Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2023 – 05:24 pm GMT

PDB ID	:	7PRV
Title	:	The glucocorticoid receptor in complex with fluticasone furoate, a PGC1a coactivator fragment and sgk 23bp
Authors	:	Postel, S.; Edman, K.; Wissler, L.
Deposited on	:	2021-09-22
Resolution	:	2.70 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:

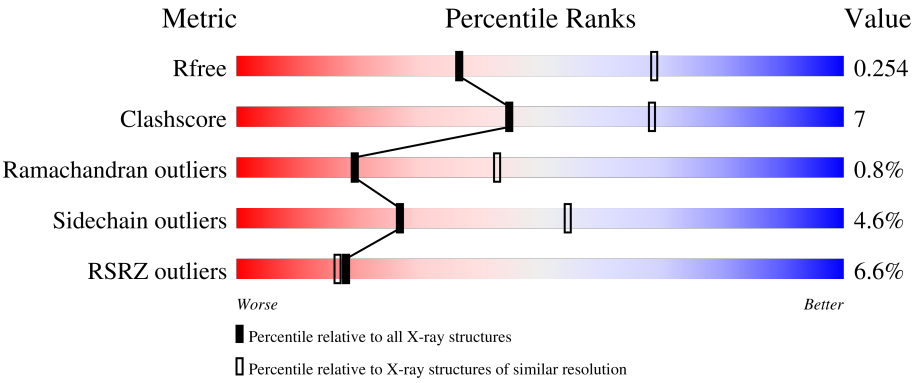
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	393	4% 64% 17% . 18%
1	B	393	8% 66% 15% . 18%
2	C	23	78% 17% .
3	D	23	74% 22% .
4	F	21	33% 24% 43%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 6278 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 Glucocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2584	1648	439	468	29			
1	B	321	Total	C	N	O	S	0	0	0
			2586	1648	440	469	29			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	404	ALA	SER	engineered mutation	UNP P04150
A	517	ASP	ASN	engineered mutation	UNP P04150
A	571	MET	VAL	engineered mutation	UNP P04150
A	602	SER	PHE	engineered mutation	UNP P04150
A	638	ASP	CYS	engineered mutation	UNP P04150
B	404	ALA	SER	engineered mutation	UNP P04150
B	517	ASP	ASN	engineered mutation	UNP P04150
B	571	MET	VAL	engineered mutation	UNP P04150
B	602	SER	PHE	engineered mutation	UNP P04150
B	638	ASP	CYS	engineered mutation	UNP P04150

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*CP*GP*AP*CP*GP*GP*AP*CP*AP*AP*AP*AP*TP*GP*TP*TP*CP*TP*GP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			450	216	84	129	21			

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*AP*CP*AP*GP*AP*AP*CP*AP*TP*TP*TP*TP*GP*TP*CP*CP*GP*TP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	22	Total	C	N	O	P	0	0	0
			446	215	79	131	21			

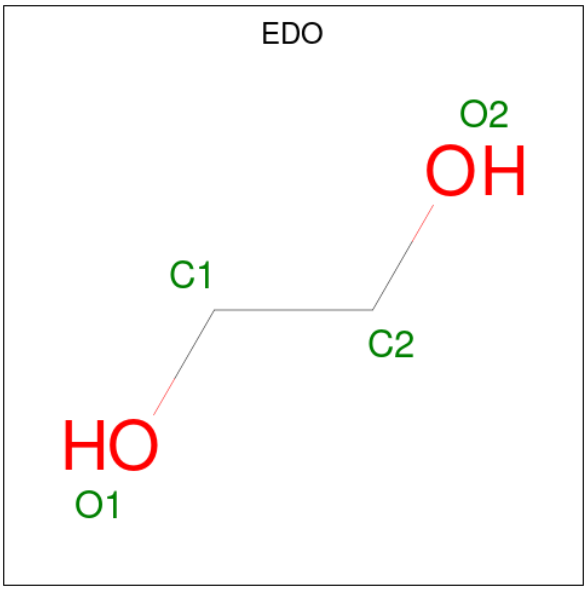
- Molecule 4 is a protein called Peroxisome proliferator-activated receptor gamma coactivator 1-alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	12	Total	C	N	O	0	0	0
			92	63	14	15			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

