



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:35 PM UTC

PDB ID : 3SLK / pdb_00003slk
Title : Structure of ketoreductase and enoylreductase didomain from modular polyketide synthase
Authors : Zheng, J.; Gay, D.C.; Keatinge-Clay, A.T.
Deposited on : 2011-06-24
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

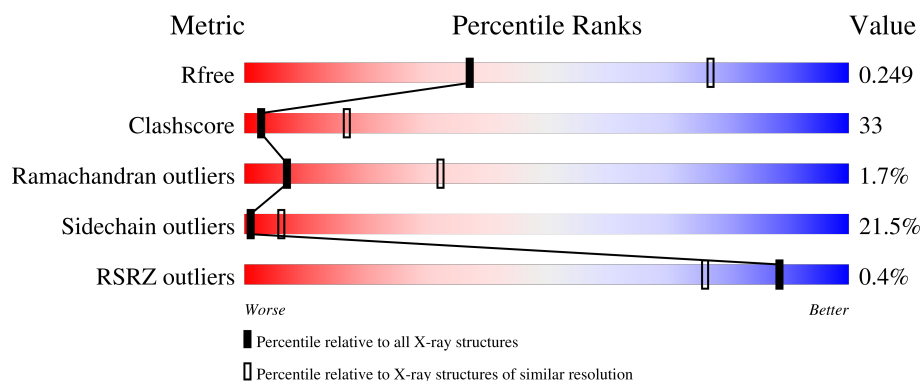
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	795	% 50% 34% 10% • 6%
1	B	795	 53% 32% 8% • 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11217 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 Polyketide synthase extender module 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	747	Total	C	N	O	S	0	0	0
			5505	3457	990	1043	15			
1	B	747	Total	C	N	O	S	0	0	0
			5505	3457	990	1043	15			

There are 42 discrepancies between the modelled and reference sequences:

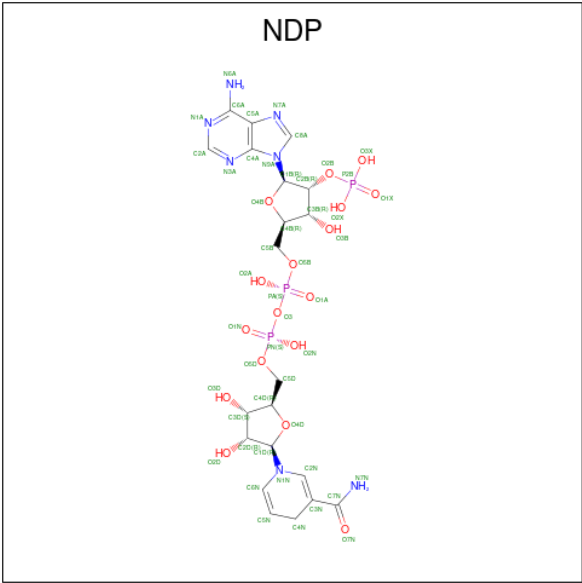
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q9ALM5
A	-19	GLY	-	expression tag	UNP Q9ALM5
A	-18	SER	-	expression tag	UNP Q9ALM5
A	-17	SER	-	expression tag	UNP Q9ALM5
A	-16	HIS	-	expression tag	UNP Q9ALM5
A	-15	HIS	-	expression tag	UNP Q9ALM5
A	-14	HIS	-	expression tag	UNP Q9ALM5
A	-13	HIS	-	expression tag	UNP Q9ALM5
A	-12	HIS	-	expression tag	UNP Q9ALM5
A	-11	HIS	-	expression tag	UNP Q9ALM5
A	-10	SER	-	expression tag	UNP Q9ALM5
A	-9	SER	-	expression tag	UNP Q9ALM5
A	-8	GLY	-	expression tag	UNP Q9ALM5
A	-7	LEU	-	expression tag	UNP Q9ALM5
A	-6	VAL	-	expression tag	UNP Q9ALM5
A	-5	PRO	-	expression tag	UNP Q9ALM5
A	-4	ARG	-	expression tag	UNP Q9ALM5
A	-3	GLY	-	expression tag	UNP Q9ALM5
A	-2	SER	-	expression tag	UNP Q9ALM5
A	-1	HIS	-	expression tag	UNP Q9ALM5
A	0	MET	-	expression tag	UNP Q9ALM5
B	-20	MET	-	expression tag	UNP Q9ALM5
B	-19	GLY	-	expression tag	UNP Q9ALM5
B	-18	SER	-	expression tag	UNP Q9ALM5
B	-17	SER	-	expression tag	UNP Q9ALM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	expression tag	UNP Q9ALM5
B	-15	HIS	-	expression tag	UNP Q9ALM5
B	-14	HIS	-	expression tag	UNP Q9ALM5
B	-13	HIS	-	expression tag	UNP Q9ALM5
B	-12	HIS	-	expression tag	UNP Q9ALM5
B	-11	HIS	-	expression tag	UNP Q9ALM5
B	-10	SER	-	expression tag	UNP Q9ALM5
B	-9	SER	-	expression tag	UNP Q9ALM5
B	-8	GLY	-	expression tag	UNP Q9ALM5
B	-7	LEU	-	expression tag	UNP Q9ALM5
B	-6	VAL	-	expression tag	UNP Q9ALM5
B	-5	PRO	-	expression tag	UNP Q9ALM5
B	-4	ARG	-	expression tag	UNP Q9ALM5
B	-3	GLY	-	expression tag	UNP Q9ALM5
B	-2	SER	-	expression tag	UNP Q9ALM5
B	-1	HIS	-	expression tag	UNP Q9ALM5
B	0	MET	-	expression tag	UNP Q9ALM5

