



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:04 AM UTC

PDB ID : 7PRW / pdb_00007prw
Title : The glucocorticoid receptor in complex with velsecorat, a PGC1a coactivator fragment and sgk 23bp
Authors : Postel, S.; Edman, K.; Wissler, L.
Deposited on : 2021-09-22
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

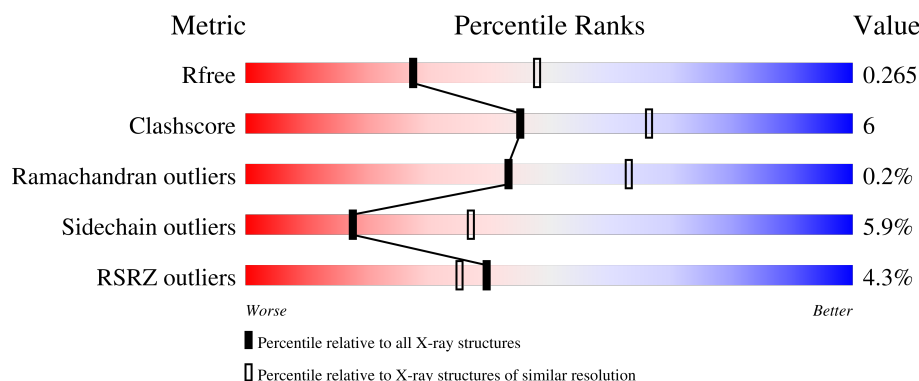
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	 4% 64% 18% 14%
1	B	393	 3% 66% 15% 16%
2	C	23	 100%
3	D	23	 78% 22%
4	F	21	 14% 33% 14% 39%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	B	805	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6429 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	326	Total	C	N	O	S	0	0	0
			2621	1671	446	475	29			
1	B	323	Total	C	N	O	S	0	1	0
			2613	1665	446	473	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*TP*GP*TP*TP*CP*TP*GP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	23	Total	C	N	O	P	0	0	0
			470	225	87	136	22			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*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	23	Total	C	N	O	P	0	0	0
			469	225	84	138	22			

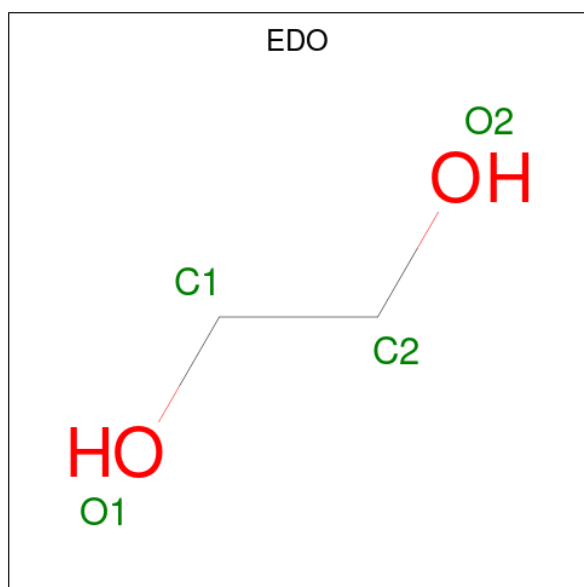
- Molecule 4 is a protein called Peroxisome proliferator-activated receptor gamma coactivator 1-alpha.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	F	10	Total	C	N	O	0	0
			76	53	12	11		0

- Molecule 5 is ZINC ION (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



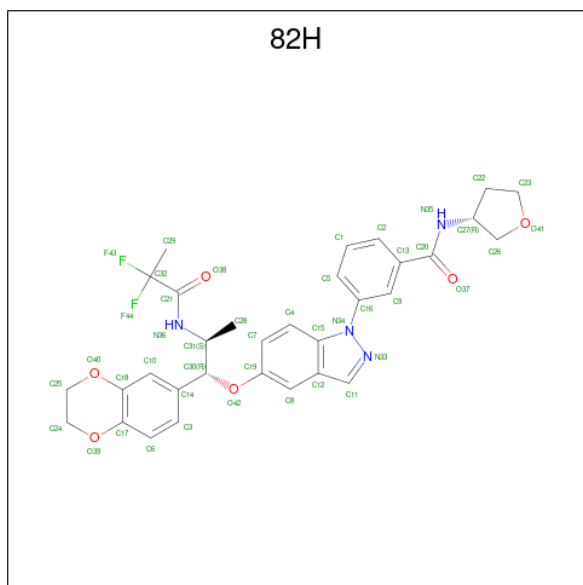
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 7 is Velsecorat (CCD ID: 82H) (formula: $C_{32}H_{32}F_2N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	0	0
			44	32	2	4	6		
7	B	1	Total	C	F	N	O	0	0
			44	32	2	4	6		