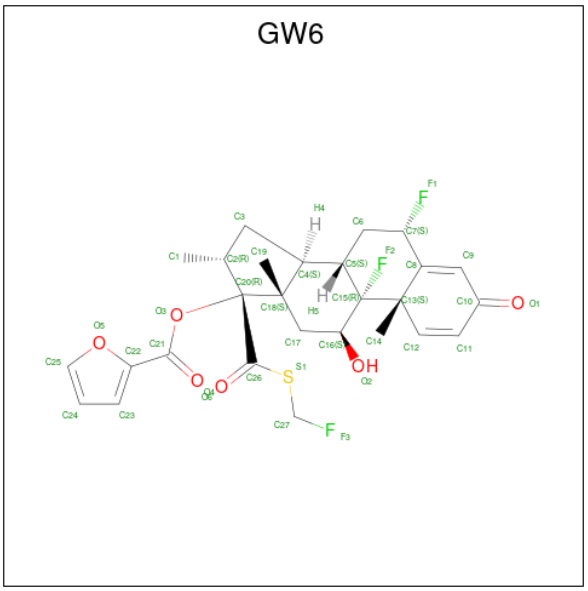
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Zn	0	0
			2	2		
5	B	2	Total	Zn	0	0
			2	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is (6alpha,11alpha,14beta,16alpha,17alpha)-6,9-difluoro-17-{[(fluoromethyl)sulfanyl]carbonyl}-11-hydroxy-16-methyl-3-oxoandrosta-1,4-dien-17-yl furan-2-carboxylate (three-letter code: GW6) (formula: $C_{27}H_{29}F_3O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C F O S 37 27 3 6 1	0	0
7	B	1	Total C F O S 37 27 3 6 1	0	0

- Molecule 8 is water.

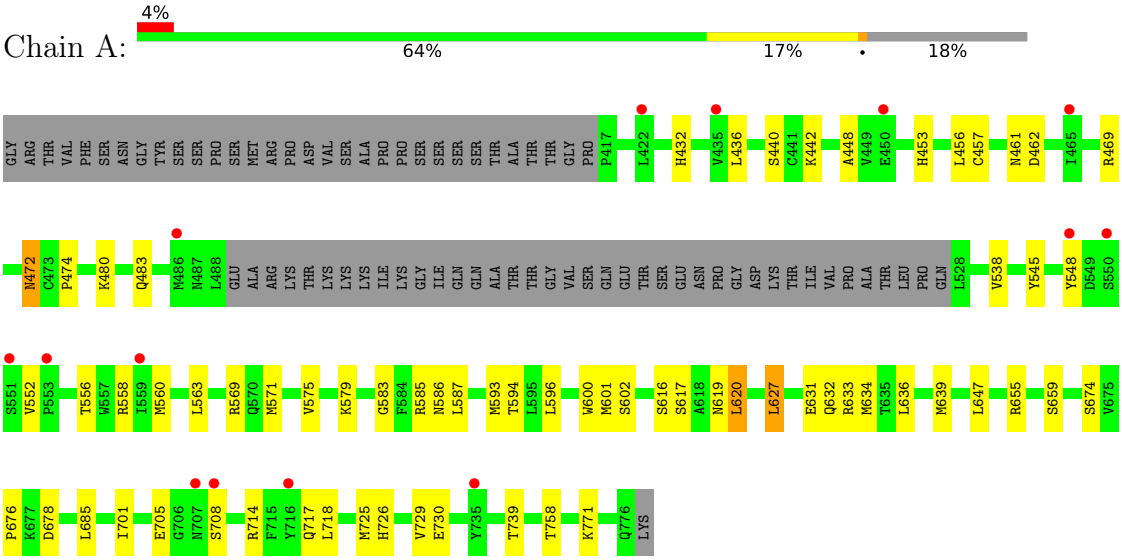
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	21	Total O 21 21	0	0
8	B	7	Total O 7 7	0	0
8	C	2	Total O 2 2	0	0

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.

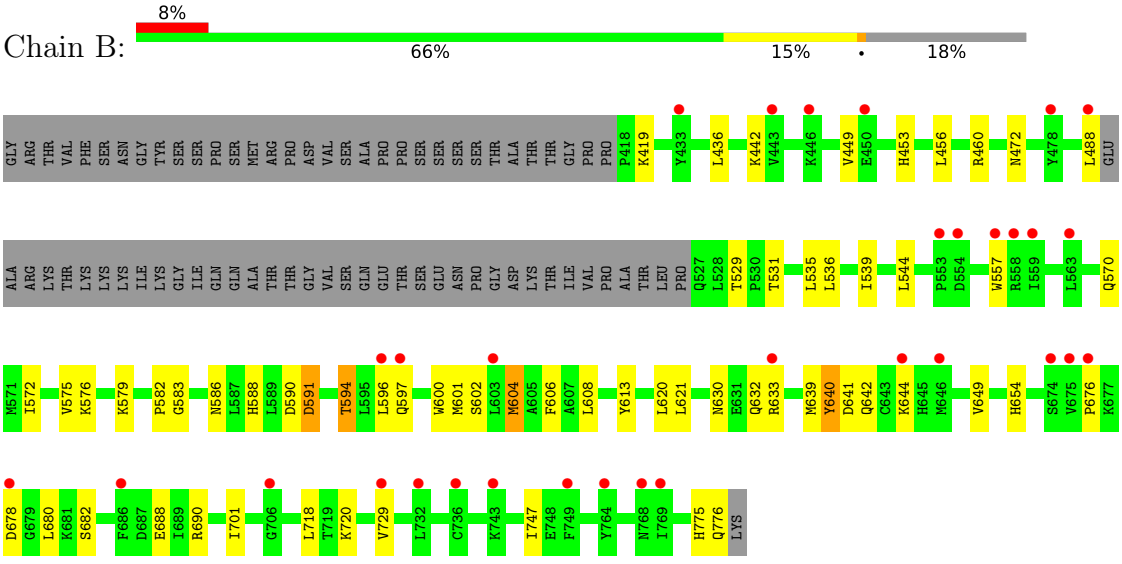
• Molecule 1: Glucocorticoid receptor

Chain A:



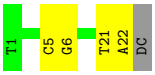
• Molecule 1: Glucocorticoid receptor

Chain B:



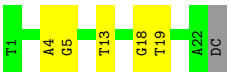
• Molecule 2: DNA (5'-D(*TP*CP*GP*AP*CP*GP*GP*AP*CP*AP*AP*AP*AP*TP*GP*TP*TP*CP*TP*GP*TP*A)-3')

Chain C:



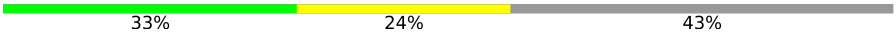
• Molecule 3: DNA (5'-D(*TP*AP*CP*AP*GP*AP*AP*CP*AP*TP*TP*TP*TP*GP*TP*CP *CP*GP*TP*CP*GP*A)-3')

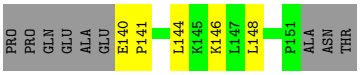
Chain D:



• Molecule 4: Peroxisome proliferator-activated receptor gamma coactivator 1-alpha

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.67Å 119.72Å 135.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.68 – 2.70 68.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	68.7 (68.68-2.70) 68.7 (68.68-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.214 , 0.253 0.216 , 0.254	Depositor DCC
R_{free} test set	1240 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	76.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6278	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.06% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ZN, GW6

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	0.42	0/2637	0.56	0/3557
1	B	0.39	0/2638	0.56	0/3557
2	C	0.81	0/505	0.94	0/778
3	D	0.84	0/499	0.89	0/768
4	F	0.40	0/93	0.52	0/125
All	All	0.50	0/6372	0.64	0/8785

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	2584	0	2596	39	0
1	B	2586	0	2597	34	0
2	C	450	0	250	3	0
3	D	446	0	251	3	0
4	F	92	0	110	4	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	12	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	37	0	29	4	0
7	B	37	0	29	1	0
8	A	21	0	0	0	0
8	B	7	0	0	0	0
8	C	2	0	0	0	0
All	All	6278	0	5880	79	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 7.

