Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 05:20 AM EDT

PDB ID	:	3JWQ
Title	:	Crystal structure of chimeric PDE5/PDE6 catalytic domain complexed with sildenafil
Authors	:	Barren, B.; Gakhar, L.; Muradov, H.; Boyd, K.K.; Ramaswamy, S.; Artemyev, N.O.
Deposited on	:	2009-09-18
Resolution	:	2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

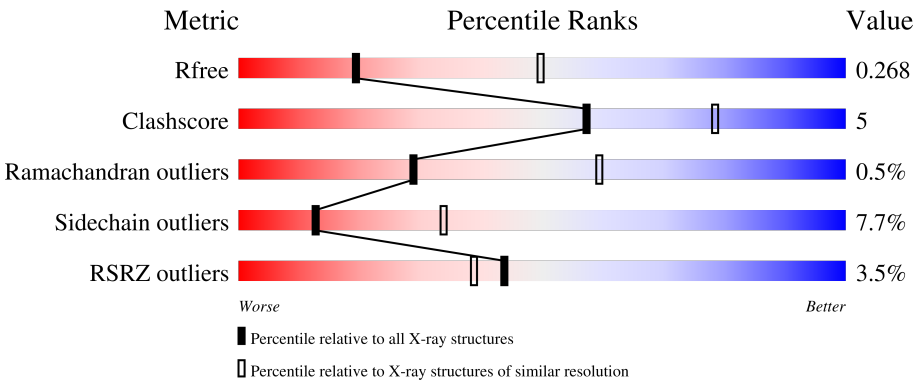
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 <=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	330	% 85% 12% • •
1	B	330	2% 82% 13% • •
1	C	330	5% 86% 11% • •
1	D	330	5% 83% 13% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10723 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 catalytic domain, Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2638	1681	459	480	18	0	0	0
1	B	324	2638	1681	459	480	18	0	0	0
1	C	327	2665	1697	464	485	19	0	0	0
1	D	323	2629	1676	458	477	18	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	531	GLY	-	expression tag	UNP O76074
A	532	SER	-	expression tag	UNP O76074
A	533	HIS	-	expression tag	UNP O76074
A	534	MET	-	expression tag	UNP O76074
B	531	GLY	-	expression tag	UNP O76074
B	532	SER	-	expression tag	UNP O76074
B	533	HIS	-	expression tag	UNP O76074
B	534	MET	-	expression tag	UNP O76074
C	531	GLY	-	expression tag	UNP O76074
C	532	SER	-	expression tag	UNP O76074
C	533	HIS	-	expression tag	UNP O76074
C	534	MET	-	expression tag	UNP O76074
D	531	GLY	-	expression tag	UNP O76074
D	532	SER	-	expression tag	UNP O76074
D	533	HIS	-	expression tag	UNP O76074
D	534	MET	-	expression tag	UNP O76074

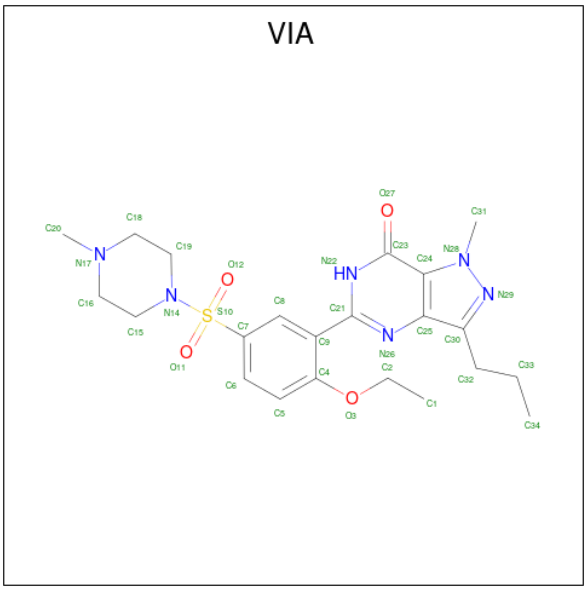
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- 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 (three-letter code: VIA) (formula: $C_{22}H_{30}N_6O_4S$).



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

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

- Molecule 5 is water.

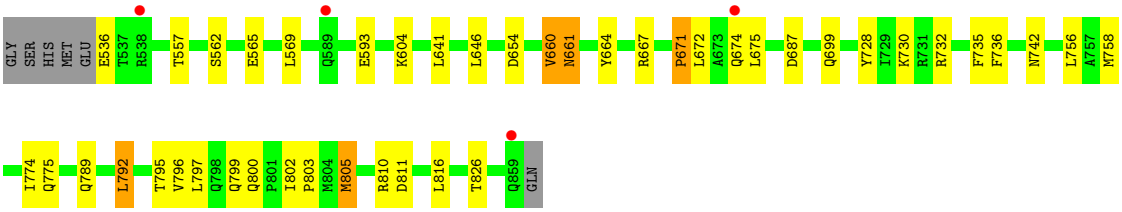
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	6	6	6	0	0
5	B	3	3	3	0	0
5	C	3	3	3	0	0
5	D	1	1	1	0	0

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.

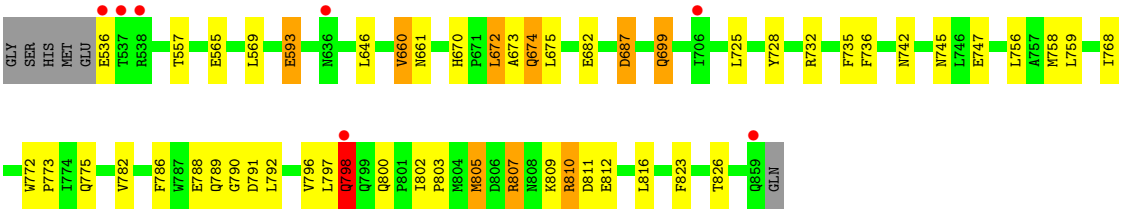
• Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase catalytic domain, Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha chimera

Chain A:



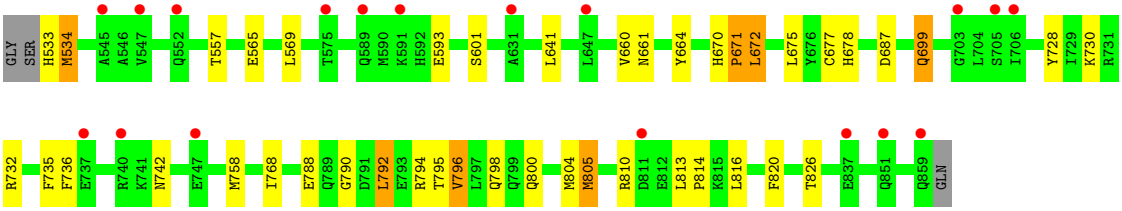
• Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase catalytic domain, Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha chimera

Chain B:



• Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase catalytic domain, Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha chimera

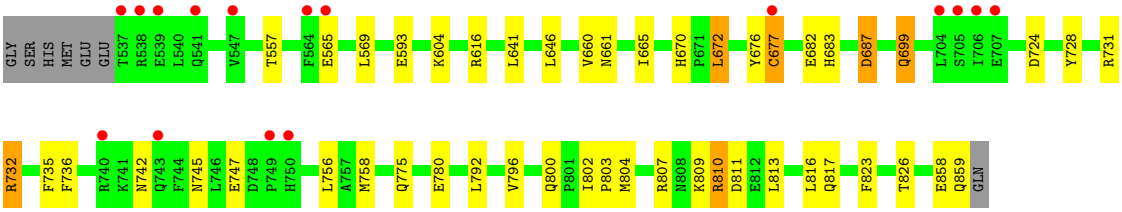
Chain C:



• Molecule 1: cGMP-specific 3',5'-cyclic phosphodiesterase catalytic domain, Cone cGMP-specific 3',5'-cyclic phosphodiesterase subunit alpha chimera

Chain D:

5%
83%
13%


GLY SER HIS MET GLU GLU T537 R538 E539 L540 Q541 V547 T557 F564 E565 L569 E593 K604 R616 L641 L646 V660 N661 I665 H670 P671 L672 Y676 C677 E682 H683 D687 Q699 L704 S705 I706 E707 D724 Y728 R731
R732 F735 F736 R740 K741 N742 Q743 F744 N745 L746 E747 D748 P749 H750 L756 A757 M758 Q775 E780 L792 V796 Q800 P801 I802 P803 M804 R807 N808 K809 R810 D811 E812 L813 L816 Q817 F823 T826 E858 Q859 GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.73Å 109.83Å 199.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.08 – 2.87 23.08 – 2.87	Depositor EDS
% Data completeness (in resolution range)	86.7 (23.08-2.87) 86.8 (23.08-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.223 , 0.275 0.218 , 0.268	Depositor DCC
R_{free} test set	1655 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	60.3	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10723	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: VIA, ZN, MG

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	0.79	0/2692	0.76	2/3640 (0.1%)
1	B	0.74	2/2692 (0.1%)	0.76	1/3640 (0.0%)
1	C	0.66	0/2720	0.72	1/3677 (0.0%)
1	D	0.67	1/2683 (0.0%)	0.71	2/3628 (0.1%)
All	All	0.72	3/10787 (0.0%)	0.74	6/14585 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	780	GLU	CG-CD	5.40	1.60	1.51
1	B	682	GLU	CG-CD	5.12	1.59	1.51
1	B	593	GLU	CG-CD	5.02	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	661	ASN	CB-CA-C	-7.37	95.66	110.40
1	D	661	ASN	CB-CA-C	-7.29	95.83	110.40
1	C	661	ASN	CB-CA-C	-6.96	96.47	110.40
1	A	661	ASN	CB-CA-C	-5.63	99.14	110.40
1	D	661	ASN	N-CA-C	5.42	125.62	111.00
1	A	654	ASP	CB-CG-OD1	5.07	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2638	0	2644	32	0
1	B	2638	0	2644	29	0
1	C	2665	0	2666	27	0
1	D	2629	0	2638	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	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
3	D	1	0	0	0	0
4	A	33	0	30	0	0
4	B	33	0	30	4	0
4	C	33	0	30	6	0
4	D	33	0	30	5	0
5	A	6	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
All	All	10723	0	10712	105	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 5.