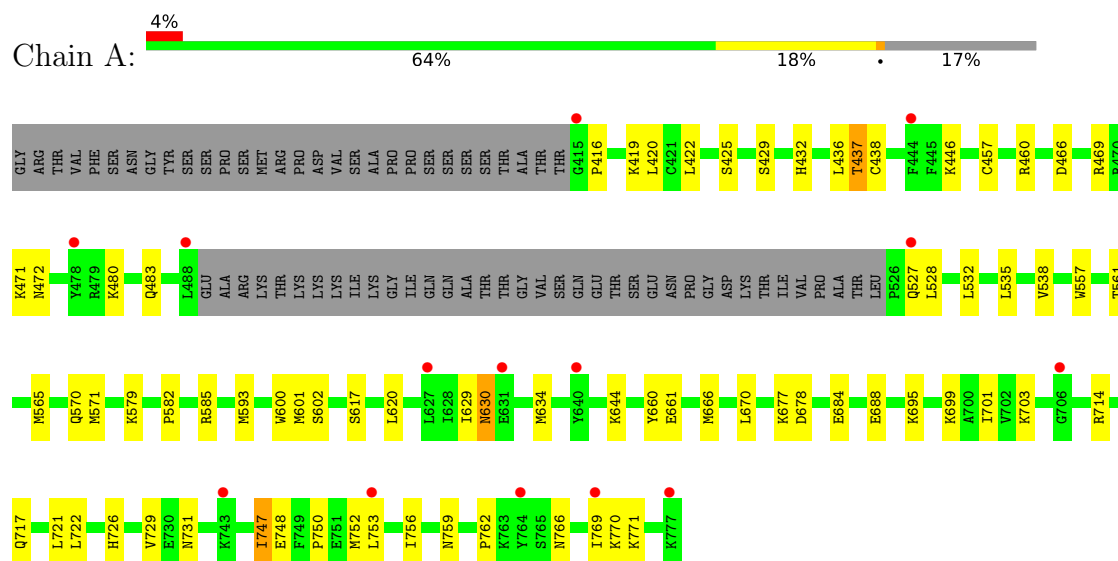
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	27	Total	O	0	0
			27	27		
8	B	33	Total	O	0	0
			33	33		
8	C	3	Total	O	0	0
			3	3		
8	D	1	Total	O	0	0
			1	1		

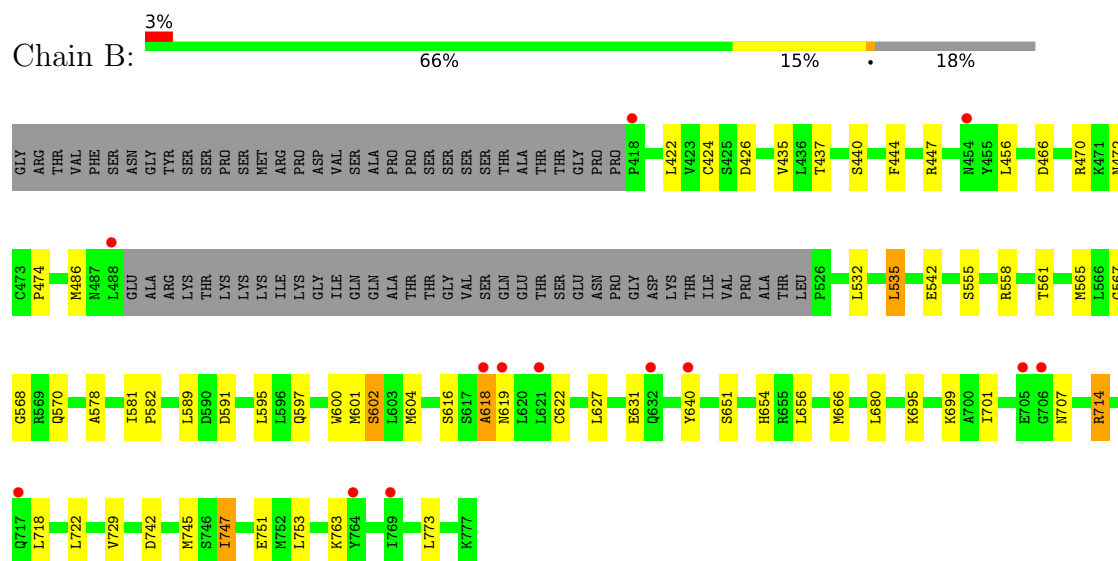
3 Residue-property plots [i](#)