All (79) 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:535:LEU:HD23	1:B:582:PRO:HG3	1.53	0.89
4:F:140:GLU:HG2	4:F:141:PRO:HA	1.61	0.81
1:A:639:MET:CE	7:A:805:GW6:H25	2.13	0.79
1:A:480:LYS:HA	1:A:483:GLN:HG2	1.68	0.75
1:A:462:ASP:OD1	1:B:460:ARG:NH2	2.19	0.74
1:A:639:MET:HE2	7:A:805:GW6:H25	1.67	0.74
1:A:583:GLY:HA2	1:A:586:ASN:HD22	1.54	0.71
1:B:535:LEU:HD23	1:B:582:PRO:CG	2.22	0.69
1:A:456:LEU:HD22	1:A:617:SER:HB3	1.74	0.69
1:B:639:MET:HG2	7:B:803:GW6:H25	1.78	0.66
6:A:803:EDO:H11	3:D:13:DT:OP1	1.96	0.65
3:D:18:DG:H2'	3:D:19:DT:C6	2.32	0.65
1:A:575:VAL:HG22	1:A:596:LEU:HD13	1.82	0.61
1:B:641:ASP:HA	1:B:644:LYS:HD2	1.84	0.58
2:C:5:DC:H5"	2:C:5:DC:H6	1.69	0.57
1:A:469:ARG:HD3	1:B:456:LEU:HB3	1.86	0.56
1:A:701:ILE:HD11	1:A:718:LEU:HD12	1.86	0.56
1:B:535:LEU:CD2	1:B:582:PRO:HG3	2.30	0.56
1:B:557:TRP:CD1	1:B:747:ILE:HD13	2.40	0.55
1:A:457:CYS:HB3	6:A:804:EDO:H21	1.88	0.55
1:B:613:TYR:HA	1:B:654:HIS:CE1	2.42	0.55
1:A:594:THR:HG21	1:A:676:PRO:HG3	1.89	0.54
1:A:616:SER:HB3	1:A:620:LEU:HD11	1.88	0.54
1:A:739:THR:HG21	7:A:805:GW6:H27A	1.90	0.54
1:B:597:GLN:O	1:B:600:TRP:HD1	1.92	0.53
1:A:655:ARG:HH12	1:A:717:GLN:HE21	1.57	0.53
1:B:419:LYS:HB3	1:B:436:LEU:HD21	1.91	0.52
1:B:449:VAL:HG21	1:B:488:LEU:HD11	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:TYR:O	1:A:569:ARG:NH1	2.44	0.51
1:A:701:ILE:HG23	1:A:714:ARG:HG2	1.93	0.50
1:B:590:ASP:O	1:B:594:THR:HB	2.12	0.50
1:A:571:MET:HE1	1:A:600:TRP:HB2	1.93	0.50
1:B:544:LEU:HD12	1:B:570:GLN:HG3	1.94	0.50
1:A:593:MET:HG3	4:F:148:LEU:HD12	1.93	0.49
1:B:701:ILE:HD11	1:B:718:LEU:HD12	1.94	0.49
1:A:726:HIS:CD2	1:A:771:LYS:HB3	2.48	0.49
1:B:570:GLN:HB3	1:B:604:MET:HE1	1.94	0.48
4:F:141:PRO:HD2	4:F:146:LYS:HE3	1.94	0.48
1:A:593:MET:HG2	4:F:144:LEU:HG	1.96	0.48
2:C:21:DT:H2"	2:C:22:DA:C8	2.49	0.47
3:D:4:DA:H2"	3:D:5:DG:C8	2.49	0.47
1:B:676:PRO:HD2	1:B:680:LEU:HG	1.96	0.47
1:B:570:GLN:HB3	1:B:604:MET:CE	2.44	0.47
1:A:705:GLU:HB3	1:A:708:SER:HB2	1.97	0.47
1:B:640:TYR:O	1:B:644:LYS:HG3	2.15	0.47
1:B:601:MET:HB3	1:B:729:VAL:HG13	1.97	0.46
1:B:606:PHE:HA	1:B:649:VAL:HG11	1.97	0.46
1:B:641:ASP:HA	1:B:644:LYS:CD	2.46	0.46
1:A:655:ARG:HH12	1:A:717:GLN:NE2	2.14	0.46
1:B:575:VAL:HG22	1:B:596:LEU:HD13	1.98	0.46
1:B:620:LEU:HD23	1:B:630:ASN:HA	1.96	0.46
1:A:472:ASN:O	1:A:474:PRO:HD3	2.16	0.45
1:A:579:LYS:HB3	1:A:585:ARG:HD2	1.98	0.45
1:A:725:MET:O	1:A:729:VAL:HG23	2.17	0.45
1:A:587:LEU:HD23	1:A:685:LEU:HD23	1.99	0.45
1:A:601:MET:HB3	1:A:729:VAL:HG13	1.98	0.45
1:A:634:MET:CE	1:A:647:LEU:HD11	2.48	0.44
1:B:597:GLN:O	1:B:600:TRP:CD1	2.71	0.44
1:B:621:LEU:HD23	1:B:621:LEU:HA	1.93	0.44
1:A:631:GLU:HA	1:A:634:MET:HE2	1.99	0.44
1:B:676:PRO:CD	1:B:680:LEU:HG	2.47	0.43
1:B:576:LYS:HA	1:B:579:LYS:HE3	2.00	0.43
1:A:432:HIS:HB3	1:A:442:LYS:HG3	2.01	0.43
1:A:571:MET:CE	1:A:600:TRP:HB2	2.48	0.43
1:A:583:GLY:O	1:A:586:ASN:HB2	2.18	0.43
1:B:536:LEU:HA	1:B:539:ILE:HG12	1.99	0.43
2:C:5:DC:H2'	2:C:6:DG:C8	2.53	0.43
1:A:448:ALA:HA	1:A:453:HIS:HD2	1.84	0.42
1:B:588:HIS:HB3	1:B:591:ASP:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:GLY:O	1:B:586:ASN:HB2	2.19	0.42
1:A:633:ARG:HD2	1:A:636:LEU:HD12	2.02	0.42
1:A:619:ASN:ND2	1:A:631:GLU:OE2	2.53	0.42
1:B:632:GLN:H	1:B:632:GLN:CD	2.23	0.41
1:A:461:ASN:HB2	1:A:659:SER:HA	2.02	0.41
1:A:563:LEU:HD21	1:A:627:LEU:HD13	2.03	0.41
1:A:560:MET:HG2	7:A:805:GW6:S1	2.61	0.41
1:B:608:LEU:HD21	1:B:621:LEU:HD22	2.03	0.41
1:A:548:TYR:CZ	1:A:558:ARG:NH2	2.89	0.40
1:B:775:HIS:O	1:B:776:GLN:HB2	2.21	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	317/393 (81%)	300 (95%)	16 (5%)	1 (0%)	41 66
1	B	317/393 (81%)	293 (92%)	20 (6%)	4 (1%)	12 30
4	F	10/21 (48%)	9 (90%)	1 (10%)	0	100 100
All	All	644/807 (80%)	602 (94%)	37 (6%)	5 (1%)	19 43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	472	ASN
1	B	453	HIS
1	B	472	ASN
1	B	640	TYR
1	B	529	THR

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	290/351 (83%)	277 (96%)	13 (4%)	27 55
1	B	290/351 (83%)	276 (95%)	14 (5%)	25 53
4	F	11/18 (61%)	11 (100%)	0	100 100
All	All	591/720 (82%)	564 (95%)	27 (5%)	27 54

