	108.67	106.69

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	903	VIA	C19-N14-S10-C7
4	C	903	VIA	C19-N14-S10-O11
4	C	903	VIA	C19-N14-S10-O12
4	C	903	VIA	C15-N14-S10-O11
4	C	903	VIA	C15-N14-S10-C7
4	C	903	VIA	C15-N14-S10-O12
4	B	902	VIA	N26-C21-C9-C4
4	B	902	VIA	N26-C21-C9-C8
4	B	902	VIA	C15-N14-S10-O12
4	B	902	VIA	N22-C21-C9-C4
4	A	901	VIA	C6-C7-S10-O12
4	A	901	VIA	N26-C21-C9-C8
4	A	901	VIA	C8-C7-S10-O12
4	B	902	VIA	N22-C21-C9-C8

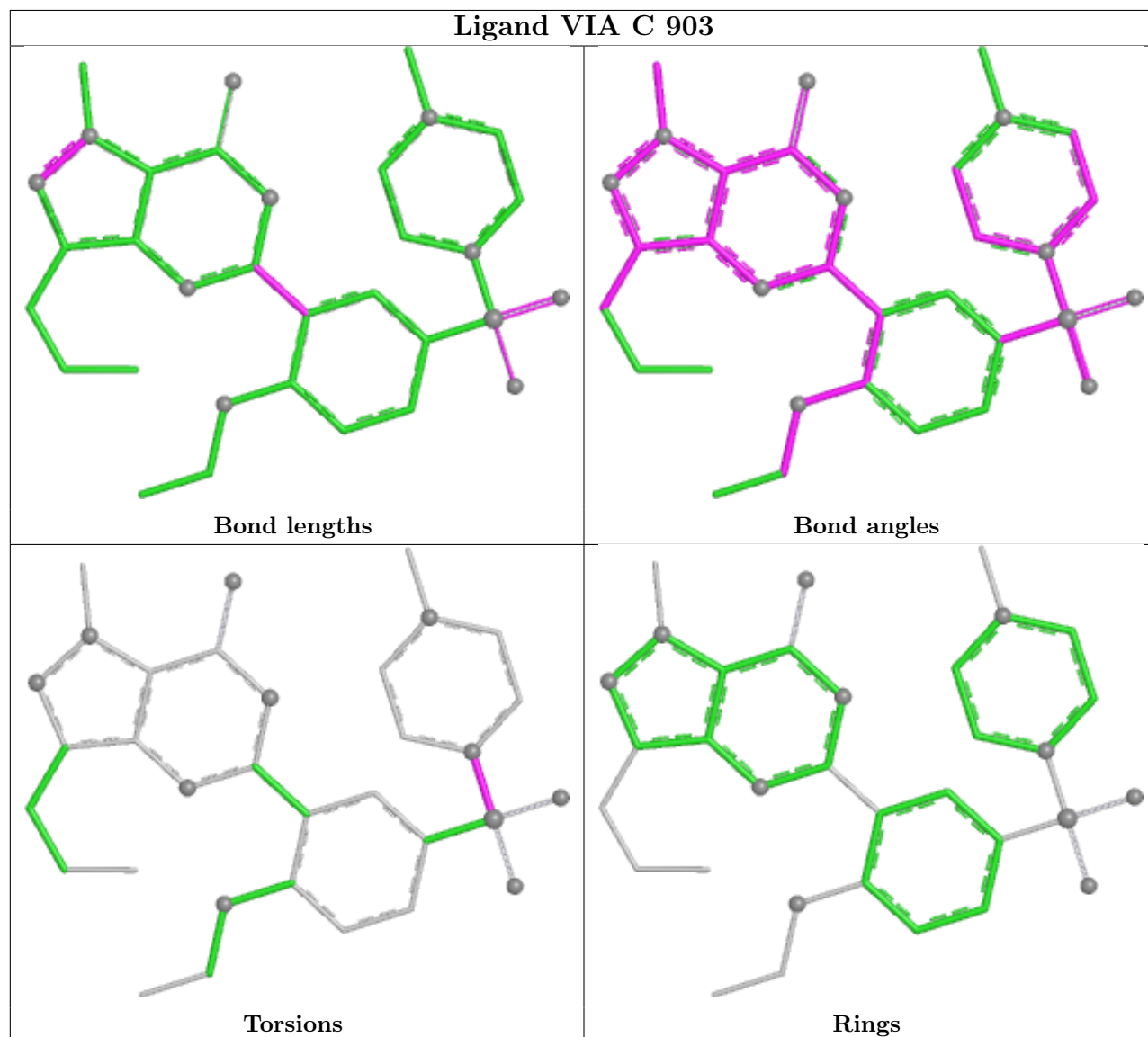
There are no ring outliers.

