Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2021 – 12:30 PM EST

PDB ID	:	6PME
Title	:	TRK-A IN COMPLEX WITH LIGAND
Authors	:	Subramanian, G.; Brown, D.G.
Deposited on	:	2019-07-01
Resolution	:	3.00 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 following versions of software and data (see references (i)) were used in the production of this report:

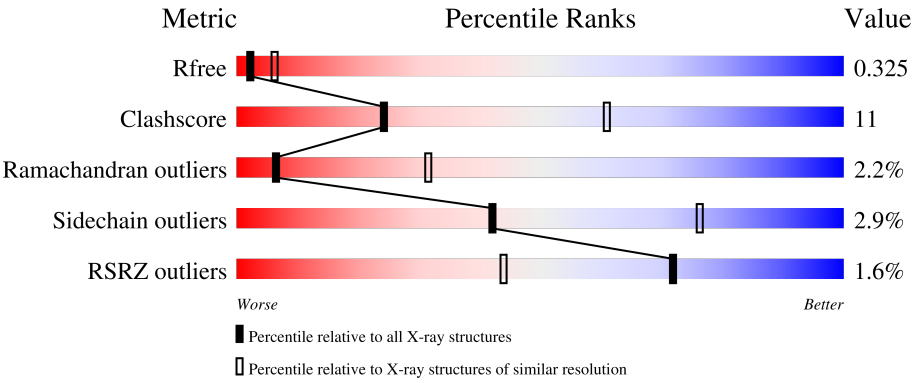
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	311	3% 59% 26% • 14%
1	B	311	% 65% 20% • 13%
1	C	311	62% 23% • 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6712 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.

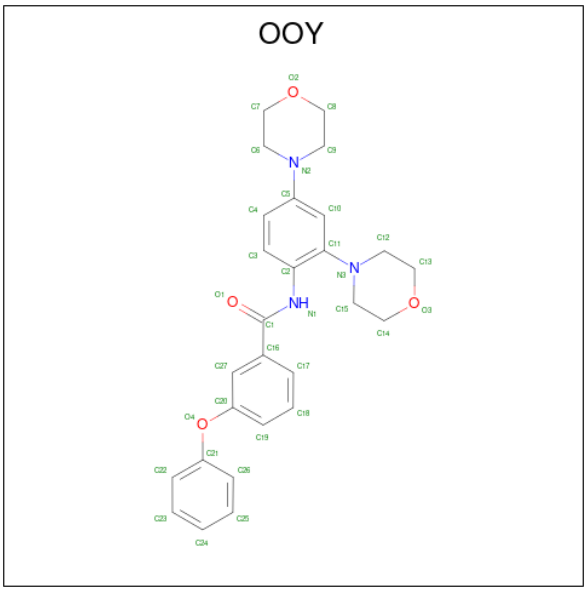
- Molecule 1 is a protein called High affinity nerve growth factor receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	P	S	32	0	0
			2164	1380	391	376	1	16			
1	B	271	Total	C	N	O	P	S	21	1	0
			2202	1404	397	384	1	16			
1	C	274	Total	C	N	O	P	S	21	1	0
			2220	1416	404	383	1	16			

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

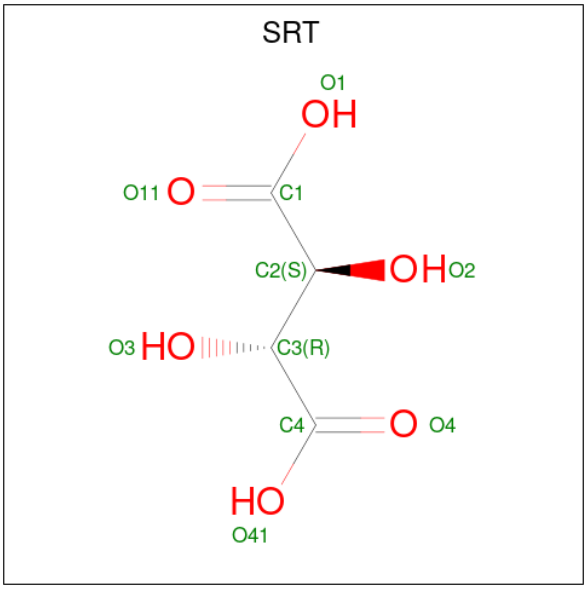
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-[2,4-bis(morpholin-4-yl)phenyl]-3-phenoxybenzamide (three-letter code: OOY) (formula: $C_{27}H_{29}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	27	3	4		
3	B	1	Total	C	N	O	0	0
			34	27	3	4		
3	C	1	Total	C	N	O	0	0
			34	27	3	4		

- Molecule 4 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is water.

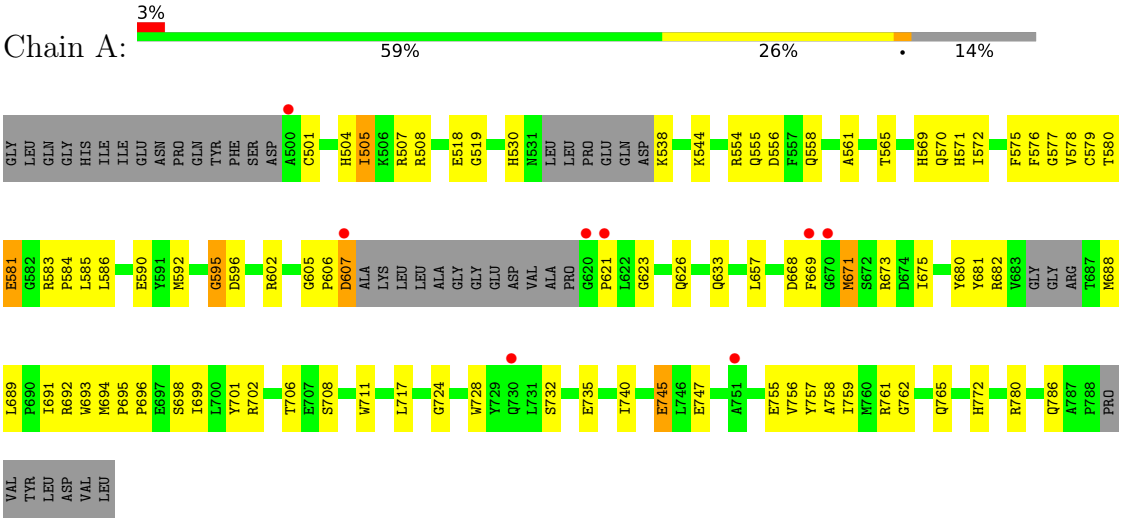
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O	0	0
			1	1		

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: High affinity nerve growth factor receptor

Chain A:

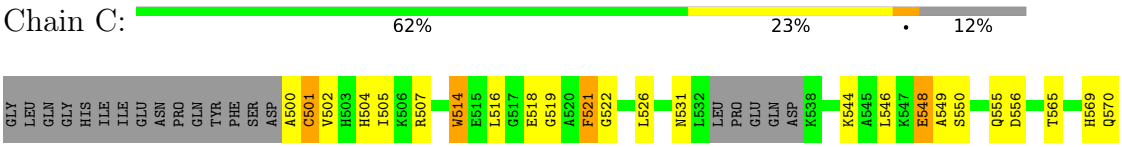


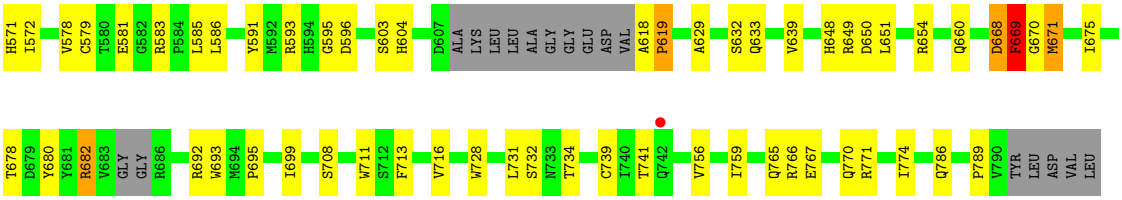
• Molecule 1: High affinity nerve growth factor receptor

Chain B:

• Molecule 1: High affinity nerve growth factor receptor

Chain C:




H571 I572 V578 C579 T580 E581 G582 R583 P584 L585 L586 Y591 M592 R593 H594 G595 D596 S603 H604 D607 ALA LYS LEU LEU ALA GLY GLY GLU ASP VAL A618 P619 A629 S632 Q633 V639 H648 R649 D650 L651 R654 Q660 D668 F669 G670 M671 I675
T678 D679 Y680 Y681 R682 V683 GLY GLY R686 R692 W693 M694 P695 I699 S708 W711 S712 F713 V716 W728 L731 S732 N733 T734 C739 I740 T741 Q742 V756 I759 Q765 R766 E767 Q770 R771 I774 Q786 P789 V790 TYR LEU ASP VAL LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	131.44Å 152.09Å 156.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 3.00 48.46 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.51-3.00) 94.8 (48.46-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.258 , 0.315 0.263 , 0.325	Depositor DCC
R_{free} test set	572 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å^2)	68.1	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 34.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6712	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, OOY, SRT, SEP

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	1.02	9/2205 (0.4%)	1.16	9/2976 (0.3%)
1	B	1.01	5/2245 (0.2%)	1.24	11/3031 (0.4%)
1	C	1.12	5/2263 (0.2%)	1.41	14/3056 (0.5%)
All	All	1.05	19/6713 (0.3%)	1.28	34/9063 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	4
1	C	0	2
All	All	0	6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	668	ASP	C-N	-25.45	0.75	1.34
1	C	669	PHE	CB-CG	20.87	1.86	1.51
1	C	682	ARG	NE-CZ	19.68	1.58	1.33
1	C	521	PHE	CB-CG	19.52	1.84	1.51
1	B	669	PHE	CB-CG	-9.83	1.34	1.51
1	A	570	GLN	CG-CD	9.76	1.73	1.51
1	C	544	LYS	CD-CE	9.66	1.75	1.51
1	A	745	GLU	CD-OE1	8.91	1.35	1.25
1	A	595	GLY	C-O	8.52	1.37	1.23
1	C	595	GLY	C-O	-7.79	1.11	1.23
1	A	682	ARG	CB-CG	7.06	1.71	1.52
1	A	757	TYR	C-O	6.87	1.36	1.23
1	B	670	GLY	C-N	-6.34	1.19	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	544	LYS	CG-CD	-6.33	1.30	1.52
1	A	745	GLU	CD-OE2	6.21	1.32	1.25
1	B	669	PHE	CA-CB	-5.78	1.41	1.53
1	A	544	LYS	CD-CE	-5.65	1.37	1.51
1	A	669	PHE	CB-CG	-5.39	1.42	1.51
1	A	607	ASP	C-O	5.19	1.33	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	669	PHE	CB-CG-CD2	-29.68	100.02	120.80
1	C	669	PHE	CB-CG-CD1	29.20	141.24	120.80
1	B	668	ASP	O-C-N	-20.97	89.15	122.70
1	C	521	PHE	CB-CG-CD2	-20.33	106.57	120.80
1	B	669	PHE	CB-CG-CD2	-19.45	107.19	120.80
1	C	521	PHE	CB-CG-CD1	19.01	134.11	120.80
1	A	669	PHE	CB-CG-CD1	-17.15	108.80	120.80
1	B	669	PHE	CB-CG-CD1	15.86	131.90	120.80
1	A	669	PHE	CB-CG-CD2	15.36	131.55	120.80
1	B	668	ASP	CA-C-N	14.46	149.02	117.20
1	B	740	ILE	CB-CG1-CD1	12.64	149.29	113.90
1	B	669	PHE	N-CA-CB	-10.53	91.65	110.60
1	A	761	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	A	682	ARG	CA-CB-CG	-9.55	92.39	113.40
1	C	682	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	A	761	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	B	669	PHE	CA-CB-CG	8.41	134.08	113.90
1	C	682	ARG	CD-NE-CZ	-8.17	112.16	123.60
1	B	669	PHE	CB-CA-C	8.14	126.68	110.40
1	C	521	PHE	CA-CB-CG	-7.85	95.05	113.90
1	C	682	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	C	507	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	544	LYS	CB-CG-CD	7.04	129.90	111.60
1	A	740	ILE	CA-CB-CG1	-7.00	97.70	111.00
1	B	668	ASP	C-N-CA	6.93	139.04	121.70
1	B	670	GLY	C-N-CA	6.80	138.70	121.70
1	A	501	CYS	CA-CB-SG	-6.50	102.30	114.00
1	A	507	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	C	669	PHE	CA-CB-CG	-6.30	98.78	113.90
1	C	514	TRP	CA-CB-CG	5.75	124.62	113.70
1	C	544	LYS	CG-CD-CE	-5.66	94.93	111.90
1	A	682	ARG	CB-CG-CD	-5.58	97.09	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	531	ASN	CB-CA-C	5.16	120.72	110.40
1	C	501	CYS	CA-CB-SG	-5.05	104.91	114.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	499	ASP	Peptide
1	B	522	GLY	Peptide
1	B	668	ASP	Mainchain
1	B	669	PHE	Sidechain
1	C	522	GLY	Peptide
1	C	682	ARG	Sidechain

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	2164	0	2145	49	0
1	B	2202	0	2170	53	0
1	C	2220	0	2208	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	34	0	0	1	0
3	B	34	0	0	0	0
3	C	34	0	0	2	0
4	A	10	0	4	0	0
4	B	10	0	4	0	0
5	C	1	0	0	0	0
All	All	6712	0	6531	144	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 11.