All (105) 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:660:VAL:CG2	1:B:789:GLN:HG3	1.96	0.96
1:D:670:HIS:CE1	1:D:672:LEU:HD22	2.12	0.85
1:D:810:ARG:HH11	1:D:810:ARG:HG3	1.43	0.83
1:B:660:VAL:HG22	1:B:789:GLN:HG3	1.59	0.83
1:A:800:GLN:HG3	1:D:803:PRO:HD2	1.59	0.83
1:A:796:VAL:HG23	1:A:797:LEU:HG	1.59	0.82
4:D:901:VIA:H8	4:D:901:VIA:H192	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:LEU:O	1:A:796:VAL:HG22	1.85	0.76
1:C:813:LEU:HB3	1:C:814:PRO:HD3	1.71	0.73
1:A:796:VAL:CG2	1:A:797:LEU:HG	2.20	0.71
1:A:730:LYS:NZ	1:B:687:ASP:OD2	2.25	0.70
1:B:660:VAL:HG23	1:B:789:GLN:HG3	1.73	0.68
1:C:804:MET:HE1	4:C:901:VIA:H191	1.77	0.66
1:C:820:PHE:HD1	4:C:901:VIA:O11	1.79	0.66
1:C:820:PHE:CD1	4:C:901:VIA:H8	2.31	0.66
4:B:901:VIA:H192	1:C:795:THR:HA	1.79	0.64
1:A:660:VAL:CG2	1:A:789:GLN:HG3	2.28	0.63
1:A:730:LYS:CE	1:B:687:ASP:OD2	2.47	0.62
1:B:646:LEU:HD11	1:B:756:LEU:HD22	1.83	0.61
1:A:660:VAL:HG23	1:A:789:GLN:HG3	1.83	0.60
1:C:533:HIS:O	1:C:534:MET:CB	2.50	0.60
1:B:660:VAL:HG22	1:B:789:GLN:CG	2.31	0.59
1:C:820:PHE:CD1	4:C:901:VIA:C8	2.85	0.59
4:B:901:VIA:O27	4:B:901:VIA:H311	2.03	0.58
4:B:901:VIA:H152	4:B:901:VIA:H8	1.85	0.58
1:C:533:HIS:O	1:C:534:MET:HB2	2.03	0.57
1:B:735:PHE:CD2	1:B:758:MET:HG3	2.40	0.57
1:B:810:ARG:O	1:B:812:GLU:N	2.38	0.57
1:D:810:ARG:HG3	1:D:810:ARG:NH1	2.10	0.57
1:D:670:HIS:CE1	1:D:672:LEU:CD2	2.88	0.55
1:A:735:PHE:CD2	1:A:758:MET:HG3	2.41	0.55
1:A:646:LEU:HD11	1:A:756:LEU:HD22	1.88	0.55
1:C:804:MET:HE1	4:C:901:VIA:C19	2.36	0.55
1:D:728:TYR:CZ	1:D:732:ARG:HD3	2.42	0.54
1:C:678:HIS:HD2	1:D:677:CYS:SG	2.30	0.54
1:B:732:ARG:HD2	1:B:736:PHE:CE1	2.42	0.54
1:B:803:PRO:HD2	1:C:800:GLN:CG	2.38	0.54
1:A:800:GLN:CG	1:D:802:ILE:HB	2.38	0.53
1:B:728:TYR:CZ	1:B:732:ARG:HD3	2.43	0.52
1:C:670:HIS:ND1	1:C:672:LEU:HB2	2.23	0.52
1:A:730:LYS:HD2	1:B:675:LEU:HD21	1.91	0.52
1:A:796:VAL:HG23	1:A:797:LEU:CG	2.35	0.52
1:C:728:TYR:CZ	1:C:732:ARG:HD3	2.44	0.52
1:D:732:ARG:HD2	1:D:736:PHE:CE1	2.45	0.52
1:D:735:PHE:CD2	1:D:758:MET:HG3	2.45	0.51
1:C:735:PHE:CD2	1:C:758:MET:HG3	2.46	0.51
1:D:804:MET:HE1	4:D:901:VIA:H152	1.92	0.51
1:B:803:PRO:HD2	1:C:800:GLN:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:ILE:HB	1:C:800:GLN:HG2	1.94	0.50
1:B:786:PHE:O	1:B:805:MET:HG3	2.10	0.50
1:A:796:VAL:CG2	1:A:797:LEU:N	2.75	0.49
1:C:732:ARG:HD2	1:C:736:PHE:CE1	2.47	0.49
1:A:800:GLN:HG2	1:D:802:ILE:HB	1.94	0.49
1:B:823:PHE:HZ	1:C:792:LEU:HD13	1.77	0.48
1:A:792:LEU:HD13	1:D:823:PHE:HZ	1.79	0.48
1:A:796:VAL:HG23	1:A:797:LEU:N	2.28	0.47
1:A:671:PRO:O	1:A:674:GLN:HG2	2.14	0.47
1:B:791:ASP:OD2	1:B:807:ARG:NH1	2.48	0.47
1:C:790:GLY:HA3	1:C:805:MET:O	2.13	0.47
4:D:901:VIA:H192	4:D:901:VIA:C8	2.40	0.46
1:A:664:TYR:CE2	1:A:796:VAL:HG21	2.50	0.46
1:D:745:ASN:HD21	1:D:747:GLU:HB2	1.80	0.46
1:A:730:LYS:HE3	1:B:687:ASP:OD2	2.16	0.46
1:A:604:LYS:HB3	1:A:604:LYS:HE2	1.71	0.45
1:A:789:GLN:HB3	1:A:805:MET:HE2	1.99	0.45
1:B:797:LEU:O	1:B:798:GLN:C	2.56	0.45
1:D:670:HIS:HE1	1:D:672:LEU:HD22	1.78	0.45
1:A:728:TYR:CZ	1:A:732:ARG:HD3	2.52	0.44
1:A:796:VAL:HG23	1:A:797:LEU:CD2	2.46	0.44
1:C:670:HIS:CD2	1:C:671:PRO:HD2	2.53	0.44
1:B:782:VAL:CG1	4:B:901:VIA:H21	2.48	0.44
1:D:731:ARG:O	1:D:732:ARG:C	2.55	0.43
1:D:616:ARG:HD3	1:D:616:ARG:HA	1.81	0.43
1:B:790:GLY:HA3	1:B:805:MET:O	2.18	0.43
1:D:682:GLU:HG2	1:D:724:ASP:HB2	2.00	0.43
1:A:732:ARG:HD2	1:A:736:PHE:CE1	2.54	0.43
1:C:699:GLN:H	1:C:699:GLN:HG2	1.59	0.43
1:C:794:ARG:O	1:C:798:GLN:HA	2.19	0.43
1:D:699:GLN:H	1:D:699:GLN:HG2	1.57	0.43
1:A:660:VAL:HG22	1:A:789:GLN:HG3	2.00	0.43
1:C:813:LEU:HB3	1:C:814:PRO:CD	2.45	0.43
1:D:817:GLN:OE1	4:D:901:VIA:O3	2.37	0.43
1:B:670:HIS:ND1	1:B:672:LEU:HB2	2.34	0.42
1:B:768:ILE:HG13	1:B:768:ILE:O	2.20	0.42
1:A:562:SER:HB2	1:A:774:ILE:HD11	2.02	0.42
1:A:800:GLN:CG	1:D:803:PRO:HD2	2.39	0.42
1:B:670:HIS:CE1	1:B:672:LEU:HD22	2.55	0.42
1:C:664:TYR:CE2	1:C:792:LEU:HB3	2.54	0.42
1:C:796:VAL:O	1:C:796:VAL:CG2	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:858:GLU:O	1:D:859:GLN:HB2	2.20	0.41
1:A:536:GLU:OE1	1:A:536:GLU:C	2.58	0.41
1:B:699:GLN:H	1:B:699:GLN:HG2	1.54	0.41
4:C:901:VIA:H5	4:C:901:VIA:H21	1.93	0.41
1:B:673:ALA:HB3	1:B:674:GLN:HE21	1.86	0.41
1:B:745:ASN:HD21	1:B:747:GLU:HB2	1.85	0.41
1:D:604:LYS:HB3	1:D:604:LYS:HE2	1.76	0.41
1:A:800:GLN:HG3	1:D:802:ILE:HB	2.02	0.41
1:B:772:TRP:O	1:B:773:PRO:C	2.58	0.41
1:A:802:ILE:O	1:A:803:PRO:C	2.59	0.41
1:C:730:LYS:HE3	1:D:687:ASP:OD2	2.21	0.41
1:D:676:TYR:CD1	1:D:683:HIS:HB3	2.56	0.41
1:A:664:TYR:CE2	1:A:792:LEU:HB3	2.56	0.41
1:C:768:ILE:O	1:C:768:ILE:HG13	2.22	0.40
1:D:817:GLN:OE1	4:D:901:VIA:C4	2.69	0.40
1:D:646:LEU:HD11	1:D:756:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/330 (98%)	307 (95%)	15 (5%)	0	100	100
1	B	322/330 (98%)	308 (96%)	11 (3%)	3 (1%)	17	45
1	C	325/330 (98%)	310 (95%)	14 (4%)	1 (0%)	41	70
1	D	321/330 (97%)	307 (96%)	12 (4%)	2 (1%)	25	55
All	All	1290/1320 (98%)	1232 (96%)	52 (4%)	6 (0%)	29	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	811	ASP
1	C	534	MET
1	D	732	ARG
1	B	798	GLN
1	B	810	ARG
1	D	677	CYS

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	290/295 (98%)	267 (92%)	23 (8%)	12	32
1	B	290/295 (98%)	266 (92%)	24 (8%)	11	30
1	C	293/295 (99%)	272 (93%)	21 (7%)	14	37
1	D	289/295 (98%)	267 (92%)	22 (8%)	13	35
All	All	1162/1180 (98%)	1072 (92%)	90 (8%)	13	34

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	557	THR
1	A	565	GLU
1	A	569	LEU
1	A	593	GLU
1	A	641	LEU
1	A	660	VAL
1	A	661	ASN
1	A	667	ARG
1	A	671	PRO
1	A	672	LEU
1	A	675	LEU
1	A	687	ASP
1	A	699	GLN
1	A	742	ASN
1	A	775	GLN
1	A	792	LEU

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Mol	Chain	Res	Type
1	A	795	THR
1	A	799	GLN
1	A	805	MET
1	A	810	ARG
1	A	811	ASP
1	A	816	LEU
1	A	826	THR
1	B	536	GLU
1	B	557	THR
1	B	565	GLU
1	B	569	LEU
1	B	593	GLU
1	B	660	VAL
1	B	672	LEU
1	B	674	GLN
1	B	687	ASP
1	B	699	GLN
1	B	725	LEU
1	B	742	ASN
1	B	759	LEU
1	B	775	GLN
1	B	788	GLU
1	B	792	LEU
1	B	796	VAL
1	B	798	GLN
1	B	800	GLN
1	B	805	MET
1	B	807	ARG
1	B	809	LYS
1	B	816	LEU
1	B	826	THR
1	C	557	THR
1	C	565	GLU
1	C	569	LEU
1	C	593	GLU
1	C	601	SER
1	C	641	LEU
1	C	660	VAL
1	C	671	PRO
1	C	672	LEU
1	C	675	LEU
1	C	677	CYS