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



• Molecule 1: Glucocorticoid receptor



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

Chain C:  100%

There are no outlier residues recorded for this chain.

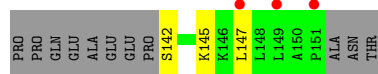
- Molecule 3: DNA (5'-D(*GP*TP*AP*CP*AP*GP*AP*AP*CP*AP*TP*TP*TP*TP*GP*TP*CP*CP*GP*TP*CP*GP*A)-3')

Chain D:  78% 22%



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

Chain F:  14% 33% 14% 52%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.21Å 122.72Å 130.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.39 – 2.50 89.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	51.1 (89.39-2.50) 51.1 (89.39-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.202 , 0.263 0.203 , 0.265	Depositor DCC
R_{free} test set	1160 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6429	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ZN, 82H

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	0.74	0/2676	1.12	6/3609 (0.2%)
1	B	0.76	1/2666 (0.0%)	1.15	11/3591 (0.3%)
2	C	0.38	0/526	0.57	0/810
3	D	0.39	0/524	0.62	0/807
4	F	0.70	0/76	1.21	0/101
All	All	0.70	1/6468 (0.0%)	1.06	17/8918 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	622	CYS	CA-C	5.43	1.59	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	763	LYS	CA-C-N	7.74	130.65	120.28
1	B	763	LYS	C-N-CA	7.74	130.65	120.28
1	B	426	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	618	ALA	CA-C-N	6.32	130.80	120.63
1	B	618	ALA	C-N-CA	6.32	130.80	120.63
1	B	466	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	654	HIS	CA-C-N	5.53	127.96	120.38
1	B	654	HIS	C-N-CA	5.53	127.96	120.38
1	A	527	GLN	CA-C-N	5.31	131.12	122.67
1	A	527	GLN	C-N-CA	5.31	131.12	122.67
1	A	416	PRO	N-CA-C	5.25	117.10	110.70
1	A	703	LYS	CA-C-N	5.24	127.61	120.54
1	A	703	LYS	C-N-CA	5.24	127.61	120.54
1	B	707	ASN	CA-CB-CG	5.21	117.81	112.60
1	B	619	ASN	N-CA-C	5.12	118.99	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	591	ASP	N-CA-C	-5.08	107.16	113.55
1	A	466	ASP	CA-CB-CG	5.00	117.60	112.60

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	2621	0	2635	38	0
1	B	2613	0	2628	31	0
2	C	470	0	261	0	0
3	D	469	0	262	4	0
4	F	76	0	97	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	8	0	12	1	0
6	B	12	0	18	5	0
6	D	4	0	6	2	0
7	A	44	0	0	0	0
7	B	44	0	0	1	0
8	A	27	0	0	1	0
8	B	33	0	0	0	0
8	C	3	0	0	0	0
8	D	1	0	0	0	0
All	All	6429	0	5919	72	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 6.

