Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 03:12 PM EDT

PDB ID	:	6PEB
Title	:	Crystal Structure of human NAMPT in complex with NVP-LTM976
Authors	:	Weihofen, W.A.
Deposited on	:	2019-06-20
Resolution	:	2.46 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

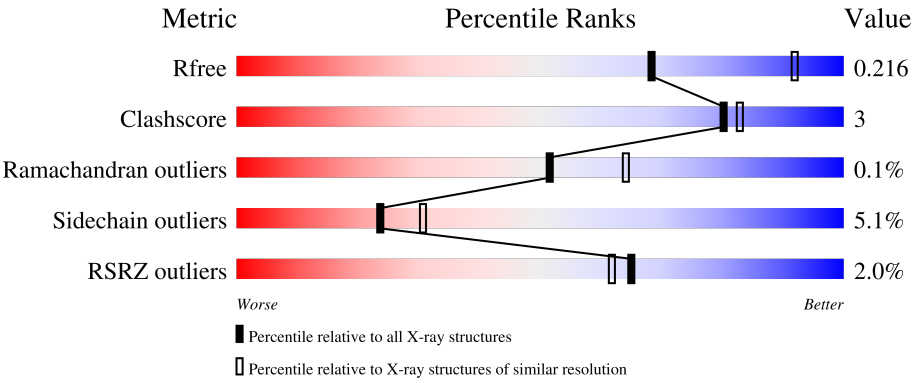
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	500	83% 10% • 6%
1	B	500	% 84% 9% • 6%
1	C	500	% 84% 9% • 6%
1	D	500	5% 81% 12% • 6%

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
3	PO4	B	604	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15757 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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3754	2416	621	710	7			
1	B	468	Total	C	N	O	S	0	0	0
			3743	2408	619	709	7			
1	C	469	Total	C	N	O	S	0	0	0
			3754	2415	620	712	7			
1	D	471	Total	C	N	O	S	0	0	0
			3768	2423	623	715	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	492	LEU	-	expression tag	UNP P43490
A	493	GLU	-	expression tag	UNP P43490
A	494	HIS	-	expression tag	UNP P43490
A	495	HIS	-	expression tag	UNP P43490
A	496	HIS	-	expression tag	UNP P43490
A	497	HIS	-	expression tag	UNP P43490
A	498	HIS	-	expression tag	UNP P43490
A	499	HIS	-	expression tag	UNP P43490
A	500	HIS	-	expression tag	UNP P43490
A	501	HIS	-	expression tag	UNP P43490
B	492	LEU	-	expression tag	UNP P43490
B	493	GLU	-	expression tag	UNP P43490
B	494	HIS	-	expression tag	UNP P43490
B	495	HIS	-	expression tag	UNP P43490
B	496	HIS	-	expression tag	UNP P43490
B	497	HIS	-	expression tag	UNP P43490
B	498	HIS	-	expression tag	UNP P43490
B	499	HIS	-	expression tag	UNP P43490
B	500	HIS	-	expression tag	UNP P43490
B	501	HIS	-	expression tag	UNP P43490
C	492	LEU	-	expression tag	UNP P43490

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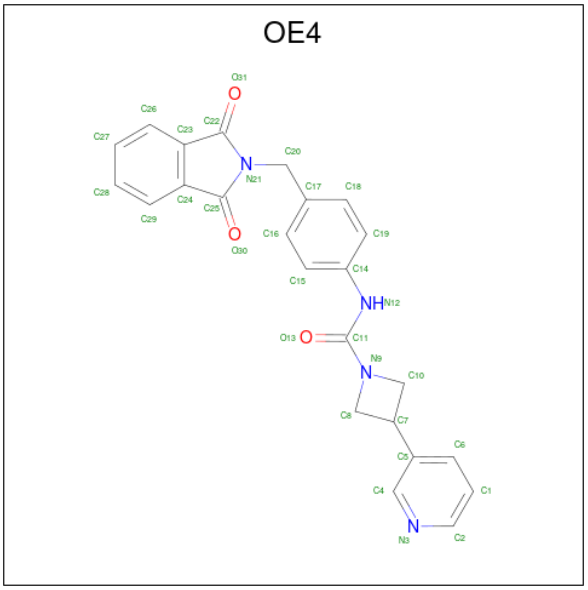
Chain	Residue	Modelled	Actual	Comment	Reference
C	493	GLU	-	expression tag	UNP P43490
C	494	HIS	-	expression tag	UNP P43490
C	495	HIS	-	expression tag	UNP P43490
C	496	HIS	-	expression tag	UNP P43490
C	497	HIS	-	expression tag	UNP P43490
C	498	HIS	-	expression tag	UNP P43490
C	499	HIS	-	expression tag	UNP P43490
C	500	HIS	-	expression tag	UNP P43490
C	501	HIS	-	expression tag	UNP P43490
D	492	LEU	-	expression tag	UNP P43490
D	493	GLU	-	expression tag	UNP P43490
D	494	HIS	-	expression tag	UNP P43490
D	495	HIS	-	expression tag	UNP P43490
D	496	HIS	-	expression tag	UNP P43490
D	497	HIS	-	expression tag	UNP P43490
D	498	HIS	-	expression tag	UNP P43490
D	499	HIS	-	expression tag	UNP P43490
D	500	HIS	-	expression tag	UNP P43490
D	501	HIS	-	expression tag	UNP P43490

- Molecule 2 is N-{4-[(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)methyl]phenyl}-3-(pyridin-3-yl)azetidine-1-carboxamide (three-letter code: OE4) (formula: $C_{24}H_{20}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	24	4	3		

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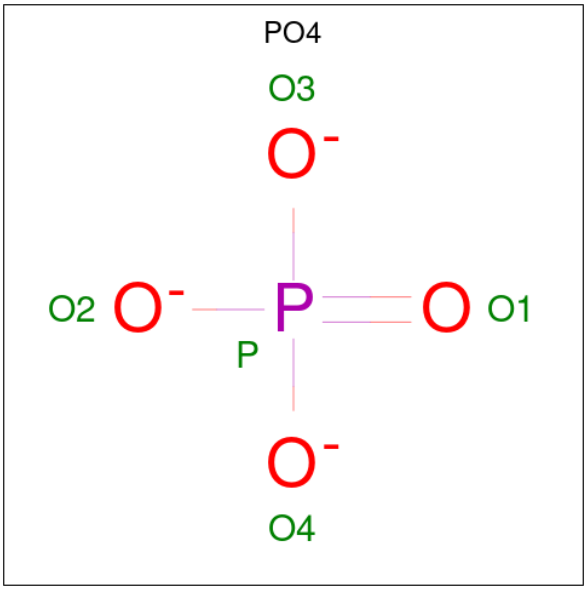
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 31 24 4 3	0	0
2	C	1	Total C N O 31 24 4 3	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0
3	D	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

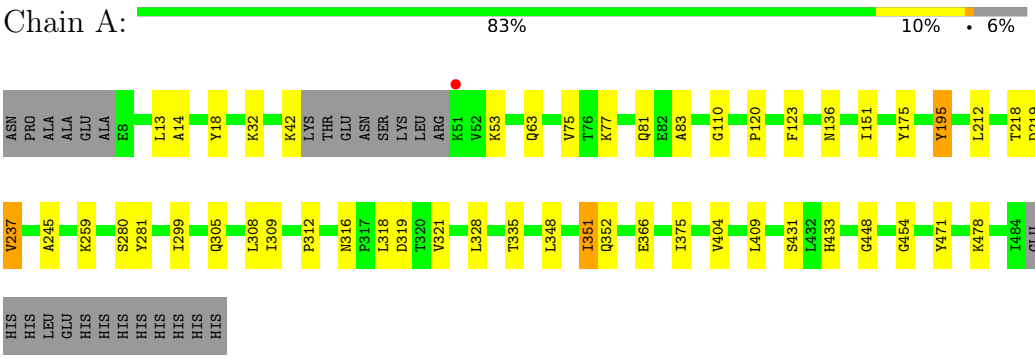
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	230	Total O 230 230	0	0
4	B	127	Total O 127 127	0	0
4	C	134	Total O 134 134	0	0
4	D	94	Total O 94 94	0	0

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.