All (144) 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:691:ILE:HA	1:A:694:MET:HE3	1.51	0.92
1:A:755:GLU:O	1:A:758:ALA:HB3	1.77	0.84
1:B:573:VAL:HG21	1:B:667:GLY:HA2	1.58	0.84
1:A:584:PRO:O	1:A:586:LEU:CD1	2.27	0.83
1:B:521:PHE:O	1:B:546:LEU:HD12	1.79	0.83
1:A:579:CYS:SG	1:A:581:GLU:HB2	2.22	0.78
1:B:681:TYR:O	1:B:688:MET:HA	1.84	0.76
1:A:569:HIS:HB3	1:A:572:ILE:HG12	1.69	0.74
1:A:747:GLU:H	1:A:747:GLU:CD	1.93	0.72
1:B:504:HIS:HE1	1:C:501:CYS:SG	2.04	0.72
1:A:673:ARG:HA	1:A:680:TYR:CE2	2.25	0.71
1:A:584:PRO:O	1:A:586:LEU:HD12	1.90	0.70
1:B:706:THR:O	1:B:710:VAL:HG23	1.94	0.68
1:B:558[A]:GLN:NE2	1:B:562:GLU:OE2	2.25	0.67
1:B:536:GLN:HE22	1:B:539:MET:HB3	1.59	0.67
1:B:508:ARG:CZ	1:C:500:ALA:O	2.43	0.66
1:B:515:GLU:OE1	1:B:518:GLU:OE1	2.14	0.66
1:C:549:ALA:HB1	1:C:583:ARG:NE	2.11	0.66
1:B:769:GLN:NE2	1:B:769:GLN:HA	2.11	0.66
1:C:579:CYS:SG	1:C:581:GLU:HB2	2.37	0.65
1:A:728:TRP:HH2	1:A:745:GLU:O	1.80	0.64
1:C:505:ILE:O	1:C:579:CYS:HB2	1.96	0.64
1:C:521:PHE:O	1:C:546:LEU:HD12	1.98	0.64
1:C:741:THR:O	1:C:766:ARG:NH2	2.31	0.64
1:A:605:GLY:O	1:A:607:ASP:N	2.31	0.63
1:C:603:SER:HB2	1:C:604:HIS:ND1	2.16	0.61
1:B:536:GLN:NE2	1:B:539:MET:HB3	2.16	0.60
1:C:504:HIS:NE2	1:C:505:ILE:O	2.34	0.60
1:C:668:ASP:O	1:C:669:PHE:O	2.20	0.60
1:B:549:ALA:HB1	1:B:583:ARG:NE	2.18	0.58
1:C:546:LEU:HD23	1:C:585:LEU:HD12	1.83	0.58
1:B:521:PHE:O	1:B:546:LEU:CD1	2.49	0.58
1:A:695:PRO:HB3	1:A:711:TRP:CD2	2.40	0.57
1:C:670:GLY:HA3	3:C:802:OOY:C26	2.35	0.57
1:C:603:SER:CB	1:C:604:HIS:ND1	2.68	0.56
1:C:593[A]:ARG:HH11	1:C:593[A]:ARG:HG2	1.70	0.56
1:A:519:GLY:HA3	1:A:671:MET:HG3	1.88	0.55
1:A:518:GLU:O	1:A:675:ILE:HD11	2.06	0.55
1:C:521:PHE:HA	1:C:548:GLU:CG	2.37	0.55
1:B:504:HIS:NE2	1:B:505:ILE:O	2.39	0.55
1:C:504:HIS:CD2	1:C:505:ILE:O	2.60	0.55
1:A:561:ALA:O	1:A:565:THR:OG1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:HIS:ND1	1:A:780:ARG:NH2	2.55	0.54
1:B:580:THR:HG22	1:B:585:LEU:HD22	1.89	0.54
1:B:504:HIS:CD2	1:B:505:ILE:O	2.61	0.53
1:B:573:VAL:HG21	1:B:657:LEU:HD12	1.91	0.53
1:C:521:PHE:HA	1:C:548:GLU:HG3	1.89	0.53
1:A:504:HIS:HE1	1:B:501:CYS:SG	2.28	0.53
1:C:786:GLN:HA	1:C:786:GLN:OE1	2.08	0.53
1:A:592:MET:O	3:A:802:OOY:C3	2.57	0.52
1:A:554:ARG:CZ	1:A:558:GLN:HE22	2.23	0.52
1:A:585:LEU:C	1:A:586:LEU:HD12	2.29	0.52
1:B:530:HIS:CE1	1:B:538:LYS:HZ1	2.28	0.52
1:B:558[A]:GLN:HG3	1:B:562:GLU:OE2	2.10	0.52
1:A:505:ILE:O	1:A:579:CYS:HB2	2.09	0.51
1:B:596:ASP:HA	1:B:656:CYS:O	2.10	0.51
1:B:667:GLY:O	1:B:668:ASP:O	2.29	0.50
1:C:708:SER:O	1:C:711:TRP:HB3	2.12	0.50
1:B:573:VAL:CG2	1:B:657:LEU:HD12	2.41	0.50
1:A:696:PRO:HD3	1:A:711:TRP:CH2	2.46	0.50
1:C:756:VAL:O	1:C:759:ILE:HB	2.11	0.50
1:C:695:PRO:HB3	1:C:711:TRP:CD2	2.46	0.50
1:B:549:ALA:HB1	1:B:583:ARG:HE	1.76	0.49
1:A:602:ARG:CZ	1:A:724:GLY:O	2.61	0.49
1:C:514:TRP:CE2	1:C:526:LEU:HD23	2.47	0.49
1:C:514:TRP:CZ2	1:C:526:LEU:HD23	2.48	0.49
1:C:650:ASP:OD2	1:C:680:TYR:OH	2.16	0.49
1:B:570:GLN:O	1:B:665:LYS:HE2	2.13	0.48
1:C:502:VAL:HG22	1:C:565:THR:HG21	1.94	0.48
1:C:569:HIS:HB3	1:C:572:ILE:HG12	1.96	0.48
1:A:756:VAL:O	1:A:759:ILE:HB	2.14	0.48
1:C:570:GLN:NE2	1:C:571:HIS:NE2	2.62	0.48
1:B:741:THR:O	1:B:766:ARG:NH1	2.38	0.48
1:B:760:MET:HE2	1:B:764:TRP:CH2	2.49	0.47
