



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:21 pm BST

PDB ID : 4PIV
Title : Human Fatty Acid Synthase Psi/KR Tri-Domain with NADPH and GSK2194069
Authors : Williams, S.P.; Wang, L.; Brown, K.K.; Parrish, C.A.; Hardwicke, M.A.
Deposited on : 2014-05-09
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

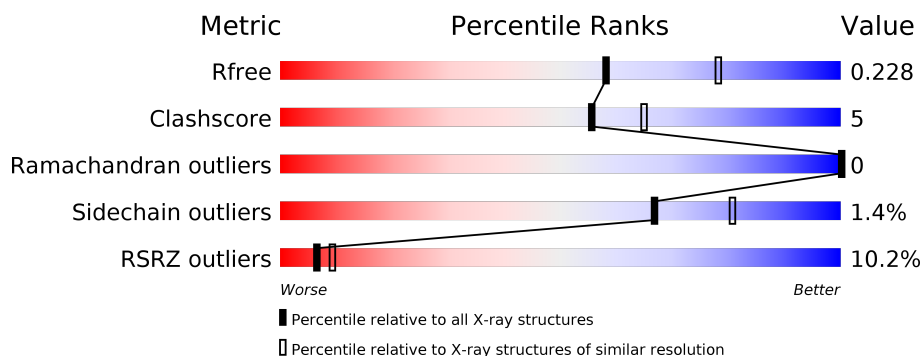
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	660	<div> <div>10%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	B	660	<div> <div>9%</div> <div>80%</div> <div>12%</div> <div>8%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9351 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.

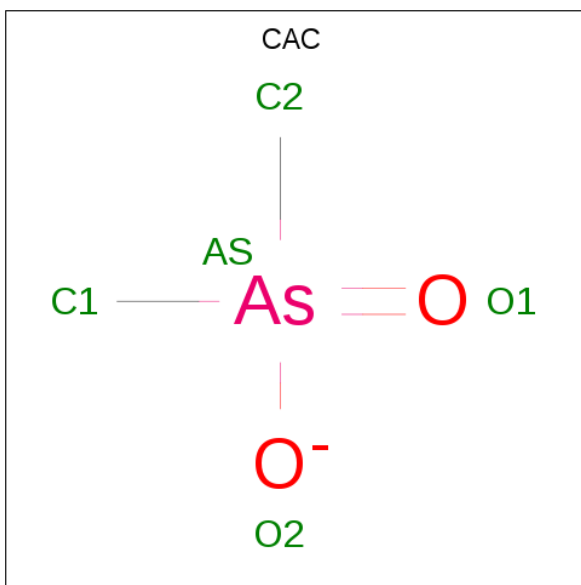
- Molecule 1 is a protein called Fatty acid synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	610	Total	C	N	O	S	0	1	0
			4462	2837	786	815	24			
1	B	610	Total	C	N	O	S	0	0	0
			4481	2847	783	827	24			

There are 16 discrepancies between the modelled and reference sequences:

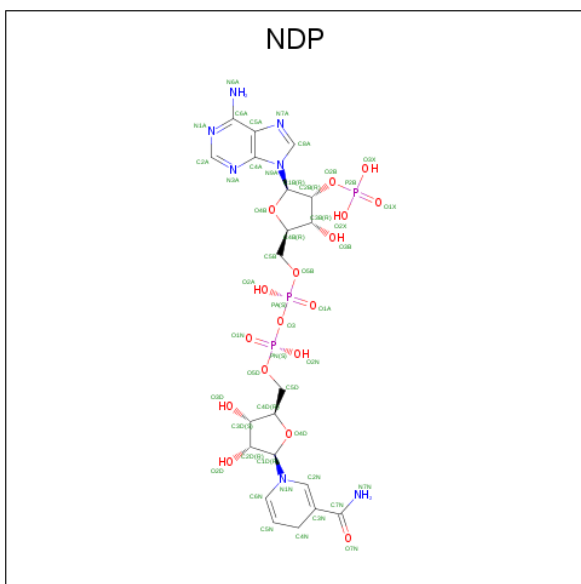
Chain	Residue	Modelled	Actual	Comment	Reference
A	1109	MET	-	initiating methionine	UNP P49327
A	1876	GLY	PRO	engineered mutation	UNP P49327
A	2115	HIS	-	expression tag	UNP P49327
A	2116	HIS	-	expression tag	UNP P49327
A	2117	HIS	-	expression tag	UNP P49327
A	2118	HIS	-	expression tag	UNP P49327
A	2119	HIS	-	expression tag	UNP P49327
A	2120	HIS	-	expression tag	UNP P49327
B	1109	MET	-	initiating methionine	UNP P49327
B	1876	GLY	PRO	engineered mutation	UNP P49327
B	2115	HIS	-	expression tag	UNP P49327
B	2116	HIS	-	expression tag	UNP P49327
B	2117	HIS	-	expression tag	UNP P49327
B	2118	HIS	-	expression tag	UNP P49327
B	2119	HIS	-	expression tag	UNP P49327
B	2120	HIS	-	expression tag	UNP P49327

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



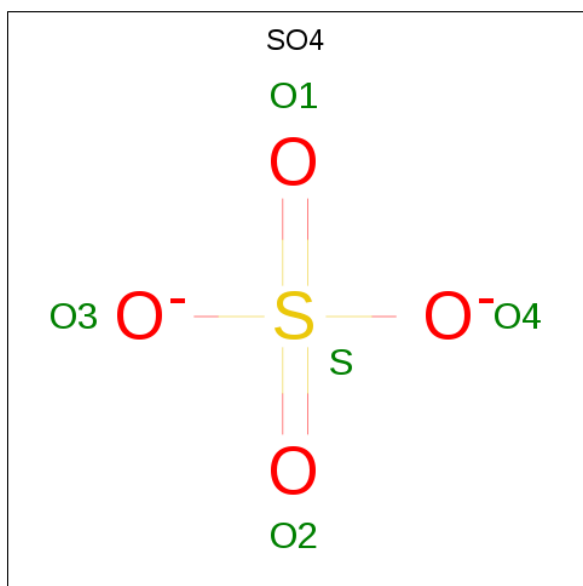
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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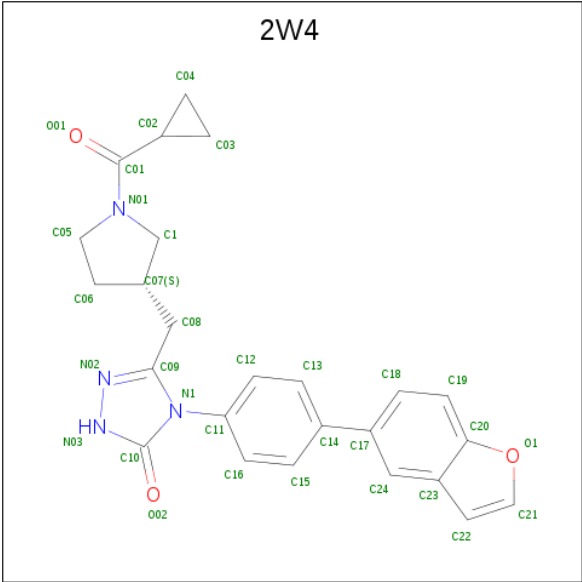
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 4-[4-(1-benzofuran-5-yl)phenyl]-5-[[[(3S)-1-(cyclopropylcarbonyl)pyrrolidin-3-yl]methyl]-2,4-dihydro-3H-1,2,4-triazol-3-one (three-letter code: 2W4) (formula: C₂₅H₂₄N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			32	25	4	3		
5	B	1	Total	C	N	O	0	0
			32	25	4	3		

