Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2020 – 09:12 AM BST

PDB ID	:	2YA7
Title	:	Crystal structure of Streptococcus pneumoniae NanA (TIGR4) in complex with Zanamivir
Authors	:	Gut, H.; Xu, G.; Taylor, G.L.; Walsh, M.A.
Deposited on	:	2011-02-18
Resolution	:	1.89 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

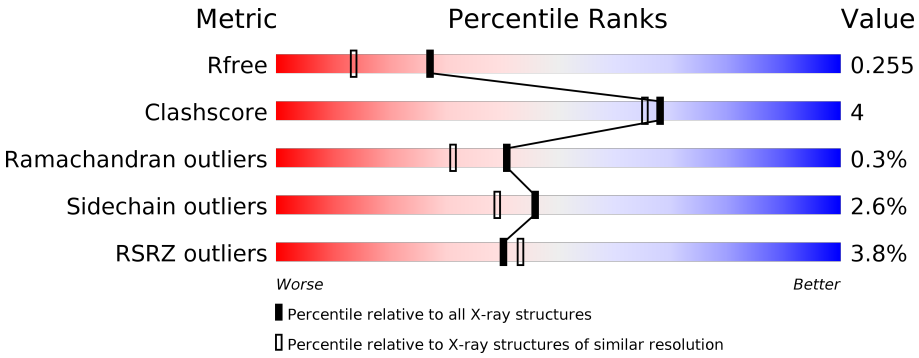
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.3.dev2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.3.dev2

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 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	493	2% 87% 8% • 5%
1	B	493	6% 83% 11% • 5%
1	C	493	2% 86% 8% • 5%
1	D	493	5% 83% 12% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16385 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 NEURAMINIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	4	0
			3744	2341	659	732	12			
1	B	468	Total	C	N	O	S	0	3	0
			3728	2333	658	725	12			
1	C	470	Total	C	N	O	S	0	5	0
			3762	2352	664	734	12			
1	D	470	Total	C	N	O	S	0	5	0
			3758	2350	663	733	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	ALA	-	expression tag	UNP B2DJD9
A	286	HIS	-	expression tag	UNP B2DJD9
A	287	HIS	-	expression tag	UNP B2DJD9
A	288	HIS	-	expression tag	UNP B2DJD9
A	289	HIS	-	expression tag	UNP B2DJD9
A	290	HIS	-	expression tag	UNP B2DJD9
A	291	HIS	-	expression tag	UNP B2DJD9
A	292	SER	-	expression tag	UNP B2DJD9
A	293	SER	-	expression tag	UNP B2DJD9
A	294	GLY	-	expression tag	UNP B2DJD9
A	295	LEU	-	expression tag	UNP B2DJD9
A	296	GLU	-	expression tag	UNP B2DJD9
A	297	VAL	-	expression tag	UNP B2DJD9
A	298	LEU	-	expression tag	UNP B2DJD9
A	299	PHE	-	expression tag	UNP B2DJD9
A	300	GLN	-	expression tag	UNP B2DJD9
A	301	GLY	-	expression tag	UNP B2DJD9
A	302	PRO	-	expression tag	UNP B2DJD9
A	440	LYS	GLU	SEE REMARK 999	UNP B2DJD9
A	584	ASP	ASN	SEE REMARK 999	UNP B2DJD9
B	285	ALA	-	expression tag	UNP B2DJD9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	286	HIS	-	expression tag	UNP B2DJD9
B	287	HIS	-	expression tag	UNP B2DJD9
B	288	HIS	-	expression tag	UNP B2DJD9
B	289	HIS	-	expression tag	UNP B2DJD9
B	290	HIS	-	expression tag	UNP B2DJD9
B	291	HIS	-	expression tag	UNP B2DJD9
B	292	SER	-	expression tag	UNP B2DJD9
B	293	SER	-	expression tag	UNP B2DJD9
B	294	GLY	-	expression tag	UNP B2DJD9
B	295	LEU	-	expression tag	UNP B2DJD9
B	296	GLU	-	expression tag	UNP B2DJD9
B	297	VAL	-	expression tag	UNP B2DJD9
B	298	LEU	-	expression tag	UNP B2DJD9
B	299	PHE	-	expression tag	UNP B2DJD9
B	300	GLN	-	expression tag	UNP B2DJD9
B	301	GLY	-	expression tag	UNP B2DJD9
B	302	PRO	-	expression tag	UNP B2DJD9
B	440	LYS	GLU	SEE REMARK 999	UNP B2DJD9
B	584	ASP	ASN	SEE REMARK 999	UNP B2DJD9
C	285	ALA	-	expression tag	UNP B2DJD9
C	286	HIS	-	expression tag	UNP B2DJD9
C	287	HIS	-	expression tag	UNP B2DJD9
C	288	HIS	-	expression tag	UNP B2DJD9
C	289	HIS	-	expression tag	UNP B2DJD9
C	290	HIS	-	expression tag	UNP B2DJD9
C	291	HIS	-	expression tag	UNP B2DJD9
C	292	SER	-	expression tag	UNP B2DJD9
C	293	SER	-	expression tag	UNP B2DJD9
C	294	GLY	-	expression tag	UNP B2DJD9
C	295	LEU	-	expression tag	UNP B2DJD9
C	296	GLU	-	expression tag	UNP B2DJD9
C	297	VAL	-	expression tag	UNP B2DJD9
C	298	LEU	-	expression tag	UNP B2DJD9
C	299	PHE	-	expression tag	UNP B2DJD9
C	300	GLN	-	expression tag	UNP B2DJD9
C	301	GLY	-	expression tag	UNP B2DJD9
C	302	PRO	-	expression tag	UNP B2DJD9
C	440	LYS	GLU	SEE REMARK 999	UNP B2DJD9
C	584	ASP	ASN	SEE REMARK 999	UNP B2DJD9
D	285	ALA	-	expression tag	UNP B2DJD9
D	286	HIS	-	expression tag	UNP B2DJD9
D	287	HIS	-	expression tag	UNP B2DJD9

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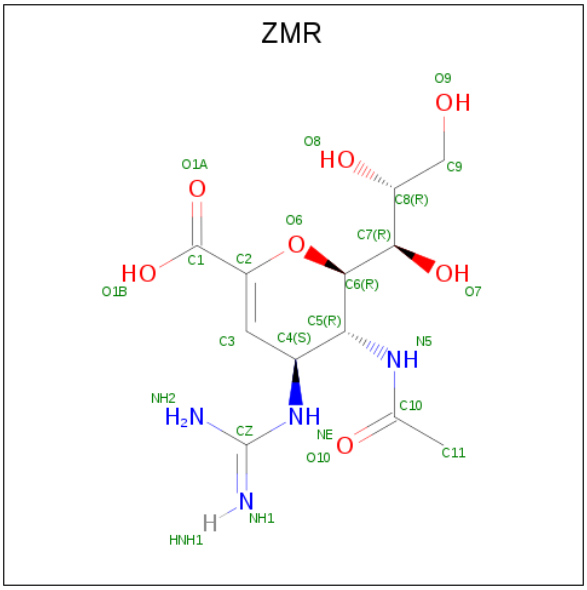
Chain	Residue	Modelled	Actual	Comment	Reference
D	288	HIS	-	expression tag	UNP B2DJD9
D	289	HIS	-	expression tag	UNP B2DJD9
D	290	HIS	-	expression tag	UNP B2DJD9
D	291	HIS	-	expression tag	UNP B2DJD9
D	292	SER	-	expression tag	UNP B2DJD9
D	293	SER	-	expression tag	UNP B2DJD9
D	294	GLY	-	expression tag	UNP B2DJD9
D	295	LEU	-	expression tag	UNP B2DJD9
D	296	GLU	-	expression tag	UNP B2DJD9
D	297	VAL	-	expression tag	UNP B2DJD9
D	298	LEU	-	expression tag	UNP B2DJD9
D	299	PHE	-	expression tag	UNP B2DJD9
D	300	GLN	-	expression tag	UNP B2DJD9
D	301	GLY	-	expression tag	UNP B2DJD9
D	302	PRO	-	expression tag	UNP B2DJD9
D	440	LYS	GLU	SEE REMARK 999	UNP B2DJD9
D	584	ASP	ASN	SEE REMARK 999	UNP B2DJD9