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	436	LEU
1	A	440	SER
1	A	538	VAL
1	A	552	VAL
1	A	556	THR
1	A	602	SER
1	A	620	LEU
1	A	627	LEU
1	A	632	GLN
1	A	674	SER
1	A	678	ASP
1	A	730	GLU
1	A	758	THR
1	B	442	LYS
1	B	531	THR
1	B	572	ILE
1	B	591	ASP
1	B	594	THR
1	B	602	SER
1	B	604	MET
1	B	633	ARG
1	B	642	GLN
1	B	678	ASP
1	B	682	SER
1	B	688	GLU
1	B	690	ARG

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Mol	Chain	Res	Type
1	B	720	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	GLN
1	A	453	HIS
1	A	586	ASN
1	A	717	GLN
1	B	453	HIS
1	B	619	ASN
1	B	713	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
6	EDO	A	804	-	3,3,3	0.53	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	GW6	A	805	-	34,41,41	1.39	6 (17%)	50,67,67	1.54	9 (18%)
6	EDO	A	806	-	3,3,3	0.93	0	2,2,2	0.20	0
6	EDO	A	803	-	3,3,3	0.66	0	2,2,2	0.23	0
7	GW6	B	803	-	34,41,41	1.48	7 (20%)	50,67,67	1.67	10 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	A	804	-	-	0/1/1/1	-
7	GW6	A	805	-	-	3/12/97/97	0/5/5/5
6	EDO	A	806	-	-	0/1/1/1	-
6	EDO	A	803	-	-	1/1/1/1	-
7	GW6	B	803	-	-	8/12/97/97	0/5/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	803	GW6	C15-C16	3.20	1.57	1.54
7	B	803	GW6	C15-C5	3.20	1.58	1.54
7	B	803	GW6	F2-C15	-3.11	1.36	1.42
7	A	805	GW6	F2-C15	-3.10	1.36	1.42
7	A	805	GW6	F1-C7	-2.82	1.35	1.40
7	A	805	GW6	C15-C5	2.77	1.57	1.54
7	A	805	GW6	O3-C21	2.40	1.39	1.34
7	B	803	GW6	F1-C7	-2.40	1.36	1.40
7	B	803	GW6	O6-C26	2.31	1.22	1.20
7	A	805	GW6	O6-C26	2.25	1.22	1.20
7	A	805	GW6	C15-C16	2.21	1.56	1.54
7	B	803	GW6	O3-C21	2.16	1.39	1.34
7	B	803	GW6	C13-C12	2.01	1.52	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	803	GW6	C18-C20-C2	-5.13	100.76	104.47
7	A	805	GW6	C20-C18-C4	-3.84	96.25	100.24
7	B	803	GW6	O2-C16-C15	3.43	114.16	109.08
7	A	805	GW6	C1-C2-C3	-3.17	108.43	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	803	GW6	C20-C18-C4	-2.98	97.15	100.24
7	A	805	GW6	C27-S1-C26	-2.97	96.81	100.48
7	A	805	GW6	C18-C20-C2	-2.85	102.41	104.47
7	A	805	GW6	O3-C21-O4	2.57	128.69	124.67
7	B	803	GW6	C13-C15-C16	2.48	117.33	115.52
7	A	805	GW6	O3-C21-C22	-2.47	107.75	111.12
7	A	805	GW6	C19-C18-C20	2.44	113.01	108.41
7	B	803	GW6	C18-C4-C5	2.41	115.63	113.73
7	A	805	GW6	C18-C4-C5	2.33	115.56	113.73
7	B	803	GW6	C2-C20-C26	-2.24	109.96	116.82
7	B	803	GW6	C1-C2-C3	-2.16	110.05	113.53
7	B	803	GW6	F1-C7-C8	2.13	112.17	109.66
7	B	803	GW6	C15-C5-C4	2.12	110.91	109.26
7	B	803	GW6	C19-C18-C20	2.08	112.34	108.41
7	A	805	GW6	O3-C20-C18	2.06	108.80	105.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	805	GW6	C20-C26-S1-C27
7	A	805	GW6	O6-C26-S1-C27
7	B	803	GW6	C26-C20-O3-C21
7	B	803	GW6	O4-C21-O3-C20
7	B	803	GW6	C22-C21-O3-C20
7	A	805	GW6	C2-C20-C26-O6
7	B	803	GW6	C2-C20-C26-O6
7	B	803	GW6	C2-C20-O3-C21
7	B	803	GW6	C18-C20-O3-C21
7	B	803	GW6	O3-C20-C26-O6
7	B	803	GW6	C18-C20-C26-O6
6	A	803	EDO	O1-C1-C2-O2