2 monomers are involved in 4 short contacts:

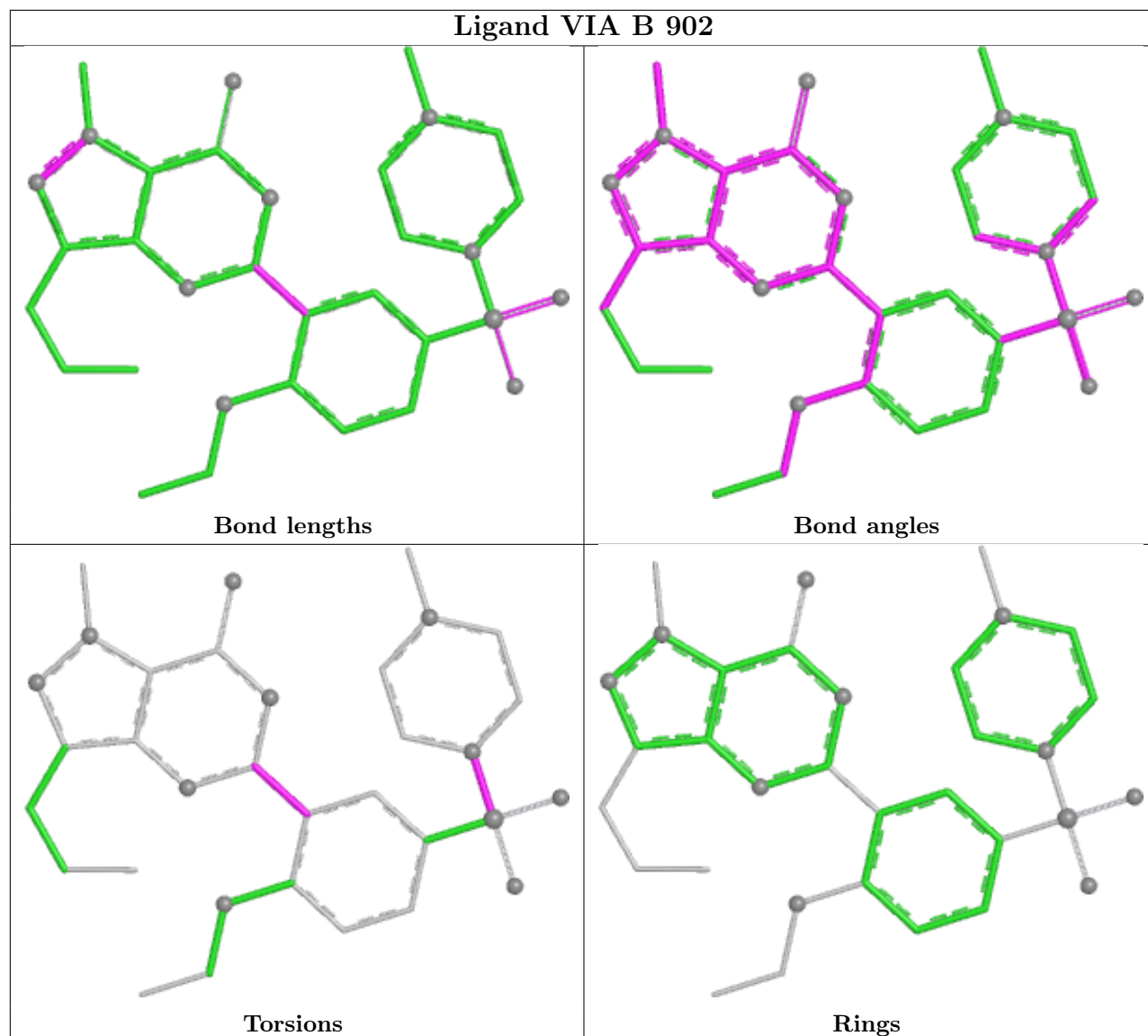
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	903	VIA	1	0
4	B	902	VIA	3	0