- Molecule 2 is ZANAMIVIR (three-letter code: ZMR) (formula: $C_{12}H_{20}N_4O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	12	4	7		
2	B	1	Total	C	N	O	0	0
			23	12	4	7		
2	C	1	Total	C	N	O	0	0
			23	12	4	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			23	12	4	7		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

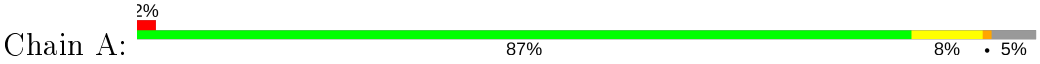
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	347	Total	O	0	2
			349	349		
4	B	297	Total	O	0	0
			297	297		
4	C	343	Total	O	0	1
			344	344		
4	D	307	Total	O	0	0
			307	307		

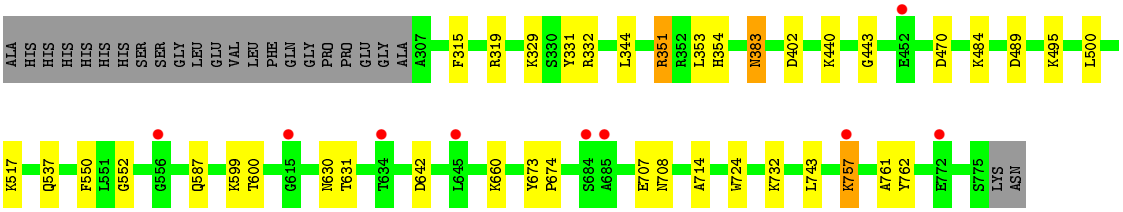
3 Residue-property plots (i)

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: NEURAMINIDASE A

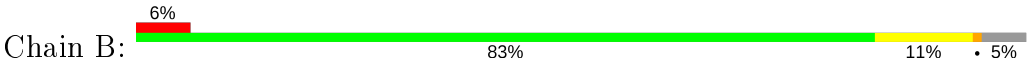
Chain A:

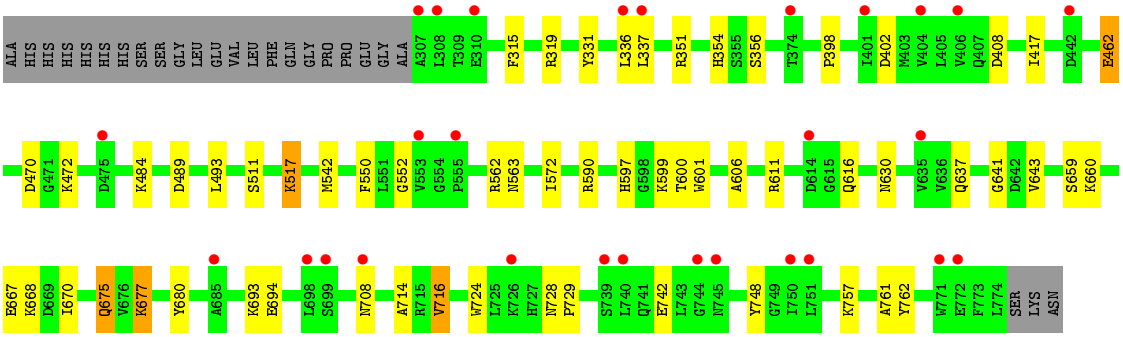




- Molecule 1: NEURAMINIDASE A

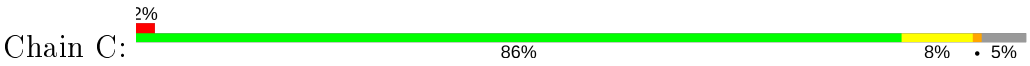
Chain B:

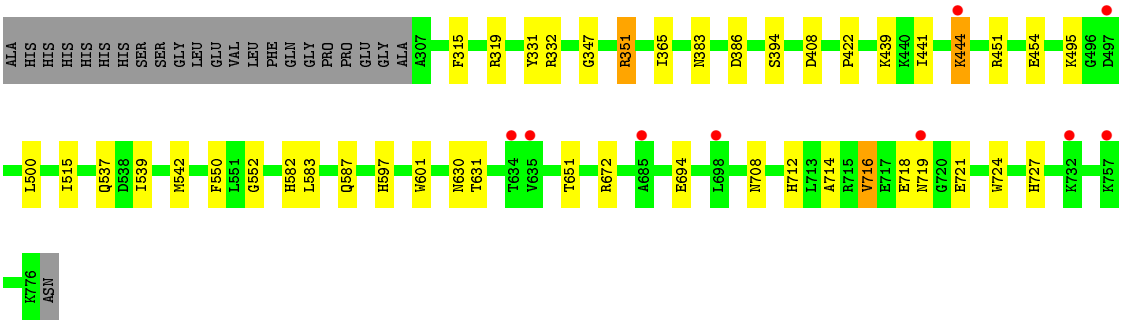




- Molecule 1: NEURAMINIDASE A

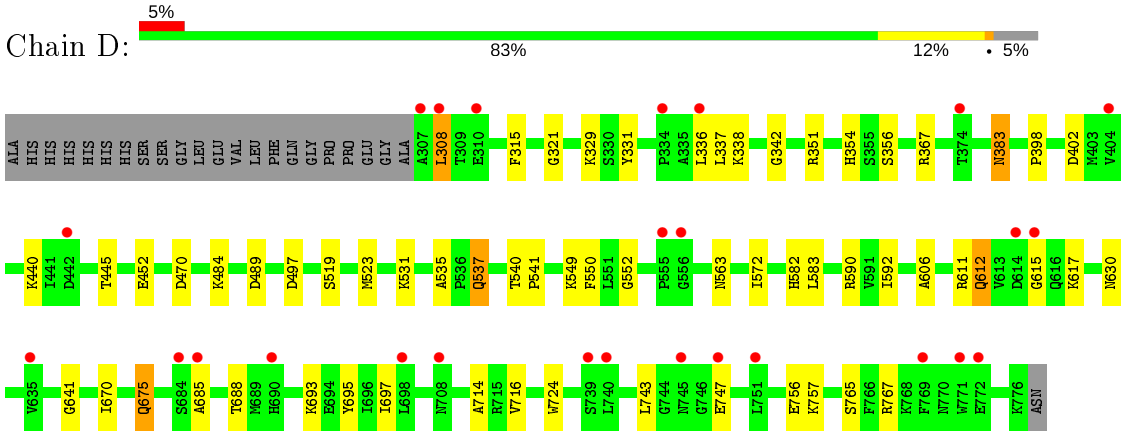
Chain C:





• Molecule 1: NEURAMINIDASE A

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.86Å 87.16Å 126.41Å 104.06° 91.04° 106.68°	Depositor
Resolution (Å)	27.81 – 1.89 27.81 – 1.89	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.81-1.89) 94.7 (27.81-1.89)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.257 0.206 , 0.255	Depositor DCC
R_{free} test set	3718 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.107 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16385	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZMR, CL

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	0.50	0/3825	0.62	0/5169
1	B	0.46	0/3809	0.61	0/5146
1	C	0.49	0/3843	0.63	0/5191
1	D	0.46	0/3839	0.61	0/5185
All	All	0.48	0/15316	0.62	0/20691

There are no bond length outliers.

There are no bond angle outliers.