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



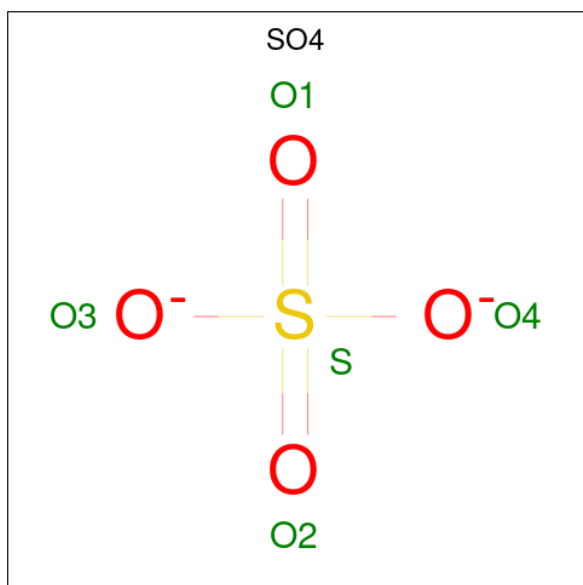
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

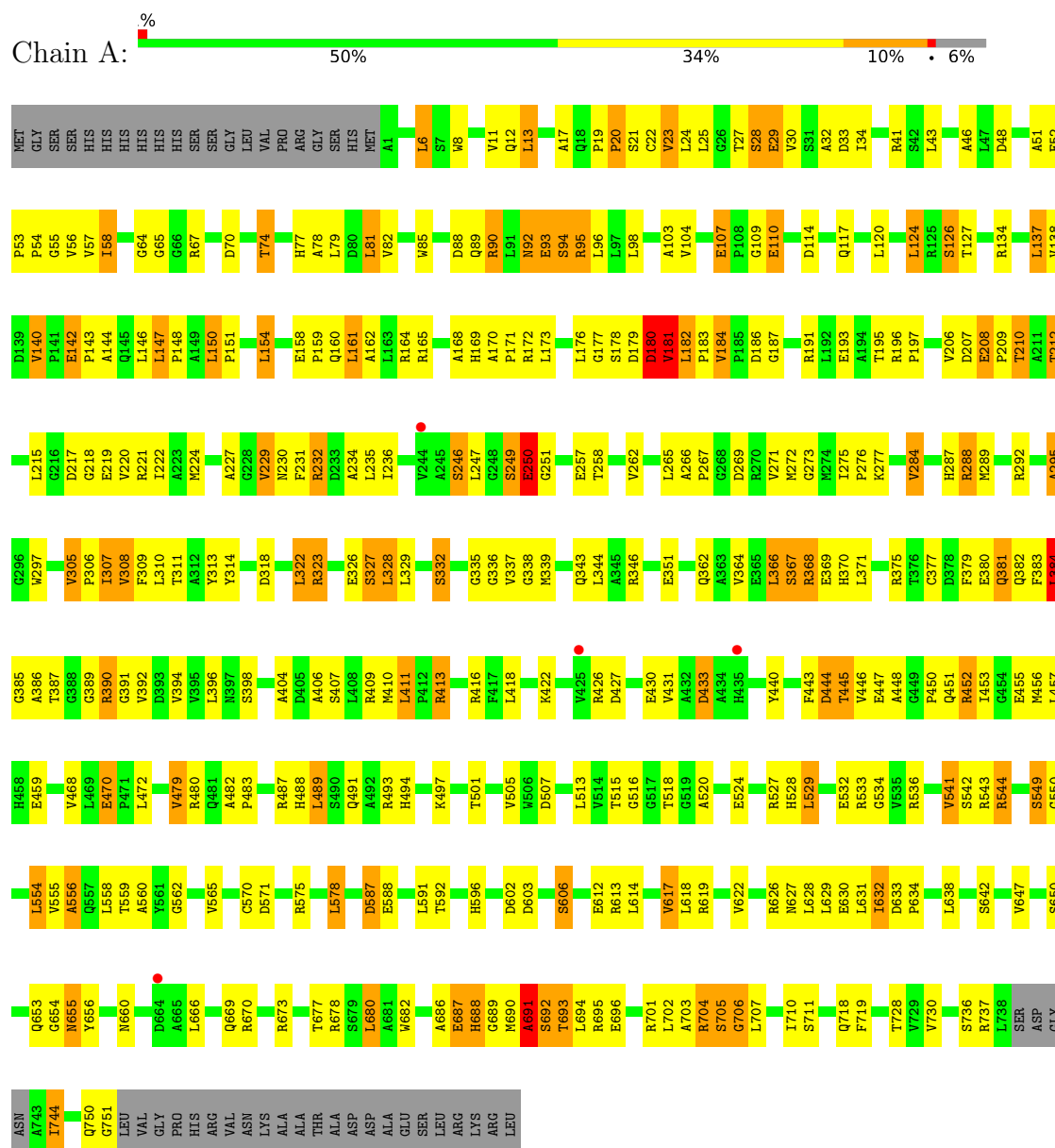


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

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: Polyketide synthase extender module 2



- Molecule 1: Polyketide synthase extender module 2

Chain B: 