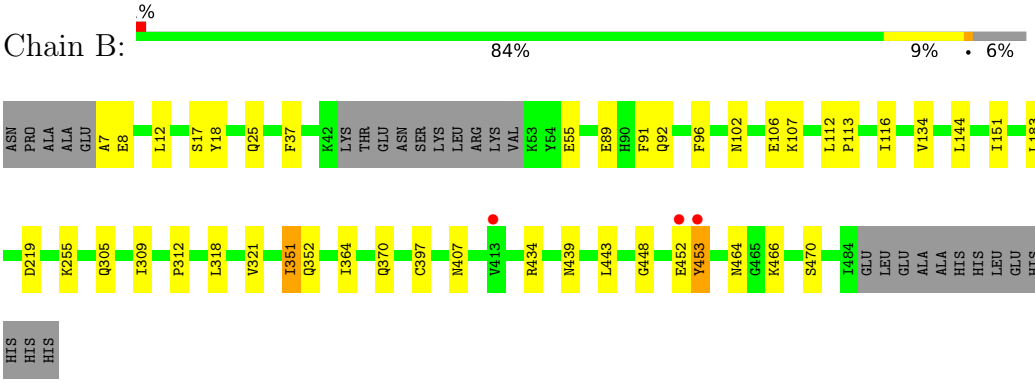
• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain A:



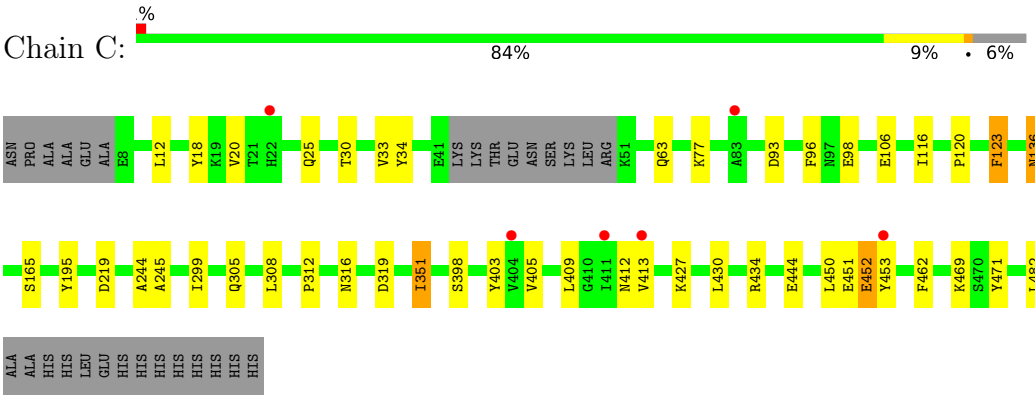
• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain B:



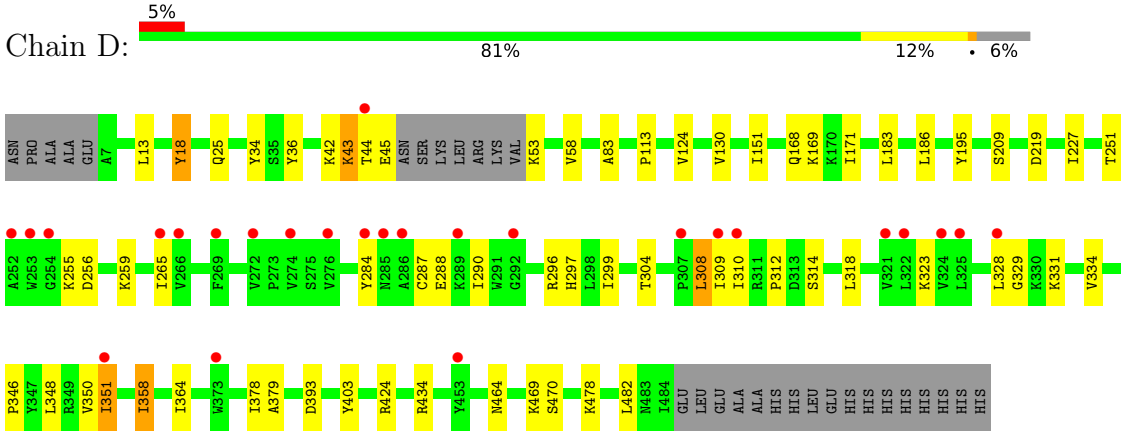
• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain C:



• Molecule 1: Nicotinamide phosphoribosyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.74Å 96.16Å 246.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.94 – 2.46 123.42 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.94-2.46) 99.9 (123.42-2.46)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.159 , 0.209 0.167 , 0.216	Depositor DCC
R_{free} test set	3962 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15757	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: OE4, PO4

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	0.52	0/3842	0.70	0/5204
1	B	0.49	0/3831	0.68	0/5190
1	C	0.52	0/3842	0.68	0/5205
1	D	0.52	0/3856	0.68	0/5223
All	All	0.51	0/15371	0.69	0/20822

