



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:34 AM UTC

PDB ID : 5YWN / pdb_00005ywn
Title : SsCR_L211H-NADP+
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Deposited on : 2017-11-29
Resolution : 2.04 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 : 4-5-2 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

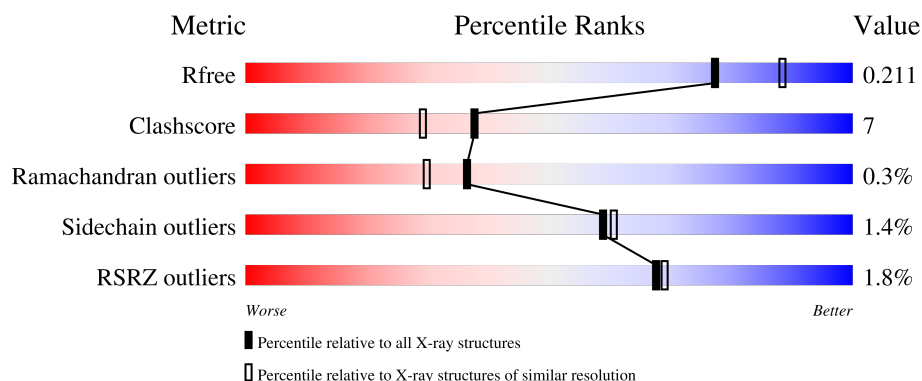
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

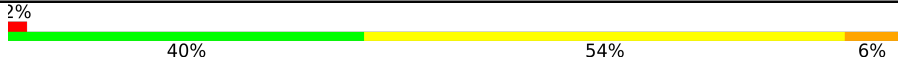
The reported resolution of this entry is 2.04 Å.

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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	334	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2910 atoms, of which 25 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 Protein induced by osmotic stress.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	2609	1673	425	508	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	HIS	LEU	engineered mutation	UNP A3LWG4

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
2	A	1	73	21	25	7	17	3	0	0

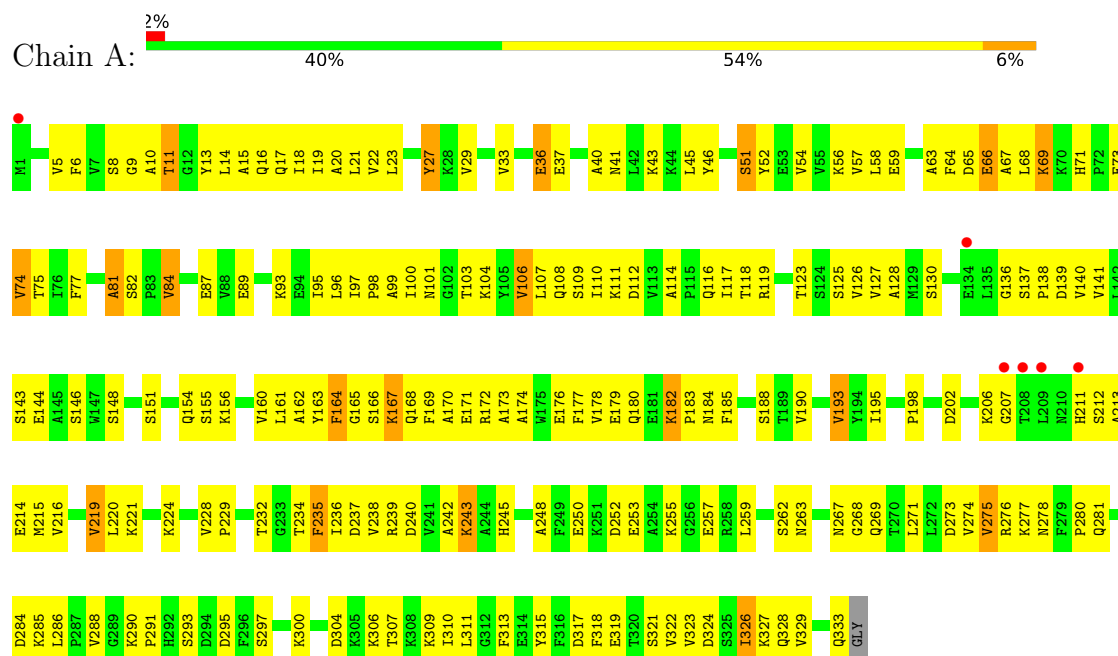
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	228	Total 228	O 228	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: Protein induced by osmotic stress



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.78Å 53.09Å 70.77Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	35.22 – 2.04 35.22 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.1 (35.22-2.04) 97.2 (35.22-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.166 , 0.223 0.183 , 0.211	Depositor DCC
R_{free} test set	1092 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2910	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% 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: NAP

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	2.30	174/2662 (6.5%)	1.17	12/3605 (0.3%)