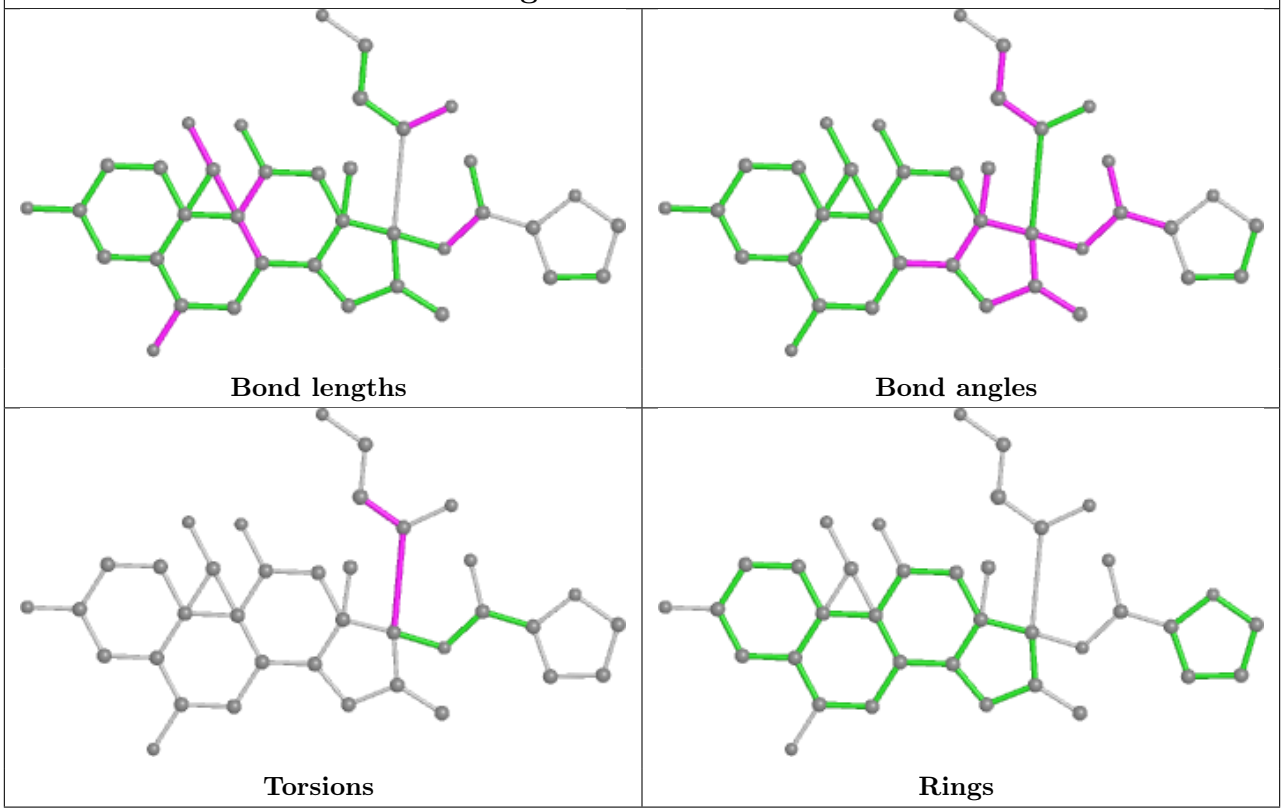
There are no ring outliers.

4 monomers are involved in 7 short contacts:

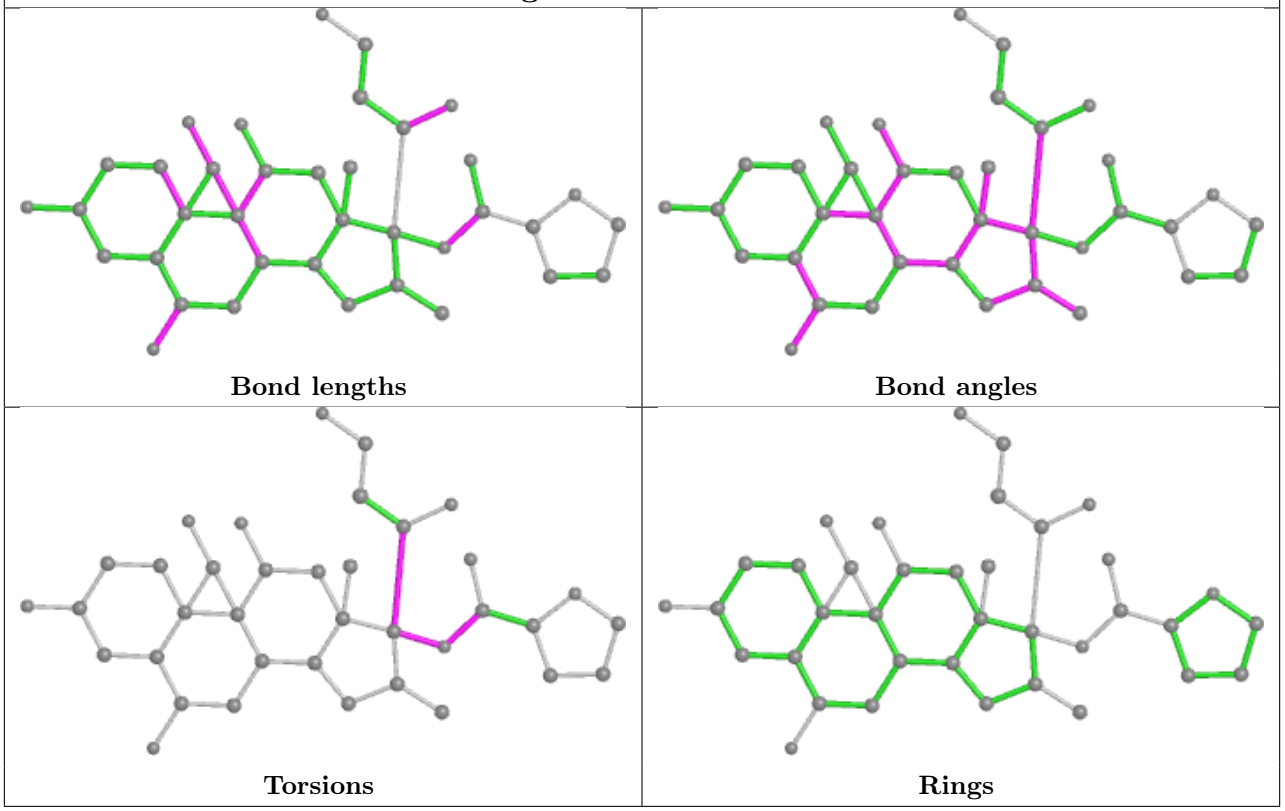
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	804	EDO	1	0
7	A	805	GW6	4	0
6	A	803	EDO	1	0
7	B	803	GW6	1	0