LEU	A686	E687	H688	G689	A691	S692	R701	R704	S705	G706	I710	S711	T712	E713	Q718	F719	T728	V729	V730	S736	R737	L738	SER	ASP	GLY	ASN	I743	I744	Q750	G751	LEU	VAL	GLY	PRO	HIS	ARG	VAL	ASN	LYS	ALA	ALA	ALA	THR	ALA	ASP	ASP	ALA	ALA	GLU	SER	LEU	ARG	LYS	ARG
	S606	L609	T610	V611	E612	L613	L614	D615	Q616	V617	L618	R619	P620	K621	R626	N627	L628	L629	E630	L631	I632	D633	P634	D635	L638	S642	S645	G649	S650	G651	G652	Q653	G654	N655	Y656	N660	S661	F662	L663	D664	A665	L666	A667	Q668	Q669	R670	Q671	S672	R673	G674	W685			
	V505	S506	D507	L513	V514	T515	G516	G517	T518	S519	A520	L521	R527	V530	E532	R533	G534	V535	R536	N537	L538	V539	L540	V541	S542	R543	R544	S549	G550	L554	Q557	L558	T559	E564	V565	C570	D571	L578	L579	K580	E588	Y591	T592	H596	D602									
	R413	G414	G415	L420	G421	K422	T423	D424	V425	R426	D427	E430	V431	Y440	D444	E447	A448	G449	R452	T453	M456	L457	H458	E459	L460	V461	L463	R467	E470	T475	D478	V479	R480	Q481	A482	P483	L489	R493	H494	V495	G496	K497	L498	M502										
	G216	D217	G218	E219	V220	R221	M224	R225	V229	N230	P231	R232	G236	Y241	V244	A245	S246	L247	V255	P260	L265	A266	P267	V271	M272	G273	N274	L275	P276	K277	Q280	P281	V284	R288	M289	V290	S304	V305	P306	I307	V308	F309	L310	T311	A312	Y313	Y314							
	V317	D318	L319	A320	G321	L322	R323	L328	L329	V330	H331	G336	V337	I342	Q343	L344	V352	Y353	A354	T355	Q362	E365	A366	S367	R368	A372	S373	S374	R375	E380	Q381	Q382	T387	R390	G391	V392	D393	V394	V395	L396	D405	A406	S407	L408	R409	M410	L411	P412						
	E142	Q145	L146	L147	P148	A149	L150	P151	G152	V153	L154	E158	P159	Q160	L161	A162	L163	R164	R165	G166	G167	A168	H169	A170	P171	R172	L176	G177	S178	D179	L182	P183	V184	P185	D186	G187	T188	G189	W190	R191	L192	E193	R196	L200	L205	V208	E208	T212	A213	P214	L215			
	A51	E52	P53	P54	G55	V56	V57	I58	A59	P60	R67	T68	A69	D70	V71	R72	E73	T74	T75	R76	L79	D80	L81	S87	D88	Q89	R90	L91	N92	E93	S94	R95	L96	L97	V104	A105	V106	E107	D114	Q117	V121	L124	R125	T127	Q128	L137	V138	D139	V140	P141				
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	A1	R5	L6	S7	W8	V11	Q12	L13	P14	T15	Q18	P19	P20	S21	G22	V23	L24	L25	G26	T27	S28	E29	V30	S31	A32	P33	I34	R41	S42	L43	T44	A45	A46	G50

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.10Å 110.19Å 202.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-3.00) 99.6 (50.00-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.210 , 0.256 0.207 , 0.249	Depositor DCC
R_{free} test set	1706 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11217	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.36 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7676e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, NDP

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	0.66	0/5614	0.81	9/7665 (0.1%)
1	B	0.66	0/5614	0.82	12/7665 (0.2%)
All	All	0.66	0/11228	0.82	21/15330 (0.1%)

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	5
1	B	0	6
All	All	0	11

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	THR	N-CA-C	-7.46	104.69	114.31
1	B	26	GLY	N-CA-C	7.16	119.64	110.20
1	A	107	GLU	CA-C-N	6.94	126.46	119.24
1	A	107	GLU	C-N-CA	6.94	126.46	119.24
1	A	184	VAL	CA-C-N	6.08	125.76	119.56

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	534	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	A	549	SER	Peptide
1	A	686	ALA	Peptide
1	A	691	ALA	Peptide
1	A	89	GLN	Peptide

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	5505	0	5524	372	0
1	B	5505	0	5524	367	1
2	A	96	0	52	12	0
2	B	96	0	52	10	0
3	A	10	0	0	1	1
3	B	5	0	0	1	0
All	All	11217	0	11152	741	1

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 33.

The worst 5 of 741 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:384:LEU:HD21	1:A:410:MET:SD	1.59	1.42
1:B:691:ALA:CB	1:B:692:SER:HB2	1.51	1.37
1:B:691:ALA:HB3	1:B:692:SER:CB	1.61	1.28
1:A:550:GLY:N	1:A:690:MET:HE3	1.50	1.26
1:A:691:ALA:HB3	1:A:692:SER:CB	1.64	1.25

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ARG:NH2	3:A:804:SO4:O1[2_564]	2.19	0.01

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	743/795 (94%)	657 (88%)	73 (10%)	13 (2%)	7	32
1	B	743/795 (94%)	684 (92%)	47 (6%)	12 (2%)	7	34
All	All	1486/1590 (94%)	1341 (90%)	120 (8%)	25 (2%)	7	32

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	ASP
1	A	691	ALA
1	B	217	ASP
1	B	691	ALA
1	A	295	ALA

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	566/605 (94%)	447 (79%)	119 (21%)	1	6
1	B	566/605 (94%)	442 (78%)	124 (22%)	1	5
All	All	1132/1210 (94%)	889 (78%)	243 (22%)	1	6

5 of 243 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	728	THR

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Mol	Chain	Res	Type
1	B	617	VAL
1	B	96	LEU
1	B	612	GLU
1	B	704	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	596	HIS
1	B	596	HIS
1	A	671	GLN
1	B	382	GLN
1	A	655	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	SO4	A	804	-	4,4,4	0.43	0	6,6,6	0.15	0
3	SO4	A	803	-	4,4,4	0.47	0	6,6,6	0.20	0
2	NDP	B	801	-	51,52,52	1.30	5 (9%)	71,80,80	1.68	12 (16%)
2	NDP	A	802	-	51,52,52	1.41	6 (11%)	71,80,80	1.78	17 (23%)
3	SO4	B	803	-	4,4,4	0.43	0	6,6,6	0.12	0
2	NDP	B	802	-	51,52,52	1.40	3 (5%)	71,80,80	1.74	15 (21%)
2	NDP	A	801	-	51,52,52	1.31	4 (7%)	71,80,80	1.63	10 (14%)