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Mol	Chain	Res	Type
1	C	687	ASP
1	C	699	GLN
1	C	742	ASN
1	C	788	GLU
1	C	792	LEU
1	C	796	VAL
1	C	805	MET
1	C	810	ARG
1	C	816	LEU
1	C	826	THR
1	D	557	THR
1	D	565	GLU
1	D	569	LEU
1	D	593	GLU
1	D	641	LEU
1	D	660	VAL
1	D	665	ILE
1	D	672	LEU
1	D	687	ASP
1	D	699	GLN
1	D	742	ASN
1	D	775	GLN
1	D	792	LEU
1	D	796	VAL
1	D	800	GLN
1	D	807	ARG
1	D	809	LYS
1	D	810	ARG
1	D	811	ASP
1	D	813	LEU
1	D	816	LEU
1	D	826	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	541	GLN
1	A	586	GLN
1	A	661	ASN
1	A	678	HIS
1	A	742	ASN
1	A	745	ASN

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Mol	Chain	Res	Type
1	B	541	GLN
1	B	586	GLN
1	B	661	ASN
1	B	666	GLN
1	B	674	GLN
1	B	678	HIS
1	B	742	ASN
1	B	745	ASN
1	C	541	GLN
1	C	586	GLN
1	C	666	GLN
1	C	678	HIS
1	C	742	ASN
1	C	745	ASN
1	C	798	GLN
1	D	541	GLN
1	D	586	GLN
1	D	661	ASN
1	D	666	GLN
1	D	742	ASN
1	D	745	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	D	901	-	31,36,36	2.45	7 (22%)	34,53,53	2.57	14 (41%)
4	VIA	C	901	-	31,36,36	2.73	8 (25%)	34,53,53	3.48	13 (38%)
4	VIA	A	901	-	31,36,36	2.42	7 (22%)	34,53,53	3.42	12 (35%)
4	VIA	B	901	-	31,36,36	2.62	8 (25%)	34,53,53	2.54	11 (32%)

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	D	901	-	-	7/18/32/32	0/4/4/4
4	VIA	C	901	-	-	10/18/32/32	0/4/4/4
4	VIA	A	901	-	-	3/18/32/32	0/4/4/4
4	VIA	B	901	-	-	9/18/32/32	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	901	VIA	S10-N14	8.70	1.75	1.63
4	A	901	VIA	O12-S10	7.93	1.52	1.43
4	A	901	VIA	O11-S10	7.83	1.52	1.43
4	B	901	VIA	O11-S10	7.33	1.51	1.43
4	D	901	VIA	O12-S10	6.78	1.51	1.43
4	B	901	VIA	S10-N14	6.35	1.72	1.63
4	D	901	VIA	O11-S10	6.34	1.50	1.43
4	D	901	VIA	S10-N14	6.17	1.72	1.63
4	B	901	VIA	O12-S10	6.06	1.50	1.43
4	C	901	VIA	O11-S10	6.02	1.50	1.43
4	C	901	VIA	O12-S10	5.41	1.49	1.43
4	C	901	VIA	C23-N22	4.96	1.41	1.33
4	D	901	VIA	C23-N22	4.55	1.41	1.33
4	B	901	VIA	C21-N22	4.46	1.43	1.35
4	B	901	VIA	C23-N22	4.25	1.40	1.33
4	C	901	VIA	C15-N14	3.99	1.52	1.47
4	D	901	VIA	C21-N22	3.66	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	901	VIA	C21-N22	3.56	1.42	1.35
4	B	901	VIA	C7-S10	-3.33	1.71	1.76
4	A	901	VIA	C21-N22	3.03	1.41	1.35
4	C	901	VIA	C30-C25	-2.98	1.38	1.43
4	B	901	VIA	C8-C9	-2.85	1.36	1.42
4	A	901	VIA	C15-N14	2.72	1.50	1.47
4	A	901	VIA	C23-N22	2.68	1.37	1.33
4	A	901	VIA	C31-N28	2.64	1.52	1.47
4	B	901	VIA	C30-C25	-2.57	1.38	1.43
4	D	901	VIA	C30-C25	-2.32	1.39	1.43
4	A	901	VIA	S10-N14	2.20	1.66	1.63
4	D	901	VIA	C8-C9	-2.14	1.37	1.42
4	C	901	VIA	C18-N17	2.04	1.50	1.46

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	901	VIA	C16-C15-N14	10.59	117.01	108.91
4	A	901	VIA	O12-S10-N14	9.28	115.15	106.69
4	A	901	VIA	C16-C15-N14	8.27	115.24	108.91
4	A	901	VIA	O12-S10-O11	-8.02	106.53	119.52
4	B	901	VIA	O11-S10-N14	7.82	113.82	106.69
4	D	901	VIA	C30-N29-N28	6.87	110.41	104.48
4	C	901	VIA	C30-N29-N28	6.74	110.29	104.48
4	C	901	VIA	C16-N17-C18	6.60	118.75	109.52
4	C	901	VIA	O12-S10-O11	-6.58	108.86	119.52
4	C	901	VIA	C7-S10-N14	6.29	114.79	107.30
4	B	901	VIA	C30-N29-N28	6.27	109.89	104.48
4	A	901	VIA	C30-N29-N28	6.06	109.70	104.48
4	D	901	VIA	C7-S10-N14	6.00	114.46	107.30
4	A	901	VIA	C15-N14-S10	-5.63	106.82	117.05
4	B	901	VIA	O12-S10-O11	-5.34	110.87	119.52
4	C	901	VIA	O12-S10-N14	5.09	111.33	106.69
4	C	901	VIA	C24-C23-N22	-4.82	116.84	123.43
4	A	901	VIA	C19-N14-S10	-4.65	108.60	117.05
4	D	901	VIA	C15-C16-N17	-4.55	105.66	110.80
4	D	901	VIA	C24-C23-N22	-4.49	117.29	123.43
4	A	901	VIA	C24-C23-N22	-4.35	117.48	123.43
4	A	901	VIA	C18-C19-N14	4.26	112.17	108.91
4	B	901	VIA	C24-C23-N22	-4.08	117.85	123.43
4	C	901	VIA	C15-N14-S10	-3.91	109.94	117.05
4	D	901	VIA	O12-S10-N14	3.69	110.06	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	VIA	C7-S10-N14	3.56	111.55	107.30
4	D	901	VIA	O12-S10-O11	-3.56	113.76	119.52
4	D	901	VIA	C16-C15-N14	-3.41	106.31	108.91
4	C	901	VIA	C19-C18-N17	3.32	114.55	110.80
4	C	901	VIA	C6-C7-S10	3.08	123.00	119.76
4	C	901	VIA	C15-C16-N17	2.91	114.09	110.80
4	B	901	VIA	O12-S10-N14	2.90	109.33	106.69
4	D	901	VIA	C18-C19-N14	2.86	111.10	108.91
4	D	901	VIA	O11-S10-C7	-2.74	104.58	108.05
4	C	901	VIA	C18-C19-N14	2.70	110.98	108.91
4	B	901	VIA	O12-S10-C7	2.59	111.33	108.05
4	B	901	VIA	C15-C16-N17	-2.50	107.98	110.80
4	D	901	VIA	C19-C18-N17	2.43	113.55	110.80
4	D	901	VIA	C15-N14-C19	-2.39	109.53	112.17
4	A	901	VIA	O11-S10-C7	2.38	111.06	108.05
4	A	901	VIA	C6-C7-S10	-2.35	117.29	119.76
4	B	901	VIA	C6-C7-S10	2.31	122.19	119.76
4	C	901	VIA	C6-C7-C8	-2.20	118.36	121.05
4	B	901	VIA	O3-C4-C9	2.15	121.02	115.01
4	D	901	VIA	C33-C32-C30	-2.14	107.41	115.27
4	D	901	VIA	O3-C4-C5	-2.14	119.75	124.46
4	D	901	VIA	C20-N17-C16	-2.12	107.49	110.66
4	A	901	VIA	C20-N17-C16	2.06	113.74	110.66
4	B	901	VIA	C8-C7-S10	-2.06	115.80	120.18
4	B	901	VIA	O3-C4-C5	-2.04	119.96	124.46