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	3754	0	3740	22	0
1	B	3743	0	3723	17	0
1	C	3754	0	3733	24	0
1	D	3768	0	3749	27	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	C	31	0	0	0	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	230	0	0	0	0
4	B	127	0	0	0	0
4	C	134	0	0	0	0
4	D	94	0	0	0	0
All	All	15757	0	14945	82	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 3.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:VAL:H	1:C:136:ASN:HD21	1.23	0.85
1:C:63:GLN:HE22	1:C:471:TYR:H	1.25	0.84
1:A:316:ASN:HD22	1:A:319:ASP:H	1.33	0.74
1:D:43:LYS:HG2	1:D:44:THR:H	1.54	0.72
1:C:450:LEU:HB3	1:C:452:GLU:HG3	1.75	0.68
1:C:245:ALA:HA	1:D:25:GLN:HE22	1.60	0.66
1:C:316:ASN:HD22	1:C:319:ASP:H	1.41	0.65
1:D:328:LEU:HD22	1:D:348:LEU:HD21	1.78	0.64
1:A:321:VAL:HG23	1:A:352:GLN:HE21	1.63	0.64
1:A:63:GLN:HE22	1:A:471:TYR:H	1.47	0.62
1:C:120:PRO:O	1:C:123:PHE:HB2	1.99	0.61
1:A:245:ALA:HA	1:B:25:GLN:HE22	1.64	0.61
1:D:304:THR:HG23	1:D:346:PRO:HB2	1.83	0.61
1:C:299:ILE:HD12	1:C:308:LEU:HD22	1.84	0.59
1:D:183:LEU:HD23	1:D:186:LEU:HD22	1.84	0.59
1:D:299:ILE:HD12	1:D:308:LEU:HD22	1.85	0.57
1:B:453:TYR:CD1	1:B:453:TYR:N	2.72	0.57
1:B:321:VAL:HG23	1:B:352:GLN:HE21	1.70	0.56
1:B:17:SER:O	1:B:91:PHE:HZ	1.89	0.55
1:A:229:LYS:NZ	1:B:7:ALA:HB2	2.22	0.55
1:C:33:VAL:H	1:C:136:ASN:ND2	1.99	0.55
1:D:113:PRO:HA	1:D:464:ASN:HD22	1.72	0.54
1:B:453:TYR:N	1:B:453:TYR:HD1	2.06	0.54
1:C:25:GLN:HG2	1:D:265:ILE:HG12	1.89	0.54
1:A:328:LEU:HD22	1:A:348:LEU:HD21	1.90	0.53
1:D:169:LYS:HG2	1:D:482:LEU:HD11	1.91	0.52
1:C:30:THR:HA	1:C:405:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:HA	1:A:136:ASN:HD21	1.75	0.51
1:A:299:ILE:HD12	1:A:308:LEU:HD22	1.91	0.51
1:B:112:LEU:O	1:B:464:ASN:HA	2.11	0.51
1:B:318:LEU:HD13	1:B:364:ILE:HA	1.93	0.50
1:C:116:ILE:HB	1:C:462:PHE:HB3	1.93	0.50
1:C:312:PRO:HD2	1:C:351:ILE:O	2.12	0.50
1:A:75:VAL:HB	1:A:110:GLY:HA2	1.94	0.50
1:A:309:ILE:HG22	1:A:351:ILE:HG22	1.92	0.49
1:D:36:TYR:HB2	1:D:130:VAL:HG23	1.94	0.49
1:B:312:PRO:HD2	1:B:351:ILE:O	2.12	0.48
1:B:443:LEU:HD23	1:B:448:GLY:HA2	1.96	0.48
1:D:296:ARG:HH12	1:D:331:LYS:C	2.17	0.48
1:A:312:PRO:HD2	1:A:351:ILE:O	2.14	0.47
1:D:297:HIS:H	1:D:297:HIS:CD2	2.33	0.46
1:D:318:LEU:HD13	1:D:364:ILE:HA	1.97	0.46
1:D:378:ILE:HG13	1:D:379:ALA:N	2.30	0.46
1:D:34:TYR:HB3	1:D:403:TYR:HB3	1.97	0.46
1:D:168:GLN:HG3	1:D:358:ILE:HD12	1.98	0.46
1:B:12:LEU:HD23	1:B:96:PHE:HZ	1.81	0.46
1:C:63:GLN:NE2	1:C:471:TYR:H	2.04	0.45
1:A:316:ASN:HB3	1:A:319:ASP:HB2	1.97	0.45
1:C:20:VAL:HG22	1:C:147:TRP:CH2	2.52	0.45
1:D:310:ILE:HB	1:D:350:VAL:HG12	1.98	0.45
1:A:212:LEU:HD11	1:A:218:THR:HG21	1.98	0.45
1:A:431:SER:OG	1:A:433:HIS:HE1	2.00	0.45
1:D:13:LEU:HD21	1:D:83:ALA:HA	1.98	0.44
1:D:58:VAL:HG22	1:D:124:VAL:HG22	1.98	0.44
1:A:195:TYR:CG	1:A:220:THR:HG23	2.52	0.44
1:C:12:LEU:HD23	1:C:96:PHE:CZ	2.53	0.44
1:D:259:LYS:HG3	1:D:290:ILE:HG23	1.99	0.44
1:A:13:LEU:HD21	1:A:83:ALA:HA	2.00	0.44
1:B:116:ILE:HG12	1:B:134:VAL:HG22	2.00	0.44
1:C:136:ASN:ND2	1:C:136:ASN:H	2.15	0.44
1:C:412:ASN:HB3	1:C:427:LYS:HB3	2.00	0.44
1:B:37:PHE:CZ	1:B:397:CYS:HB3	2.53	0.44
1:A:237:VAL:HG22	1:B:89:GLU:HB3	1.99	0.43
1:C:136:ASN:H	1:C:136:ASN:HD22	1.66	0.43
1:D:329:GLY:HA2	1:D:334:VAL:HG13	1.99	0.43
1:D:168:GLN:HA	1:D:171:ILE:HD12	1.99	0.43
1:B:309:ILE:HG22	1:B:351:ILE:HG22	2.01	0.42
1:C:413:VAL:HB	1:D:251:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:TYR:HB3	1:C:403:TYR:HB3	2.02	0.42
1:C:244:ALA:HB3	1:D:18:TYR:HB2	2.02	0.42
1:D:312:PRO:HD2	1:D:351:ILE:O	2.19	0.42
1:A:431:SER:OG	1:A:448:GLY:HA3	2.20	0.42
1:A:14:ALA:HA	1:B:195:TYR:OH	2.19	0.41
1:B:113:PRO:HD2	1:B:144:LEU:CD2	2.50	0.41
1:C:482:LEU:HB2	1:C:485:GLU:HG3	2.02	0.41
1:A:120:PRO:O	1:A:123:PHE:HB2	2.20	0.41
1:A:433:HIS:HD2	1:A:454:GLY:O	2.03	0.41
1:D:43:LYS:CG	1:D:44:THR:H	2.28	0.41
1:A:175:TYR:HB3	1:A:375:ILE:HG13	2.02	0.41
1:C:12:LEU:HD23	1:C:96:PHE:HZ	1.84	0.41
1:C:430:LEU:HD23	1:C:444:GLU:HA	2.03	0.40
1:D:209:SER:HA	1:D:227:ILE:HD11	2.03	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	465/500 (93%)	452 (97%)	13 (3%)	0	100	100
1	B	464/500 (93%)	449 (97%)	14 (3%)	1 (0%)	47	57
1	C	465/500 (93%)	451 (97%)	14 (3%)	0	100	100
1	D	467/500 (93%)	447 (96%)	19 (4%)	1 (0%)	47	57
All	All	1861/2000 (93%)	1799 (97%)	60 (3%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	43	LYS

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Mol	Chain	Res	Type
1	B	8	GLU

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	413/439 (94%)	393 (95%)	20 (5%)	25	33
1	B	411/439 (94%)	389 (95%)	22 (5%)	22	28
1	C	413/439 (94%)	394 (95%)	19 (5%)	27	35
1	D	414/439 (94%)	390 (94%)	24 (6%)	20	25
All	All	1651/1756 (94%)	1566 (95%)	85 (5%)	24	31