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	NDP	B	801	-	-	12/34/77/77	0/5/5/5
2	NDP	B	802	-	-	3/34/77/77	0/5/5/5
2	NDP	A	801	-	-	11/34/77/77	0/5/5/5
2	NDP	A	802	-	-	4/34/77/77	0/5/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	NDP	C4N-C3N	-6.18	1.38	1.50
2	A	802	NDP	C4N-C3N	-6.04	1.38	1.50
2	A	801	NDP	C4N-C3N	-5.91	1.38	1.50
2	B	801	NDP	C4N-C3N	-5.82	1.39	1.50
2	A	802	NDP	C4N-C5N	-4.08	1.38	1.49

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	NDP	C5A-C4A-N3A	-5.64	118.95	126.72
2	B	801	NDP	C5A-C4A-N3A	-5.45	119.21	126.72
2	B	802	NDP	N3A-C2A-N1A	-5.08	120.90	128.58
2	A	801	NDP	N3A-C2A-N1A	-5.03	120.96	128.58
2	B	801	NDP	N3A-C2A-N1A	-4.94	121.11	128.58

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

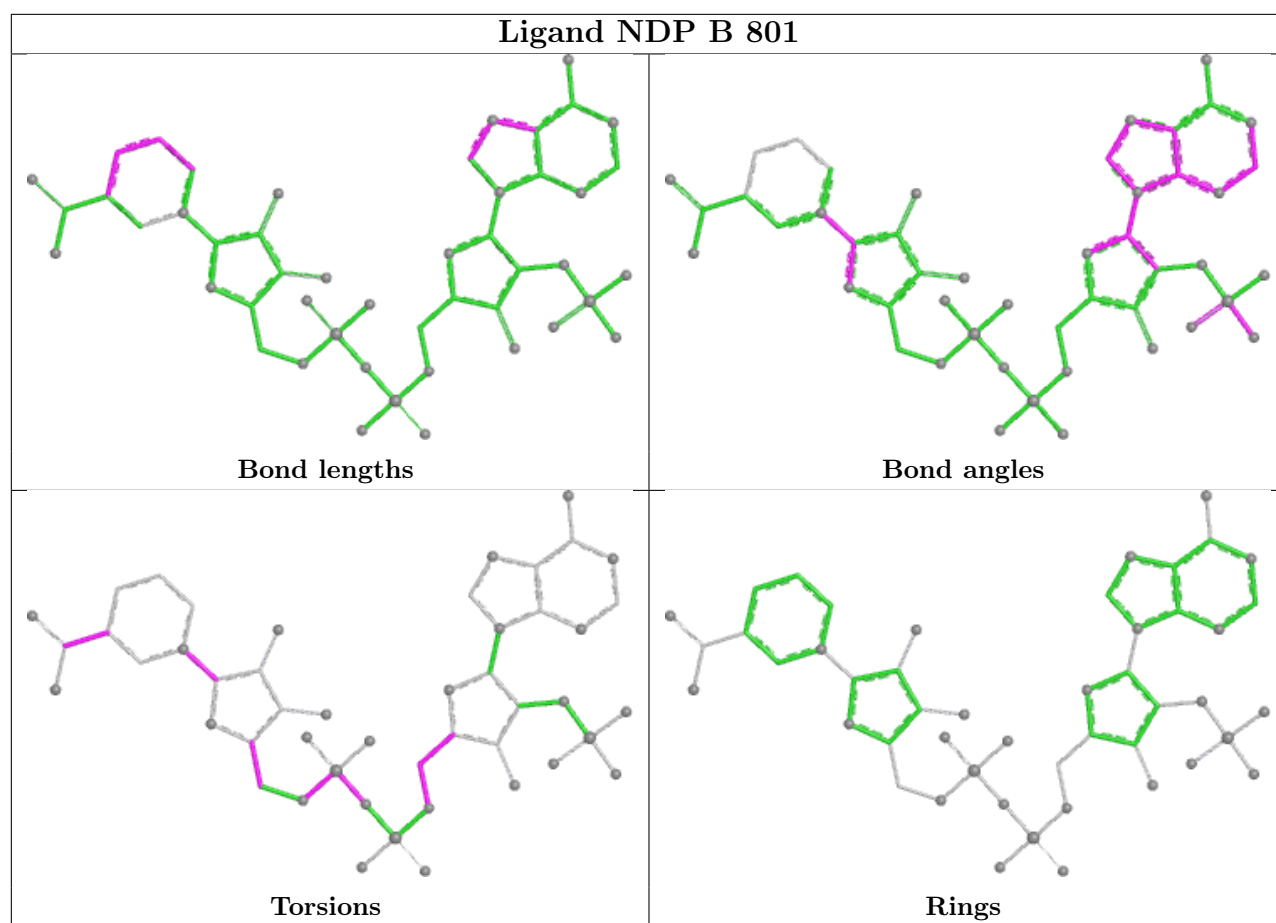
Mol	Chain	Res	Type	Atoms
2	A	801	NDP	C5B-O5B-PA-O1A
2	B	801	NDP	C5D-O5D-PN-O2N
2	B	801	NDP	O4D-C4D-C5D-O5D
2	A	802	NDP	O4D-C1D-N1N-C6N
2	B	802	NDP	O4D-C1D-N1N-C6N