All (72) 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:A:695:LYS:HE2	1:A:699:LYS:NZ	2.01	0.74
1:B:444:PHE:HA	6:B:805:EDO:H22	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ARG:HD2	6:B:805:EDO:H11	1.73	0.71
1:A:419:LYS:HD3	1:A:436:LEU:HD11	1.76	0.67
1:A:666:MET:HE1	1:A:721:LEU:HD23	1.80	0.64
1:B:444:PHE:CA	6:B:805:EDO:H22	2.28	0.62
1:A:677:LYS:HA	1:A:770:LYS:HB2	1.82	0.62
3:D:4:DC:H2"	3:D:5:DA:C8	2.37	0.60
1:B:656:LEU:O	1:B:714:ARG:NH1	2.35	0.60
1:B:437:THR:HG21	1:B:486:MET:HE2	1.84	0.59
1:B:701:ILE:HD11	1:B:718:LEU:HD12	1.85	0.59
1:B:595:LEU:HD21	1:B:680:LEU:HD11	1.85	0.58
1:B:561:THR:O	1:B:565:MET:HG2	2.03	0.58
1:A:762:PRO:O	1:A:766:ASN:HB2	2.04	0.57
1:B:447:ARG:CD	6:B:805:EDO:H11	2.34	0.57
1:A:620:LEU:HD22	1:A:630:ASN:HA	1.88	0.56
1:B:555:SER:HB3	1:B:558:ARG:HB2	1.87	0.56
1:A:561:THR:HG23	1:A:748:GLU:HB2	1.88	0.55
1:A:469:ARG:O	1:A:472:ASN:HB2	2.06	0.55
1:A:717:GLN:HG2	1:B:640:TYR:HE2	1.71	0.55
1:A:419:LYS:HG2	1:A:436:LEU:HD21	1.88	0.55
1:A:571:MET:HE3	1:A:756:ILE:HD12	1.89	0.54
1:B:666:MET:HB3	1:B:722:LEU:HD21	1.89	0.53
1:B:578:ALA:HA	1:B:581:ILE:HD12	1.90	0.53
1:A:432:HIS:HA	3:D:5:DA:OP2	2.08	0.53
1:A:457:CYS:HB3	6:A:803:EDO:H12	1.91	0.52
1:A:471:LYS:HB2	6:D:101:EDO:H12	1.91	0.52
1:B:618:ALA:HB2	1:B:651:SER:HA	1.93	0.51
1:B:745:MET:HB3	1:B:747:ILE:HD12	1.92	0.51
1:A:480:LYS:HA	1:A:483:GLN:HG2	1.93	0.51
1:A:717:GLN:HE22	1:B:631:GLU:HG2	1.76	0.50
1:A:695:LYS:HG2	1:A:699:LYS:NZ	2.25	0.50
1:A:460:ARG:HD3	1:A:660:TYR:CD1	2.47	0.50
1:A:666:MET:HB3	1:A:722:LEU:HD21	1.94	0.50
1:B:570:GLN:HB2	1:B:604:MET:HE3	1.94	0.49
4:F:142:SER:HA	4:F:145:LYS:CD	2.42	0.49
3:D:14:DT:OP1	6:D:101:EDO:H21	2.13	0.49
1:B:567:GLY:HA2	1:B:604:MET:HE1	1.95	0.48
1:B:472:ASN:O	1:B:474:PRO:HD3	2.14	0.48
1:B:597:GLN:O	1:B:600:TRP:HD1	1.97	0.48
1:A:695:LYS:HG2	1:A:699:LYS:HZ1	1.78	0.48
