Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2025 – 03:48 am BST

PDB ID	:	8QO6 / pdb_00008qo6
Title	:	OPR3 variant R283D in complex with NADH4
Authors	:	Bijelic, A.; Macheroux, P.; Kerschbaumer, B.
Deposited on	:	2023-09-28
Resolution	:	2.37 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:

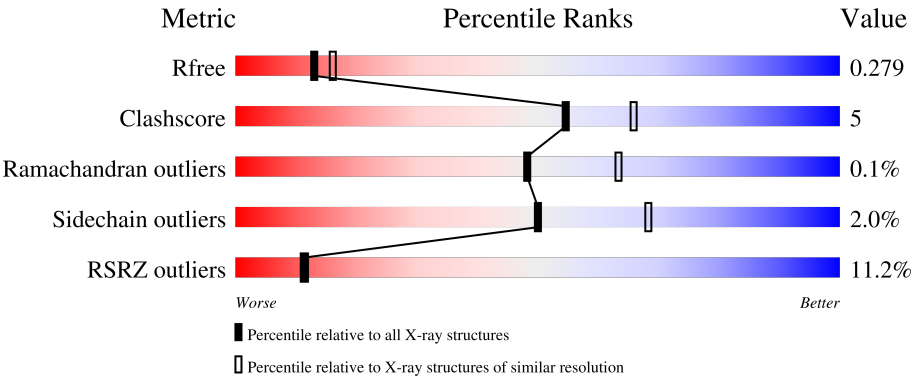
MolProbity	:	4.02b-467
Mogul	:	?.? (???), CSD ??CSD?? (????)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.37 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}	164625	6699 (2.40-2.36)
Clashscore	180529	7414 (2.40-2.36)
Ramachandran outliers	177936	7337 (2.40-2.36)
Sidechain outliers	177891	7338 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

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	402	10% 77% 12% 11%
1	B	402	10% 79% 9% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5771 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.

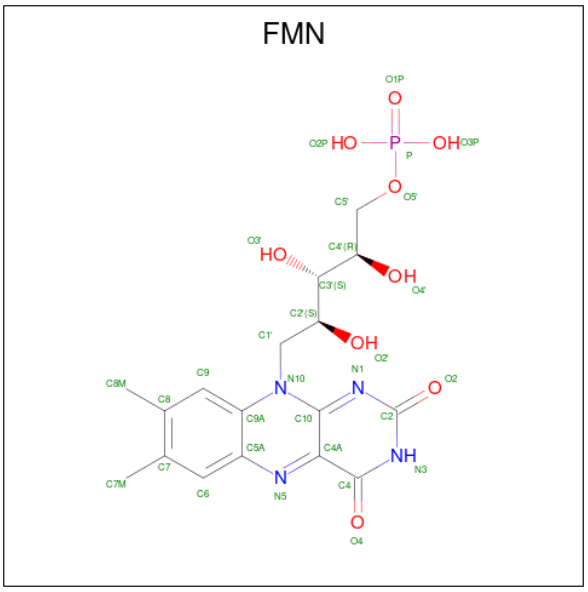
- Molecule 1 is a protein called 12-oxophytodienoate reductase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2747	1746	487	503	11			
1	B	356	Total	C	N	O	S	0	0	0
			2714	1727	480	496	11			

There are 14 discrepancies between the modelled and reference sequences:

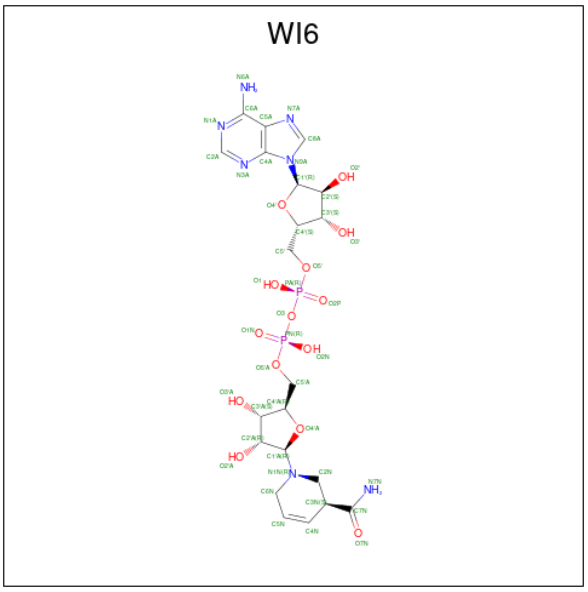
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q9FEW9
A	-4	HIS	-	expression tag	UNP Q9FEW9
A	-3	HIS	-	expression tag	UNP Q9FEW9
A	-2	HIS	-	expression tag	UNP Q9FEW9
A	-1	HIS	-	expression tag	UNP Q9FEW9
A	0	HIS	-	expression tag	UNP Q9FEW9
A	283	ASP	ARG	engineered mutation	UNP Q9FEW9
B	-5	HIS	-	expression tag	UNP Q9FEW9
B	-4	HIS	-	expression tag	UNP Q9FEW9
B	-3	HIS	-	expression tag	UNP Q9FEW9
B	-2	HIS	-	expression tag	UNP Q9FEW9
B	-1	HIS	-	expression tag	UNP Q9FEW9
B	0	HIS	-	expression tag	UNP Q9FEW9
B	283	ASP	ARG	engineered mutation	UNP Q9FEW9

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is 1,4,5,6-Tetrahydronicotinamide adenine dinucleotide (CCD ID: WI6) (formula: $C_{21}H_{31}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			26	11	2	11	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

- Molecule 4 is water.

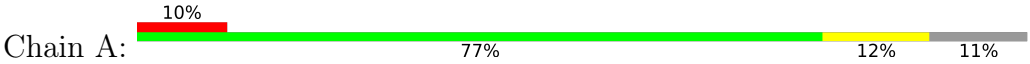
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	95	Total	O	0	0
			95	95		

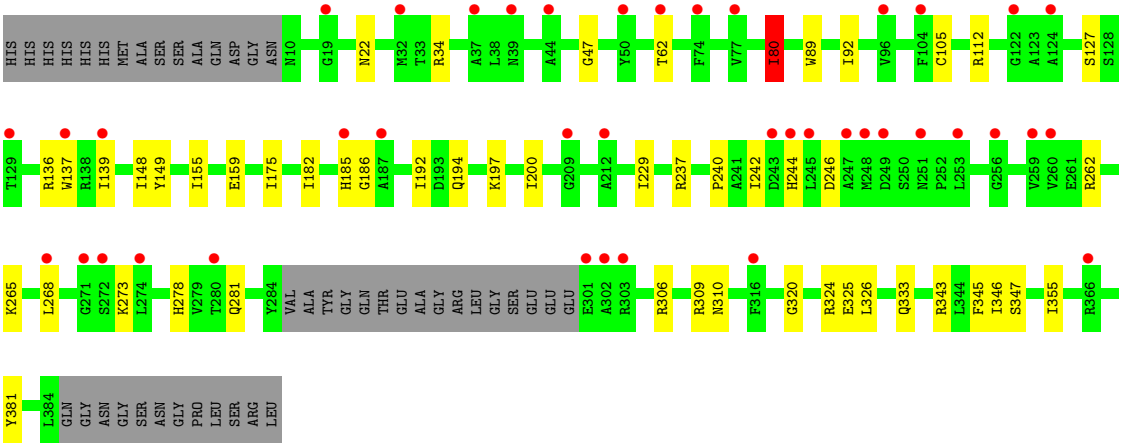
3 Residue-property plots (i)

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: 12-oxophytodienoate reductase 3

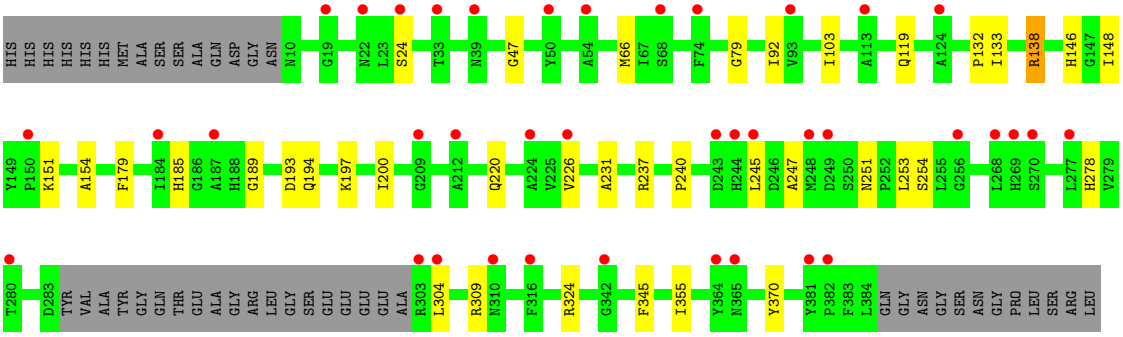
Chain A:





• Molecule 1: 12-oxophytodienoate reductase 3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.56Å 92.85Å 89.77Å 90.00° 97.86° 90.00°	Depositor
Resolution (Å)	45.71 – 2.37 45.71 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.2 (45.71-2.37) 90.6 (45.71-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.37Å)	Xtriage
Refinement program	PHENIX (dev_4761: ???)	Depositor
R, R_{free}	0.234 , 0.276 0.234 , 0.279	Depositor DCC
R_{free} test set	1075 reflections (3.29%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.864	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5771	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.07% 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: WI6, FMN

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	0.28	0/2811	0.48	0/3825
1	B	0.26	0/2778	0.48	0/3783
All	All	0.27	0/5589	0.48	0/7608

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	ARG	Sidechain

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	2747	0	2684	28	0
1	B	2714	0	2645	22	0
2	A	31	0	19	0	0
2	B	31	0	19	2	0
3	A	26	0	0	0	0
3	B	22	0	0	0	0
4	A	105	0	0	7	0
4	B	95	0	0	3	0
All	All	5771	0	5367	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (51) 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:119:GLN:NE2	4:B:504:HOH:O	2.16	0.79
1:B:220:GLN:NE2	4:B:501:HOH:O	2.07	0.74
1:B:154:ALA:O	4:B:503:HOH:O	2.15	0.63
1:B:226:VAL:HG22	1:B:231:ALA:HA	1.80	0.62
1:B:253:LEU:HD13	1:B:304:LEU:HD23	1.82	0.62
1:A:62:THR:HB	1:A:105:CYS:HA	1.81	0.61
1:A:273:LYS:NZ	4:A:505:HOH:O	2.31	0.61
1:A:262:ARG:NE	4:A:512:HOH:O	2.33	0.60
1:B:133:ILE:HD13	1:B:245:LEU:HB3	1.85	0.57
2:B:401:FMN:O5'	2:B:401:FMN:O3'	2.22	0.57
1:A:175:ILE:HD11	1:A:229:ILE:HD12	1.87	0.56
1:B:324:ARG:HG3	1:B:355:ILE:HG23	1.86	0.56
1:A:22:ASN:ND2	4:A:504:HOH:O	2.28	0.53
1:B:251:ASN:HB3	1:B:254:SER:HB3	1.91	0.53
1:B:132:PRO:HB3	1:B:151:LYS:HA	1.91	0.52
1:A:197:LYS:HE2	1:A:240:PRO:HA	1.90	0.52
1:A:281:GLN:HG2	1:A:320:GLY:HA3	1.92	0.50
1:B:138:ARG:HB3	1:B:146:HIS:HB3	1.92	0.50
1:A:324:ARG:HG3	1:A:355:ILE:HG23	1.94	0.49
1:B:200:ILE:HD11	1:B:247:ALA:HA	1.97	0.47
1:A:137:TRP:NE1	1:A:246:ASP:OD1	2.45	0.46
1:A:47:GLY:HA2	1:A:92:ILE:HG23	1.97	0.46
1:A:34:ARG:NH1	1:A:346:ILE:HG12	2.31	0.46
1:A:237:ARG:HA	1:A:278:HIS:O	2.16	0.46
1:B:237:ARG:HA	1:B:278:HIS:O	2.16	0.46
1:A:194:GLN:HG2	1:A:200:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ILE:HG12	1:B:179:PHE:HE1	1.81	0.45
1:A:155:ILE:HB	1:A:159:GLU:HB3	1.98	0.45
1:B:237:ARG:HG3	1:B:278:HIS:HB3	2.00	0.44
1:B:47:GLY:HA2	1:B:92:ILE:HG23	1.98	0.44
1:B:66:MET:HB2	1:B:79:GLY:HA2	1.99	0.44
1:A:112:ARG:HB3	1:A:127:SER:HB2	2.00	0.43
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.88	0.43
1:B:103:ILE:HG12	1:B:179:PHE:CE1	2.54	0.43
1:A:80:ILE:HD12	1:A:89:TRP:CD1	2.54	0.43
1:A:325:GLU:HG2	4:A:521:HOH:O	2.19	0.43
1:A:242:ILE:HG22	1:A:244:HIS:H	1.84	0.43
1:A:182:ILE:HG12	1:A:229:ILE:HD11	2.01	0.42
1:A:186:GLY:HA2	1:A:192:ILE:HB	2.01	0.42
1:B:148:ILE:HD13	1:B:148:ILE:HA	1.85	0.42
1:A:273:LYS:HG2	4:A:505:HOH:O	2.18	0.41
1:A:306:ARG:NH2	1:A:333:GLN:O	2.53	0.41
1:B:197:LYS:HE2	1:B:240:PRO:HA	2.02	0.41
1:A:148:ILE:HG12	4:A:552:HOH:O	2.19	0.41
1:B:370:TYR:CZ	2:B:401:FMN:HM72	2.55	0.41
1:A:139:ILE:HB	1:A:149:TYR:CE1	2.55	0.41
1:B:194:GLN:HG2	1:B:200:ILE:HG21	2.02	0.41
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.88	0.40
1:B:189:GLY:HA2	1:B:193:ASP:HB3	2.04	0.40
1:A:310:ASN:OD1	4:A:502:HOH:O	2.22	0.40
1:A:347:SER:HA	1:A:381:TYR:CG	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	355/402 (88%)	337 (95%)	17 (5%)	1 (0%)	37 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	352/402 (88%)	338 (96%)	14 (4%)	0	100 100
All	All	707/804 (88%)	675 (96%)	31 (4%)	1 (0%)	48 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ILE