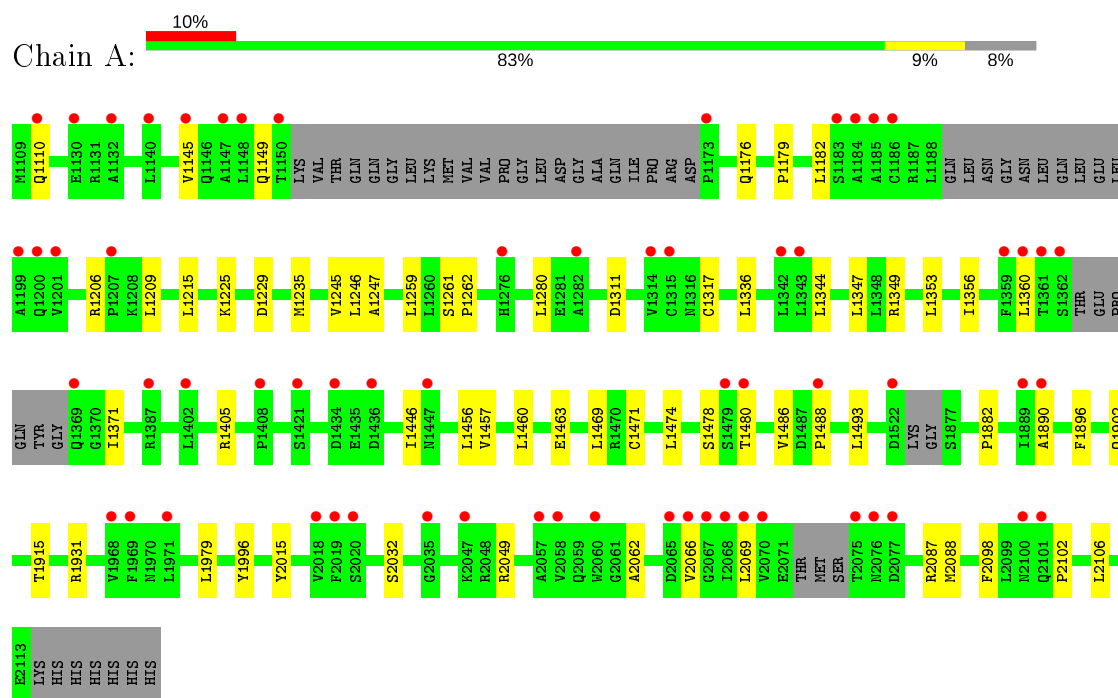
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	102	Total	O	0	0
			102	102		
6	B	118	Total	O	0	0
			118	118		

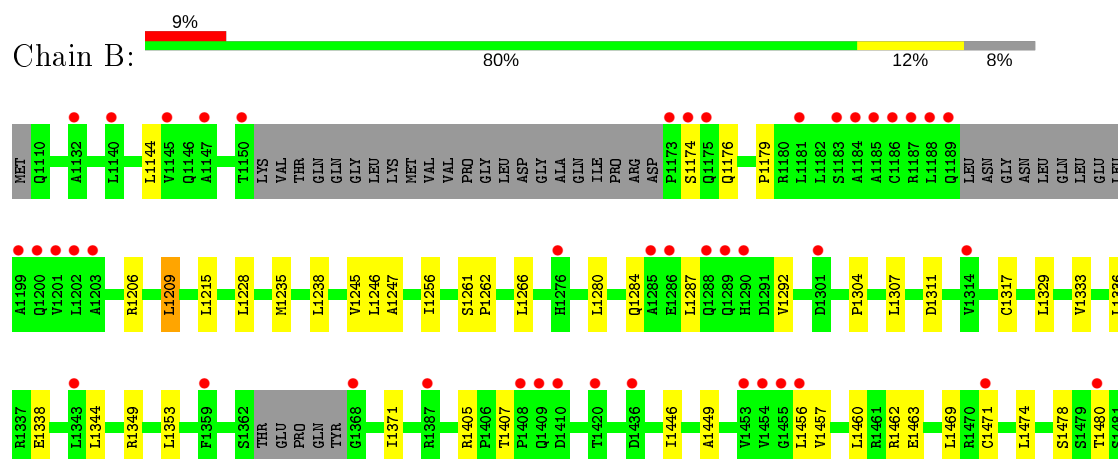
3 Residue-property plots [i](#)

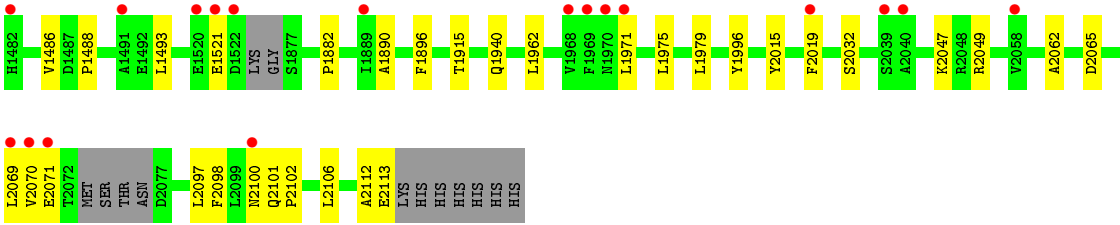
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Fatty acid synthase



• Molecule 1: Fatty acid synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.22Å 85.76Å 86.00Å 65.49° 89.96° 87.22°	Depositor
Resolution (Å)	28.55 – 2.30 28.55 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (28.55-2.30) 95.5 (28.55-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0109, BUSTER	Depositor
R, R_{free}	0.214 , 0.246 0.199 , 0.228	Depositor DCC
R_{free} test set	3898 reflections (7.34%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9351	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, NDP, 2W4, SO4

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	0.33	0/4552	0.55	0/6200
1	B	0.33	0/4568	0.55	0/6216
All	All	0.33	0/9120	0.55	0/12416