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	TYR
1	A	42	LYS
1	A	53	LYS
1	A	77	LYS
1	A	81	GLN
1	A	151	ILE
1	A	195	TYR
1	A	219	ASP
1	A	237	VAL
1	A	259	LYS
1	A	280	SER
1	A	281	TYR
1	A	305	GLN
1	A	318	LEU
1	A	335	THR
1	A	351	ILE
1	A	366	GLU
1	A	404	VAL
1	A	409	LEU
1	A	478	LYS

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Mol	Chain	Res	Type
1	B	18	TYR
1	B	55	GLU
1	B	92	GLN
1	B	102	ASN
1	B	106	GLU
1	B	107	LYS
1	B	151	ILE
1	B	183	LEU
1	B	195	TYR
1	B	199	SER
1	B	219	ASP
1	B	255	LYS
1	B	305	GLN
1	B	351	ILE
1	B	370	GLN
1	B	407	ASN
1	B	434	ARG
1	B	439	ASN
1	B	452	GLU
1	B	453	TYR
1	B	466	LYS
1	B	470	SER
1	C	18	TYR
1	C	77	LYS
1	C	93	ASP
1	C	98	GLU
1	C	106	GLU
1	C	123	PHE
1	C	136	ASN
1	C	165	SER
1	C	195	TYR
1	C	219	ASP
1	C	305	GLN
1	C	351	ILE
1	C	398	SER
1	C	409	LEU
1	C	434	ARG
1	C	451	GLU
1	C	452	GLU
1	C	453	TYR
1	C	469	LYS
1	D	18	TYR

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Mol	Chain	Res	Type
1	D	42	LYS
1	D	45	GLU
1	D	53	LYS
1	D	151	ILE
1	D	195	TYR
1	D	219	ASP
1	D	255	LYS
1	D	256	ASP
1	D	284	TYR
1	D	287	CYS
1	D	288	GLU
1	D	308	LEU
1	D	309	ILE
1	D	314	SER
1	D	323	LYS
1	D	351	ILE
1	D	358	ILE
1	D	393	ASP
1	D	424	ARG
1	D	434	ARG
1	D	469	LYS
1	D	470	SER
1	D	478	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	136	ASN
1	A	164	ASN
1	A	316	ASN
1	A	352	GLN
1	A	433	HIS
1	A	464	ASN
1	B	25	GLN
1	B	92	GLN
1	B	164	ASN
1	B	439	ASN
1	C	63	GLN
1	C	136	ASN
1	C	164	ASN
1	C	268	GLN

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Mol	Chain	Res	Type
1	C	305	GLN
1	C	316	ASN
1	C	352	GLN
1	C	433	HIS
1	C	459	HIS
1	C	464	ASN
1	D	25	GLN
1	D	164	ASN
1	D	297	HIS
1	D	352	GLN
1	D	464	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 monosaccharides in this entry.

5.6 Ligand geometry

15 ligands 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	$\#\|Z\| > 2$
3	PO4	B	602	-	4,4,4	2.46	1 (25%)	6,6,6	0.74	0
3	PO4	C	604	-	4,4,4	2.56	1 (25%)	6,6,6	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PO4	D	603	-	4,4,4	2.11	1 (25%)	6,6,6	0.35	0
3	PO4	A	604	-	4,4,4	2.07	2 (50%)	6,6,6	0.82	0
3	PO4	C	602	-	4,4,4	2.53	1 (25%)	6,6,6	0.74	0
3	PO4	C	603	-	4,4,4	2.51	2 (50%)	6,6,6	0.66	0
3	PO4	D	602	-	4,4,4	1.97	0	6,6,6	0.65	0
3	PO4	B	603	-	4,4,4	2.46	1 (25%)	6,6,6	0.51	0
3	PO4	A	602	-	4,4,4	1.72	1 (25%)	6,6,6	1.01	0
3	PO4	A	603	-	4,4,4	2.48	1 (25%)	6,6,6	0.58	0
3	PO4	D	601	-	4,4,4	2.43	2 (50%)	6,6,6	0.79	0
3	PO4	B	604	-	4,4,4	1.77	2 (50%)	6,6,6	1.66	2 (33%)
2	OE4	C	601	-	35,35,35	1.30	3 (8%)	45,50,50	1.78	14 (31%)
2	OE4	A	601	-	35,35,35	1.41	4 (11%)	45,50,50	2.10	14 (31%)
2	OE4	B	601	-	35,35,35	1.38	6 (17%)	45,50,50	2.12	15 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OE4	C	601	-	-	0/12/40/40	0/5/5/5
2	OE4	A	601	-	-	0/12/40/40	0/5/5/5
2	OE4	B	601	-	-	0/12/40/40	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	604	PO4	P-O1	4.32	1.61	1.50
3	B	603	PO4	P-O1	4.12	1.60	1.50
3	C	602	PO4	P-O1	4.12	1.60	1.50
3	B	602	PO4	P-O1	4.08	1.60	1.50
3	C	603	PO4	P-O1	4.07	1.60	1.50
3	A	603	PO4	P-O1	4.07	1.60	1.50
3	D	601	PO4	P-O1	3.96	1.60	1.50
2	C	601	OE4	C22-N21	-3.55	1.35	1.39
2	A	601	OE4	C10-N9	-3.07	1.44	1.47
2	B	601	OE4	C25-N21	-2.91	1.36	1.39
2	C	601	OE4	C25-N21	-2.90	1.36	1.39
2	B	601	OE4	C10-N9	-2.80	1.44	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	OE4	C22-N21	-2.71	1.36	1.39
3	D	603	PO4	P-O1	2.54	1.56	1.50
2	A	601	OE4	C25-N21	-2.49	1.36	1.39
3	A	604	PO4	P-O1	2.41	1.56	1.50
2	B	601	OE4	C22-N21	-2.40	1.36	1.39
2	B	601	OE4	C4-C5	2.38	1.42	1.39
2	B	601	OE4	C6-C5	2.30	1.42	1.39
2	C	601	OE4	C10-N9	-2.18	1.45	1.47
2	A	601	OE4	C8-N9	-2.10	1.45	1.47
3	D	601	PO4	P-O4	2.07	1.60	1.54
3	A	602	PO4	P-O4	2.05	1.60	1.54
2	B	601	OE4	C8-N9	-2.05	1.45	1.47
3	B	604	PO4	P-O3	2.04	1.60	1.54
3	B	604	PO4	P-O2	2.02	1.60	1.54
3	A	604	PO4	P-O3	2.01	1.60	1.54
3	C	603	PO4	P-O3	2.01	1.60	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	OE4	C23-C22-N21	5.07	109.48	105.88
2	B	601	OE4	C23-C22-N21	4.67	109.19	105.88
2	A	601	OE4	C24-C25-N21	4.42	109.02	105.88
2	A	601	OE4	N12-C11-N9	4.28	120.78	115.89
2	A	601	OE4	O31-C22-N21	4.18	128.88	124.81
2	B	601	OE4	C5-C4-N3	-4.11	117.69	124.14
2	B	601	OE4	O31-C22-N21	4.04	128.75	124.81
2	B	601	OE4	C24-C25-N21	4.02	108.73	105.88
2	C	601	OE4	C24-C25-N21	4.00	108.72	105.88
2	A	601	OE4	O30-C25-N21	3.87	128.58	124.81
2	C	601	OE4	O30-C25-N21	3.81	128.52	124.81
2	C	601	OE4	C23-C22-N21	3.80	108.58	105.88
2	A	601	OE4	O31-C22-C23	-3.68	121.52	128.68
2	B	601	OE4	C2-N3-C4	3.58	123.04	116.85
2	B	601	OE4	O31-C22-C23	-3.42	122.03	128.68
2	B	601	OE4	C8-C7-C10	3.40	97.37	88.31
2	B	601	OE4	O13-C11-N9	-3.37	117.05	121.78
2	B	601	OE4	N12-C11-N9	3.36	119.74	115.89
2	C	601	OE4	C8-C7-C10	3.34	97.21	88.31
2	A	601	OE4	O30-C25-C24	-3.23	122.39	128.68
2	C	601	OE4	O30-C25-C24	-3.04	122.76	128.68
2	A	601	OE4	C25-N21-C22	-2.99	109.59	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	OE4	O13-C11-N9	-2.99	117.59	121.78
2	C	601	OE4	C2-N3-C4	2.97	121.99	116.85
2	A	601	OE4	C8-C7-C10	2.82	95.81	88.31
2	C	601	OE4	C24-C23-C22	-2.78	105.85	108.26
2	A	601	OE4	C24-C23-C22	-2.78	105.85	108.26
2	B	601	OE4	C6-C5-C4	2.76	119.82	116.88
2	B	601	OE4	C24-C23-C22	-2.75	105.87	108.26
2	C	601	OE4	C23-C24-C25	-2.75	105.88	108.26
3	B	604	PO4	O4-P-O1	-2.75	100.84	110.89
3	B	604	PO4	O4-P-O2	2.70	116.64	107.97
2	A	601	OE4	C23-C24-C25	-2.69	105.92	108.26
2	B	601	OE4	O30-C25-N21	2.69	127.43	124.81
2	A	601	OE4	C2-N3-C4	2.60	121.35	116.85
2	B	601	OE4	O30-C25-C24	-2.49	123.83	128.68
2	B	601	OE4	C23-C24-C25	-2.45	106.14	108.26
2	B	601	OE4	C25-N21-C22	-2.43	110.04	112.03
2	C	601	OE4	O31-C22-N21	2.40	127.15	124.81
2	C	601	OE4	O31-C22-C23	-2.30	124.21	128.68
2	C	601	OE4	O13-C11-N9	-2.15	118.77	121.78
2	C	601	OE4	N12-C11-N9	2.13	118.33	115.89
2	C	601	OE4	C5-C4-N3	-2.13	120.80	124.14
2	A	601	OE4	C14-N12-C11	2.05	130.24	126.12
2	C	601	OE4	C28-C29-C24	-2.04	115.97	119.81