1:C:593[A]:ARG:HG2	1:C:593[A]:ARG:NH1	2.29	0.47
1:C:578:VAL:HG23	1:C:586:LEU:O	2.14	0.47
1:A:519:GLY:CA	1:A:671:MET:HG3	2.44	0.47
1:B:570:GLN:H	1:B:570:GLN:CD	2.18	0.47
1:C:670:GLY:HA3	3:C:802:OOY:C25	2.45	0.46
1:A:576:PHE:HE2	1:A:590:GLU:HA	1.80	0.46
1:A:595:GLY:O	1:A:657:LEU:HA	2.15	0.46
1:A:698:SER:O	1:A:702:ARG:HA	2.15	0.46
1:B:573:VAL:CG2	1:B:667:GLY:HA2	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:GLN:O	1:C:556:ASP:C	2.54	0.46
1:B:571:HIS:CE1	1:B:633:GLN:HG2	2.51	0.46
1:B:573:VAL:HG23	1:B:666:ILE:O	2.16	0.46
1:C:618:ALA:HA	1:C:619:PRO:C	2.36	0.46
1:A:504:HIS:HA	1:A:578:VAL:O	2.16	0.46
1:B:730:GLN:HG2	1:B:731:LEU:HD13	1.98	0.46
1:A:728:TRP:CH2	1:A:745:GLU:O	2.64	0.46
1:A:695:PRO:HB3	1:A:711:TRP:CE3	2.51	0.45
1:A:623:GLY:O	1:A:626:GLN:N	2.44	0.45
1:A:681:TYR:O	1:A:688:MET:HA	2.16	0.45
1:A:732:SER:O	1:A:735:GLU:HG2	2.16	0.45
1:C:639:VAL:HG22	1:C:774:ILE:HG23	1.98	0.45
1:A:689:LEU:HB3	1:A:694:MET:HE1	1.99	0.44
1:A:695:PRO:HG3	1:A:708:SER:HA	2.00	0.44
1:C:519:GLY:HA3	1:C:671:MET:HG3	2.00	0.44
1:C:692:ARG:NH1	1:C:728:TRP:O	2.50	0.44
1:B:671:MET:HG2	1:B:671:MET:O	2.18	0.44
1:C:518:GLU:O	1:C:675:ILE:HD11	2.18	0.43
1:C:591:TYR:CZ	1:C:593[A]:ARG:HA	2.52	0.43
1:A:583:ARG:N	1:B:562:GLU:OE1	2.51	0.43
1:C:713:PHE:O	1:C:716:VAL:HB	2.19	0.43
1:C:765:GLN:HB2	1:C:771:ARG:HG3	2.01	0.43
1:B:530:HIS:CE1	1:B:538:LYS:NZ	2.86	0.43
1:A:571:HIS:CE1	1:A:633:GLN:HG2	2.53	0.43
1:B:554:ARG:CZ	1:B:558[B]:GLN:NE2	2.82	0.43
1:C:516:LEU:HD21	1:C:526:LEU:HB2	2.00	0.43
1:A:692:ARG:HB2	1:A:693:TRP:CZ3	2.54	0.43
1:A:762:GLY:HA2	1:A:765:GLN:HE21	1.84	0.43
1:B:760:MET:HE2	1:B:764:TRP:HH2	1.84	0.43
1:A:755:GLU:N	1:A:755:GLU:OE1	2.38	0.42
1:B:681:TYR:CD2	1:B:733:ASN:HB3	2.53	0.42
1:C:629:ALA:O	1:C:633:GLN:HG3	2.19	0.42
1:B:573:VAL:HG21	1:B:667:GLY:CA	2.40	0.42
1:B:505:ILE:O	1:B:579:CYS:HB2	2.20	0.42
1:C:648:HIS:O	1:C:649:ARG:HB2	2.18	0.42
1:A:580:THR:HG22	1:A:585:LEU:HD22	2.01	0.42
1:A:508:ARG:HG2	1:B:501:CYS:O	2.20	0.42
1:B:653:THR:OG1	1:B:719:GLU:OE1	2.34	0.42
1:C:603:SER:HB3	1:C:604:HIS:ND1	2.35	0.42
1:B:653:THR:HG1	1:B:719:GLU:CD	2.23	0.42
1:C:654:ARG:NH1	1:C:693:TRP:CH2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:PHE:CZ	1:A:577:GLY:HA2	2.54	0.42
1:B:560:GLU:O	1:B:564:LEU:HG	2.20	0.41
1:B:579:CYS:SG	1:B:581:GLU:HB2	2.60	0.41
1:B:499:ASP:OD2	1:B:558[A]:GLN:NE2	2.53	0.41
1:C:651:LEU:HG	1:C:716:VAL:HG21	2.01	0.41
1:A:586:LEU:N	1:A:586:LEU:HD12	2.35	0.41
1:A:717:LEU:HA	1:A:717:LEU:HD12	1.78	0.41
1:B:697:GLU:HA	1:B:701:TYR:CD2	2.55	0.41
1:A:555:GLN:O	1:A:556:ASP:C	2.59	0.41
1:B:604:HIS:O	1:B:621:PRO:HA	2.20	0.41
1:B:648:HIS:O	1:B:649:ARG:HB2	2.21	0.41
1:B:559:ARG:HA	1:B:559:ARG:HD3	1.96	0.41
1:A:689:LEU:HB3	1:A:694:MET:CE	2.50	0.41
1:C:731:LEU:HD21	1:C:739:CYS:SG	2.61	0.41
1:C:767:GLU:HG3	1:C:770:GLN:NE2	2.36	0.41
1:B:698:SER:O	1:B:702:ARG:HA	2.20	0.40
1:B:530:HIS:ND1	1:B:530:HIS:N	2.68	0.40
1:A:702:ARG:HG3	1:A:702:ARG:O	2.21	0.40
1:B:760:MET:CE	1:B:764:TRP:CH2	3.05	0.40
1:A:530:HIS:CD2	1:A:538:LYS:HE3	2.57	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	259/311 (83%)	234 (90%)	21 (8%)	4 (2%)	10	42
1	B	263/311 (85%)	241 (92%)	17 (6%)	5 (2%)	8	36
1	C	266/311 (86%)	240 (90%)	18 (7%)	8 (3%)	4	24
All	All	788/933 (84%)	715 (91%)	56 (7%)	17 (2%)	6	31