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	4462	0	4365	39	0
1	B	4481	0	4404	51	0
2	A	4	0	0	2	0
2	B	4	0	0	2	0
3	A	48	0	26	1	0
3	B	48	0	26	1	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	32	0	24	1	0
5	B	32	0	24	2	0
6	A	102	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	118	0	0	1	0
All	All	9351	0	8869	92	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 (92) 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:1110:GLN:HE22	1:A:2087:ARG:H	1.25	0.84
1:A:2062:ALA:HB1	1:A:2069:LEU:HD21	1.65	0.78
1:B:1338:GLU:HB3	1:B:1407:THR:HG22	1.66	0.75
1:B:2101:GLN:OE1	1:B:2101:GLN:HA	1.89	0.72
1:A:1110:GLN:NE2	1:A:2087:ARG:H	1.89	0.71
1:B:1478:SER:OG	1:B:1480:THR:HG22	1.91	0.70
1:A:1446:ILE:HG23	1:A:1474:LEU:HD12	1.76	0.68
1:B:1449:ALA:HB1	1:B:2047:LYS:HE3	1.77	0.67
1:A:1478:SER:OG	1:A:1480:THR:HG22	1.96	0.64
1:B:1209:LEU:HD22	1:B:1215:LEU:CD1	2.30	0.61
1:B:1456:LEU:HD12	1:B:2032:SER:HB2	1.82	0.61
1:A:1456:LEU:HD12	1:A:2032:SER:HB2	1.83	0.61
1:A:1486:VAL:O	1:A:1493:LEU:HD22	2.02	0.60
1:B:1446:ILE:HG23	1:B:1474:LEU:HD12	1.84	0.59
1:B:1209:LEU:HD22	1:B:1215:LEU:HD12	1.84	0.59
1:B:1215:LEU:HD23	1:B:1353:LEU:HD21	1.83	0.59
1:B:1349:ARG:HB2	1:B:1371:ILE:HG22	1.85	0.58
1:B:1304:PRO:HD2	1:B:1307:LEU:HD12	1.84	0.58
1:B:1486:VAL:O	1:B:1493:LEU:HD22	2.03	0.57
1:B:1462:ARG:NH2	6:B:2355:HOH:O	2.20	0.57
1:A:2062:ALA:HB1	1:A:2069:LEU:CD2	2.33	0.57
1:A:1215:LEU:HD23	1:A:1353:LEU:HD21	1.87	0.56
1:A:1446:ILE:HG23	1:A:1474:LEU:CD1	2.36	0.56
1:A:1488:PRO:HA	1:A:1493:LEU:HD23	1.87	0.55
1:A:2049:ARG:NH2	1:A:2102:PRO:O	2.39	0.54
1:B:1521:GLU:CB	1:B:2101:GLN:HE22	2.20	0.54
3:A:2202:NDP:H41N	5:A:2205:2W4:C01	2.38	0.54
1:A:2015:TYR:CE2	2:A:2201:CAC:C1	2.91	0.53
1:B:1317:CYS:SG	1:B:1344:LEU:HD11	2.49	0.53
1:B:2062:ALA:HB1	1:B:2069:LEU:CD2	2.39	0.52
1:B:1176:GLN:HA	1:B:1176:GLN:NE2	2.24	0.52
1:B:2049:ARG:NH2	1:B:2102:PRO:O	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:CYS:SG	1:A:1344:LEU:HD11	2.50	0.52
1:B:1463:GLU:HG2	1:B:1979:LEU:HD22	1.93	0.51
1:A:1457:VAL:HG21	1:A:1471:CYS:HB3	1.92	0.51
1:B:1971:LEU:HD22	1:B:2019:PHE:CG	2.45	0.51
1:B:1457:VAL:HG21	1:B:1471:CYS:HB3	1.92	0.50
1:A:1176:GLN:NE2	1:A:1176:GLN:HA	2.27	0.50
1:A:1463:GLU:HG2	1:A:1979:LEU:HD22	1.93	0.50
1:B:1971:LEU:HD22	1:B:2019:PHE:CD2	2.46	0.50
1:A:1145:VAL:HG21	1:A:1356:ILE:HG12	1.93	0.50
1:A:1176:GLN:O	1:A:1179:PRO:HD2	2.12	0.50
1:B:1176:GLN:O	1:B:1179:PRO:HD2	2.13	0.49
1:B:2062:ALA:HB1	1:B:2069:LEU:HD21	1.93	0.49
1:A:1110:GLN:HE22	1:A:2087:ARG:N	2.03	0.49
3:B:2202:NDP:H41N	5:B:2205:2W4:C01	2.43	0.48
1:A:1225:LYS:NZ	1:A:1229:ASP:OD2	2.46	0.48
1:B:1940:GLN:HG3	1:B:1962:LEU:HD11	1.95	0.48
1:B:2015:TYR:CE2	2:B:2201:CAC:C2	2.97	0.47
1:B:1488:PRO:HA	1:B:1493:LEU:HD23	1.96	0.47
1:B:1235:MET:SD	1:B:1311:ASP:HB3	2.55	0.47
1:A:1182:LEU:HD23	1:A:1360:LEU:HD13	1.97	0.47
1:B:1521:GLU:HB2	1:B:2101:GLN:HE22	1.78	0.47
1:B:1460:LEU:HB3	1:B:1469:LEU:HD13	1.96	0.47
1:B:1238:LEU:O	1:B:1266:LEU:HD12	2.15	0.46
1:B:1975:LEU:HD11	5:B:2205:2W4:H7	1.98	0.46
1:A:1890:ALA:HA	1:A:1915:THR:OG1	2.15	0.46
1:A:1235:MET:SD	1:A:1311:ASP:HB3	2.56	0.46
1:B:1890:ALA:HA	1:B:1915:THR:OG1	2.15	0.46
1:B:2112:ALA:O	1:B:2113:GLU:C	2.54	0.46
1:B:1882:PRO:HD2	2:B:2201:CAC:C2	2.45	0.46
1:A:1902:GLN:HE22	1:A:1931:ARG:HH22	1.64	0.45
1:A:2066:VAL:HG22	1:A:2088:MET:HE3	1.99	0.45
1:B:1228:LEU:HD11	1:B:1256:ILE:HG12	1.99	0.44
1:A:1261:SER:N	1:A:1262:PRO:CD	2.81	0.44
1:B:1247:ALA:HB3	1:B:1280:LEU:HD21	1.99	0.44
1:A:1209:LEU:HG	1:A:1215:LEU:CD1	2.48	0.44
1:B:1261:SER:N	1:B:1262:PRO:CD	2.81	0.44