1:A:432:HIS:CD2	1:A:437:THR:HG22	2.50	0.47
1:A:630:ASN:HD22	1:A:630:ASN:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ARG:HB3	1:A:660:TYR:HB2	1.96	0.46
1:A:535:LEU:HD22	1:A:582:PRO:HD3	1.98	0.46
1:A:432:HIS:HD2	1:A:437:THR:HG22	1.81	0.46
1:B:701:ILE:HG23	1:B:714:ARG:HG2	1.97	0.46
1:B:535:LEU:HD23	1:B:582:PRO:HG3	1.98	0.46
1:B:422:LEU:HD12	1:B:435:VAL:HG13	1.97	0.45
1:A:602:SER:HB3	1:A:670:LEU:HD13	1.97	0.45
1:A:561:THR:O	1:A:565:MET:HG2	2.16	0.44
1:B:437:THR:HG21	1:B:486:MET:CE	2.48	0.44
1:A:601:MET:HB3	1:A:729:VAL:HG13	2.00	0.43
1:A:579:LYS:HD2	1:A:585:ARG:HH11	1.83	0.43
1:B:604:MET:HE2	7:B:806:82H:C15	2.48	0.43
1:B:568:GLY:HA2	1:B:753:LEU:HG	2.00	0.43
4:F:142:SER:HA	4:F:145:LYS:HD2	2.01	0.42
1:A:429:SER:H	1:A:438:CYS:HA	1.85	0.42
1:A:629:ILE:HG22	1:A:634:MET:HG3	2.01	0.42
1:A:726:HIS:ND1	1:A:771:LYS:HB3	2.34	0.42
1:B:424:CYS:SG	1:B:470:ARG:NH1	2.93	0.42
3:D:1:DG:H2"	3:D:2:DT:H71	2.01	0.42
1:A:750:PRO:HG2	1:A:753:LEU:HB2	2.02	0.41
1:A:557:TRP:HD1	1:A:747:ILE:HD12	1.84	0.41
1:A:695:LYS:HE2	1:A:699:LYS:HZ2	1.82	0.41
1:A:661:GLU:HG3	8:A:904:HOH:O	2.20	0.41
1:A:701:ILE:HG23	1:A:714:ARG:HG2	2.03	0.41
1:A:571:MET:HE1	1:A:600:TRP:CG	2.55	0.40
1:B:444:PHE:CB	6:B:805:EDO:H22	2.51	0.40
1:B:695:LYS:NZ	1:B:699:LYS:HE2	2.36	0.40
1:B:602:SER:HA	1:B:729:VAL:HG21	2.03	0.40
1:B:601:MET:HB3	1:B:729:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/393 (82%)	301 (94%)	21 (6%)	0	100	100
1	B	320/393 (81%)	299 (93%)	20 (6%)	1 (0%)	36	55
4	F	8/21 (38%)	8 (100%)	0	0	100	100
All	All	650/807 (80%)	608 (94%)	41 (6%)	1 (0%)	43	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	616	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/351 (84%)	273 (93%)	21 (7%)	13	29
1	B	293/351 (84%)	280 (96%)	13 (4%)	25	50
4	F	9/18 (50%)	8 (89%)	1 (11%)	6	12
All	All	596/720 (83%)	561 (94%)	35 (6%)	18	37