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	621	PRO
1	A	668	ASP
1	B	573	VAL
1	B	668	ASP
1	C	548	GLU
1	C	668	ASP
1	C	669	PHE
1	C	789	PRO
1	B	548	GLU
1	C	550	SER
1	B	675	ILE
1	C	660	GLN
1	A	606	PRO
1	B	550	SER
1	A	699	ILE
1	C	699	ILE
1	C	619	PRO

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	226/260 (87%)	219 (97%)	7 (3%)	40	75
1	B	230/260 (88%)	223 (97%)	7 (3%)	41	75
1	C	232/260 (89%)	226 (97%)	6 (3%)	46	78
All	All	688/780 (88%)	668 (97%)	20 (3%)	42	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	505	ILE
1	A	581	GLU
1	A	596	ASP
1	A	671	MET

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Mol	Chain	Res	Type
1	A	701	TYR
1	A	706	THR
1	A	786	GLN
1	B	559	ARG
1	B	575	PHE
1	B	581	GLU
1	B	668	ASP
1	B	671	MET
1	B	747	GLU
1	B	759	ILE
1	C	596	ASP
1	C	632	SER
1	C	671	MET
1	C	678	THR
1	C	732	SER
1	C	734	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	555	GLN
1	A	558	GLN
1	A	742	GLN
1	A	765	GLN
1	A	778	HIS
1	A	786	GLN
1	B	536	GLN
1	B	742	GLN
1	B	769	GLN
1	B	778	HIS
1	C	570	GLN
1	C	742	GLN
1	C	769	GLN
1	C	770	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	SEP	A	677	1	8,9,10	0.59	0	8,12,14	0.84	0
1	SEP	B	677	1	8,9,10	0.65	0	8,12,14	1.09	0
1	SEP	C	677	1	8,9,10	0.57	0	8,12,14	0.86	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
1	SEP	A	677	1	-	1/5/8/10	-
1	SEP	B	677	1	-	1/5/8/10	-
1	SEP	C	677	1	-	1/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	677	SEP	N-CA-CB-OG
1	A	677	SEP	N-CA-CB-OG
1	B	677	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
4	SRT	A	803	-	3,9,9	0.37	0	6,12,12	0.79	0
4	SRT	B	803	-	3,9,9	0.41	0	6,12,12	0.89	0
3	OOY	A	802	-	38,38,38	0.71	1 (2%)	50,51,51	0.92	3 (6%)
3	OOY	B	802	-	38,38,38	0.70	1 (2%)	50,51,51	0.97	2 (4%)
3	OOY	C	802	-	38,38,38	0.62	0	50,51,51	1.09	3 (6%)

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	SRT	A	803	-	-	0/4/12/12	-
4	SRT	B	803	-	-	4/4/12/12	-
3	OOY	A	802	-	-	2/20/36/36	0/5/5/5
3	OOY	B	802	-	-	1/20/36/36	0/5/5/5
3	OOY	C	802	-	-	2/20/36/36	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	OOY	C2-C11	2.09	1.43	1.40
3	B	802	OOY	C2-C11	2.06	1.42	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	802	OOY	C10-C11-N3	-3.03	118.03	122.52
3	A	802	OOY	C15-N3-C11	2.69	122.65	116.27
3	B	802	OOY	C15-N3-C12	2.66	117.39	111.52
3	A	802	OOY	C12-N3-C11	2.66	122.57	116.27
3	C	802	OOY	C12-N3-C11	2.49	122.17	116.27
3	B	802	OOY	C13-C12-N3	2.37	114.39	110.02
3	C	802	OOY	C2-N1-C1	2.33	133.31	126.93
3	A	802	OOY	C2-N1-C1	2.03	132.48	126.93

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	803	SRT	C1-C2-C3-C4
4	B	803	SRT	O2-C2-C3-O3
4	B	803	SRT	C1-C2-C3-O3
3	C	802	OOY	C10-C11-N3-C12
3	B	802	OOY	C10-C11-N3-C12
3	A	802	OOY	C10-C11-N3-C15
3	A	802	OOY	C10-C11-N3-C12
3	C	802	OOY	C2-C11-N3-C12
4	B	803	SRT	O2-C2-C3-C4

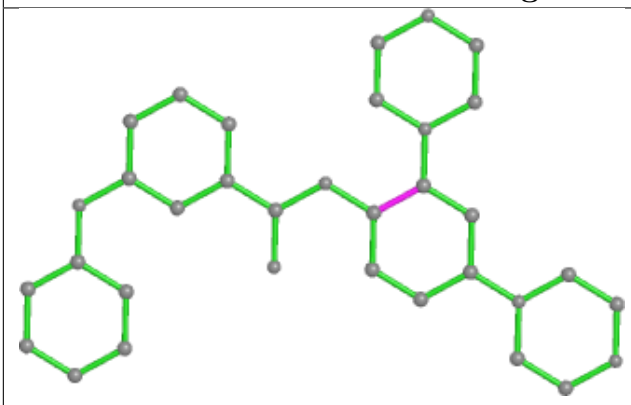
There are no ring outliers.

2 monomers are involved in 3 short contacts:

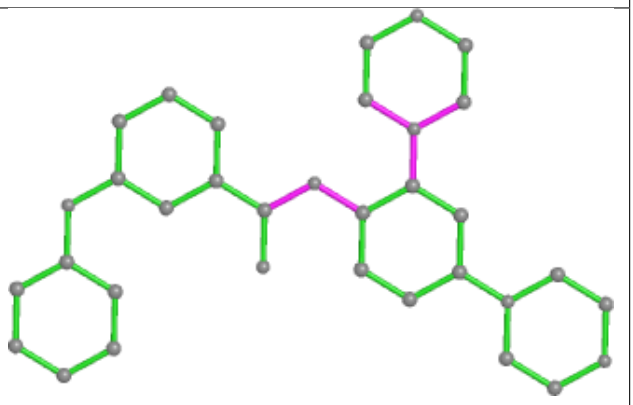
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	OOY	1	0
3	C	802	OOY	2	0

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.