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	3744	0	3635	18	0
1	B	3728	0	3632	28	0
1	C	3762	0	3659	30	0
1	D	3758	0	3659	36	0
2	A	23	0	19	0	0
2	B	23	0	19	0	0
2	C	23	0	19	0	0
2	D	23	0	19	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	349	0	0	1	0
4	B	297	0	0	3	0
4	C	344	0	0	8	0
4	D	307	0	0	5	0
All	All	16385	0	14661	112	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 4.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:HIS:HD2	1:C:727:HIS:HD2	1.13	0.91
1:C:672:ARG:NH1	4:C:2291:HOH:O	2.07	0.85
1:C:712:HIS:HD2	1:C:727:HIS:CD2	1.96	0.83
1:C:712:HIS:CD2	1:C:727:HIS:HD2	1.97	0.81
1:A:383:ASN:ND2	4:A:2047:HOH:O	2.19	0.76
1:B:484:LYS:HD2	1:B:489:ASP:HB3	1.70	0.72
1:B:319:ARG:HH12	1:B:757:LYS:HB2	1.56	0.70
1:D:338:LYS:NZ	1:D:342:GLY:HA2	2.07	0.68
1:A:440:LYS:HE2	1:A:443:GLY:HA2	1.75	0.68
1:C:386[A]:ASP:OD1	4:C:2041:HOH:O	2.12	0.67
1:D:338:LYS:HZ1	1:D:342:GLY:HA2	1.62	0.65
1:C:383:ASN:OD1	4:C:2036:HOH:O	2.14	0.64
1:D:354:HIS:CE1	1:D:356:SER:HB2	2.33	0.64
1:D:756:GLU:HG3	1:D:757:LYS:HD2	1.80	0.62
1:D:550:PHE:CZ	1:D:552:GLY:HA3	2.35	0.62
1:D:765:SER:OG	4:D:2303:HOH:O	2.16	0.62
1:D:383:ASN:ND2	4:D:2033:HOH:O	2.36	0.59
1:D:338:LYS:HE2	1:D:743:LEU:O	2.03	0.58
1:C:651:THR:HB	1:C:672:ARG:NH2	2.19	0.57
1:C:719:ASN:HB2	4:C:2320:HOH:O	2.04	0.57
1:C:651:THR:HB	1:C:672:ARG:HH21	1.70	0.57
1:D:440:LYS:HG2	1:D:445:THR:HG22	1.86	0.56
1:B:643:VAL:HB	1:B:659[A]:SER:OG	2.07	0.55
1:D:675:GLN:HG3	1:D:724:TRP:HB2	1.89	0.55
1:A:319:ARG:HH21	1:A:757:LYS:HB2	1.70	0.55
1:D:452:GLU:HA	1:D:452:GLU:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:GLU:HG2	1:B:716:VAL:HG13	1.87	0.55
1:B:742:GLU:HG3	1:B:748:TYR:CE1	2.42	0.55
1:A:495:LYS:HB2	1:A:500:LEU:HD11	1.90	0.54
1:C:451:ARG:HD3	1:C:454:GLU:OE2	2.08	0.54
1:B:550:PHE:CZ	1:B:552:GLY:HA3	2.44	0.53
1:C:439:LYS:HE2	1:C:441:ILE:HD11	1.90	0.53
1:C:539:ILE:HB	1:C:542:MET:CE	2.38	0.53
1:A:714:ALA:HB2	1:A:724:TRP:CE3	2.44	0.53
1:C:550:PHE:CZ	1:C:552:GLY:HA3	2.44	0.52
1:C:694:GLU:HG2	1:C:716:VAL:HG13	1.91	0.52
1:D:572:ILE:HB	1:D:592:ILE:HG13	1.91	0.52
1:A:599:LYS:HG3	1:A:600:THR:HG23	1.92	0.52
1:C:422:PRO:HG3	1:C:515:ILE:HD11	1.93	0.51
1:D:523:MET:O	1:D:537:GLN:HG2	2.10	0.51
1:B:694:GLU:HG2	1:B:716:VAL:CG1	2.40	0.51
1:A:315:PHE:HB3	1:A:331:TYR:CG	2.45	0.50
1:A:329:LYS:HE2	1:A:353:LEU:O	2.11	0.50
1:D:484:LYS:HD2	1:D:489:ASP:HB3	1.93	0.50
1:C:694:GLU:HG2	1:C:716:VAL:CG1	2.42	0.49
1:A:329:LYS:HD2	1:A:354:HIS:HA	1.94	0.49
1:D:321:GLY:O	1:D:329:LYS:HE3	2.12	0.49
1:C:315:PHE:HB3	1:C:331:TYR:CG	2.47	0.49
1:C:719:ASN:HB3	1:C:721:GLU:H	1.77	0.49
1:C:587:GLN:HB3	1:C:631:THR:HG22	1.95	0.49
1:D:714:ALA:HB2	1:D:724:TRP:CE3	2.48	0.49
1:B:714:ALA:HB2	1:B:724:TRP:CE3	2.48	0.48
1:A:550:PHE:CZ	1:A:552:GLY:HA3	2.49	0.48
1:B:408:ASP:OD2	1:B:597:HIS:HD2	1.97	0.48
1:D:535:ALA:O	1:D:537:GLN:NE2	2.47	0.48
1:C:542:MET:HE1	1:C:601:TRP:HD1	1.80	0.47
1:C:714:ALA:HB2	1:C:724:TRP:CE3	2.49	0.47
1:C:408:ASP:OD2	1:C:597:HIS:HD2	1.97	0.47
1:D:497:ASP:HB2	4:D:2132:HOH:O	2.14	0.47
1:D:540:THR:N	1:D:541:PRO:HD2	2.30	0.47
1:D:354:HIS:ND1	1:D:356:SER:HB2	2.29	0.47
1:D:308:LEU:HD21	1:D:767:ARG:HD3	1.96	0.47
1:B:562:ARG:H	1:B:637:GLN:NE2	2.12	0.46
1:C:347:GLY:HA2	1:C:365:ILE:HG22	1.96	0.46
1:A:587:GLN:HB3	1:A:631:THR:HG22	1.98	0.46
1:B:675:GLN:HG3	1:B:724:TRP:HB2	1.97	0.46
1:D:367:ARG:NH2	1:D:531:LYS:HE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:ARG:CZ	1:B:670:ILE:HD12	2.46	0.45
1:C:332:ARG:HG3	1:C:351:ARG:CZ	2.46	0.45
1:C:454:GLU:HB3	4:C:2103:HOH:O	2.16	0.45
1:C:672:ARG:CZ	4:C:2291:HOH:O	2.58	0.45
1:D:563:ASN:OD1	1:D:641:GLY:HA2	2.16	0.45
1:B:562:ARG:H	1:B:637:GLN:HE22	1.65	0.45
1:B:677:LYS:HE3	4:B:2255:HOH:O	2.17	0.45
1:A:484:LYS:HD2	1:A:489:ASP:HB3	1.97	0.45
1:B:660:LYS:HE2	1:B:667:GLU:OE2	2.18	0.44
1:D:338:LYS:HD3	1:D:743:LEU:HA	1.99	0.44
1:B:728:ASN:HA	1:B:729:PRO:HD2	1.86	0.44
1:C:495:LYS:HB2	1:C:500:LEU:HD11	2.00	0.43
1:D:582:HIS:CG	1:D:583:LEU:H	2.36	0.43
1:B:493:LEU:HD12	1:B:511:SER:HB2	2.00	0.43
1:B:517:LYS:HD3	4:B:2144:HOH:O	2.18	0.43
1:A:642:ASP:OD2	1:A:660:LYS:NZ	2.49	0.43
1:A:332:ARG:HG3	1:A:351:ARG:CZ	2.49	0.43
1:D:315:PHE:HB3	1:D:331:TYR:CG	2.53	0.43
1:A:761:ALA:HA	1:A:762:TYR:HA	1.70	0.43
1:C:444:LYS:HA	4:C:2088[A]:HOH:O	2.19	0.43
1:C:708:ASN:ND2	4:C:2315:HOH:O	2.52	0.42
1:D:590:ARG:HB3	1:D:606:ALA:HA	2.02	0.42
1:D:612:GLN:HE22	1:D:615:GLY:HA2	1.83	0.42
1:D:611:ARG:CZ	1:D:670:ILE:HD12	2.50	0.42
1:B:315:PHE:HB3	1:B:331:TYR:CG	2.54	0.42
1:D:688:THR:HG23	1:D:695:TYR:HB2	2.02	0.42
1:D:612:GLN:HG2	1:D:617:LYS:HD3	2.02	0.42
1:D:685:ALA:HA	1:D:697:ILE:O	2.20	0.42
1:B:563:ASN:OD1	1:B:641:GLY:HA2	2.19	0.42
1:B:590:ARG:HB3	1:B:606:ALA:HA	2.02	0.42
1:C:582:HIS:CG	1:C:583:LEU:H	2.38	0.41
1:B:462:GLU:O	1:B:462:GLU:OE1	2.39	0.41
1:A:673:TYR:HA	1:A:674:PRO:HD2	1.93	0.41
1:B:542:MET:HE1	1:B:601:TRP:HD1	1.85	0.41
1:A:344:LEU:HD21	1:A:743:LEU:CD2	2.51	0.41
1:D:338:LYS:HZ2	1:D:342:GLY:HA2	1.83	0.41
1:D:549:LYS:HD3	1:D:582:HIS:ND1	2.36	0.41
1:B:761:ALA:HA	1:B:762:TYR:HA	1.77	0.41
1:B:417:ILE:HD12	1:B:572:ILE:HG13	2.03	0.41
1:B:354:HIS:CE1	1:B:356:SER:HB2	2.56	0.41
1:B:599:LYS:HG3	1:B:600:THR:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:GLU:HG3	1:A:708:ASN:ND2	2.36	0.40
1:D:398:PRO:HG2	4:D:2035:HOH:O	2.22	0.40
1:B:398:PRO:HG2	4:B:2036:HOH:O	2.21	0.40
1:D:747:GLU:HB2	4:D:2298:HOH:O	2.22	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	471/493 (96%)	444 (94%)	25 (5%)	2 (0%)	34 24
1	B	469/493 (95%)	446 (95%)	20 (4%)	3 (1%)	25 15
1	C	473/493 (96%)	454 (96%)	19 (4%)	0	100 100
1	D	473/493 (96%)	446 (94%)	26 (6%)	1 (0%)	47 38
All	All	1886/1972 (96%)	1790 (95%)	90 (5%)	6 (0%)	41 31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	757	LYS
1	B	680	TYR
1	D	402	ASP
1	B	402	ASP
1	A	402	ASP
1	B	708	ASN