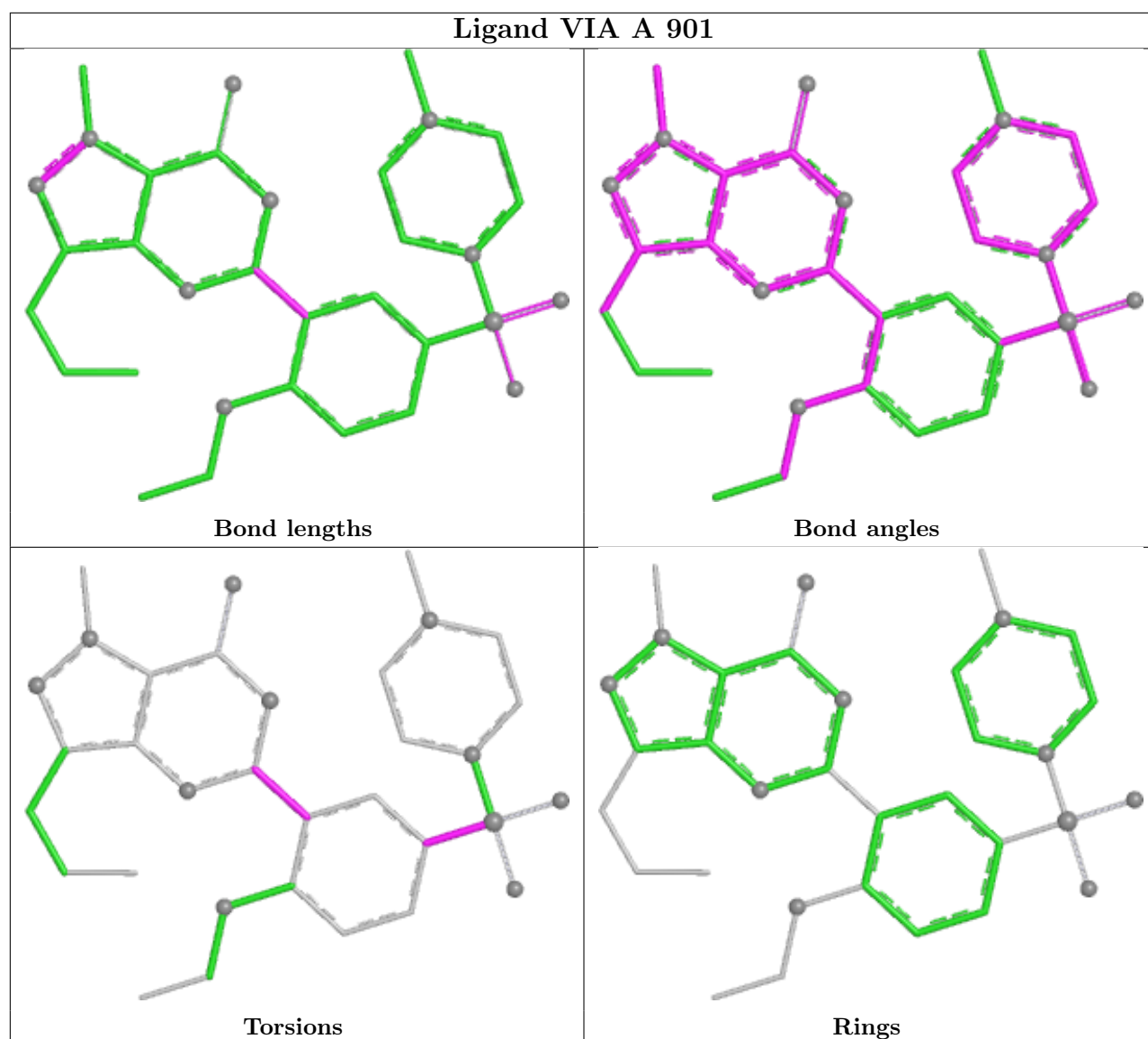
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand VIA B 902