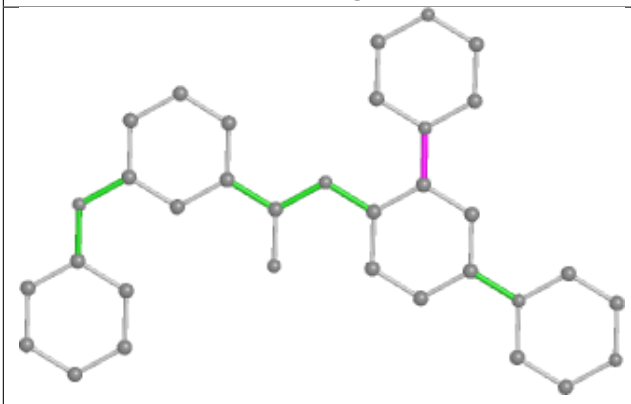
Ligand OOY A 802



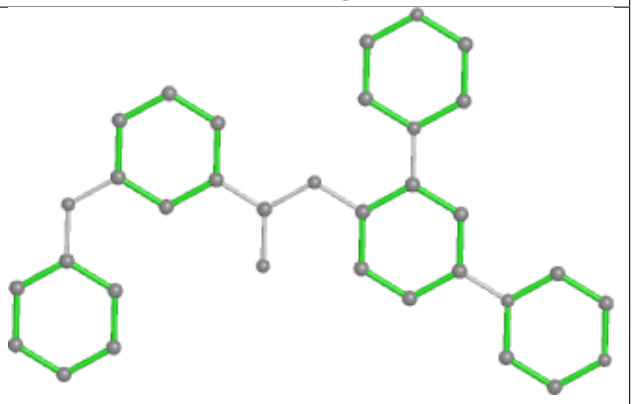
Bond lengths



Bond angles

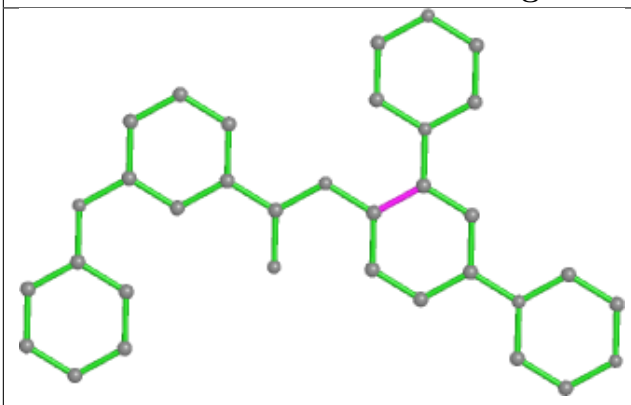


Torsions

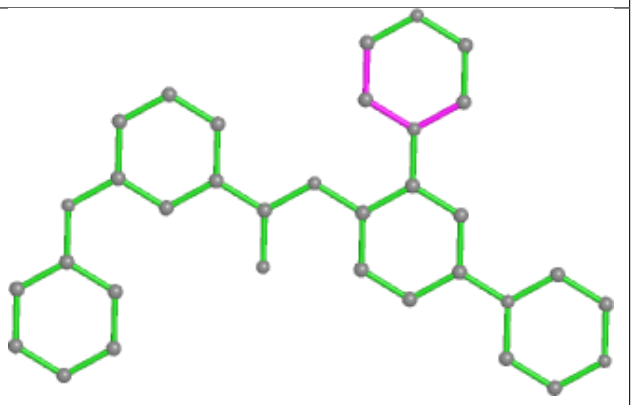


Rings

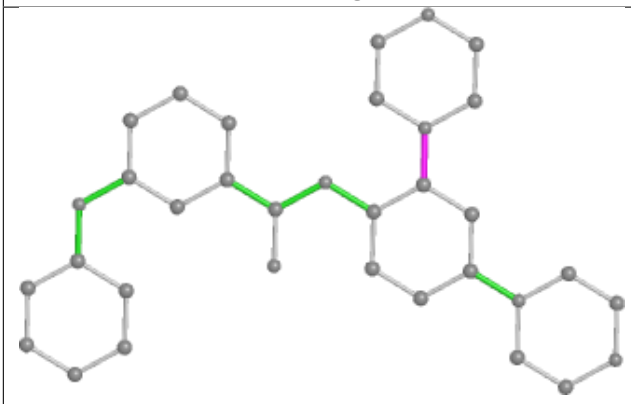
Ligand OOY B 802



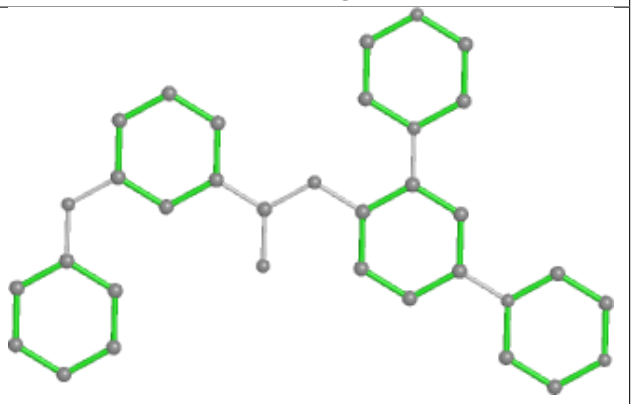
Bond lengths



Bond angles

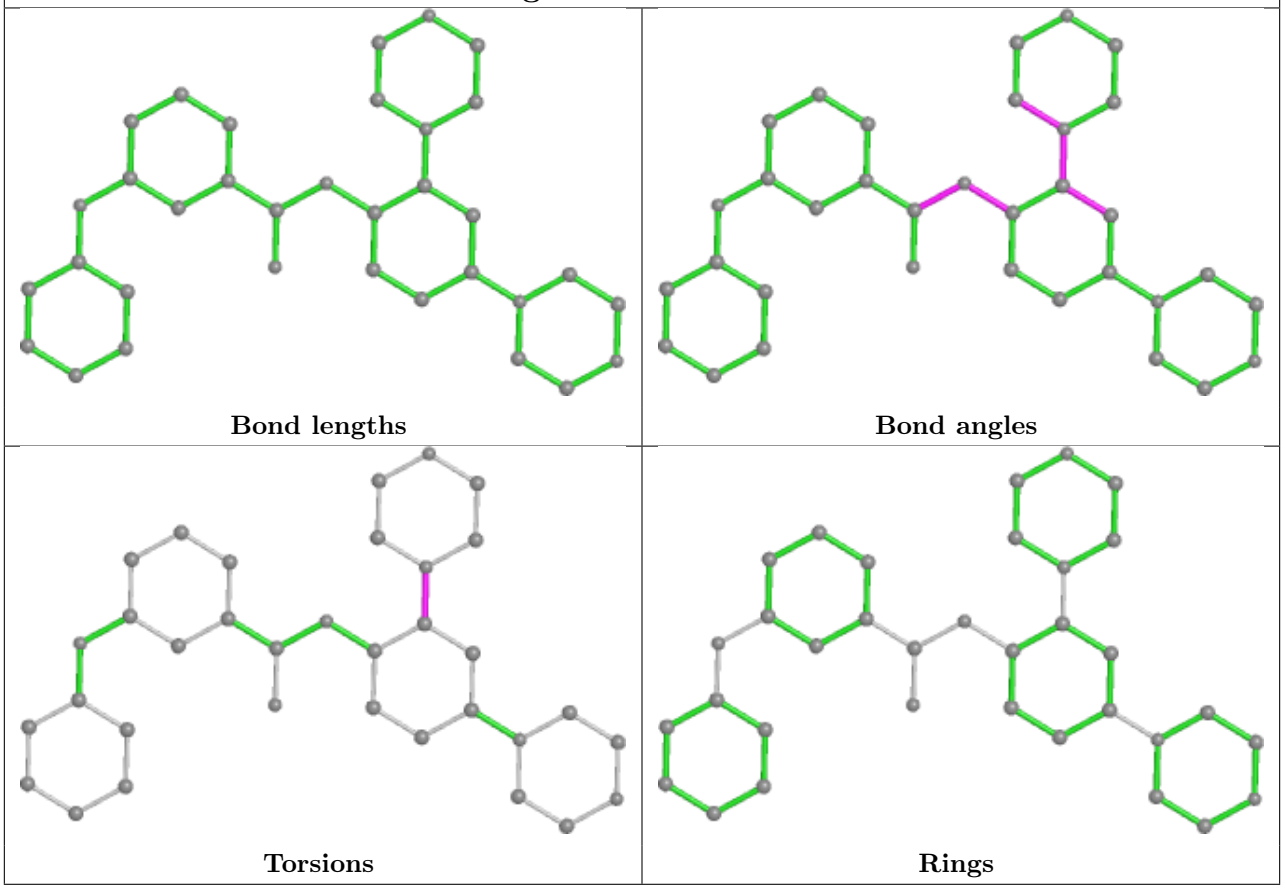


Torsions



Rings

Ligand OOY C 802



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	670:GLY	C	671:MET	N	1.19
1	B	668:ASP	C	669:PHE	N	0.75

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	267/311 (85%)	0.21	8 (2%)	50	22	26, 42, 69, 120	9 (3%)
1	B	269/311 (86%)	0.16	4 (1%)	73	46	25, 44, 71, 96	4 (1%)
1	C	273/311 (87%)	0.09	1 (0%)	92	79	26, 44, 74, 104	5 (1%)
All	All	809/933 (86%)	0.15	13 (1%)	72	44	25, 43, 72, 120	18 (2%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	669	PHE	5.0