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/420 (96%)	397 (98%)	8 (2%)	55	51
1	B	403/420 (96%)	389 (96%)	14 (4%)	36	27
1	C	407/420 (97%)	397 (98%)	10 (2%)	47	41
1	D	407/420 (97%)	394 (97%)	13 (3%)	39	30
All	All	1622/1680 (96%)	1577 (97%)	45 (3%)	46	36

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	ARG
1	A	383	ASN
1	A	470	ASP
1	A	517	LYS
1	A	537[A]	GLN
1	A	537[B]	GLN
1	A	630	ASN
1	A	732	LYS
1	B	336	LEU
1	B	337	LEU
1	B	351	ARG
1	B	462	GLU
1	B	470	ASP
1	B	472	LYS
1	B	517	LYS
1	B	616	GLN
1	B	630	ASN
1	B	668	LYS
1	B	675	GLN
1	B	677	LYS
1	B	693	LYS
1	B	716	VAL
1	C	319	ARG
1	C	351	ARG
1	C	394[A]	SER
1	C	394[B]	SER
1	C	444	LYS
1	C	537[A]	GLN

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Mol	Chain	Res	Type
1	C	537[B]	GLN
1	C	630	ASN
1	C	716	VAL
1	C	718	GLU
1	D	308	LEU
1	D	336	LEU
1	D	337	LEU
1	D	351	ARG
1	D	383	ASN
1	D	470	ASP
1	D	519	SER
1	D	537	GLN
1	D	612	GLN
1	D	630	ASN
1	D	675	GLN
1	D	693	LYS
1	D	716	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	ASN
1	B	322	ASN
1	B	371	ASN
1	B	579	ASN
1	B	587	GLN
1	B	597	HIS
1	B	616	GLN
1	B	637	GLN
1	B	690	HIS
1	C	597	HIS
1	C	712	HIS
1	C	727	HIS
1	D	322	ASN
1	D	383	ASN
1	D	579	ASN
1	D	655	GLN

5.3.3 RNA

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 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
2	ZMR	A	1776	-	19,23,23	1.79	3 (15%)	19,32,32	1.81	1 (5%)
2	ZMR	B	1776	-	19,23,23	1.65	2 (10%)	19,32,32	1.55	1 (5%)
2	ZMR	C	1776	-	19,23,23	1.60	2 (10%)	19,32,32	1.67	2 (10%)
2	ZMR	D	1776	-	19,23,23	1.53	1 (5%)	19,32,32	1.58	1 (5%)

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
2	ZMR	A	1776	-	-	0/18/38/38	0/1/1/1
2	ZMR	B	1776	-	-	0/18/38/38	0/1/1/1
2	ZMR	C	1776	-	-	0/18/38/38	0/1/1/1
2	ZMR	D	1776	-	-	0/18/38/38	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1776	ZMR	C3-C2	6.15	1.40	1.32
2	A	1776	ZMR	C3-C2	5.75	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1776	ZMR	C3-C2	5.68	1.39	1.32
2	C	1776	ZMR	C3-C2	5.44	1.39	1.32
2	A	1776	ZMR	C4-C3	2.90	1.54	1.50
2	C	1776	ZMR	C4-C3	2.64	1.54	1.50
2	B	1776	ZMR	C4-C3	2.17	1.53	1.50
2	A	1776	ZMR	C5-N5	2.12	1.49	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1776	ZMR	C3-C4-NE	-7.21	100.71	111.00
2	D	1776	ZMR	C3-C4-NE	-6.39	101.88	111.00
2	C	1776	ZMR	C3-C4-NE	-5.98	102.47	111.00
2	B	1776	ZMR	C3-C4-NE	-5.73	102.82	111.00
2	C	1776	ZMR	O6-C6-C7	-2.55	101.24	105.91

There are no chirality outliers.

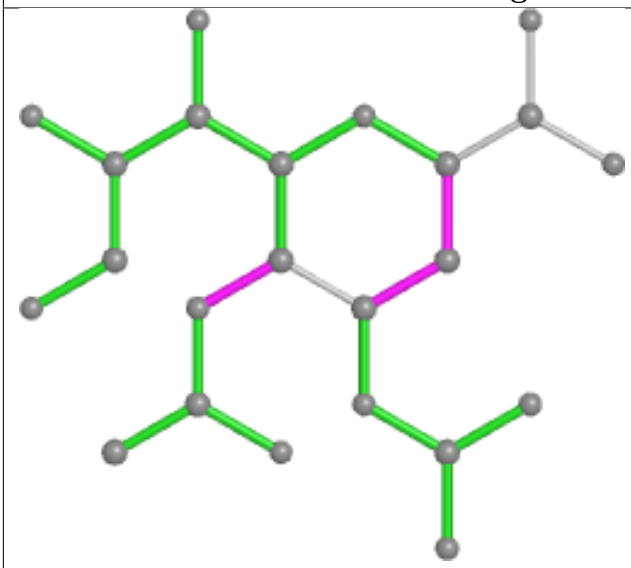
There are no torsion outliers.

There are no ring outliers.

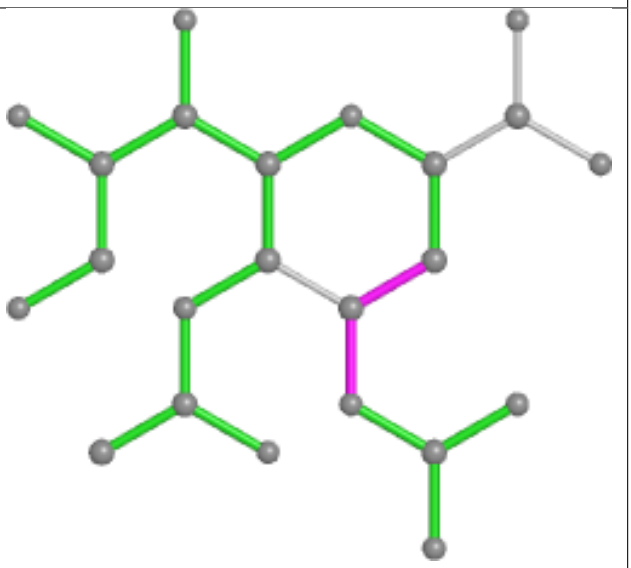
No monomer is involved in short contacts.

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 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.