1:A:1336:LEU:O	1:A:1405:ARG:NH2	2.51	0.43
1:B:2098:PHE:CD1	1:B:2106:LEU:HD13	2.53	0.43
1:B:1336:LEU:O	1:B:1405:ARG:NH1	2.51	0.43
1:A:1245:VAL:HG12	1:A:1246:LEU:HG	2.01	0.43
1:B:1287:LEU:HD22	1:B:1292:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1209:LEU:O	1:A:1215:LEU:HD12	2.18	0.43
1:B:1209:LEU:HD22	1:B:1215:LEU:HD11	1.98	0.43
1:B:2065:ASP:N	1:B:2070:VAL:HG21	2.34	0.43
1:B:2097:LEU:O	1:B:2101:GLN:HG2	2.19	0.43
1:B:2101:GLN:OE1	1:B:2101:GLN:CA	2.62	0.43
1:B:1287:LEU:HD22	1:B:1292:VAL:CG1	2.49	0.42
1:B:1446:ILE:HG23	1:B:1474:LEU:CD1	2.47	0.42
1:A:1882:PRO:HD2	2:A:2201:CAC:C1	2.50	0.42
1:A:1215:LEU:HD22	1:A:1347:LEU:HD11	2.01	0.42
1:A:1247:ALA:HB3	1:A:1280:LEU:HD21	2.02	0.41
1:A:1460:LEU:HB3	1:A:1469:LEU:HD13	2.01	0.41
1:A:1259:LEU:HD11	6:A:2324:HOH:O	2.19	0.41
1:B:1329:LEU:O	1:B:1333:VAL:HG23	2.21	0.41
1:A:1349:ARG:HB2	1:A:1371:ILE:HG22	2.01	0.41
1:A:2098:PHE:CD1	1:A:2106:LEU:HD13	2.56	0.41
1:B:1209:LEU:O	1:B:1215:LEU:HD12	2.21	0.41
1:B:1460:LEU:CB	1:B:1469:LEU:HD13	2.51	0.41
1:B:1245:VAL:HG12	1:B:1246:LEU:HG	2.02	0.40
1:A:1176:GLN:C	1:A:1179:PRO:HD2	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/660 (91%)	588 (98%)	11 (2%)	0	100	100
1	B	598/660 (91%)	587 (98%)	11 (2%)	0	100	100
All	All	1197/1320 (91%)	1175 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	454/548 (83%)	450 (99%)	4 (1%)	78	89
1	B	462/548 (84%)	453 (98%)	9 (2%)	57	73
All	All	916/1096 (84%)	903 (99%)	13 (1%)	67	81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1149	GLN
1	A	1206	ARG
1	A	1896	PHE
1	A	1996	TYR
1	B	1144	LEU
1	B	1174	SER
1	B	1206	ARG
1	B	1209	LEU
1	B	1284	GLN
1	B	1896	PHE
1	B	1996	TYR
1	B	2071	GLU
1	B	2100	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1110	GLN
1	A	1176	GLN
1	B	1135	GLN
1	B	1176	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
2	CAC	A	2201	1	0,3,4	0.00	-	0,3,6	0.00	-
3	NDP	B	2202	-	45,52,52	0.77	1 (2%)	53,80,80	1.66	8 (15%)
4	SO4	A	2204	-	4,4,4	0.38	0	6,6,6	0.06	0
5	2W4	A	2205	-	31,37,37	0.68	1 (3%)	36,54,54	0.80	1 (2%)
5	2W4	B	2205	-	31,37,37	0.62	1 (3%)	36,54,54	0.79	1 (2%)
3	NDP	A	2202	-	45,52,52	0.77	1 (2%)	53,80,80	1.62	8 (15%)
2	CAC	B	2201	1	0,3,4	0.00	-	0,3,6	0.00	-
4	SO4	B	2203	-	4,4,4	0.31	0	6,6,6	0.22	0
4	SO4	B	2204	-	4,4,4	0.35	0	6,6,6	0.11	0
4	SO4	A	2203	-	4,4,4	0.33	0	6,6,6	0.09	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
5	2W4	A	2205	-	-	0/20/31/31	0/6/6/6
3	NDP	B	2202	-	-	8/30/77/77	0/4/5/5
3	NDP	A	2202	-	-	8/30/77/77	0/4/5/5
5	2W4	B	2205	-	-	0/20/31/31	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2202	NDP	O4B-C1B	2.43	1.44	1.41
3	B	2202	NDP	O4B-C1B	2.32	1.44	1.41
5	A	2205	2W4	C23-C20	-2.17	1.38	1.43
5	B	2205	2W4	C23-C20	-2.11	1.39	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2202	NDP	C1D-N1N-C6N	-5.12	109.79	120.83
3	A	2202	NDP	N3A-C2A-N1A	-4.92	120.99	128.68
3	B	2202	NDP	N3A-C2A-N1A	-4.70	121.33	128.68
3	A	2202	NDP	C1D-N1N-C6N	-4.41	111.33	120.83
3	B	2202	NDP	O4D-C1D-N1N	4.13	116.13	108.06
3	A	2202	NDP	C1D-N1N-C2N	-3.89	114.63	121.11
3	B	2202	NDP	O2B-P2B-O1X	-3.65	95.31	109.39
3	A	2202	NDP	O4D-C1D-N1N	3.57	115.03	108.06
3	A	2202	NDP	O2B-C2B-C1B	3.39	122.31	110.10
3	B	2202	NDP	C3N-C2N-N1N	-3.07	118.71	123.10
3	A	2202	NDP	C3N-C2N-N1N	-2.92	118.92	123.10
5	B	2205	2W4	C10-N03-N02	2.61	113.20	106.15
5	A	2205	2W4	C10-N03-N02	2.60	113.17	106.15
3	A	2202	NDP	C1B-N9A-C4A	-2.37	122.47	126.64
3	B	2202	NDP	PN-O3-PA	-2.30	124.94	132.83
3	B	2202	NDP	C1D-N1N-C2N	-2.30	117.29	121.11
3	B	2202	NDP	O2B-C2B-C1B	2.19	118.00	110.10
3	A	2202	NDP	C4A-C5A-N7A	-2.17	107.13	109.40