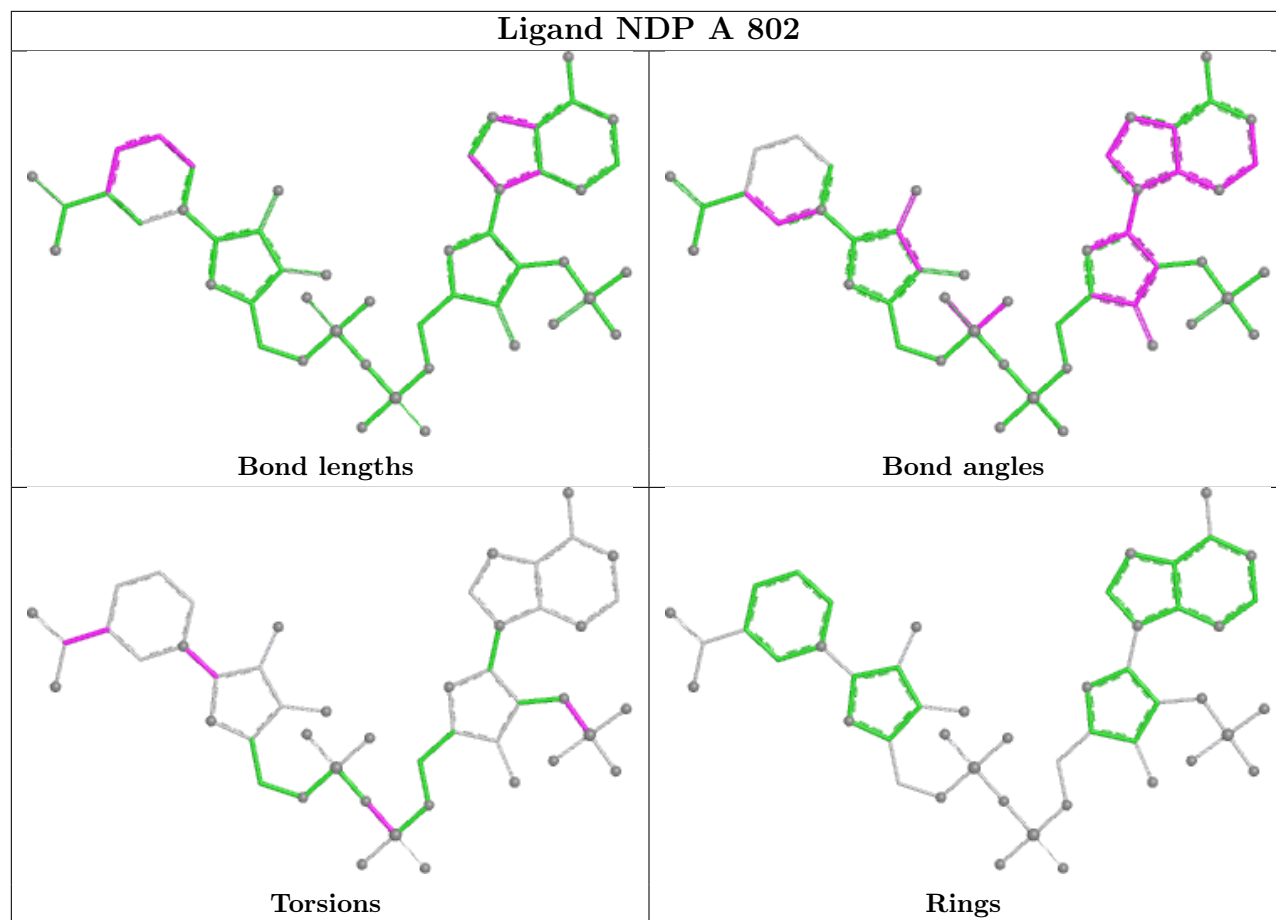
There are no ring outliers.

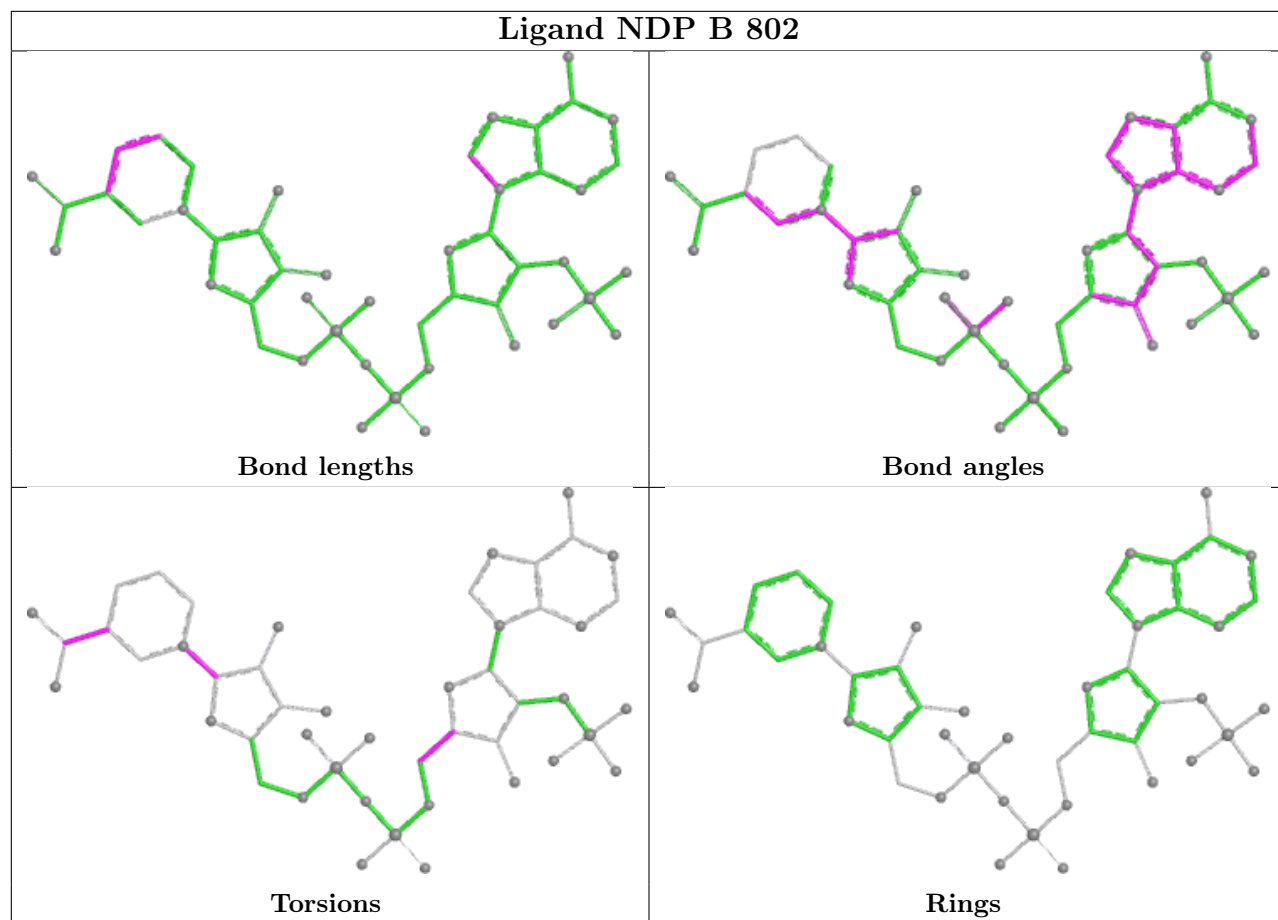
7 monomers are involved in 25 short contacts:

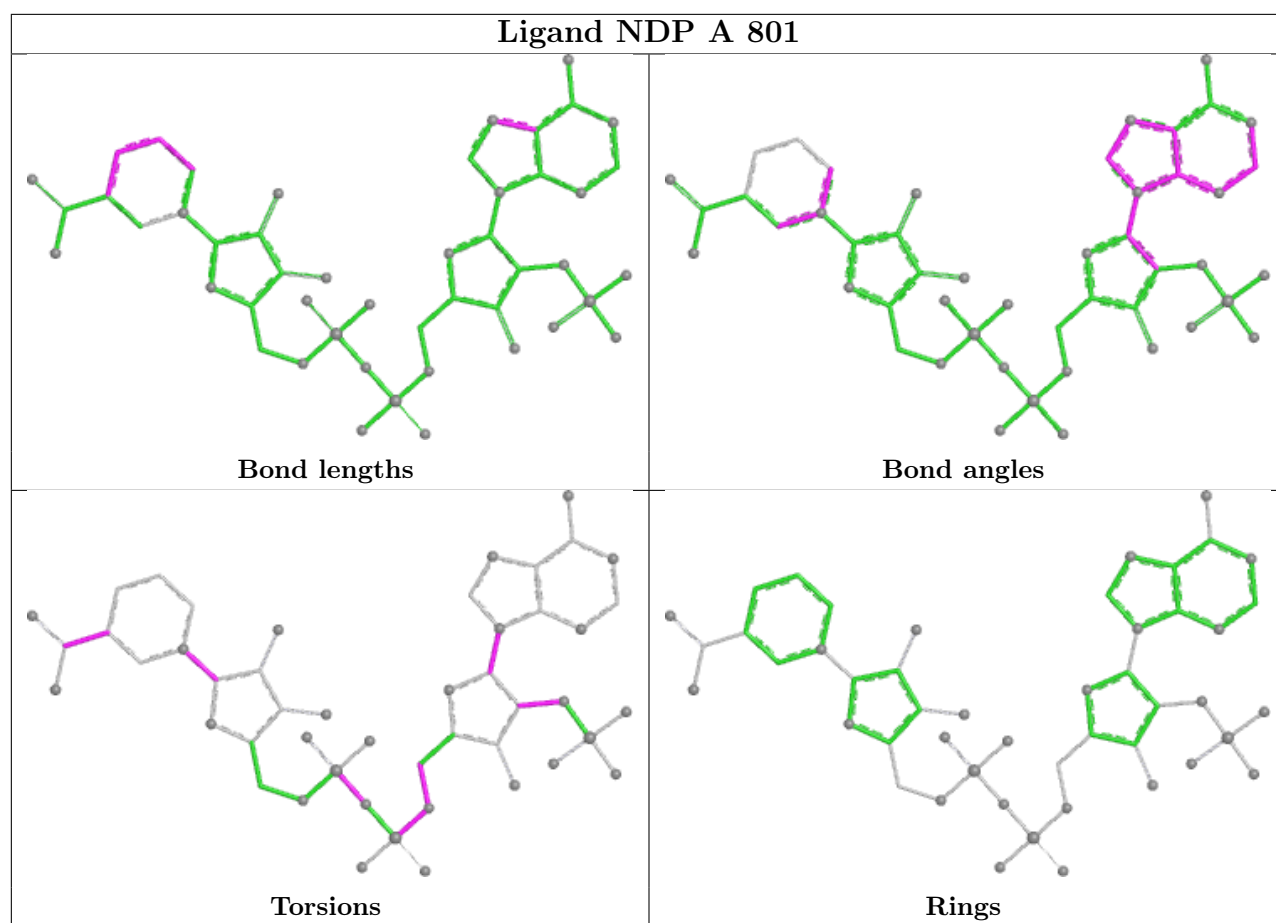
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	SO4	0	1
3	A	803	SO4	1	0
2	B	801	NDP	4	0
2	A	802	NDP	5	0
3	B	803	SO4	1	0
2	B	802	NDP	6	0
2	A	801	NDP	7	0