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	420	LEU
1	A	422	LEU
1	A	425	SER
1	A	437	THR
1	A	446	LYS
1	A	528	LEU
1	A	532	LEU
1	A	538	VAL
1	A	570	GLN
1	A	593	MET
1	A	617	SER
1	A	630	ASN

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Mol	Chain	Res	Type
1	A	644	LYS
1	A	678	ASP
1	A	684	GLU
1	A	688	GLU
1	A	731	ASN
1	A	747	ILE
1	A	752	MET
1	A	759	ASN
1	A	769	ILE
1	B	440	SER
1	B	456	LEU
1	B	532	LEU
1	B	535	LEU
1	B	542	GLU
1	B	589	LEU
1	B	602	SER
1	B	627	LEU
1	B	714	ARG
1	B	742	ASP
1	B	747	ILE
1	B	751	GLU
1	B	773	LEU
4	F	147	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	ASN
1	A	630	ASN
1	A	713	GLN
1	A	759	ASN
1	A	760	GLN
1	B	453	HIS
1	B	461	ASN
1	B	619	ASN
1	B	630	ASN
1	B	632	GLN
1	B	707	ASN
1	B	711	ASN
1	B	738	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	B	804	-	3,3,3	0.55	0	2,2,2	0.26	0
6	EDO	D	101	-	3,3,3	0.53	0	2,2,2	0.05	0
6	EDO	B	803	-	3,3,3	0.68	0	2,2,2	0.21	0
7	82H	A	804	-	48,49,49	1.12	6 (12%)	66,71,71	1.72	14 (21%)
6	EDO	A	803	-	3,3,3	0.43	0	2,2,2	0.37	0
6	EDO	B	805	-	3,3,3	0.83	0	2,2,2	0.17	0
7	82H	B	806	-	48,49,49	1.13	5 (10%)	66,71,71	1.46	9 (13%)
6	EDO	A	805	-	3,3,3	0.53	0	2,2,2	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	804	-	-	1/1/1/1	-
6	EDO	D	101	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	803	-	-	0/1/1/1	-
7	82H	A	804	-	-	5/34/48/48	0/6/6/6
6	EDO	A	803	-	-	1/1/1/1	-
6	EDO	B	805	-	-	0/1/1/1	-
7	82H	B	806	-	-	5/34/48/48	0/6/6/6
6	EDO	A	805	-	-	0/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	804	82H	N34-N33	-3.44	1.34	1.38
7	B	806	82H	N34-N33	-3.37	1.34	1.38
7	B	806	82H	C32-C21	-3.15	1.50	1.54
7	A	804	82H	C32-C21	-2.72	1.51	1.54
7	B	806	82H	C30-C31	-2.65	1.51	1.54
7	A	804	82H	C21-N36	2.43	1.38	1.34
7	A	804	82H	C16-N34	-2.34	1.39	1.42
7	A	804	82H	C30-C31	-2.23	1.52	1.54
7	B	806	82H	C21-N36	2.22	1.38	1.34
7	B	806	82H	C20-N35	2.19	1.39	1.34
7	A	804	82H	C20-N35	2.04	1.39	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	804	82H	C16-N34-N33	-5.05	114.90	119.15
7	A	804	82H	C30-C31-N36	4.20	116.38	110.03
7	A	804	82H	C28-C31-C30	-3.90	108.70	112.81
7	A	804	82H	O37-C20-N35	3.78	129.65	122.47
7	B	806	82H	C28-C31-C30	-3.71	108.90	112.81
7	A	804	82H	C11-N33-N34	-3.70	103.78	106.14
7	B	806	82H	C30-C31-N36	3.56	115.42	110.03
7	A	804	82H	F43-C32-C21	3.20	114.81	109.84
7	A	804	82H	C15-N34-N33	3.12	113.83	111.33
7	B	806	82H	C9-C16-N34	3.07	122.77	119.46
7	B	806	82H	C16-N34-N33	-2.92	116.69	119.15
7	B	806	82H	C11-N33-N34	-2.62	104.47	106.14
7	B	806	82H	C26-C27-N35	2.58	115.11	112.03
7	B	806	82H	C31-N36-C21	-2.58	119.02	122.88
7	A	804	82H	C22-C27-N35	2.51	117.12	111.98
7	A	804	82H	C4-C7-C19	2.45	122.53	119.73
7	B	806	82H	C12-C8-C19	-2.42	117.72	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	804	82H	C2-C13-C9	2.40	122.03	119.25
7	B	806	82H	O37-C20-N35	2.33	126.89	122.47
7	A	804	82H	C27-N35-C20	2.31	126.93	122.56
7	A	804	82H	O37-C20-C13	-2.19	116.56	120.90
7	A	804	82H	C3-C14-C30	-2.05	116.80	120.62
7	A	804	82H	O40-C18-C17	-2.04	120.20	122.02

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	804	82H	C22-C27-N35-C20
7	A	804	82H	C14-C30-C31-N36
7	B	806	82H	C22-C27-N35-C20
7	B	806	82H	C14-C30-C31-N36
7	A	804	82H	C9-C16-N34-N33
7	B	806	82H	C9-C16-N34-N33
7	B	806	82H	C5-C16-N34-N33
7	A	804	82H	C5-C16-N34-N33
7	A	804	82H	O42-C30-C31-N36
7	B	806	82H	O42-C30-C31-N36
6	A	803	EDO	O1-C1-C2-O2
6	B	804	EDO	O1-C1-C2-O2