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	283/328 (86%)	277 (98%)	6 (2%)	48 67
1	B	279/328 (85%)	274 (98%)	5 (2%)	54 72
All	All	562/656 (86%)	551 (98%)	11 (2%)	50 68

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ILE
1	A	136	ARG
1	A	185	HIS
1	A	265	LYS
1	A	309	ARG
1	A	345	PHE
1	B	24	SER
1	B	138	ARG
1	B	185	HIS
1	B	309	ARG
1	B	345	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

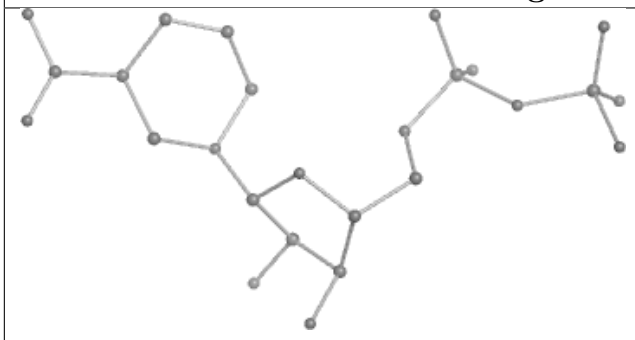
There are no torsion outliers.

There are no ring outliers.

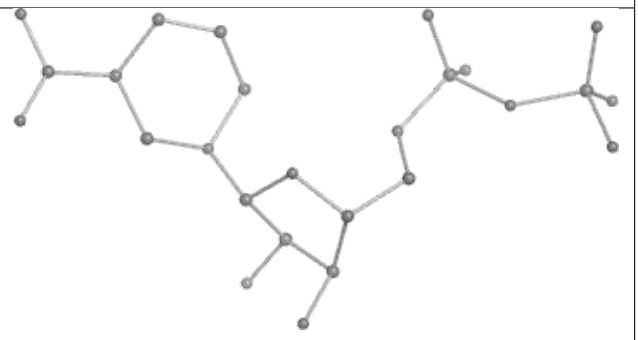
No monomer is involved in short contacts.

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.