1	A	620	GLY	3.8
1	A	669	PHE	3.1
1	B	620	GLY	3.0
1	A	500	ALA	2.8
1	B	531	ASN	2.6
1	A	621	PRO	2.6
1	C	742	GLN	2.5
1	A	751	ALA	2.4
1	A	607	ASP	2.3
1	A	670	GLY	2.2
1	B	499	ASP	2.1
1	A	730	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	SEP	A	677	10/11	0.60	0.34	71,81,94,95	0
1	SEP	B	677	10/11	0.79	0.27	70,84,102,105	0
1	SEP	C	677	10/11	0.87	0.27	63,69,84,84	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

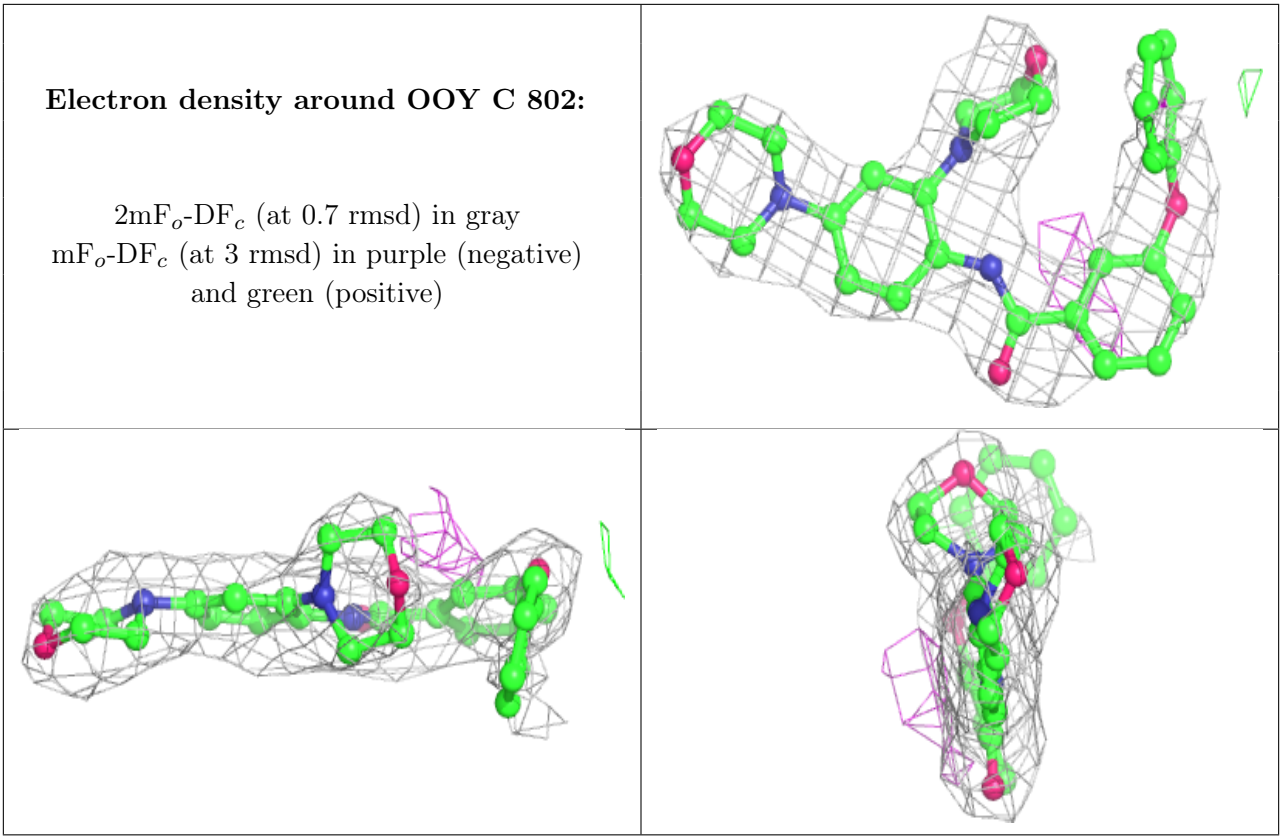
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	SRT	A	803	10/10	0.77	0.35	80,95,103,105	0
4	SRT	B	803	10/10	0.89	0.35	42,64,78,98	0
3	OOY	C	802	34/34	0.89	0.35	44,60,80,83	0
3	OOY	B	802	34/34	0.90	0.30	47,57,80,87	0
3	OOY	A	802	34/34	0.92	0.34	46,49,80,83	0
2	ZN	A	801	1/1	0.96	0.13	46,46,46,46	0
2	ZN	C	801	1/1	0.98	0.13	48,48,48,48	0
2	ZN	B	801	1/1	0.99	0.13	49,49,49,49	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.