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 GW6 A 805



Ligand GW6 B 803



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	321/393 (81%)	0.52	14 (4%) 34 33	42, 87, 130, 139	0
1	B	321/393 (81%)	0.66	32 (9%) 7 5	57, 110, 158, 164	0
2	C	22/23 (95%)	-0.21	0 100 100	85, 128, 143, 150	0
3	D	22/23 (95%)	-0.35	0 100 100	86, 127, 154, 159	0
4	F	12/21 (57%)	-0.31	0 100 100	127, 130, 133, 139	0
All	All	698/853 (81%)	0.52	46 (6%) 18 16	42, 100, 155, 164	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	ILE	6.4
1	B	446	LYS	5.5
1	B	736	CYS	5.4
1	B	764	TYR	5.4
1	A	550	SER	5.0
1	B	596	LEU	4.8
1	B	554	ASP	4.6
1	A	553	PRO	4.5
1	B	768	ASN	4.4
1	A	551	SER	4.1
1	B	644	LYS	3.7
1	A	708	SER	3.4
1	B	769	ILE	3.2
1	B	563	LEU	3.1
1	A	422	LEU	3.1
1	B	675	VAL	3.1
1	B	678	ASP	2.9
1	A	435	VAL	2.9
1	B	686	PHE	2.8
1	B	732	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	553	PRO	2.7
1	B	603	LEU	2.7
1	A	707	ASN	2.7
1	A	548	TYR	2.7
1	B	557	TRP	2.7
1	B	478	TYR	2.6
1	B	633	ARG	2.5
1	A	450	GLU	2.5
1	B	729	VAL	2.5
1	B	676	PRO	2.4
1	B	646	MET	2.4
1	B	450	GLU	2.4
1	A	559	ILE	2.3
1	B	433	TYR	2.3
1	B	749	PHE	2.3
1	B	706	GLY	2.3
1	A	735	TYR	2.2
1	A	486	MET	2.2
1	B	443	VAL	2.2
1	B	597	GLN	2.2
1	B	674	SER	2.1
1	A	465	ILE	2.1
1	B	743	LYS	2.1
1	A	716	TYR	2.1
1	B	488	LEU	2.0
1	B	558	ARG	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)

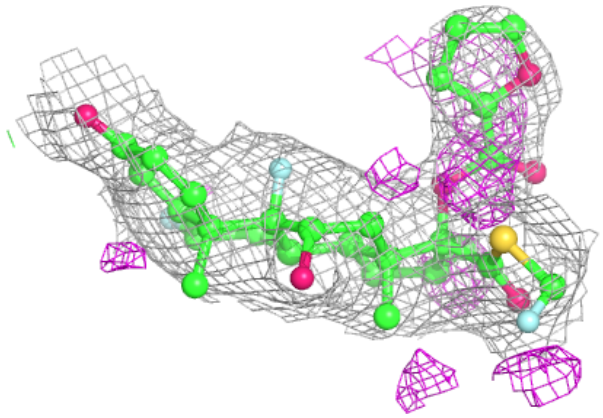
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

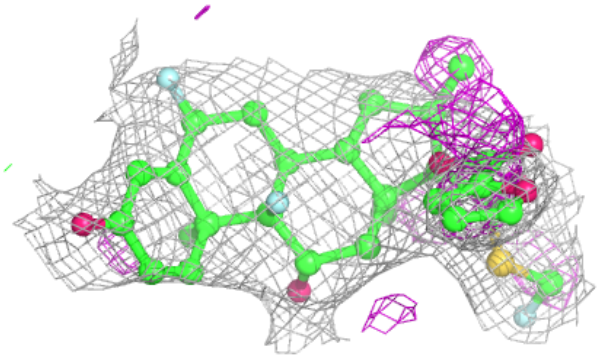
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	806	4/4	0.89	0.23	76,76,76,76	0
7	GW6	B	803	37/37	0.89	0.35	138,140,143,143	0
6	EDO	A	803	4/4	0.91	0.52	86,87,87,87	0
7	GW6	A	805	37/37	0.93	0.29	87,89,96,96	0
6	EDO	A	804	4/4	0.97	0.32	57,58,58,58	0
5	ZN	B	802	1/1	0.99	0.23	68,68,68,68	0
5	ZN	A	801	1/1	0.99	0.21	94,94,94,94	0
5	ZN	A	802	1/1	1.00	0.23	58,58,58,58	0
5	ZN	B	801	1/1	1.00	0.19	77,77,77,77	0