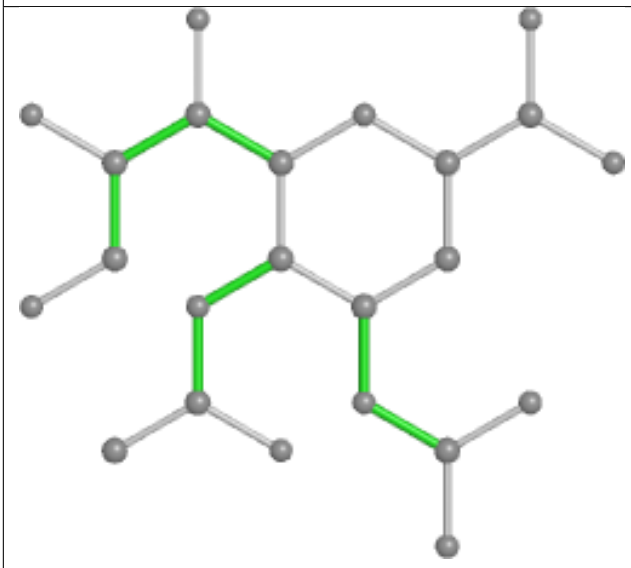
Ligand ZMR A 1776



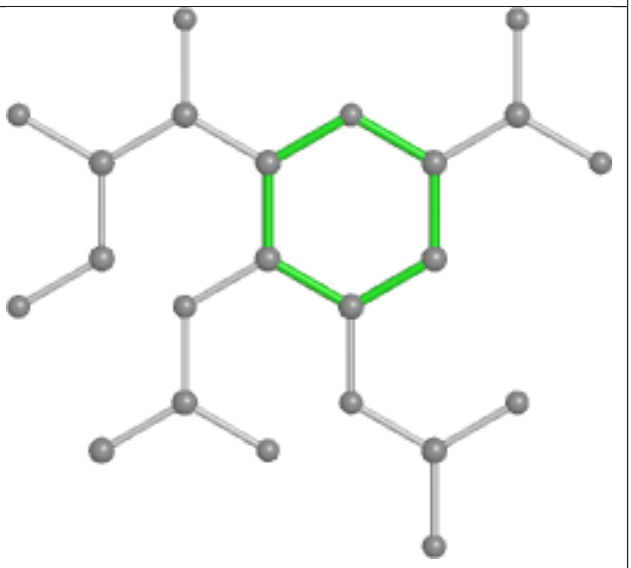
Bond lengths



Bond angles

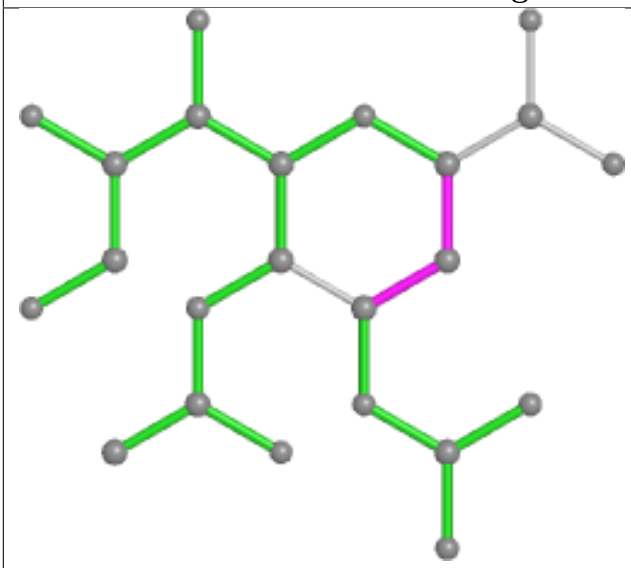


Torsions

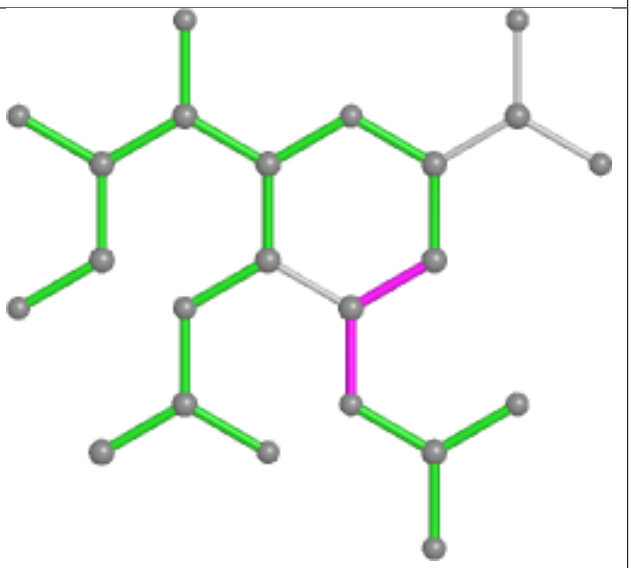


Rings

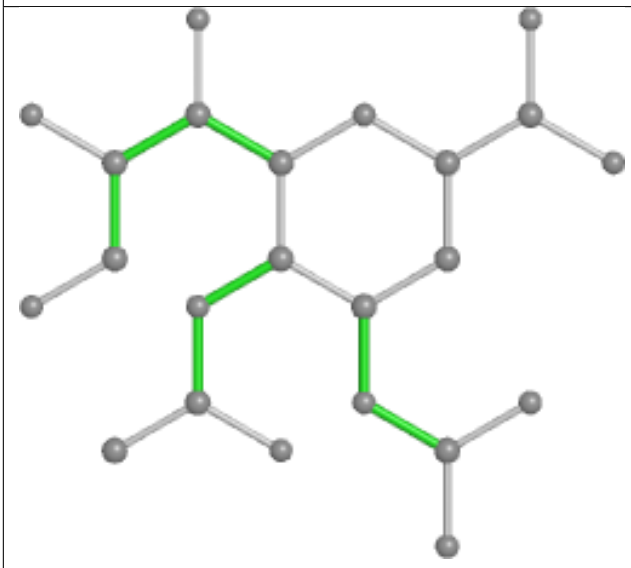
Ligand ZMR B 1776



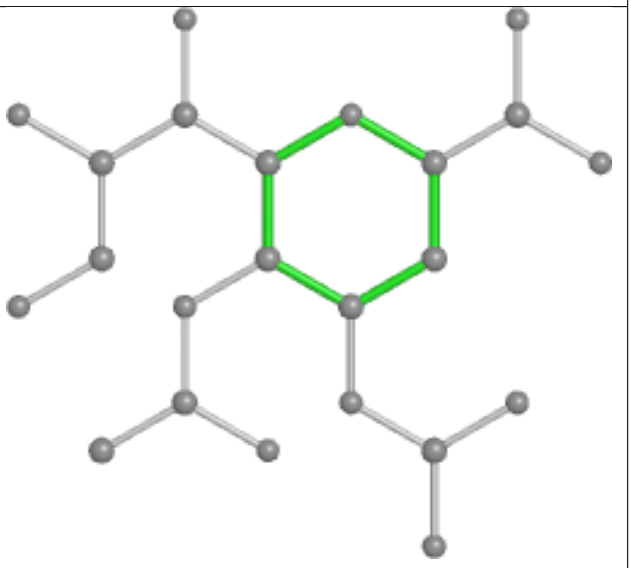
Bond lengths



Bond angles

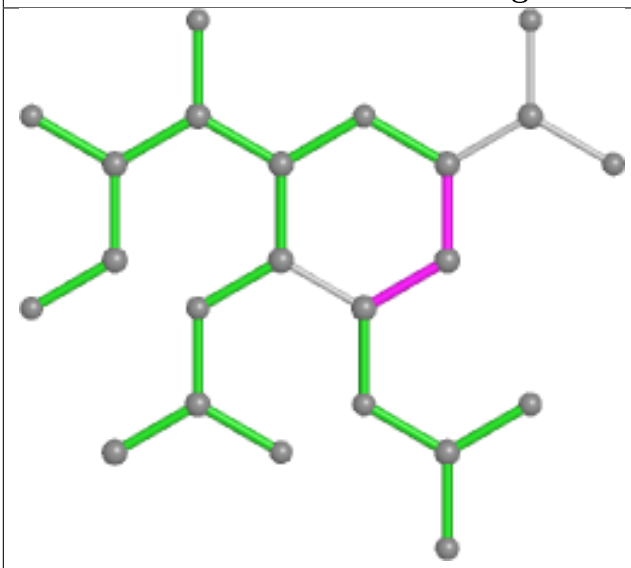


Torsions

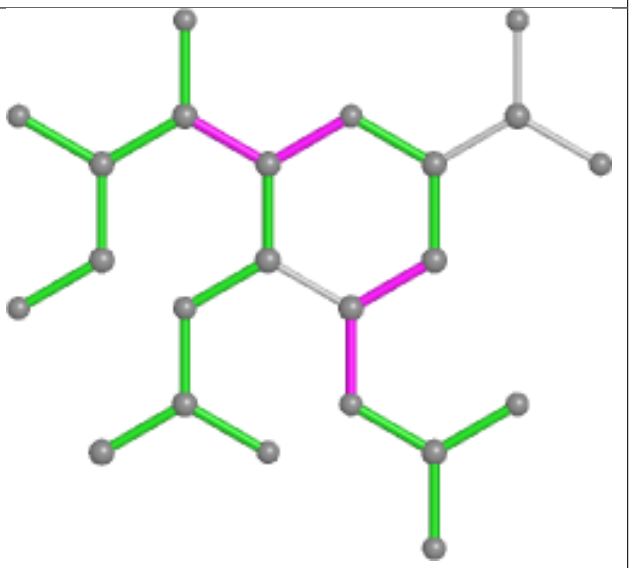


Rings

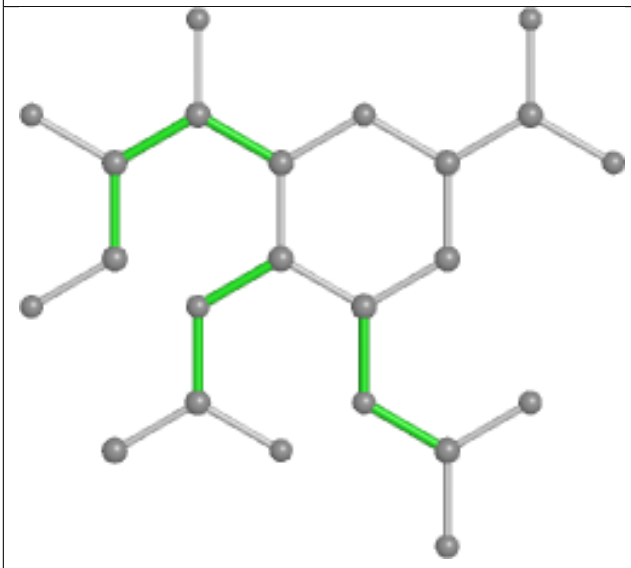
Ligand ZMR C 1776



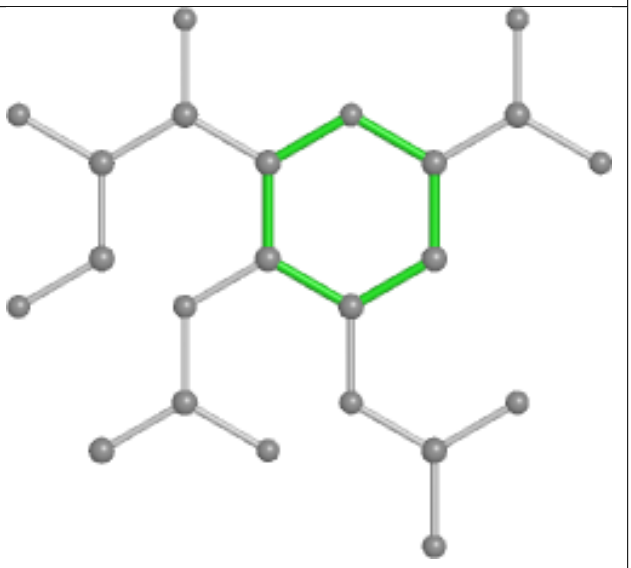
Bond lengths



Bond angles

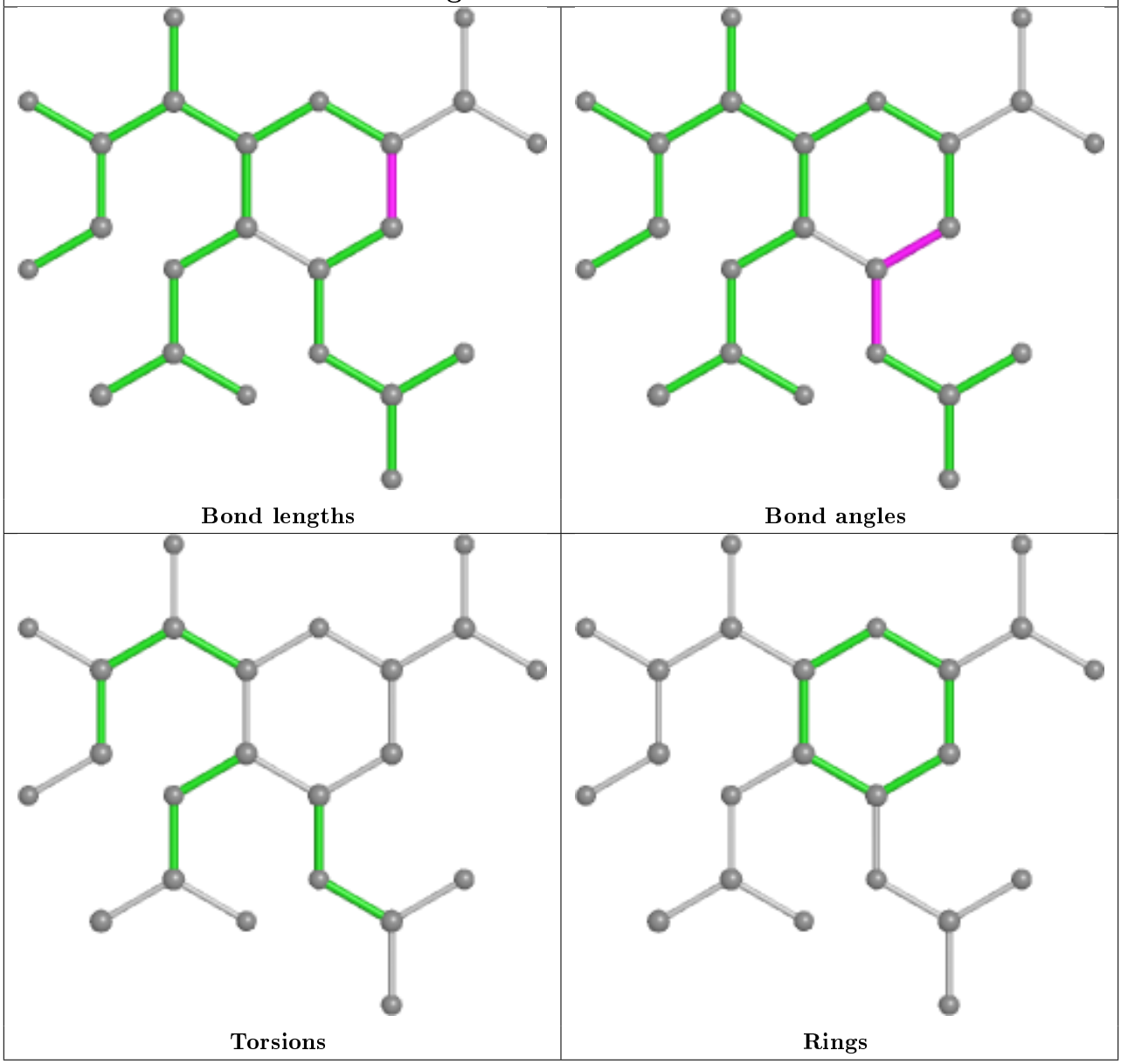


Torsions



Rings

Ligand ZMR D 1776



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, 95^{th} 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	469/493 (95%)	0.08	9 (1%) 66 69	17, 28, 41, 49	0
1	B	468/493 (94%)	0.33	28 (5%) 21 24	19, 32, 51, 59	0
1	C	470/493 (95%)	0.11	9 (1%) 66 69	19, 29, 43, 57	0