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









5.7 Other polymers [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	747/795 (93%)	-0.11	4 (0%)	87 72	33, 73, 144, 182	0
1	B	747/795 (93%)	-0.27	2 (0%)	90 79	36, 63, 112, 171	0
All	All	1494/1590 (93%)	-0.19	6 (0%)	88 76	33, 67, 136, 182	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	LEU	2.5
1	A	664	ASP	2.5
1	B	743	ALA	2.3
1	A	244	VAL	2.2
1	A	425	VAL	2.2

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

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

6.3 Carbohydrates [i](#)

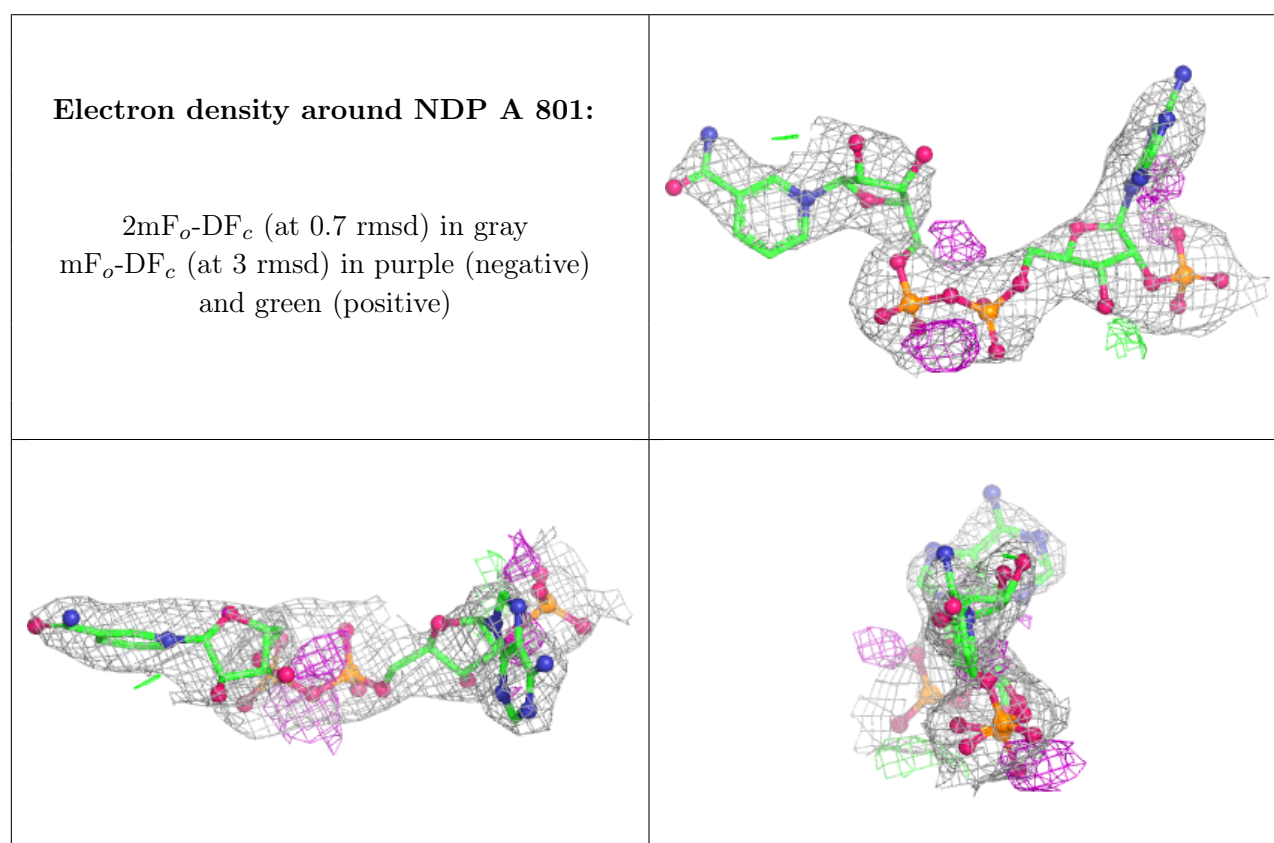
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

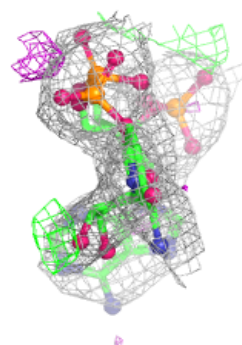
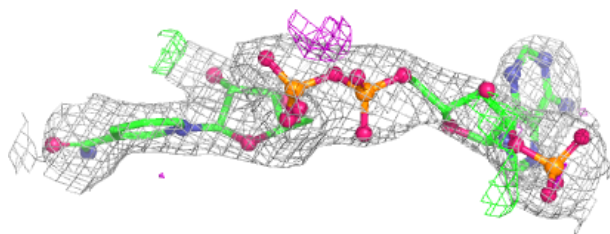
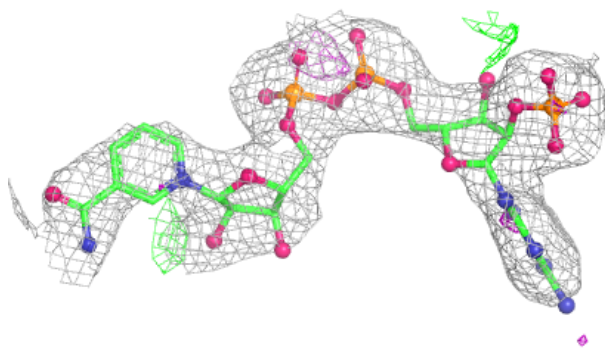
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	A	801	48/48	0.84	0.12	83,100,111,119	0
2	NDP	B	801	48/48	0.88	0.11	64,83,95,98	0
3	SO4	B	803	5/5	0.89	0.10	69,69,94,111	0
2	NDP	A	802	48/48	0.96	0.07	25,31,37,40	0
2	NDP	B	802	48/48	0.97	0.07	24,29,34,40	0
3	SO4	A	804	5/5	0.98	0.08	42,45,47,48	0
3	SO4	A	803	5/5	0.98	0.07	25,27,33,36	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.