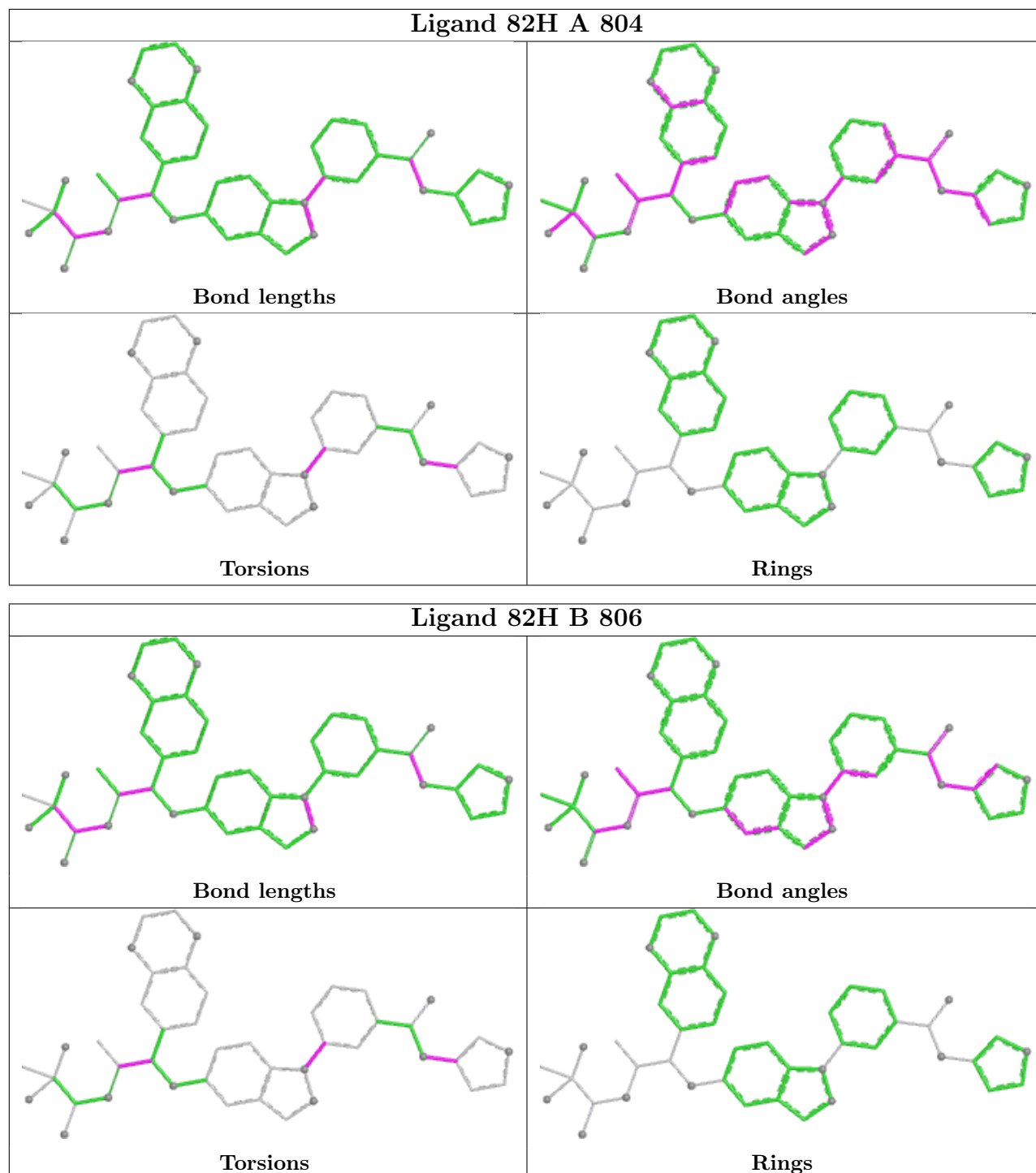
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	101	EDO	2	0
6	A	803	EDO	1	0
6	B	805	EDO	5	0
7	B	806	82H	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/393 (82%)	0.57	14 (4%) 40 35	33, 82, 129, 141	0
1	B	323/393 (82%)	0.45	13 (4%) 42 38	27, 78, 122, 137	1 (0%)
2	C	23/23 (100%)	0.17	0 100 100	74, 120, 165, 173	0
3	D	23/23 (100%)	0.21	0 100 100	68, 133, 153, 163	0
4	F	10/21 (47%)	1.69	3 (30%) 1 1	126, 132, 137, 138	0
All	All	705/853 (82%)	0.50	30 (4%) 40 35	27, 83, 133, 173	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	LEU	6.6
1	A	764	TYR	4.8
1	B	764	TYR	4.0
1	A	478	TYR	3.8
1	A	706	GLY	3.3
4	F	147	LEU	3.1
1	B	418	PRO	3.1
1	A	769	ILE	3.1
1	B	769	ILE	3.1
4	F	151	PRO	2.9
1	B	706	GLY	2.8
1	A	753	LEU	2.7
1	A	640	TYR	2.6
1	B	618	ALA	2.6
1	B	640	TYR	2.5
4	F	149	LEU	2.5
1	A	631	GLU	2.5
1	B	717	GLN	2.4
1	A	743	LYS	2.3
1	B	454	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	627	LEU	2.2
1	B	632	GLN	2.2
1	A	527	GLN	2.2
1	B	619	ASN	2.1
1	A	444	PHE	2.1
1	B	488	LEU	2.0
1	A	777	LYS	2.0
1	B	621	LEU	2.0
1	B	705	GLU	2.0
1	A	415	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