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	901	VIA	N29-C30-C32-C33
4	C	901	VIA	C30-C32-C33-C34
4	D	901	VIA	C30-C32-C33-C34
4	C	901	VIA	C15-N14-S10-C7
4	C	901	VIA	C15-N14-S10-O12
4	C	901	VIA	C19-N14-S10-O11
4	A	901	VIA	C19-N14-S10-O11
4	B	901	VIA	C19-N14-S10-O11
4	C	901	VIA	C15-N14-S10-O11
4	C	901	VIA	C19-N14-S10-C7
4	A	901	VIA	C19-N14-S10-C7
4	B	901	VIA	C19-N14-S10-C7

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Mol	Chain	Res	Type	Atoms
4	B	901	VIA	C5-C4-O3-C2
4	B	901	VIA	C9-C4-O3-C2
4	C	901	VIA	C19-N14-S10-O12
4	D	901	VIA	C19-N14-S10-O11
4	D	901	VIA	C8-C7-S10-O11
4	D	901	VIA	C6-C7-S10-O11
4	D	901	VIA	C8-C7-S10-N14
4	D	901	VIA	C6-C7-S10-N14
4	D	901	VIA	C19-N14-S10-C7
4	A	901	VIA	C15-N14-S10-O12
4	C	901	VIA	C9-C4-O3-C2
4	C	901	VIA	C5-C4-O3-C2
4	B	901	VIA	C1-C2-O3-C4
4	B	901	VIA	C8-C7-S10-O11
4	C	901	VIA	C1-C2-O3-C4
4	B	901	VIA	C6-C7-S10-O11
4	B	901	VIA	C25-C30-C32-C33

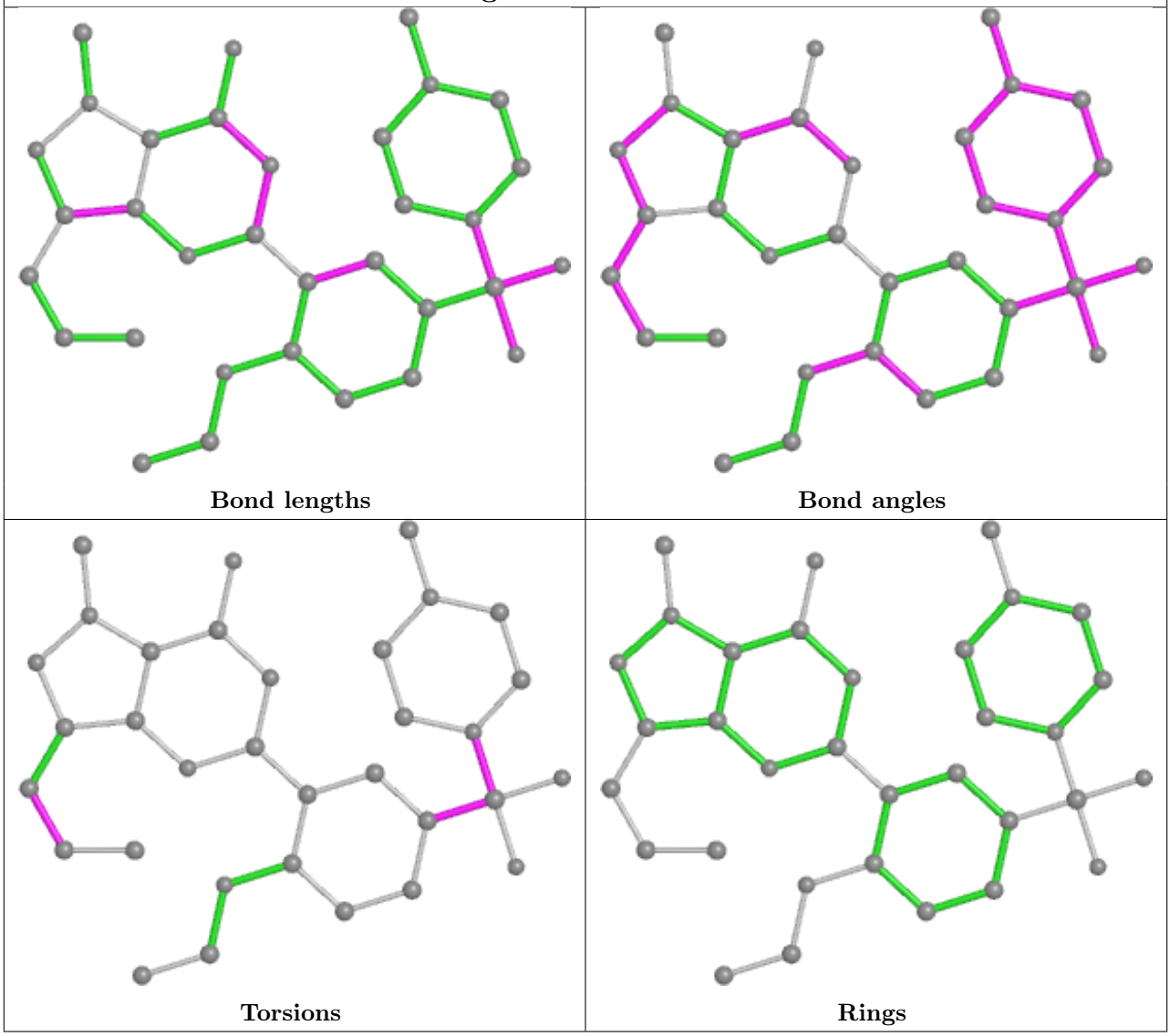
There are no ring outliers.

3 monomers are involved in 15 short contacts:

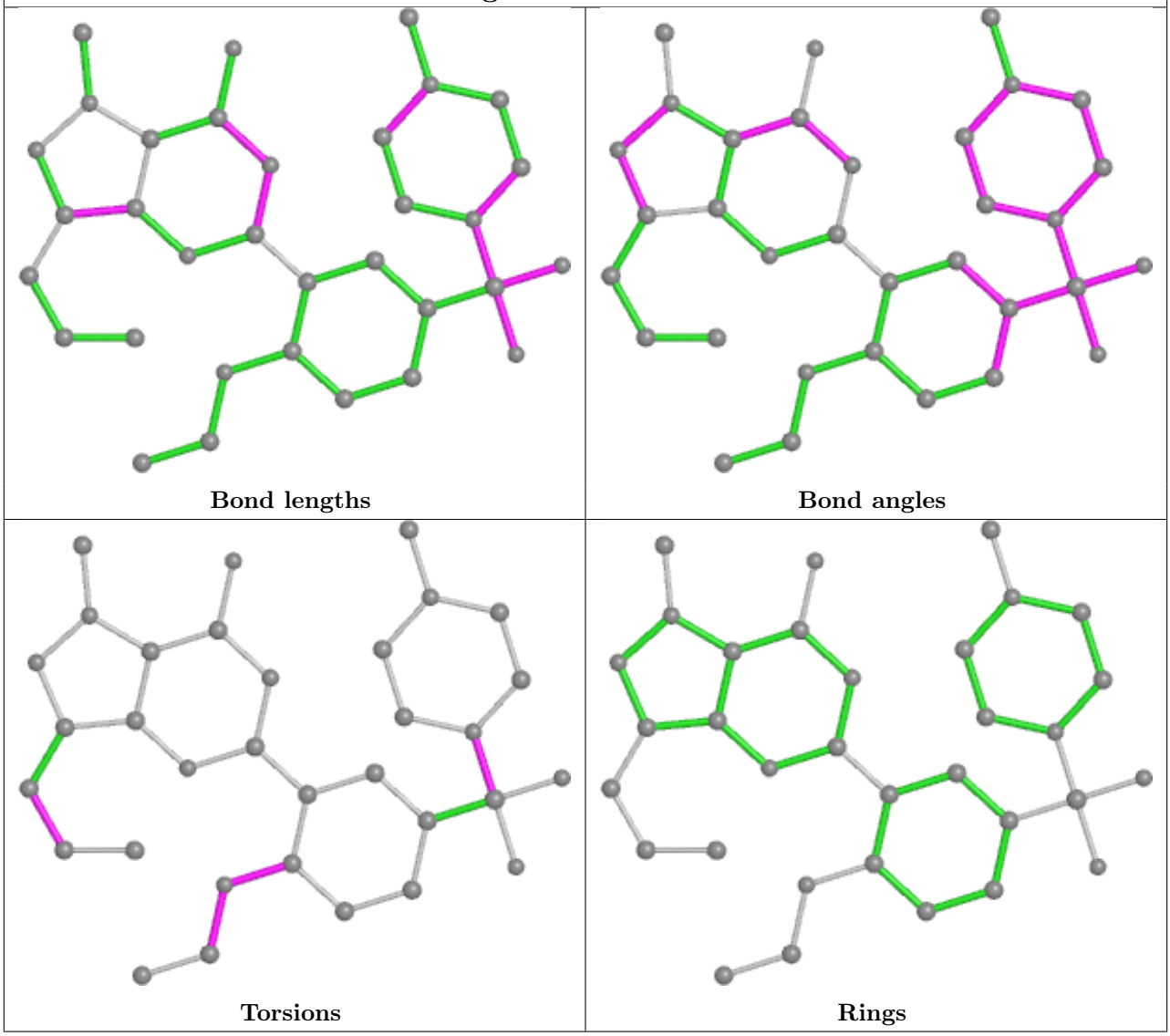
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	901	VIA	5	0
4	C	901	VIA	6	0
4	B	901	VIA	4	0

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 then 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.