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2202	NDP	C5D-O5D-PN-O2N
3	A	2202	NDP	C5D-O5D-PN-O2N
3	B	2202	NDP	C1B-C2B-O2B-P2B
3	B	2202	NDP	C3B-C2B-O2B-P2B
3	B	2202	NDP	C5D-O5D-PN-O3
3	A	2202	NDP	C5D-O5D-PN-O3
3	B	2202	NDP	C5D-O5D-PN-O1N
3	A	2202	NDP	C5D-O5D-PN-O1N
3	B	2202	NDP	O4D-C1D-N1N-C6N
3	A	2202	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	A	2202	NDP	C1B-C2B-O2B-P2B
3	B	2202	NDP	C2D-C1D-N1N-C6N
3	A	2202	NDP	C2D-C1D-N1N-C6N
3	B	2202	NDP	O4B-C4B-C5B-O5B
3	A	2202	NDP	PN-O3-PA-O2A
3	A	2202	NDP	O4B-C4B-C5B-O5B

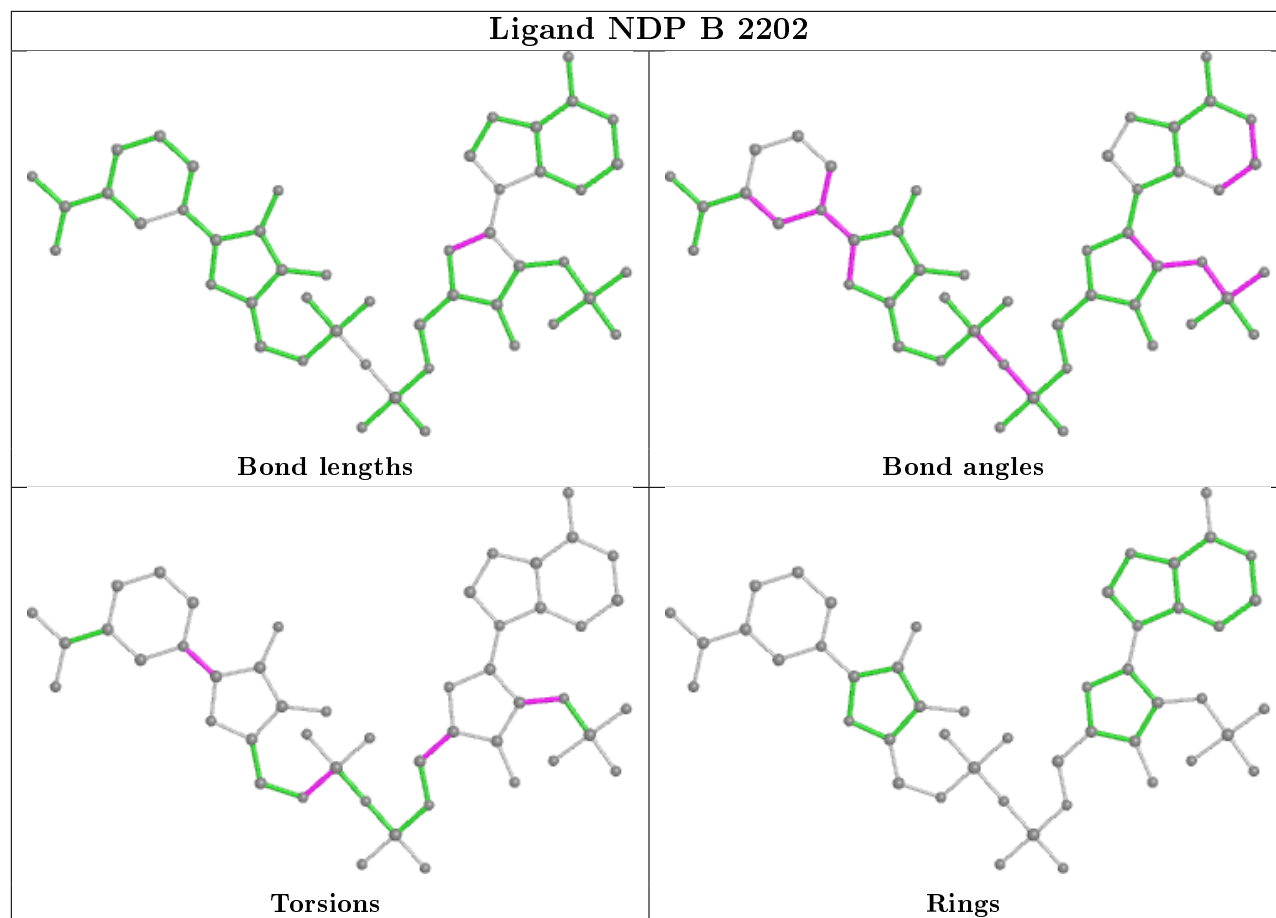
There are no ring outliers.

6 monomers are involved in 7 short contacts:

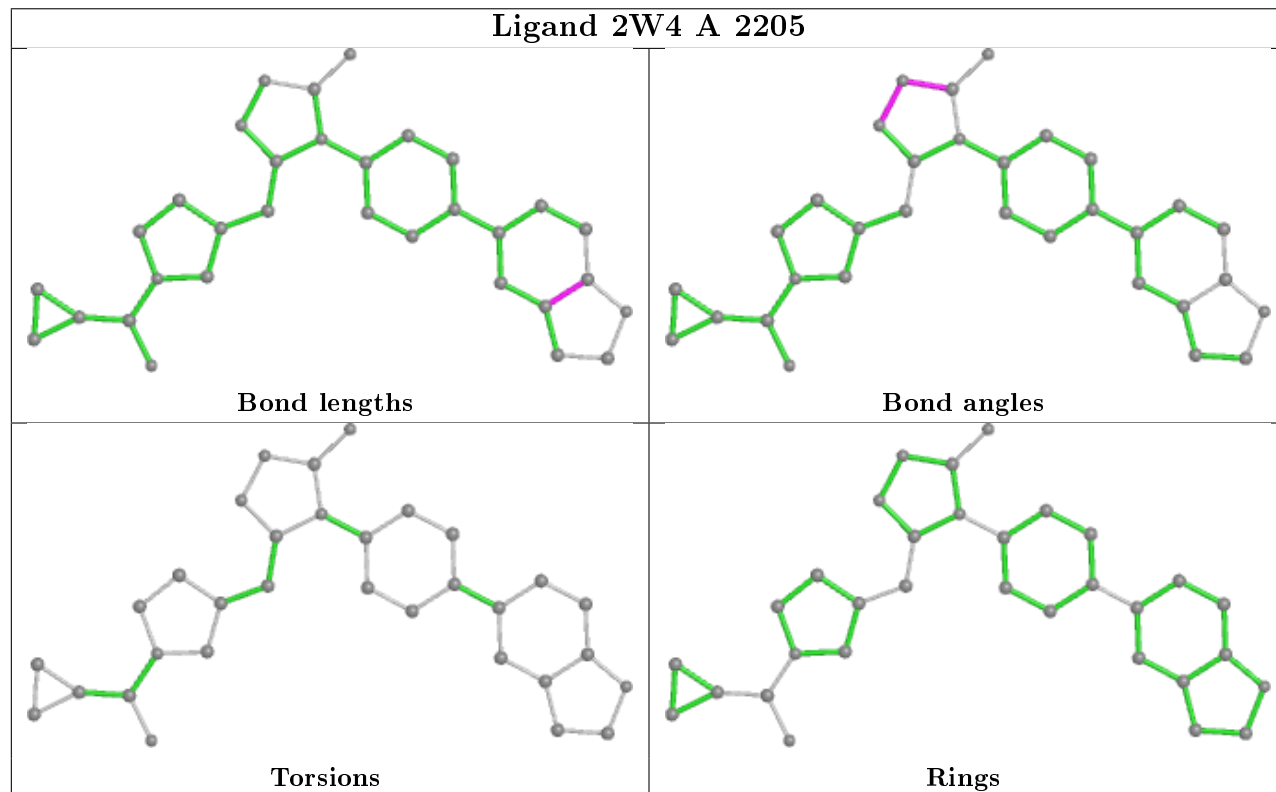
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2201	CAC	2	0
3	B	2202	NDP	1	0
5	A	2205	2W4	1	0
5	B	2205	2W4	2	0
3	A	2202	NDP	1	0
2	B	2201	CAC	2	0