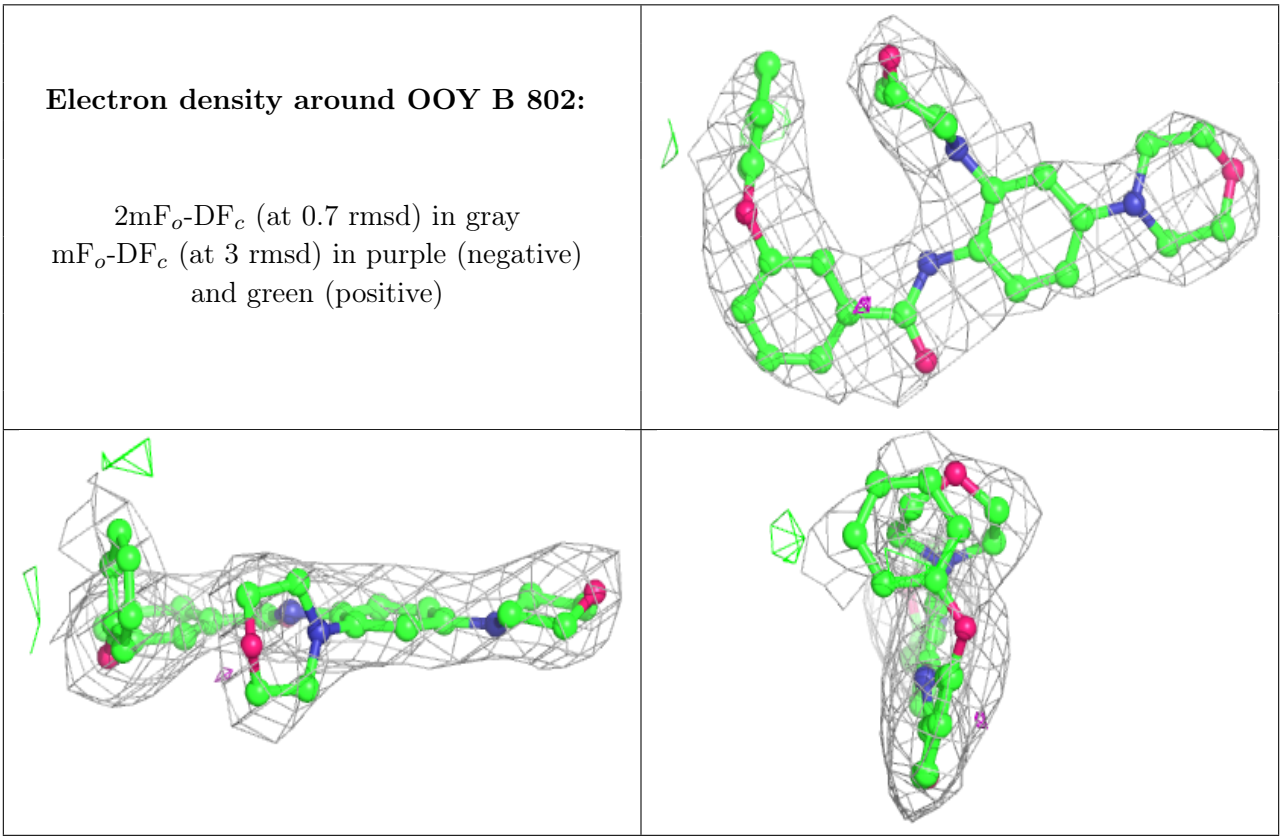
Electron density around OOY C 802:

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



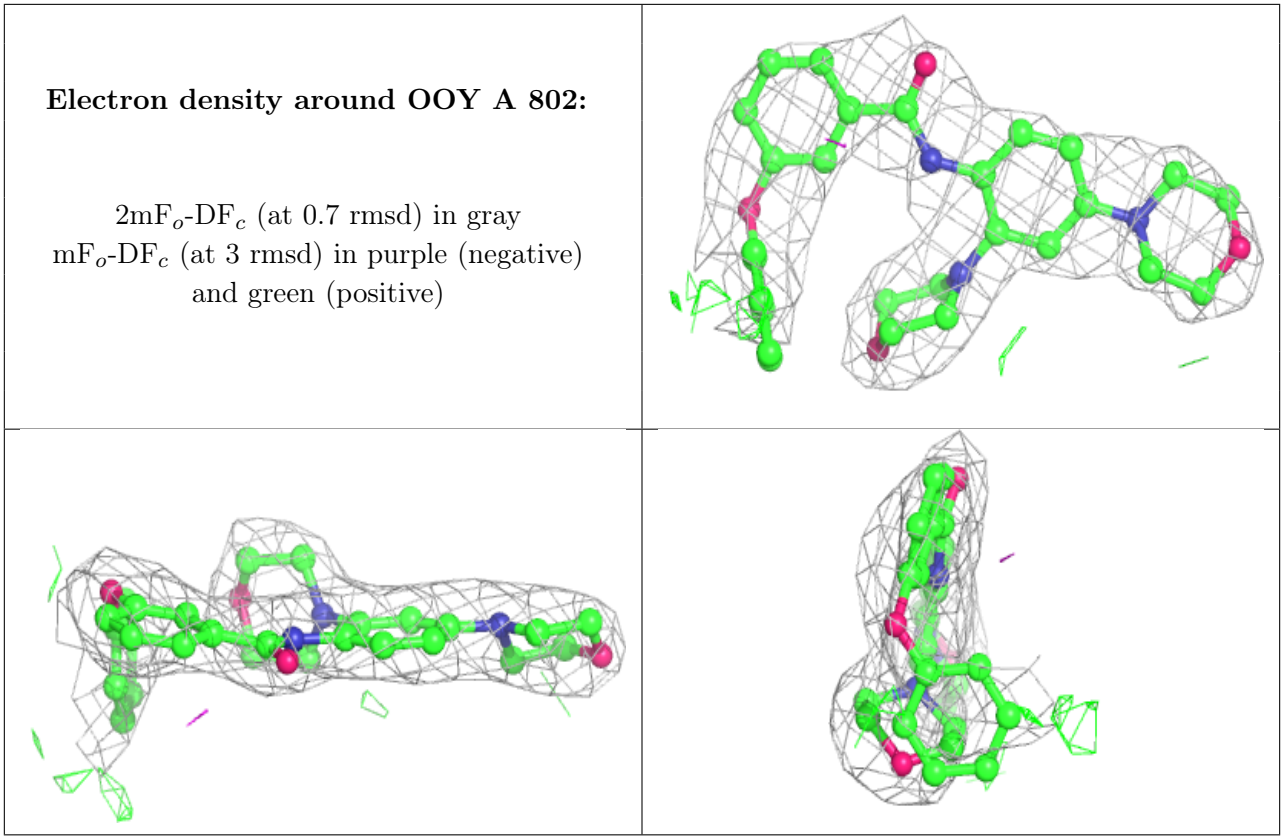
Electron density around OOY B 802:

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



Electron density around OOY A 802:

$2mF_o$-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.