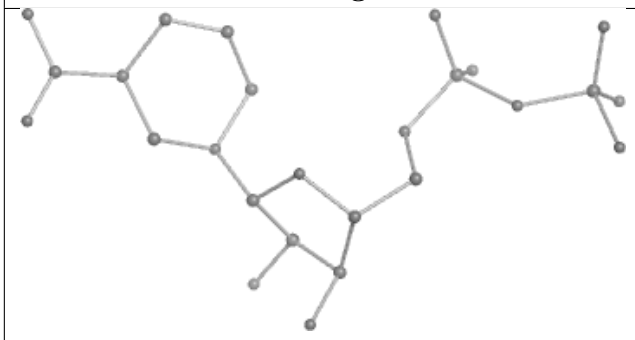
Ligand WI6 A 402



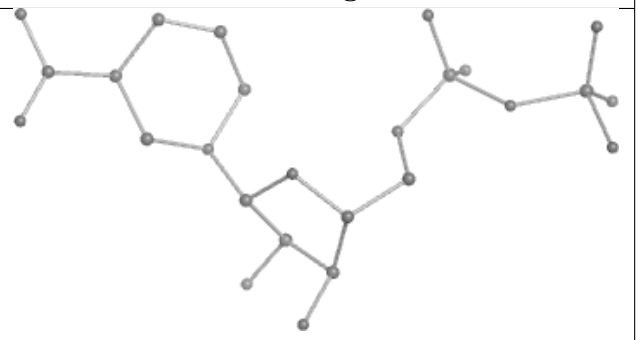
Bond lengths



Bond angles

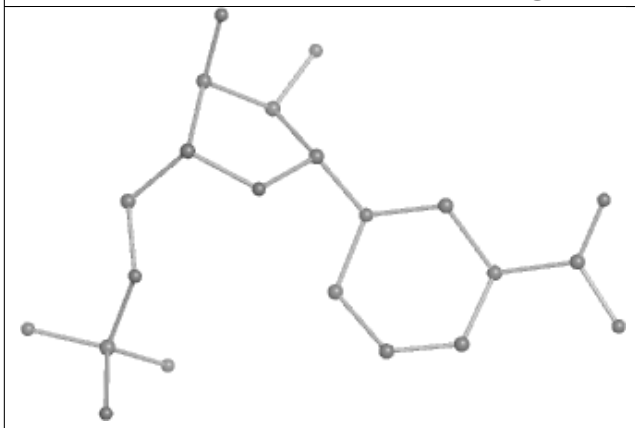


Torsions

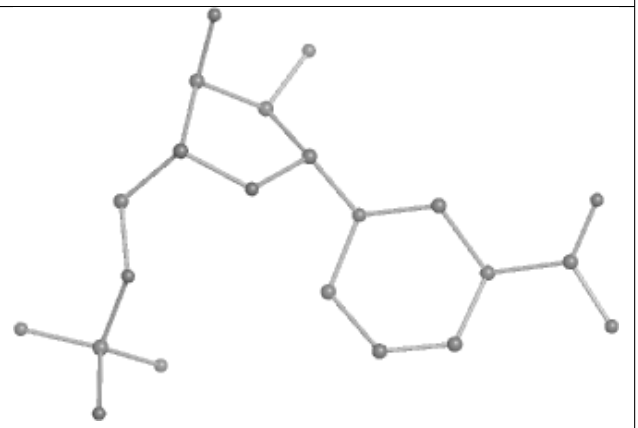


Rings

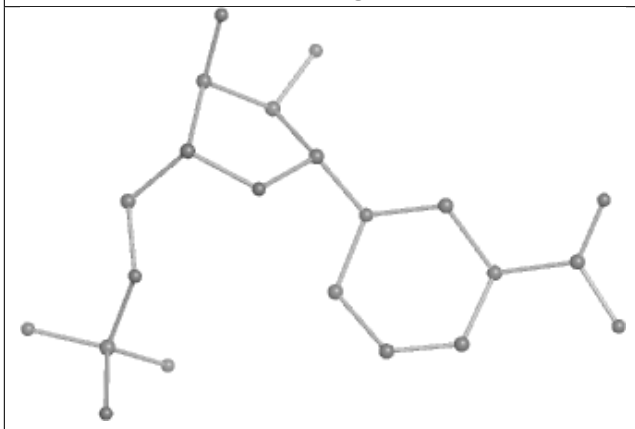
Ligand WI6 B 402



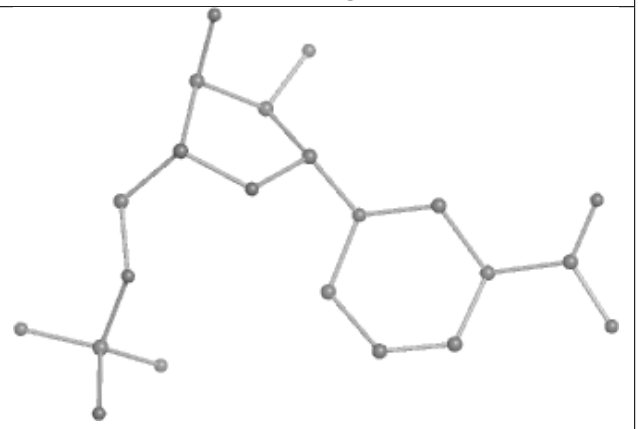
Bond lengths



Bond angles



Torsions



Rings

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	359/402 (89%)	0.97	41 (11%)	11	11	21, 32, 46, 61	0
1	B	356/402 (88%)	1.05	39 (10%)	12	11	22, 34, 46, 55	0
All	All	715/804 (88%)	1.01	80 (11%)	11	11	21, 34, 46, 61	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	ASP	4.0
1	B	304	LEU	3.8
1	B	277	LEU	3.6
1	A	96	VAL	3.5
1	A	302	ALA	3.5
1	B	124	ALA	3.3
1	A	316	PHE	3.1
1	A	248	MET	3.1
1	B	248	MET	3.0
1	A	249	ASP	2.9
1	B	54	ALA	2.8
1	A	212	ALA	2.8
1	A	243	ASP	2.8
1	B	316	PHE	2.8
1	A	247	ALA	2.8
1	B	303	ARG	2.7
1	B	268	LEU	2.7
1	B	187	ALA	2.7
1	B	224	ALA	2.7
1	B	280	THR	2.6
1	B	269	HIS	2.6
1	A	62	THR	2.6
1	A	280	THR	2.6