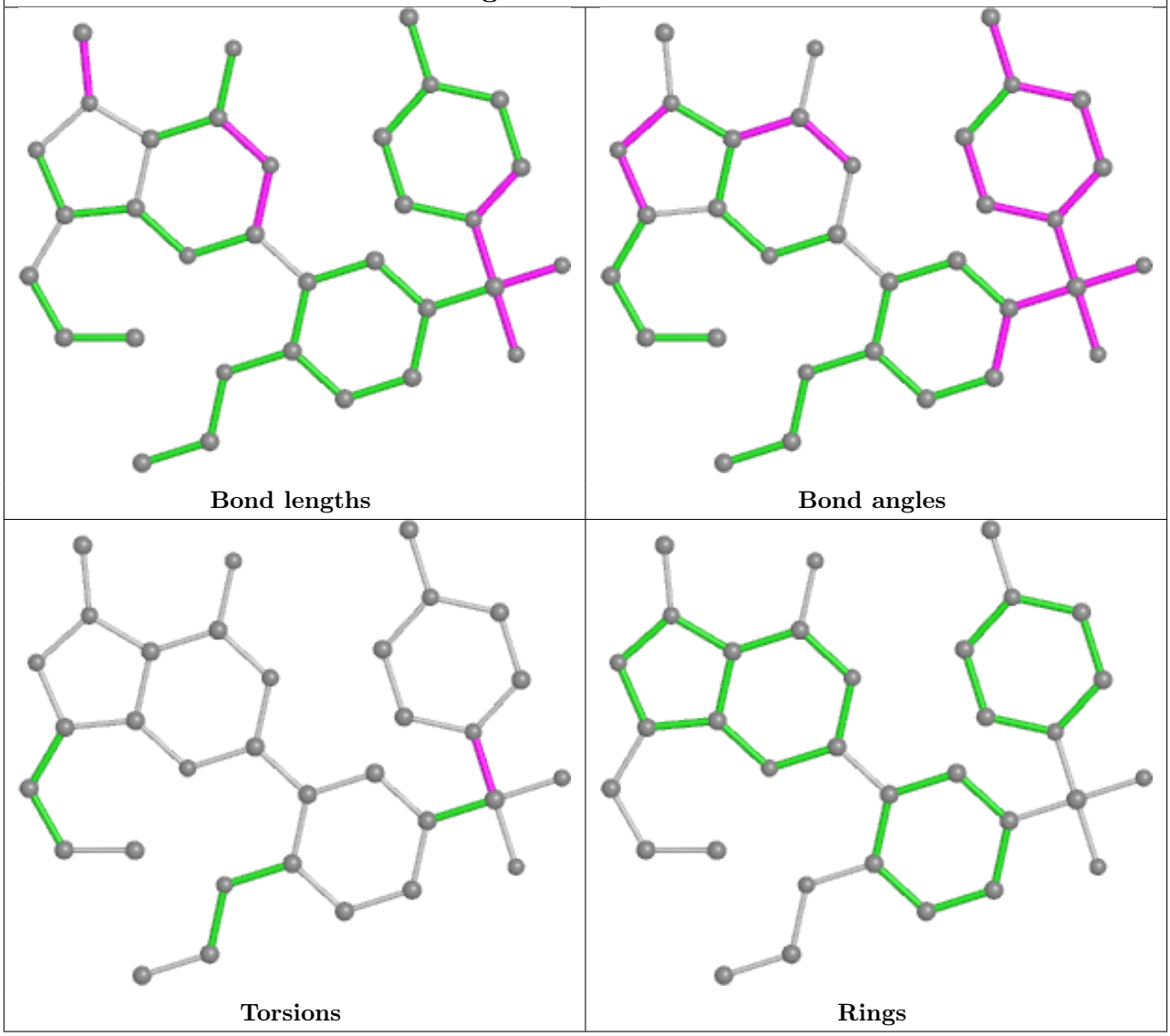
Ligand VIA D 901



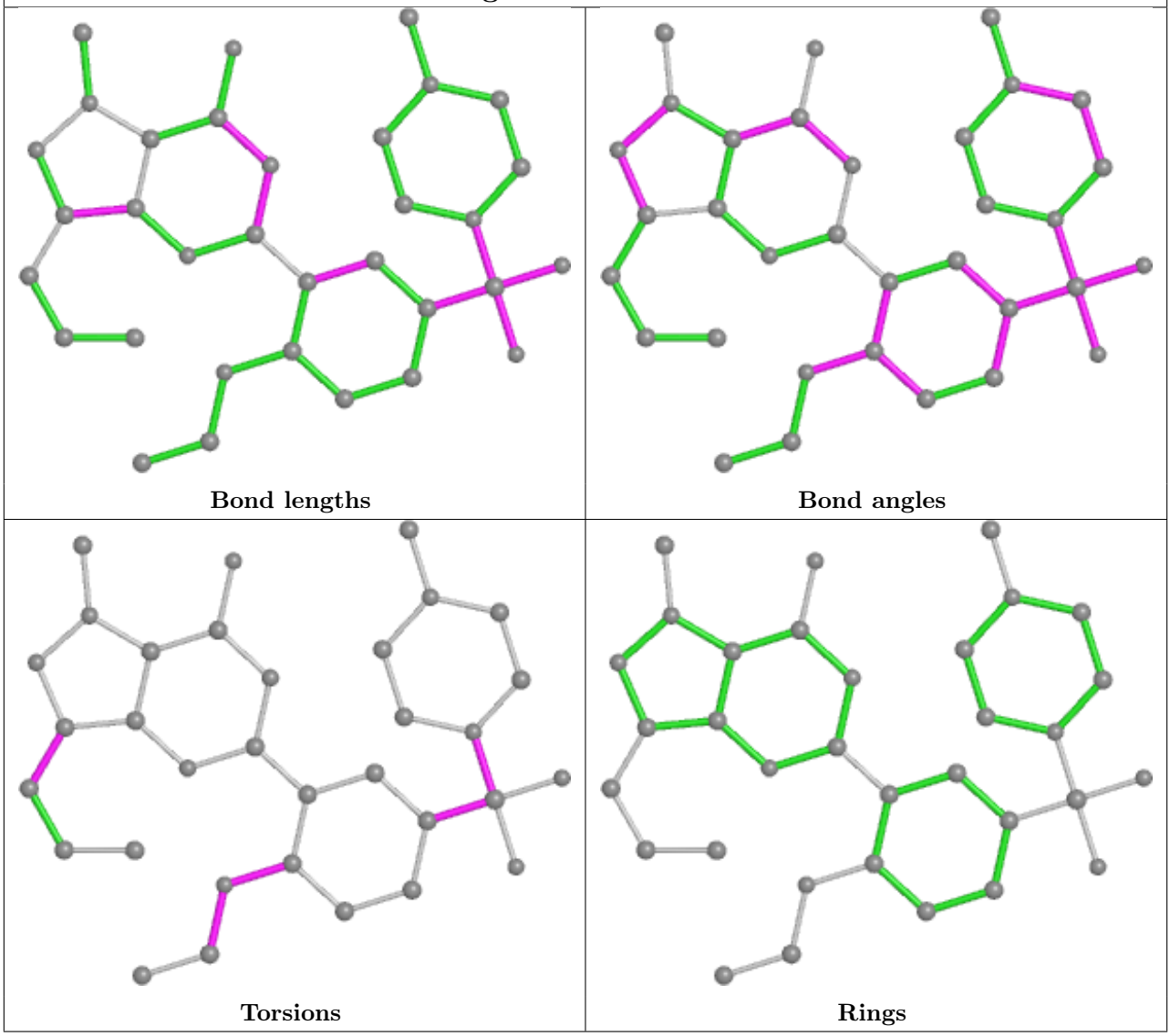
Ligand VIA C 901



Ligand VIA A 901



Ligand VIA B 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	324/330 (98%)	-0.12	4 (1%)	79	78	14, 22, 32, 43	0
1	B	324/330 (98%)	0.09	7 (2%)	62	60	14, 22, 32, 43	0
1	C	327/330 (99%)	0.17	18 (5%)	25	21	14, 22, 32, 43	0
1	D	323/330 (97%)	0.13	16 (4%)	28	25	14, 22, 32, 43	0
All	All	1298/1320 (98%)	0.07	45 (3%)	44	39	14, 22, 32, 43	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	798	GLN	5.0
1	D	538	ARG	4.2
1	D	706	ILE	4.2
1	C	631	ALA	3.6
1	A	859	GLN	3.6
1	A	538	ARG	3.5
1	D	705	SER	3.5
1	C	575	THR	3.4
1	C	703	GLY	3.4
1	B	636	ASN	3.4
1	C	547	VAL	3.2
1	D	677	CYS	3.1
1	D	564	PHE	3.0
1	D	539	GLU	3.0
1	C	747	GLU	2.9
1	A	674	GLN	2.8
1	B	537	THR	2.8
1	B	538	ARG	2.8
1	C	859	GLN	2.7
1	D	565	GLU	2.7
1	C	706	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	704	LEU	2.7
1	D	541	GLN	2.7
1	B	536	GLU	2.7
1	D	547	VAL	2.7
1	D	740	ARG	2.6
1	D	749	PRO	2.6
1	D	743	GLN	2.4
1	D	750	HIS	2.4
1	C	737	GLU	2.4
1	D	707	GLU	2.4
1	C	705	SER	2.4
1	C	647	LEU	2.3
1	C	552	GLN	2.3
1	B	706	ILE	2.2
1	C	740	ARG	2.2
1	C	851	GLN	2.2
1	C	811	ASP	2.2
1	B	859	GLN	2.1
1	C	837	GLU	2.1
1	A	589	GLN	2.1
1	C	589	GLN	2.1
1	C	545	ALA	2.1
1	D	537	THR	2.1
1	C	591	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

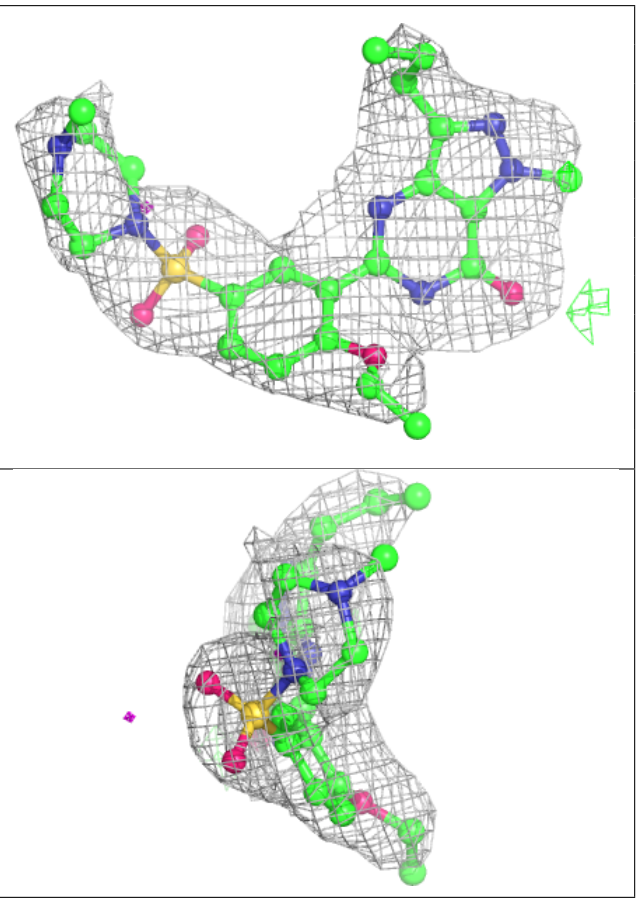
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	VIA	C	901	33/33	0.89	0.27	61,65,78,79	0
3	MG	D	900	1/1	0.90	0.33	54,54,54,54	0
4	VIA	A	901	33/33	0.92	0.20	36,40,60,62	0
3	MG	C	900	1/1	0.93	0.20	28,28,28,28	0
3	MG	A	900	1/1	0.94	0.26	17,17,17,17	0
4	VIA	B	901	33/33	0.95	0.30	47,52,64,66	0
3	MG	B	900	1/1	0.95	0.16	29,29,29,29	0
4	VIA	D	901	33/33	0.96	0.24	42,48,56,59	0
2	ZN	C	899	1/1	0.97	0.12	50,50,50,50	0
2	ZN	D	899	1/1	0.99	0.11	42,42,42,42	0
2	ZN	B	899	1/1	0.99	0.12	34,34,34,34	0
2	ZN	A	899	1/1	0.99	0.12	28,28,28,28	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.