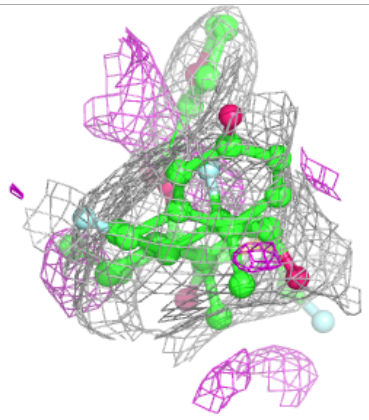
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GW6 B 803:

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

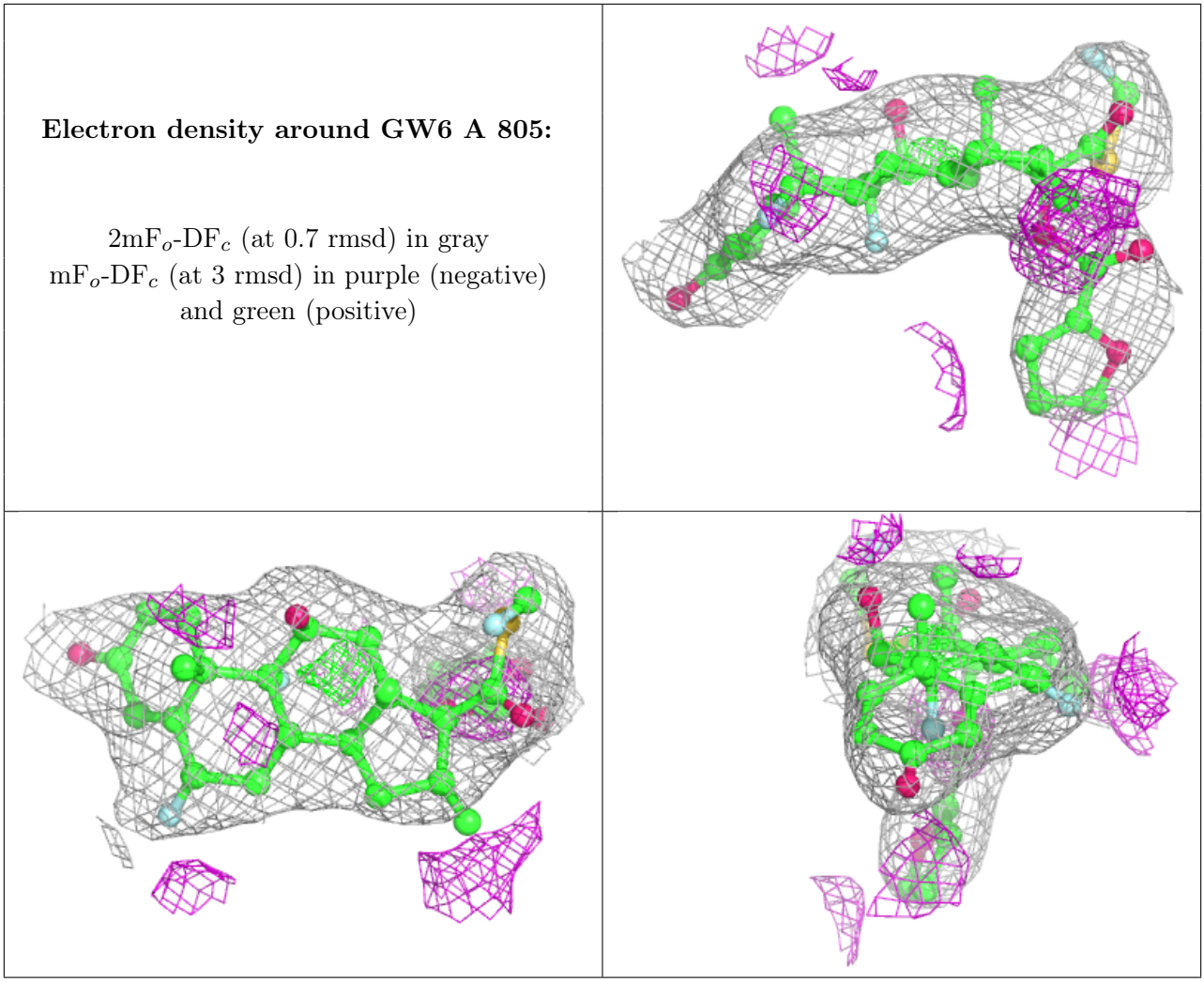






Electron density around GW6 A 805:

$2mF_o$-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.