There are no chirality outliers.

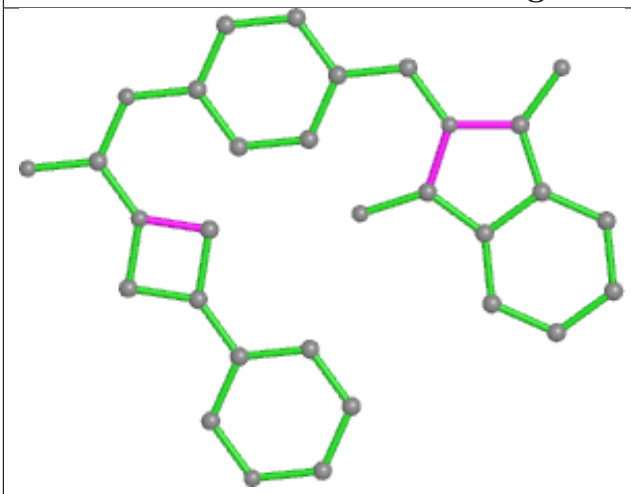
There are no torsion outliers.

There are no ring outliers.

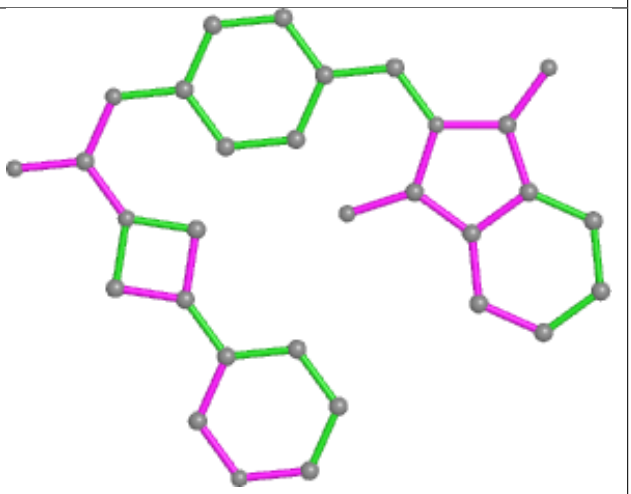
No monomer is involved in short contacts.

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.