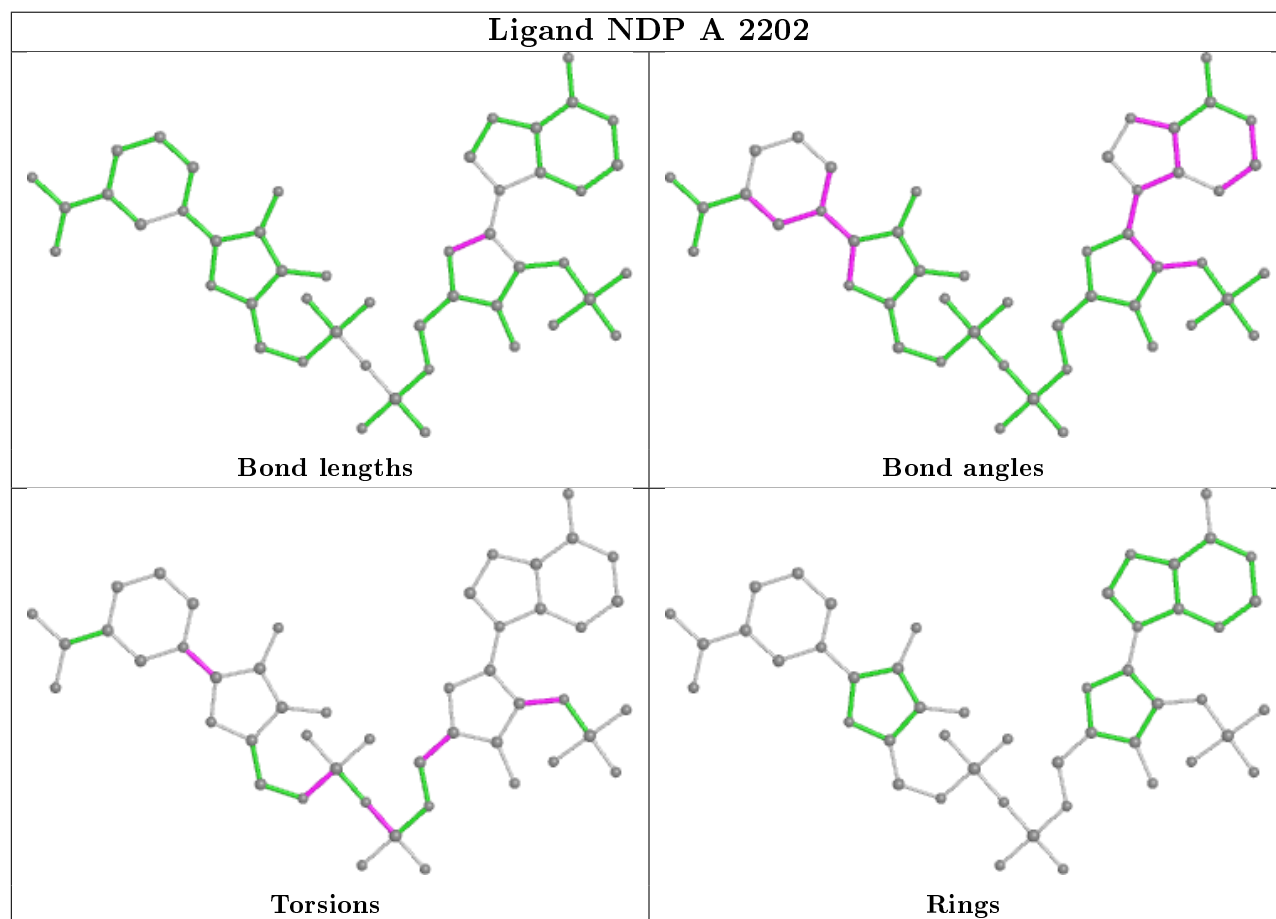
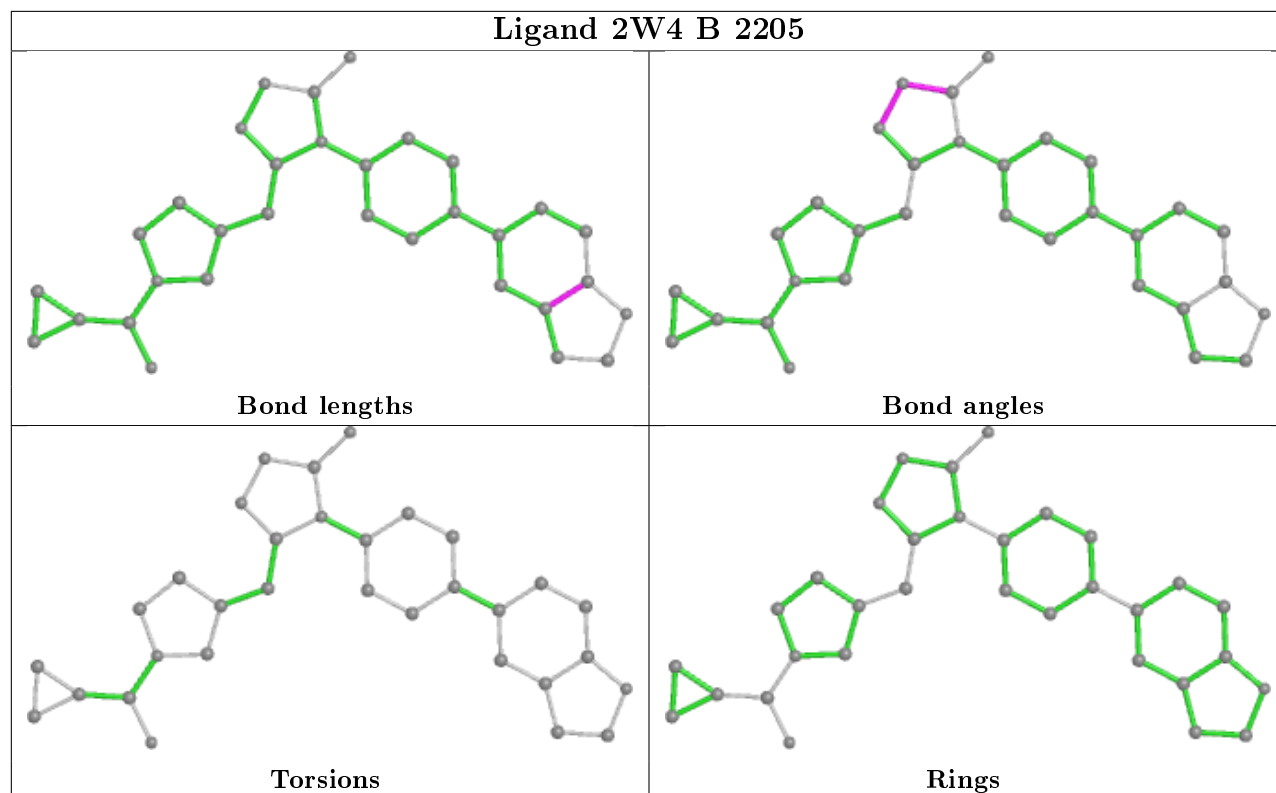
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NDP B 2202