1	D	470/493 (95%)	0.31	26 (5%) 25 28	19, 33, 51, 66	0
All	All	1877/1972 (95%)	0.21	72 (3%) 40 43	17, 31, 48, 66	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	ALA	4.6
1	B	740	LEU	3.9
1	B	614	ASP	3.8
1	D	740	LEU	3.7
1	D	310	GLU	3.7
1	B	744	GLY	3.6
1	A	757	LYS	3.6
1	D	308	LEU	3.6
1	B	308	LEU	3.4
1	B	475	ASP	3.4
1	D	745	ASN	3.3
1	A	634	THR	3.2
1	D	374	THR	3.2
1	A	556	GLY	3.2
1	B	404	VAL	3.2
1	D	771	TRP	3.1
1	B	374	THR	3.1
1	B	442	ASP	3.0
1	B	698	LEU	3.0
1	C	757	LYS	3.0
1	D	307	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	739	SER	2.9
1	B	745	ASN	2.8
1	D	404	VAL	2.8
1	D	698	LEU	2.8
1	B	401	ILE	2.8
1	D	635	VAL	2.8
1	B	751	LEU	2.7
1	B	336	LEU	2.7
1	D	685	ALA	2.7
1	D	739	SER	2.6
1	B	685	ALA	2.6
1	D	772	GLU	2.6
1	D	615	GLY	2.6
1	B	553	VAL	2.6
1	C	685	ALA	2.5
1	D	751	LEU	2.5
1	C	497	ASP	2.5
1	B	772	GLU	2.5
1	D	334	PRO	2.4
1	C	635	VAL	2.4
1	D	556	GLY	2.4
1	B	635	VAL	2.4
1	D	555	PRO	2.4
1	A	685	ALA	2.4
1	C	698	LEU	2.3
1	B	310	GLU	2.3
1	C	719	ASN	2.3