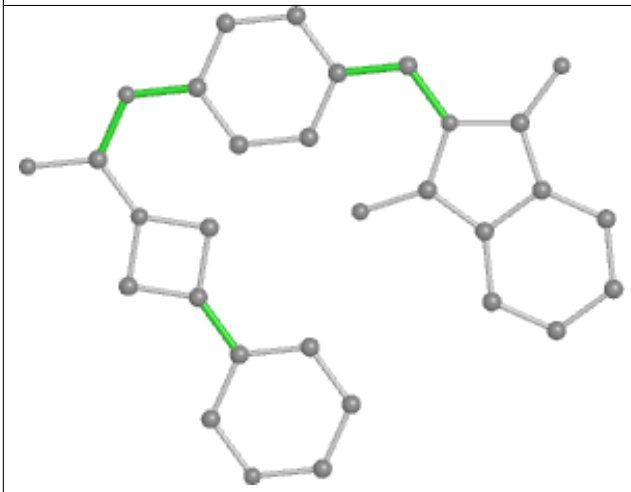
Ligand OE4 C 601



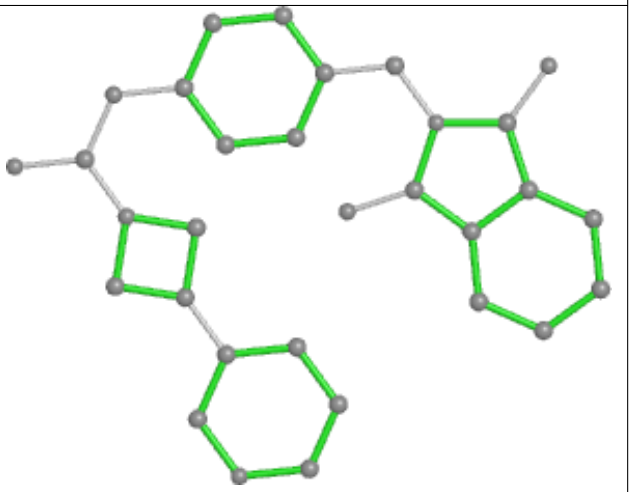
Bond lengths



Bond angles

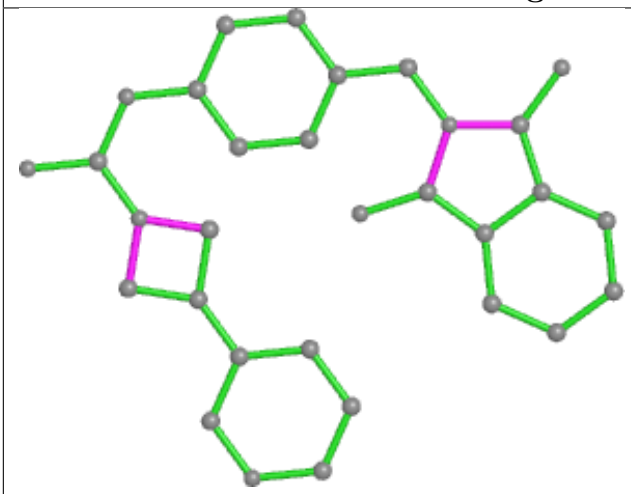


Torsions

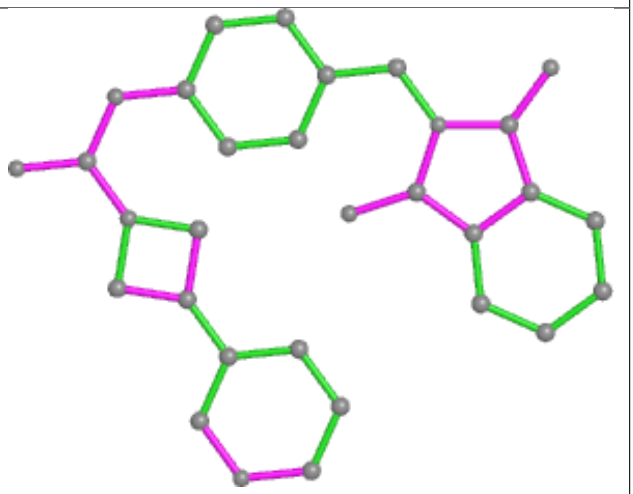


Rings

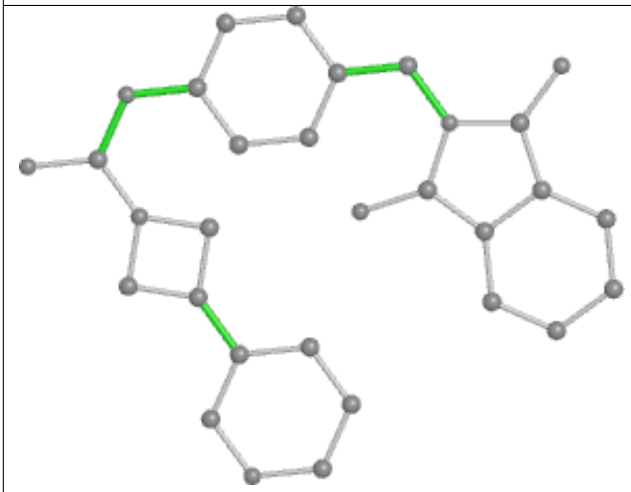
Ligand OE4 A 601



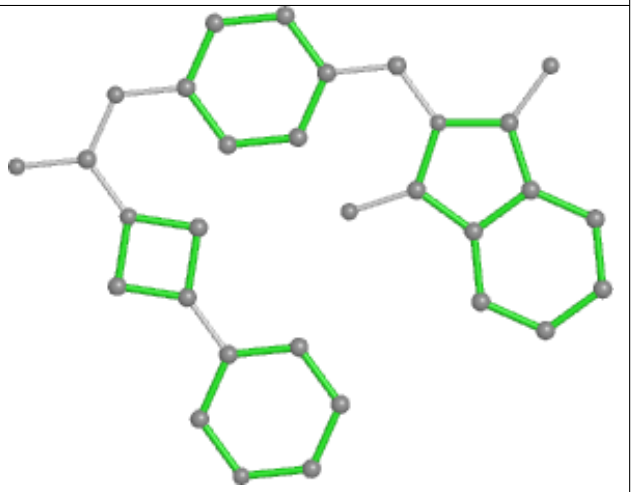
Bond lengths



Bond angles

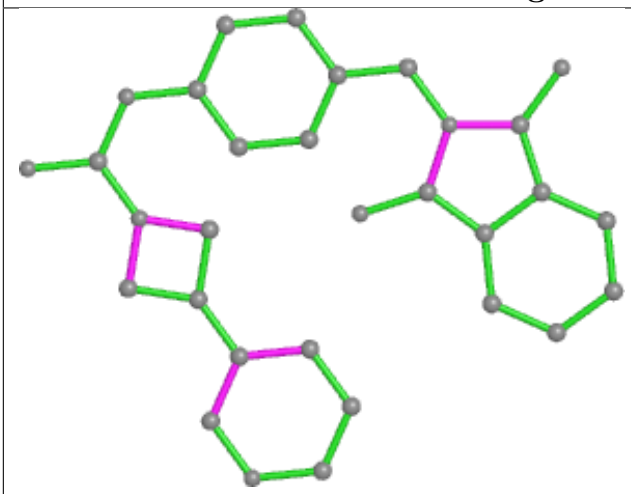


Torsions

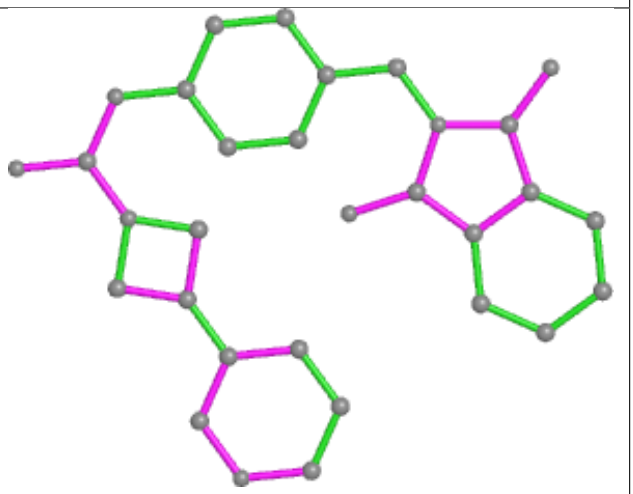


Rings

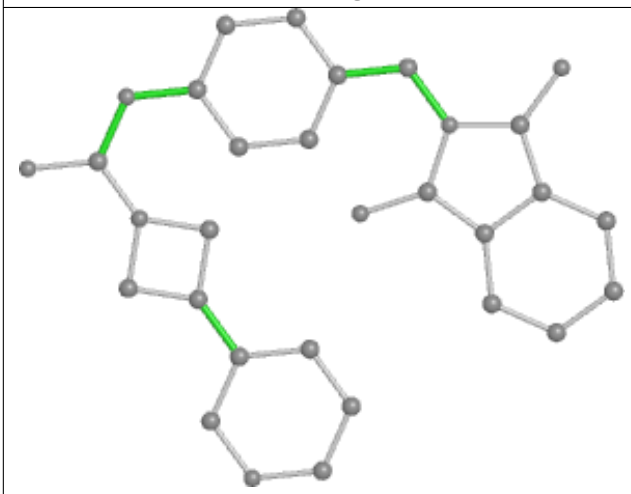
Ligand OE4 B 601



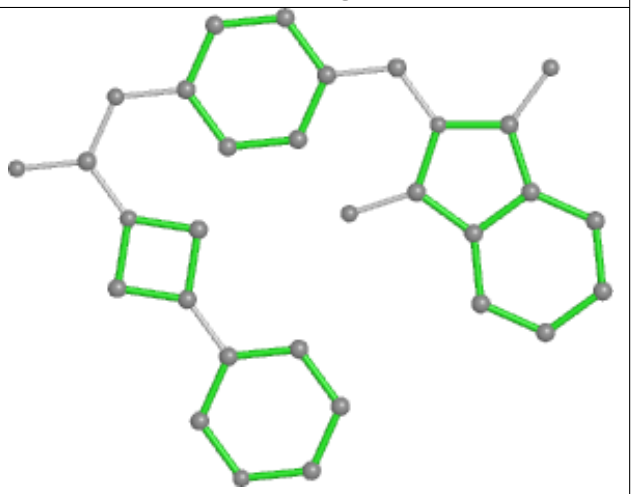
Bond lengths



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	469/500 (93%)	-0.26	1 (0%)	95	95	33, 53, 101, 122	0
1	B	468/500 (93%)	-0.26	3 (0%)	89	89	39, 64, 95, 132	0
1	C	469/500 (93%)	-0.13	7 (1%)	73	71	40, 68, 121, 161	0
1	D	471/500 (94%)	0.05	26 (5%)	25	22	47, 80, 144, 160	0
All	All	1877/2000 (93%)	-0.15	37 (1%)	65	62	33, 67, 126, 161	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	321	VAL	5.5
1	D	284	TYR	5.4
1	B	453	TYR	5.2
1	D	253	TRP	3.6
1	D	325	LEU	3.6
1	D	292	GLY	3.5
1	D	324	VAL	3.3
1	D	272	VAL	3.2
1	C	411	ILE	3.0
1	D	351	ILE	3.0
1	D	276	VAL	2.7
1	B	413	VAL	2.7
1	D	328	LEU	2.5
1	C	22	HIS	2.5
1	D	322	LEU	2.5
1	D	265	ILE	2.5
1	D	254	GLY	2.5