1	A	185	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	209	GLY	2.6
1	B	19	GLY	2.6
1	A	268	LEU	2.6
1	A	245	LEU	2.5
1	B	245	LEU	2.5
1	B	22	ASN	2.5
1	A	253	LEU	2.5
1	B	244	HIS	2.5
1	B	381	TYR	2.5
1	B	243	ASP	2.5
1	A	244	HIS	2.5
1	A	129	THR	2.4
1	A	303	ARG	2.4
1	A	256	GLY	2.4
1	B	342	GLY	2.4
1	A	124	ALA	2.4
1	A	274	LEU	2.4
1	B	212	ALA	2.4
1	A	32	MET	2.3
1	A	37	ALA	2.3
1	A	74	PHE	2.3
1	B	226	VAL	2.3
1	B	150	PRO	2.3
1	B	270	SER	2.3
1	A	301	GLU	2.3
1	B	113	ALA	2.3
1	A	77	VAL	2.3
1	A	122	GLY	2.3
1	B	39	ASN	2.2
1	B	209	GLY	2.2
1	B	184	ILE	2.2
1	A	271	GLY	2.2
1	A	187	ALA	2.2
1	B	93	VAL	2.2
1	A	272	SER	2.2
1	A	19	GLY	2.2
1	A	137	TRP	2.2
1	B	50	TYR	2.2
1	B	74	PHE	2.2
1	A	50	TYR	2.1
1	A	104	PHE	2.1
1	A	251	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	259	VAL	2.1
1	B	364	TYR	2.1
1	A	366	ARG	2.1
1	A	39	ASN	2.1
1	B	310	ASN	2.1
1	B	382	PRO	2.1
1	A	44	ALA	2.1
1	B	33	THR	2.1
1	A	260	VAL	2.0
1	B	256	GLY	2.0
1	B	24	SER	2.0
1	B	68	SER	2.0
1	A	139	ILE	2.0
1	B	365	ASN	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)