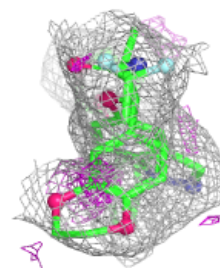
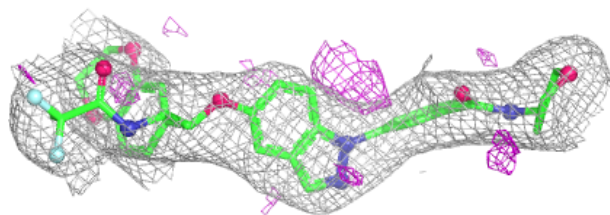
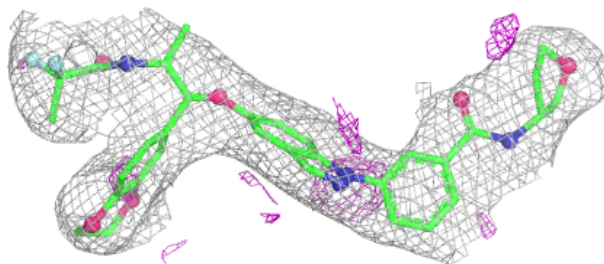
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	B	805	4/4	0.84	0.30	58,58,59,59	0
6	EDO	B	803	4/4	0.86	0.13	77,77,78,78	0
6	EDO	B	804	4/4	0.90	0.10	67,68,68,68	0
6	EDO	A	805	4/4	0.90	0.10	67,67,67,67	0
7	82H	B	806	44/44	0.94	0.10	68,73,80,80	0
7	82H	A	804	44/44	0.96	0.07	54,57,62,62	0
6	EDO	D	101	4/4	0.96	0.09	68,69,69,69	0
6	EDO	A	803	4/4	0.99	0.05	27,28,28,28	0
5	ZN	A	801	1/1	0.99	0.09	84,84,84,84	0
5	ZN	B	802	1/1	1.00	0.04	49,49,49,49	0
5	ZN	A	802	1/1	1.00	0.04	39,39,39,39	0
5	ZN	B	801	1/1	1.00	0.05	60,60,60,60	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.

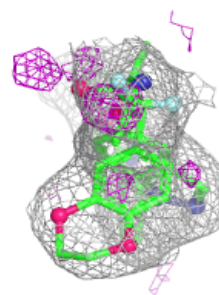
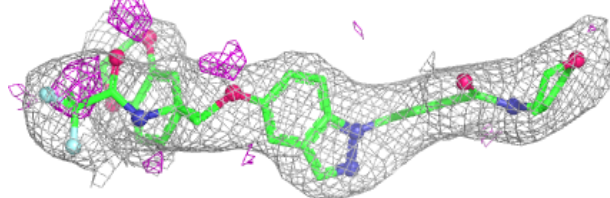
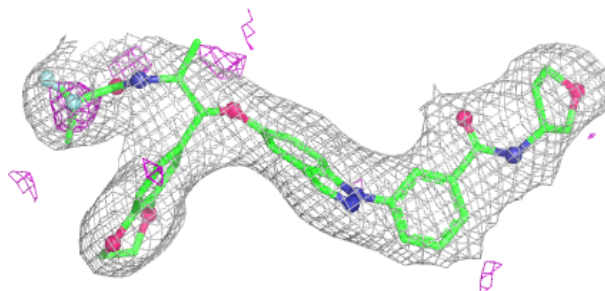
Electron density around 82H B 806:

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



Electron density around 82H A 804:

$2mF_o-DF_c$ (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.