1	D	309	ILE	2.4
1	D	252	ALA	2.4
1	D	44	THR	2.4
1	C	83	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	310	ILE	2.3
1	D	286	ALA	2.3
1	D	307	PRO	2.3
1	C	404	VAL	2.3
1	D	285	ASN	2.2
1	C	413	VAL	2.2
1	D	453	TYR	2.2
1	D	266	VAL	2.1
1	B	452	GLU	2.1
1	D	289	LYS	2.1
1	C	151	ILE	2.0
1	D	373	TRP	2.0
1	D	274	VAL	2.0
1	C	453	TYR	2.0
1	D	269	PHE	2.0
1	A	51	LYS	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	PO4	D	603	5/5	0.76	0.35	134,134,135,137	0
3	PO4	D	602	5/5	0.82	0.21	142,142,143,144	0
3	PO4	A	603	5/5	0.84	0.22	133,133,134,136	0
3	PO4	B	604	5/5	0.88	0.31	73,82,85,90	0
3	PO4	C	602	5/5	0.88	0.18	110,110,111,112	0
3	PO4	C	603	5/5	0.90	0.18	108,111,111,111	0
3	PO4	B	603	5/5	0.92	0.17	107,108,111,113	0

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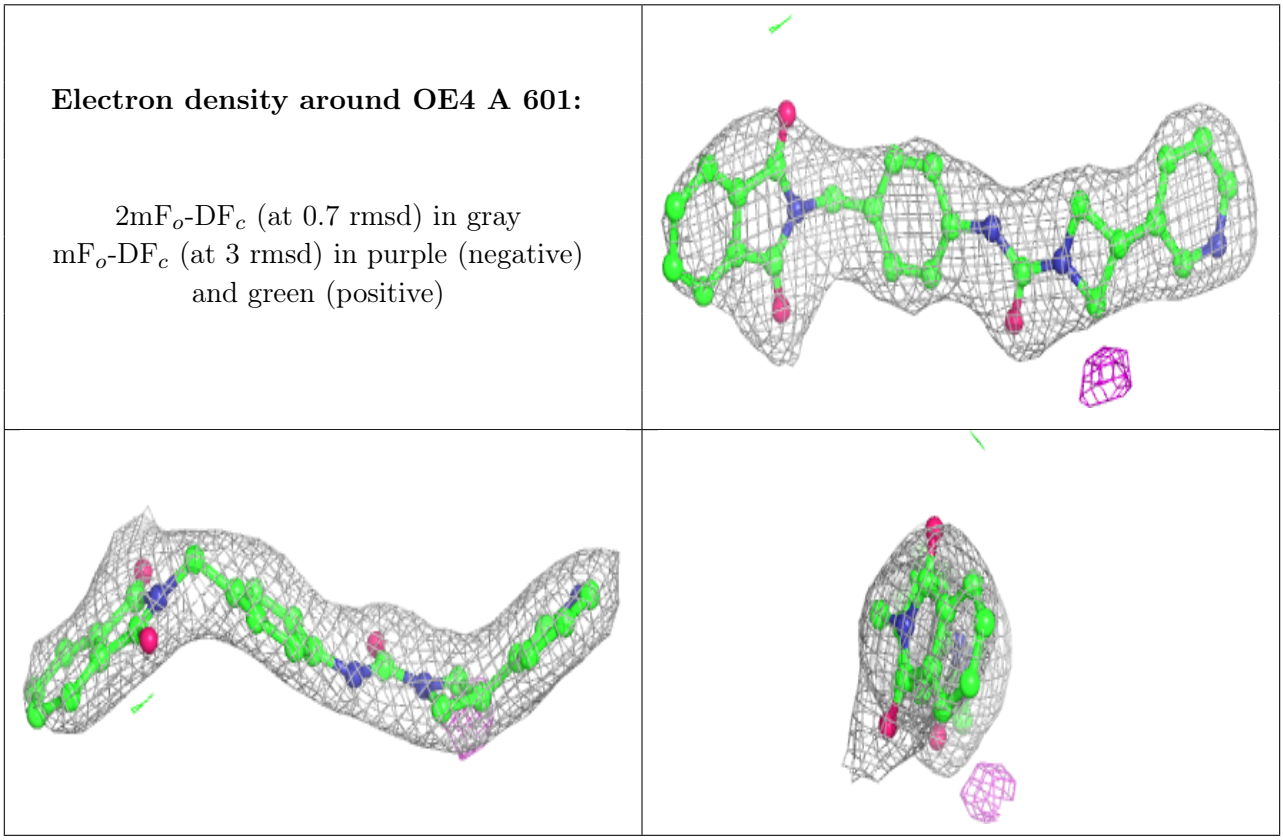
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	A	604	5/5	0.93	0.31	94,95,99,103	0
3	PO4	B	602	5/5	0.94	0.19	80,86,89,89	0
3	PO4	C	604	5/5	0.95	0.24	62,77,81,82	0
2	OE4	A	601	31/31	0.96	0.16	44,62,83,85	0
2	OE4	B	601	31/31	0.96	0.17	35,65,78,80	0
3	PO4	D	601	5/5	0.97	0.17	71,74,76,77	0
2	OE4	C	601	31/31	0.97	0.15	40,52,68,69	0
3	PO4	A	602	5/5	0.97	0.16	59,63,65,69	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.