1	B	771	TRP	2.3
1	A	645	LEU	2.3
1	B	708	ASN	2.3
1	C	444	LYS	2.3
1	B	555	PRO	2.3
1	C	732	LYS	2.2
1	B	699	SER	2.2
1	A	684	SER	2.2
1	A	615	GLY	2.2
1	B	406	VAL	2.2
1	B	337	LEU	2.2
1	A	772	GLU	2.2
1	D	747	GLU	2.1
1	B	726	LYS	2.1
1	D	442	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	452	GLU	2.1
1	D	614	ASP	2.1
1	B	750	ILE	2.1
1	C	634	THR	2.1
1	D	684	SER	2.0
1	D	690	HIS	2.0
1	D	708	ASN	2.0
1	D	769	PHE	2.0
1	D	336	LEU	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)

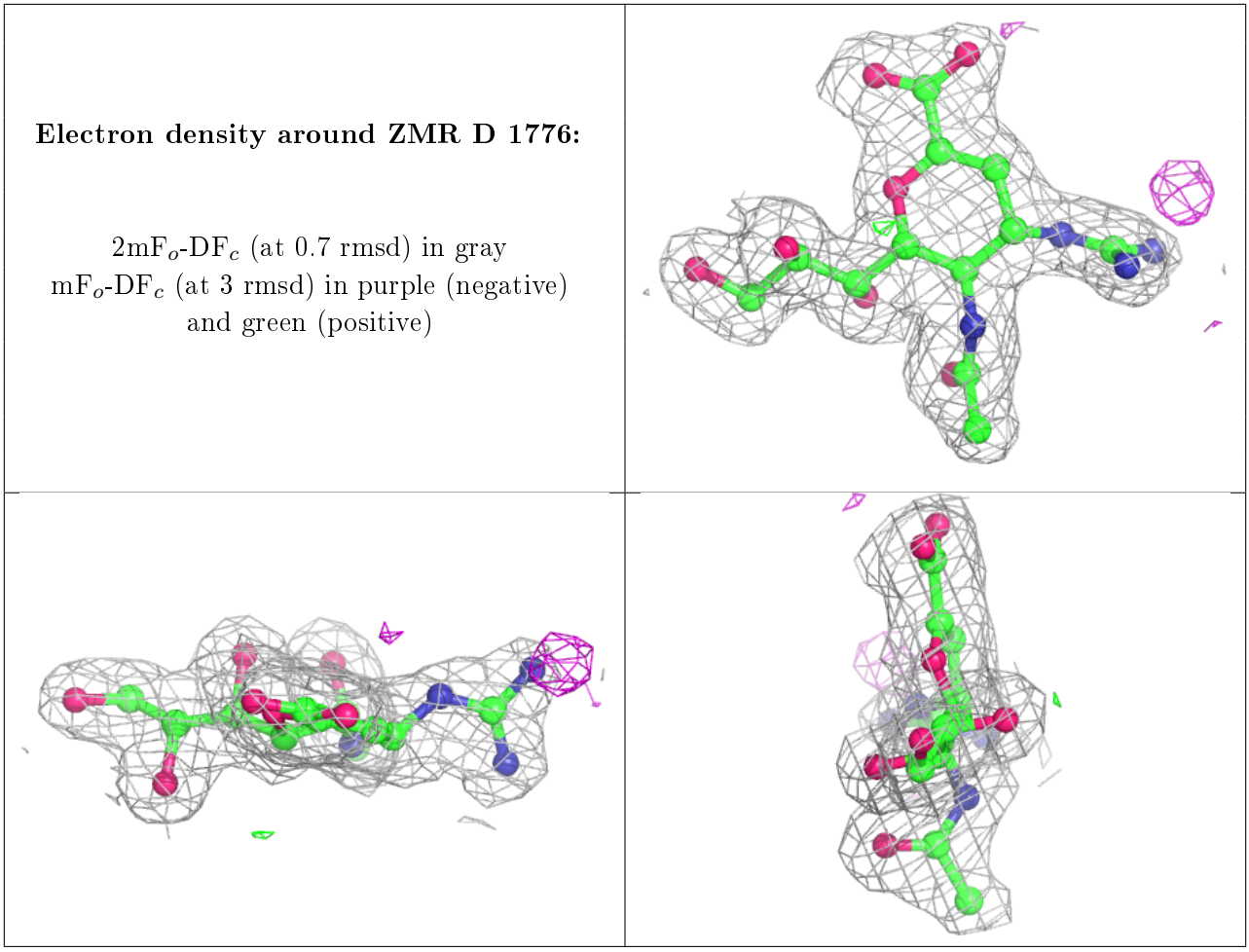
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	ZMR	D	1776	23/23	0.92	0.11	25,27,30,32	0
2	ZMR	B	1776	23/23	0.94	0.09	22,26,29,32	0
2	ZMR	A	1776	23/23	0.95	0.09	20,23,25,27	0
2	ZMR	C	1776	23/23	0.95	0.08	22,24,26,27	0
3	CL	B	1777	1/1	0.99	0.04	27,27,27,27	0
3	CL	C	1777	1/1	0.99	0.03	28,28,28,28	0
3	CL	D	1777	1/1	0.99	0.05	29,29,29,29	0
3	CL	A	1777	1/1	1.00	0.02	27,27,27,27	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.