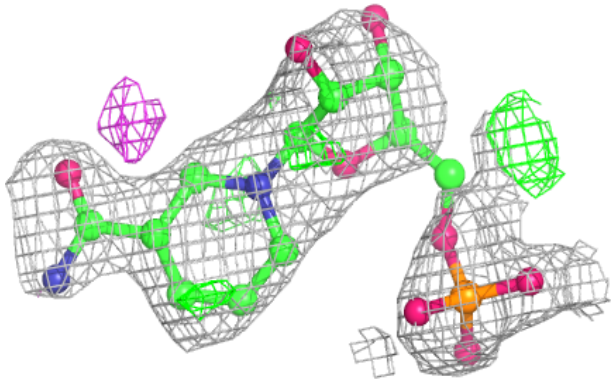
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

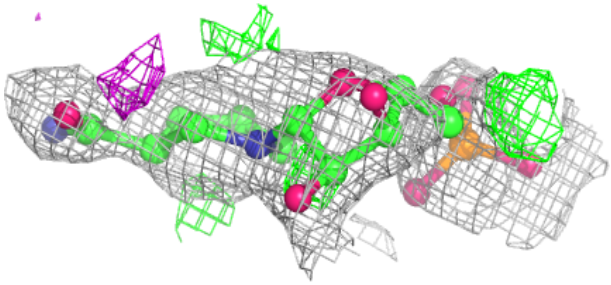
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	WI6	B	402	22/44	0.73	0.21	27,46,62,73	22
3	WI6	A	402	26/44	0.83	0.15	23,44,75,76	26
2	FMN	B	401	31/31	0.83	0.17	21,30,45,47	0
2	FMN	A	401	31/31	0.85	0.16	24,32,39,47	0

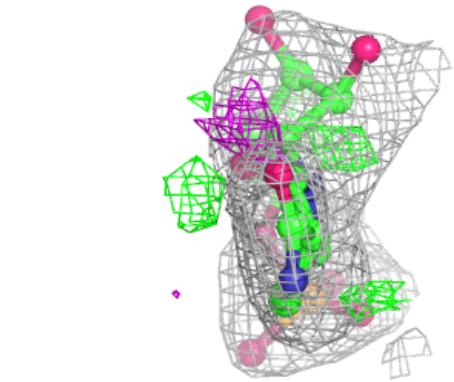
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WI6 B 402:

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

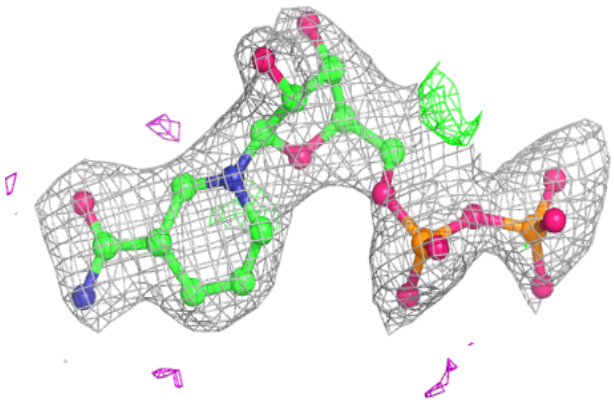


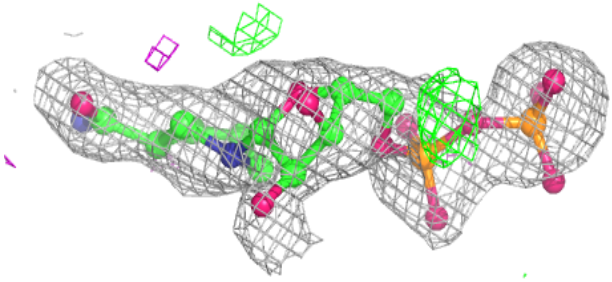


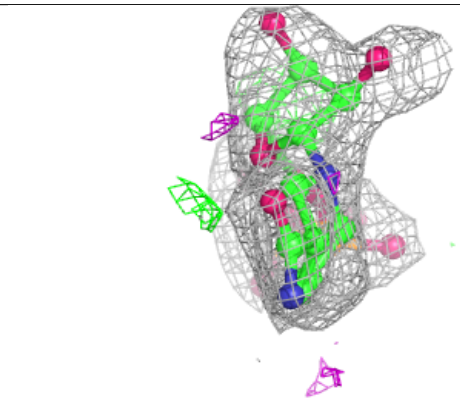


Electron density around WI6 A 402:

$2mF_o$-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.