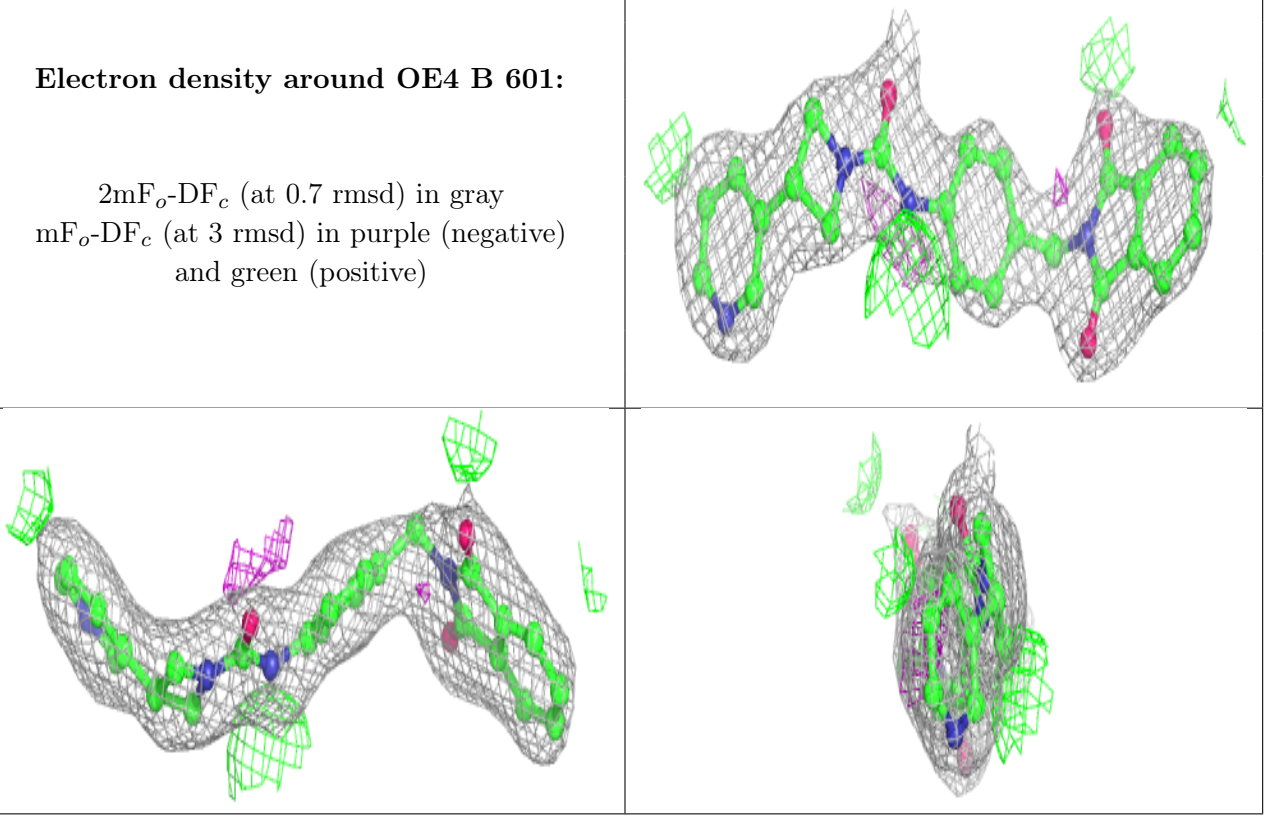
Electron density around OE4 A 601:

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



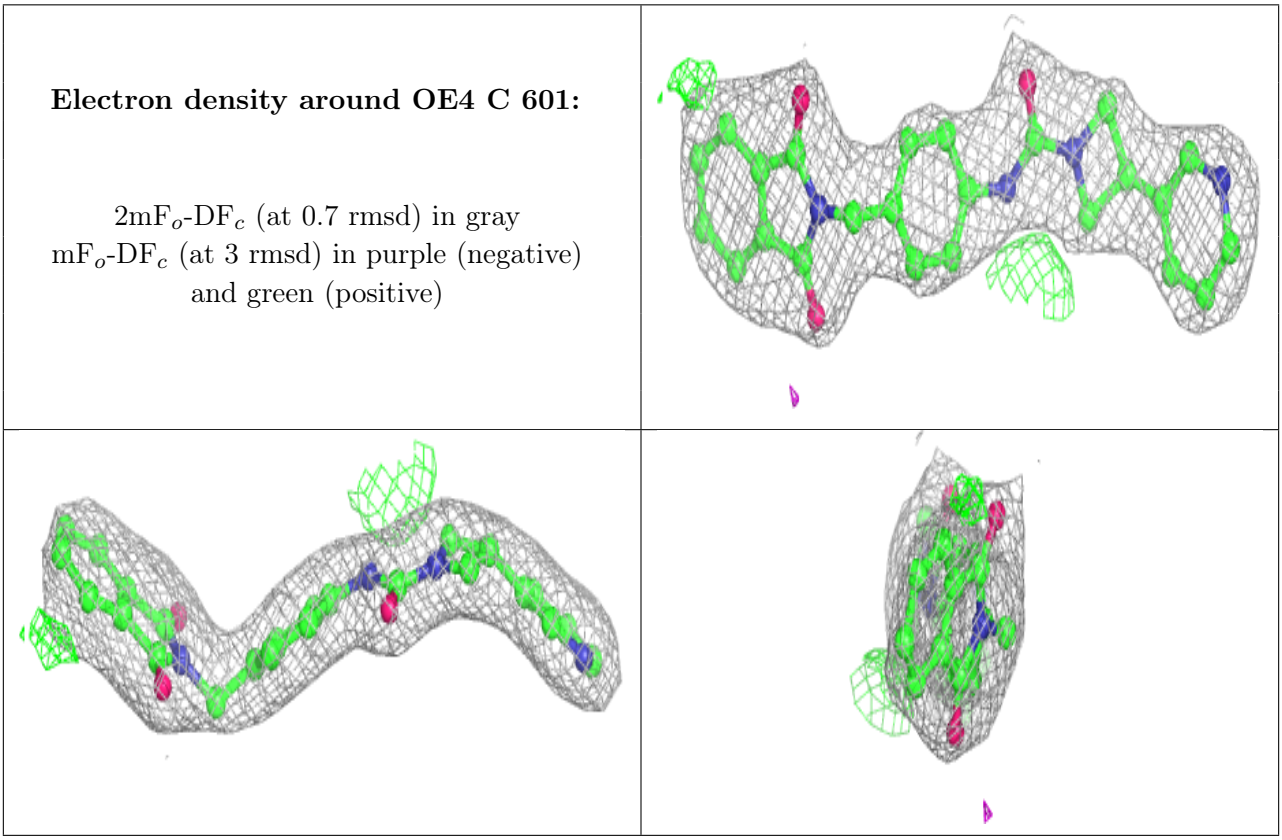
Electron density around OE4 B 601:

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



Electron density around OE4 C 601:

$2mF_o$-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.