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	326/326 (100%)	0.16	11 (3%) 48 50	17, 29, 45, 71	0
1	B	317/326 (97%)	0.08	21 (6%) 24 26	16, 24, 45, 71	0
1	C	317/326 (97%)	0.04	12 (3%) 44 46	13, 24, 42, 60	0
All	All	960/978 (98%)	0.09	44 (4%) 37 39	13, 25, 45, 71	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	860	GLN	9.1
1	B	860	GLN	6.8
1	B	677	CYS	6.5
1	C	677	CYS	6.2
1	B	678	HIS	5.4
1	A	860	GLN	5.3
1	B	667	ARG	5.1
1	A	859	GLN	4.1
1	C	859	GLN	4.0
1	C	535	GLU	3.5
1	A	677	CYS	3.5
1	C	678	HIS	3.2
1	B	536	GLU	3.2
1	C	536	GLU	3.2
1	A	665	ILE	3.2
1	B	679	SER	3.1
1	B	680	ILE	3.0
1	B	609	ASN	2.9
1	B	859	GLN	2.8
1	A	538	ARG	2.8
1	C	667	ARG	2.7
1	A	678	HIS	2.7
1	B	636	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	665	ILE	2.7
1	B	834	HIS	2.6
1	B	665	ILE	2.6
1	B	663	SER	2.6
1	C	664	TYR	2.6
1	B	537	THR	2.5
1	C	636	ASN	2.3
1	B	742	ASN	2.3
1	C	795	LYS	2.3
1	B	810	LYS	2.2
1	B	706	ILE	2.2
1	B	798	ASN	2.2
1	A	565	GLU	2.2
1	B	778	ILE	2.2
1	A	680	ILE	2.1
1	B	538	ARG	2.1
1	B	666	GLN	2.1
1	A	798	ASN	2.1
1	A	676	TYR	2.1
1	A	851	GLN	2.0
1	C	798	ASN	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 ⓘ

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($\text{\AA}^2$)	Q<0.9
2	ZN	B	503	1/1	0.63	0.45	45,45,45,45	0
3	MG	B	504	1/1	0.68	0.15	38,38,38,38	0