Ligand 2W4 A 2205





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	610/660 (92%)	0.53	63 (10%) 6 9	25, 39, 67, 86	2 (0%)
1	B	610/660 (92%)	0.49	62 (10%) 6 9	22, 37, 70, 92	3 (0%)
All	All	1220/1320 (92%)	0.51	125 (10%) 6 9	22, 38, 70, 92	5 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2075	THR	11.5
1	A	2070	VAL	9.1
1	A	2066	VAL	7.7
1	A	1145	VAL	6.9
1	B	1150	THR	6.8
1	A	1185	ALA	6.5
1	A	2067	GLY	5.9
1	A	2069	LEU	5.5
1	A	1968	VAL	5.0
1	B	1189	GLN	5.0
1	B	1201	VAL	4.9
1	B	1184	ALA	4.9
1	A	2076	ASN	4.9
1	B	1173	PRO	4.8
1	B	1175	GLN	4.8
1	B	1368	GLY	4.7
1	B	1359	PHE	4.6
1	B	1188	LEU	4.6
1	A	2068	ILE	4.4
1	A	1362	SER	4.4
1	A	1200	GLN	4.2
1	A	2077	ASP	4.1
1	B	1174	SER	4.1
1	A	2058	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1359	PHE	4.0
1	B	1186	CYS	3.9
1	A	1140	LEU	3.9
1	B	1202	LEU	3.8
1	B	1183	SER	3.8
1	B	1200	GLN	3.8
1	A	1522	ASP	3.8
1	B	1187	ARG	3.7
1	B	1491	ALA	3.7
1	B	1132	ALA	3.6
1	A	1184	ALA	3.6
1	B	1482	HIS	3.6
1	A	1361	THR	3.6
1	B	2070	VAL	3.6
1	B	1185	ALA	3.5
1	B	1140	LEU	3.5
1	A	1132	ALA	3.3
1	A	1148	LEU	3.2
1	A	1436	ASP	3.2
1	A	1186	CYS	3.1
1	B	1522	ASP	3.1
1	B	1276	HIS	3.1
1	A	1480	THR	3.1
1	A	1369	GLN	3.1
1	A	1147	ALA	3.1
1	A	2019	PHE	3.0
1	A	1343	LEU	3.0
1	A	1282	ALA	3.0
1	B	1520	GLU	3.0
1	B	2039	SER	3.0
1	B	1145	VAL	3.0
1	B	1289	GLN	2.9
1	A	1199	ALA	2.9
1	A	2065	ASP	2.9
1	B	1290	HIS	2.9
1	B	1436	ASP	2.8
1	A	2020	SER	2.8
1	A	1890	ALA	2.8
1	B	1521	GLU	2.8
1	A	1387	ARG	2.8
1	A	2018	VAL	2.8
1	B	1408	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1889	ILE	2.7
1	B	1454	VAL	2.7
1	A	1488	PRO	2.6
1	A	2060	TRP	2.6
1	B	2058	VAL	2.6
1	B	1285	ALA	2.6
1	B	1455	GLY	2.6
1	A	1276	HIS	2.6
1	B	2040	ALA	2.6
1	A	1447	ASN	2.6
1	B	1410	ASP	2.5
1	B	1453	VAL	2.5
1	B	1471	CYS	2.5
1	B	1409	GLN	2.5
1	A	1342	LEU	2.5
1	B	1199	ALA	2.5
1	A	2100	ASN	2.5
1	A	1173	PRO	2.5
1	A	1408	PRO	2.5
1	B	1969	PHE	2.4
1	A	1971	LEU	2.4
1	B	2071	GLU	2.4
1	B	1480	THR	2.4
1	A	1315	CYS	2.4
1	A	1201	VAL	2.4
1	B	1889	ILE	2.4
1	B	1456	LEU	2.4
1	B	1203	ALA	2.4
1	A	1130	GLU	2.4
1	A	1969	PHE	2.4
1	A	2057	ALA	2.3
1	B	2069	LEU	2.3
1	A	2047	LYS	2.3
1	B	1181	LEU	2.3
1	B	1314	VAL	2.3
1	A	1150	THR	2.2
1	A	1479	SER	2.2
1	A	1402	LEU	2.2
1	B	1971	LEU	2.2
1	A	1314	VAL	2.2
1	B	1968	VAL	2.2
1	A	2035	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1387	ARG	2.2
1	B	1147	ALA	2.2
1	B	1970	ASN	2.2
1	B	1301	ASP	2.1
1	A	1183	SER	2.1
1	A	1360	LEU	2.1
1	A	1110	GLN	2.1
1	B	1343	LEU	2.1
1	A	2101	GLN	2.1
1	B	1288	GLN	2.0
1	A	1434	ASP	2.0
1	B	1286	GLU	2.0
1	A	1207	PRO	2.0
1	B	2019	PHE	2.0
1	B	2100	ASN	2.0
1	A	1421	SER	2.0
1	B	1420	THR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

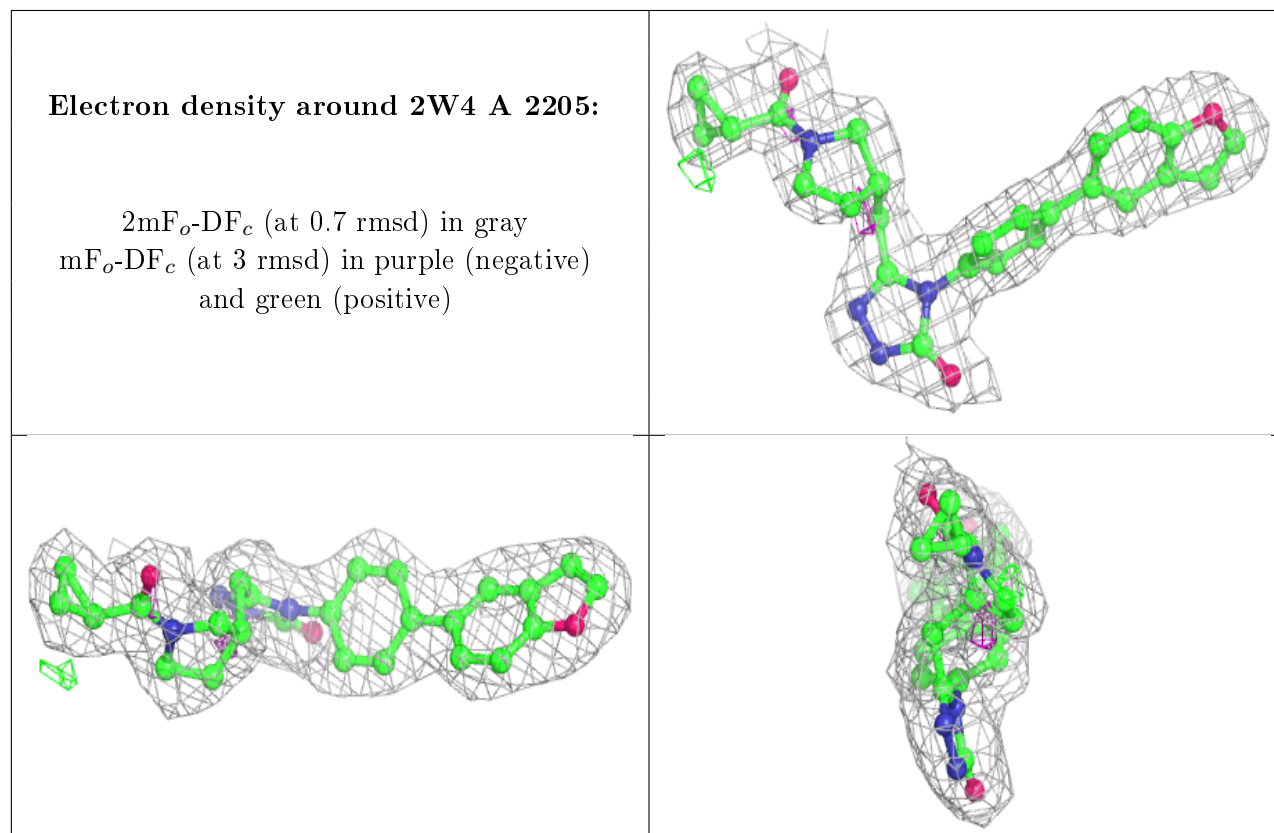
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	2204	5/5	0.88	0.18	74,74,77,78	0
5	2W4	A	2205	32/32	0.94	0.13	26,27,28,29	0
5	2W4	B	2205	32/32	0.94	0.13	24,25,28,30	0
4	SO4	B	2204	5/5	0.94	0.12	65,65,70,72	0
4	SO4	A	2203	5/5	0.94	0.23	60,63,65,66	0
3	NDP	A	2202	48/48	0.95	0.14	26,29,33,34	0