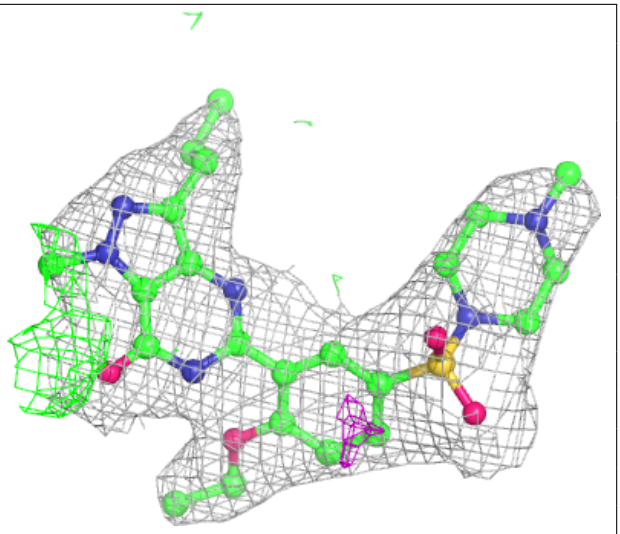
Electron density around VIA C 901:

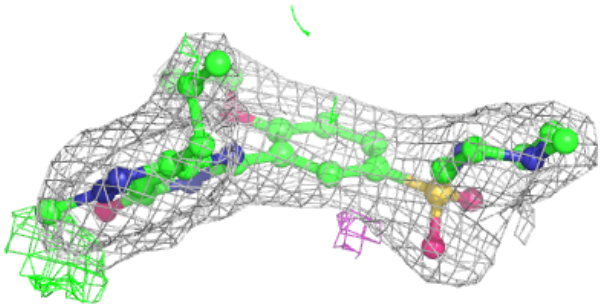
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

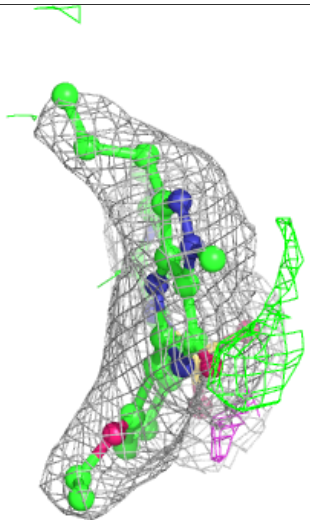


Electron density around VIA A 901:

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

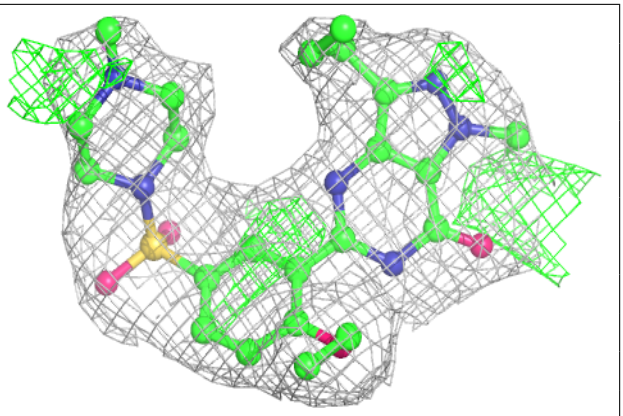


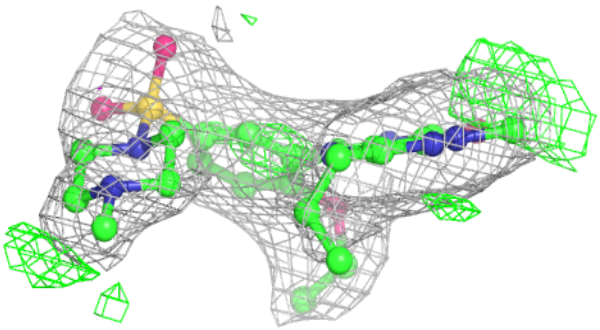


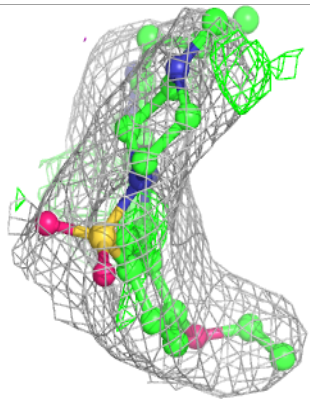


Electron density around VIA B 901:

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

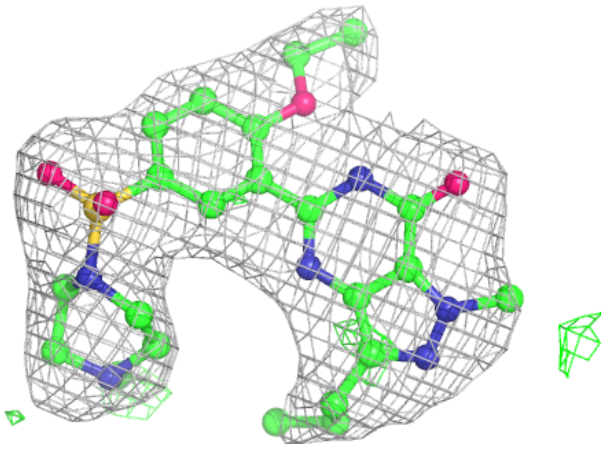


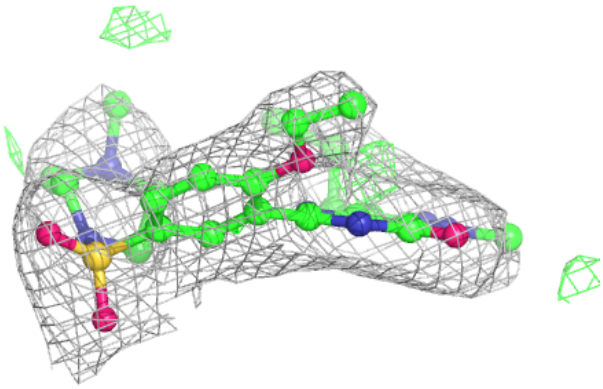


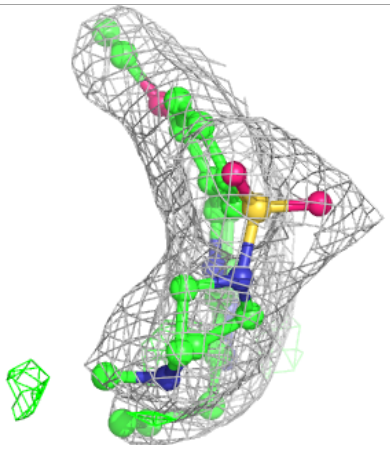


Electron density around VIA D 901:

$2mF_o$-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.