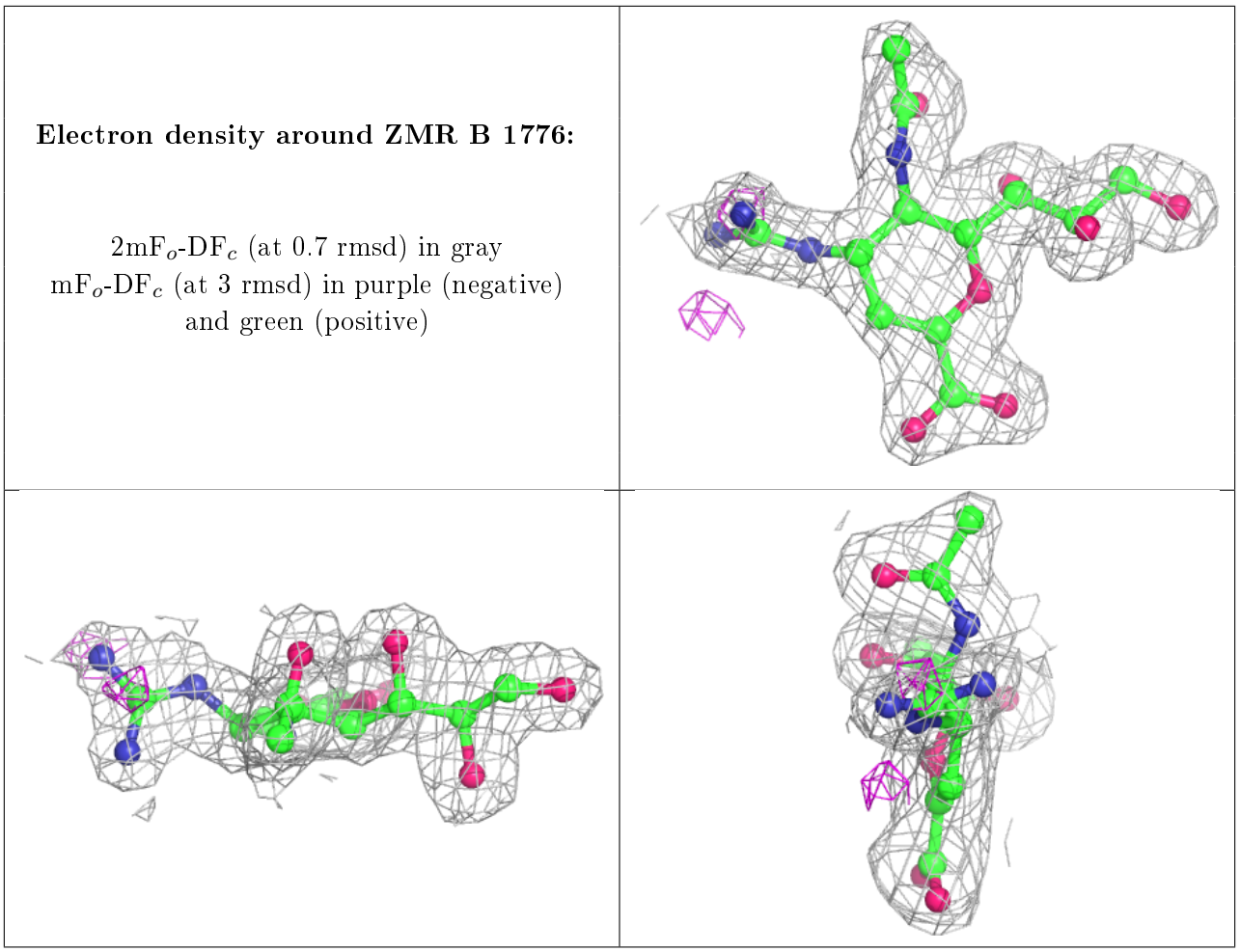
Electron density around ZMR D 1776:

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



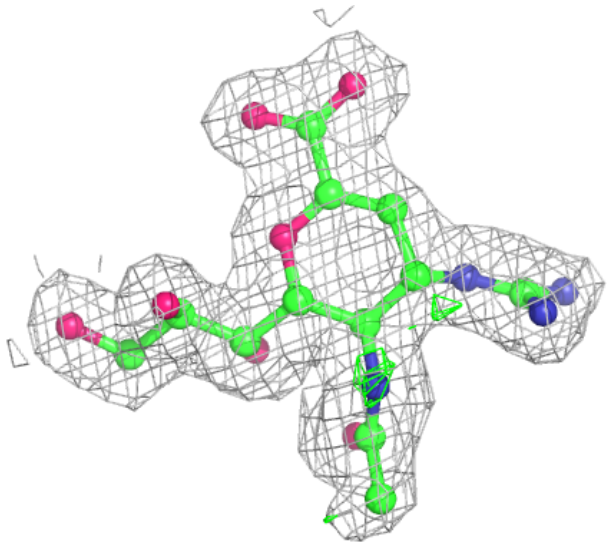
Electron density around ZMR B 1776:

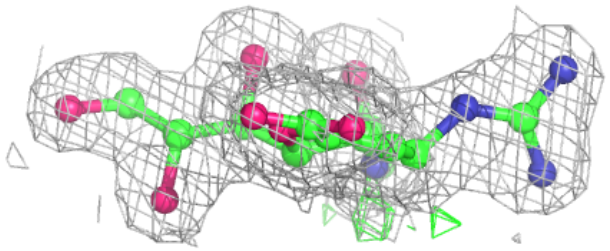
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

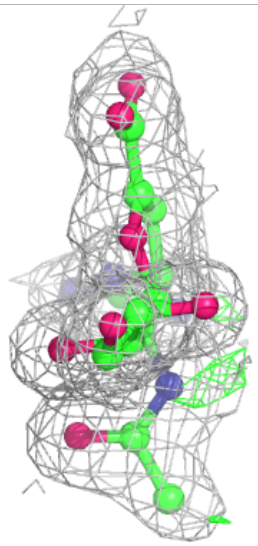


Electron density around ZMR A 1776:

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

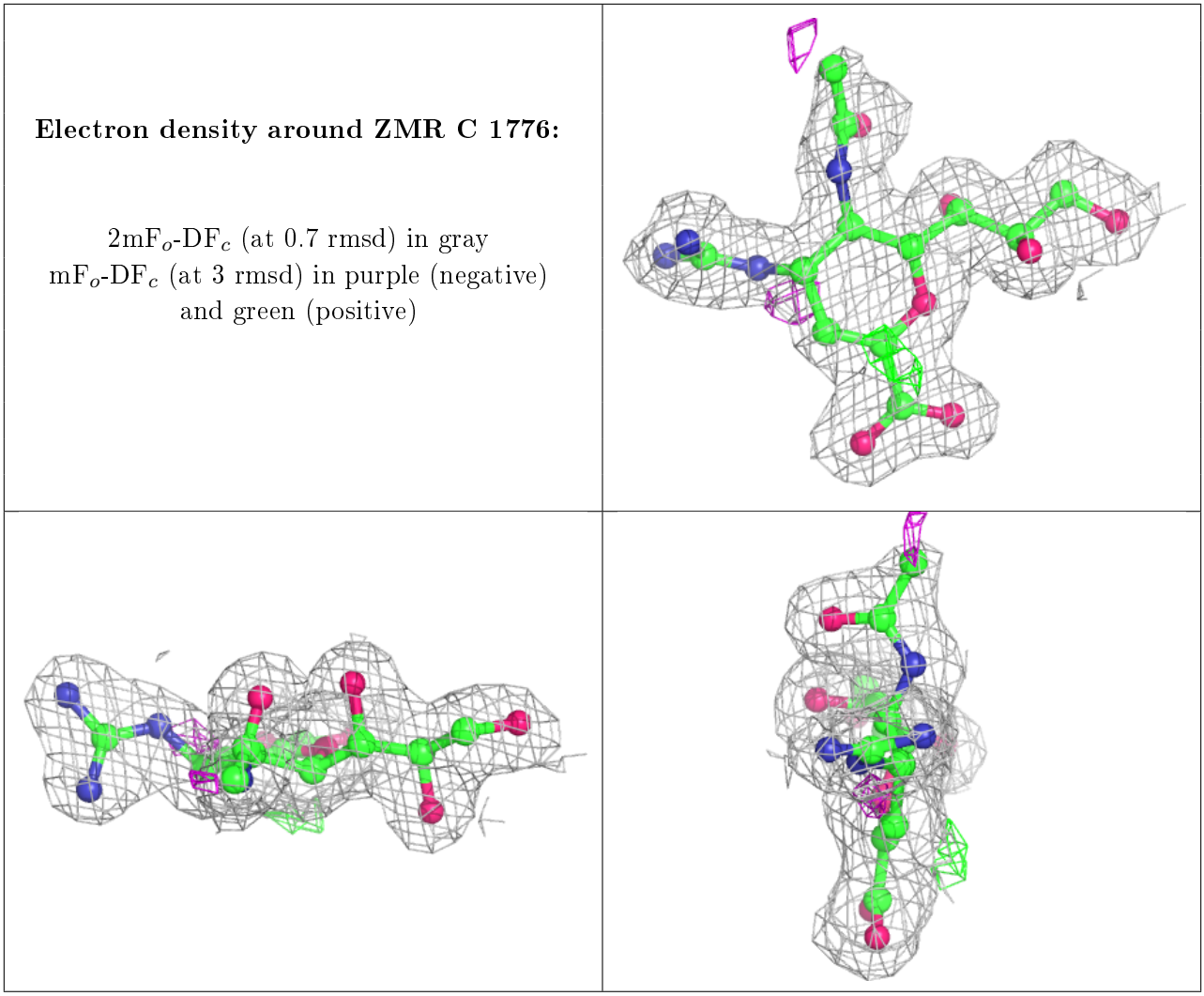






Electron density around ZMR C 1776:

$2mF_o$-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

There are no such residues in this entry.