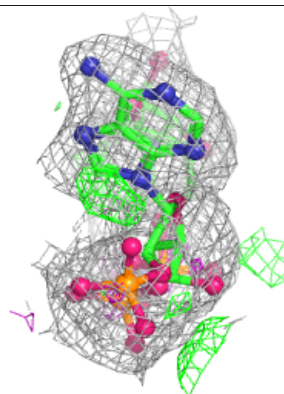
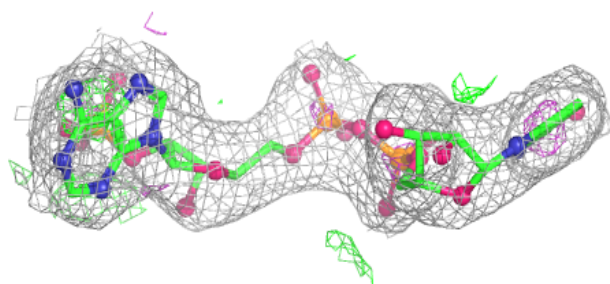
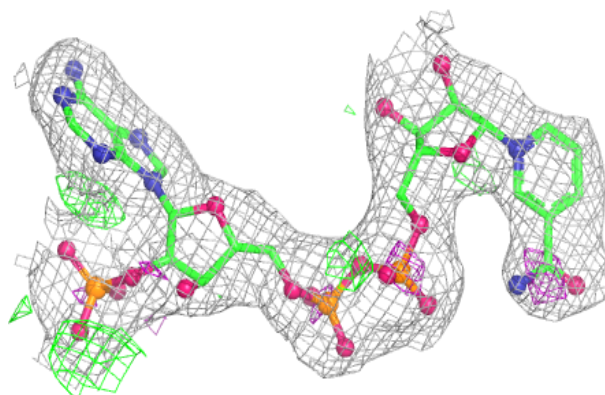


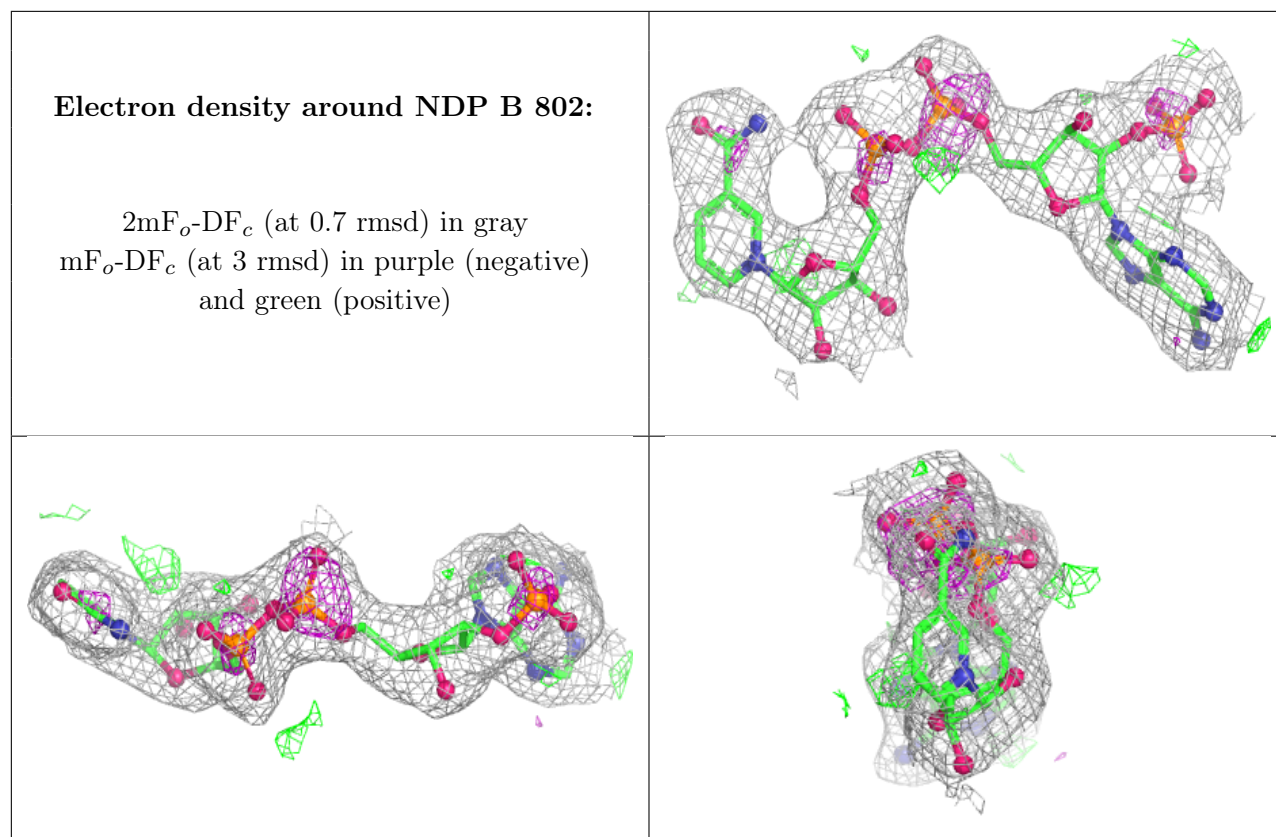
Electron density around NDP B 801:

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

**Electron density around NDP A 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.