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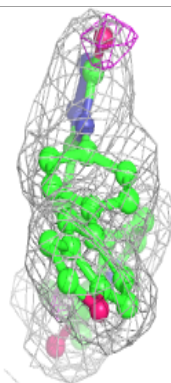
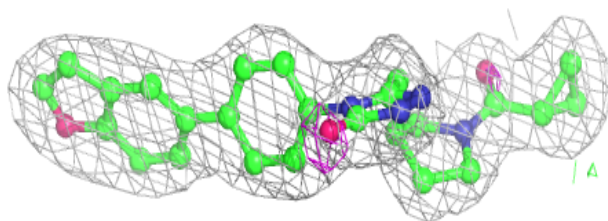
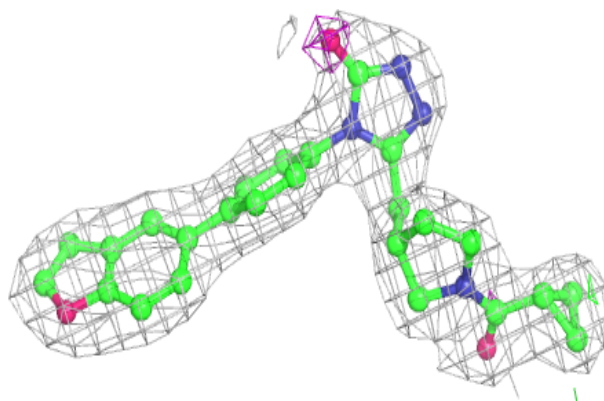
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NDP	B	2202	48/48	0.96	0.12	24,26,30,31	0
4	SO4	B	2203	5/5	0.97	0.17	49,51,52,54	0
2	CAC	A	2201	4/5	0.97	0.15	38,38,40,41	0
2	CAC	B	2201	4/5	0.97	0.15	39,40,43,44	0

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.

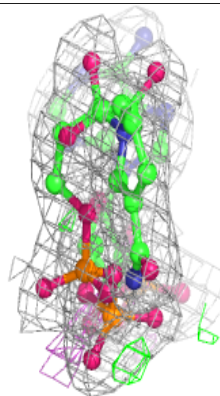
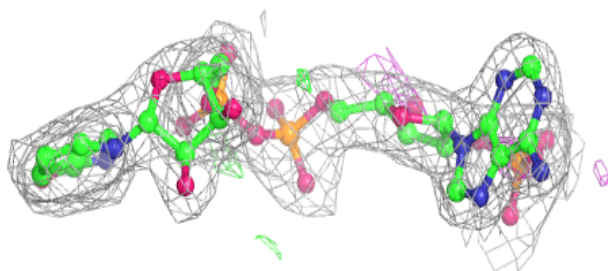
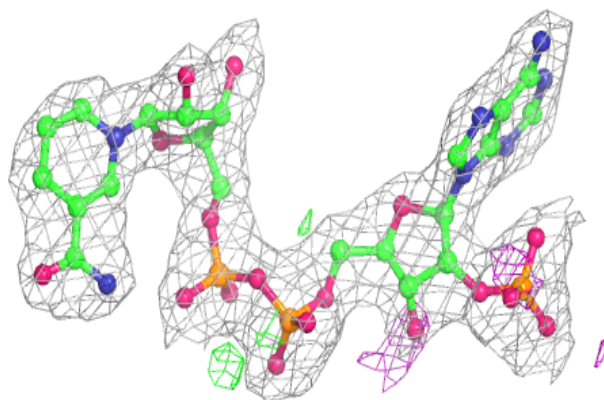


Electron density around 2W4 B 2205:

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

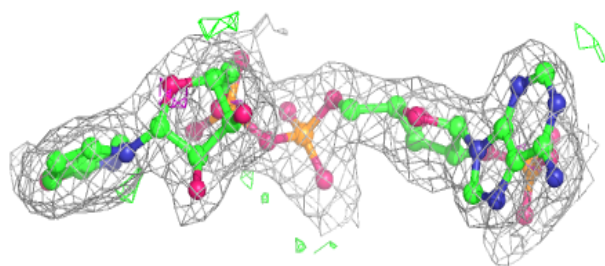
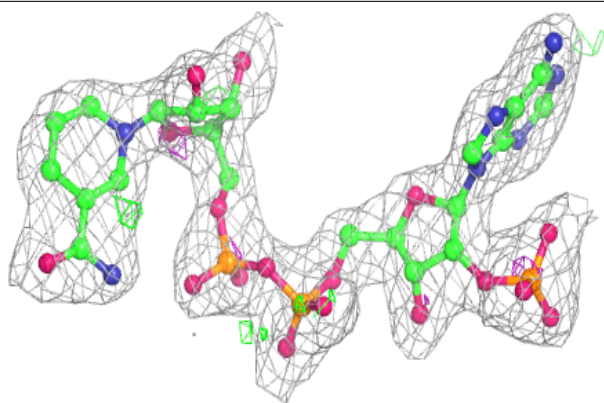
**Electron density around NDP A 2202:**

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



Electron density around NDP B 2202:

$2mF_o-DF_c$ (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.