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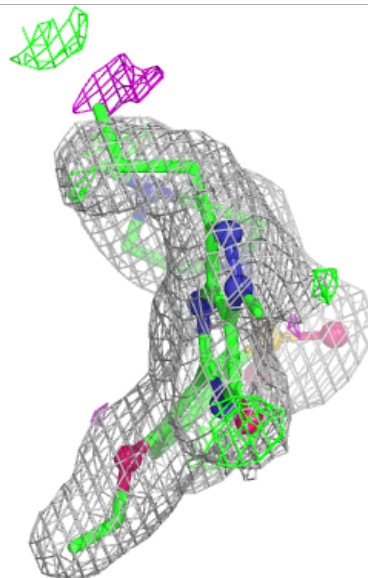
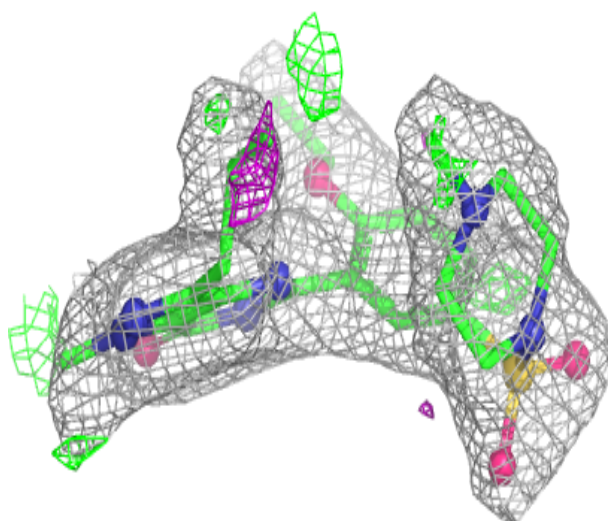
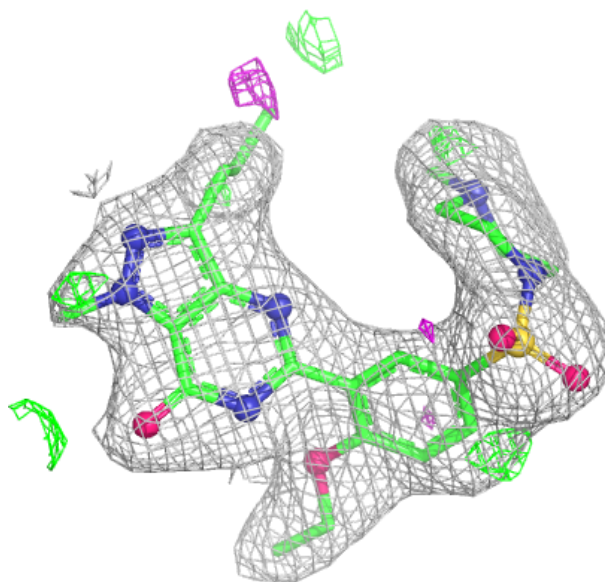
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	502	1/1	0.69	0.17	38,38,38,38	0
2	ZN	C	505	1/1	0.75	0.50	46,46,46,46	0
3	MG	C	506	1/1	0.75	0.15	35,35,35,35	0
4	VIA	A	901	33/33	0.91	0.11	29,33,35,37	0
2	ZN	A	501	1/1	0.93	0.21	42,42,42,42	0
4	VIA	C	903	33/33	0.93	0.11	23,25,35,35	0
4	VIA	B	902	33/33	0.96	0.08	22,25,28,31	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.

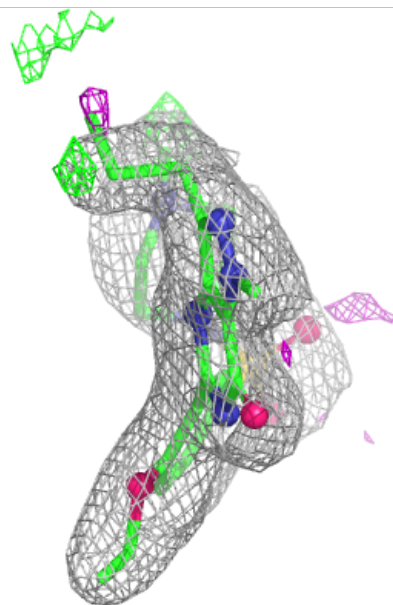
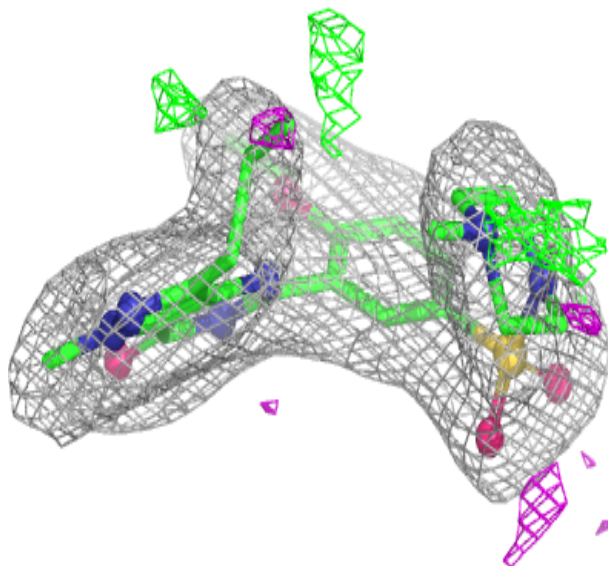
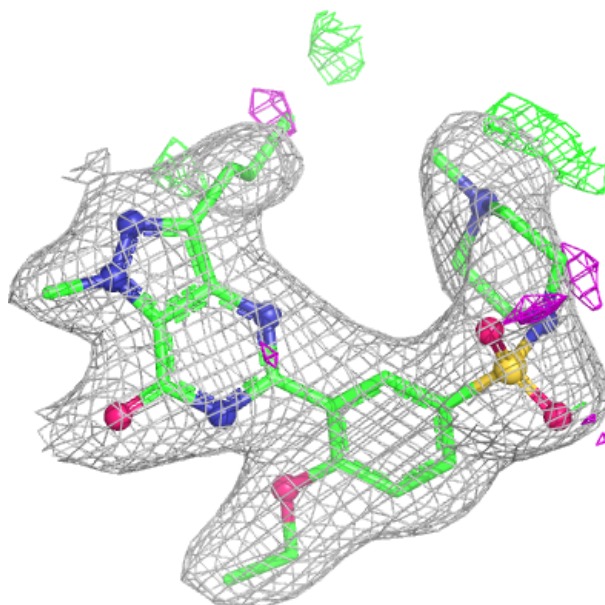
Electron density around VIA A 901:

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



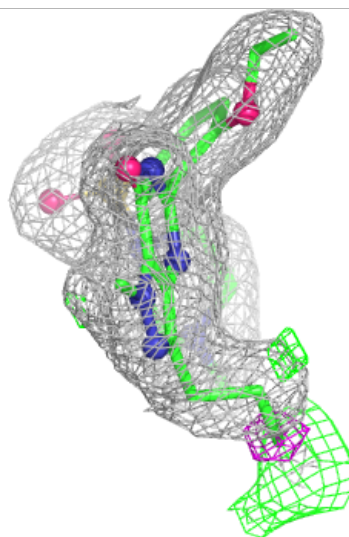
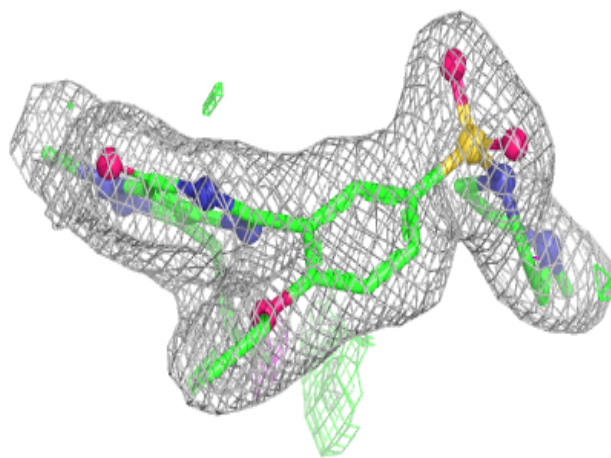
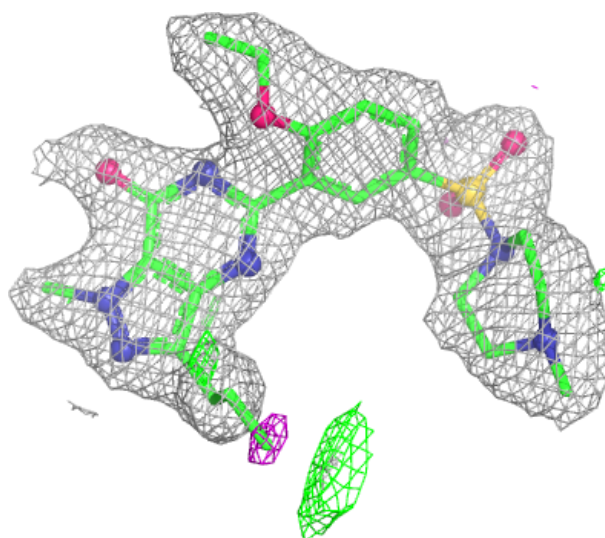
Electron density around VIA C 903:

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



Electron density around VIA B 902:

$2mF_o-DF_c$ (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.