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	ILE	C-O	-9.02	1.16	1.24
1	A	19	ILE	C-O	-8.15	1.15	1.24
1	A	29	VAL	C-O	-8.14	1.16	1.24
1	A	16	GLN	C-O	-8.14	1.14	1.24
1	A	117	ILE	C-O	-8.00	1.16	1.23
1	A	323	VAL	C-O	-7.76	1.15	1.24
1	A	96	LEU	C-O	-7.73	1.15	1.24
1	A	168	GLN	C-O	-7.68	1.15	1.24
1	A	322	VAL	C-O	-7.68	1.15	1.24
1	A	126	VAL	C-O	-7.61	1.14	1.24
1	A	288	VAL	C-O	-7.47	1.16	1.23
1	A	219	VAL	C-O	-7.45	1.15	1.24
1	A	184	ASN	C-O	-7.43	1.14	1.24
1	A	17	GLN	C-O	-7.38	1.15	1.24
1	A	170	ALA	C-O	-7.34	1.15	1.24
1	A	182	LYS	C-O	-7.20	1.20	1.23
1	A	274	VAL	C-O	-7.20	1.16	1.24
1	A	162	ALA	C-O	-7.18	1.15	1.24
1	A	161	LEU	C-O	-7.13	1.15	1.24
1	A	36	GLU	C-O	-7.11	1.16	1.24
1	A	214	GLU	C-O	-7.07	1.14	1.24
1	A	103	THR	C-O	-7.03	1.16	1.24
1	A	136	GLY	C-O	-7.03	1.17	1.24
1	A	277	LYS	C-O	-7.00	1.16	1.24
1	A	281	GLN	C-O	-6.99	1.15	1.24
1	A	33	VAL	C-O	-6.98	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	LYS	C-O	-6.96	1.15	1.23
1	A	172	ARG	C-O	-6.95	1.16	1.24
1	A	18	ILE	C-O	-6.93	1.16	1.24
1	A	242	ALA	C-O	-6.93	1.16	1.24
1	A	309	LYS	C-O	-6.92	1.16	1.24
1	A	163	TYR	C-O	-6.84	1.16	1.24
1	A	229	PRO	C-O	-6.81	1.15	1.23
1	A	69	LYS	C-O	-6.78	1.16	1.24
1	A	315	TYR	C-O	-6.76	1.15	1.23
1	A	56	LYS	C-O	-6.67	1.16	1.24
1	A	95	ILE	C-O	-6.67	1.16	1.24
1	A	5	VAL	C-O	-6.67	1.16	1.24
1	A	319	GLU	C-O	-6.67	1.16	1.24
1	A	212	SER	C-O	-6.62	1.16	1.24
1	A	74	VAL	C-O	-6.60	1.17	1.24
1	A	278	ASN	C-O	-6.53	1.15	1.24
1	A	160	VAL	C-O	-6.53	1.16	1.24
1	A	58	LEU	C-O	-6.52	1.16	1.24
1	A	106	VAL	C-O	-6.52	1.16	1.24
1	A	100	ILE	C-O	-6.50	1.17	1.24
1	A	15	ALA	C-O	-6.49	1.16	1.24
1	A	250	GLU	C-O	-6.45	1.16	1.24
1	A	144	GLU	C-O	-6.45	1.15	1.24
1	A	173	ALA	C-O	-6.45	1.16	1.24
1	A	166	SER	C-O	-6.42	1.16	1.24
1	A	84	VAL	C-O	-6.38	1.16	1.24
1	A	128	ALA	C-O	-6.34	1.15	1.24
1	A	63	ALA	C-O	-6.28	1.16	1.24
1	A	224	LYS	C-O	-6.27	1.16	1.24
1	A	23	LEU	C-O	-6.25	1.16	1.24
1	A	21	LEU	C-O	-6.24	1.16	1.24
1	A	107	LEU	C-O	-6.23	1.16	1.24
1	A	169	PHE	C-O	-6.12	1.16	1.24
1	A	112	ASP	C-O	-6.12	1.17	1.24
1	A	324	ASP	C-O	-6.10	1.17	1.24
1	A	93	LYS	C-O	-6.09	1.16	1.24
1	A	111	LYS	C-O	-6.08	1.17	1.24
1	A	155	SER	C-O	-6.08	1.16	1.24
1	A	98	PRO	C-O	-6.07	1.16	1.24
1	A	252	ASP	C-O	-6.06	1.17	1.24
1	A	253	GLU	C-O	-6.05	1.16	1.24
1	A	114	ALA	C-O	-6.03	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	ILE	C-O	-6.01	1.18	1.24
1	A	243	LYS	C-O	-6.01	1.17	1.24
1	A	240	ASP	C-O	-6.00	1.17	1.24
1	A	311	LEU	C-O	-5.99	1.17	1.24
1	A	65	ASP	C-O	-5.95	1.17	1.24
1	A	245	HIS	C-O	-5.94	1.17	1.24
1	A	179	GLU	C-O	-5.94	1.17	1.24
1	A	327	LYS	C-O	-5.94	1.17	1.24
1	A	167	LYS	C-O	-5.88	1.17	1.24
1	A	13	TYR	C-O	-5.88	1.17	1.24
1	A	268	GLY	C-O	-5.87	1.16	1.23
1	A	130	SER	C-O	-5.87	1.17	1.23
1	A	165	GLY	C-O	-5.87	1.16	1.23
1	A	164	PHE	C-O	-5.86	1.17	1.24
1	A	185	PHE	C-O	-5.83	1.16	1.23
1	A	321	SER	C-O	-5.83	1.17	1.24
1	A	140	VAL	C-O	-5.82	1.17	1.24
1	A	123	THR	C-O	-5.82	1.16	1.23
1	A	14	LEU	C-O	-5.80	1.17	1.24
1	A	71	HIS	C-O	-5.80	1.17	1.24
1	A	101	ASN	C-O	-5.80	1.17	1.24
1	A	273	ASP	C-O	-5.77	1.17	1.24
1	A	297	SER	C-O	-5.77	1.16	1.24
1	A	267	ASN	C-O	-5.76	1.17	1.24
1	A	269	GLN	C-O	-5.76	1.17	1.24
1	A	54	VAL	C-O	-5.75	1.17	1.24
1	A	10	ALA	C-O	-5.73	1.16	1.24
1	A	66	GLU	C-O	-5.69	1.17	1.24
1	A	99	ALA	C-O	-5.69	1.17	1.24
1	A	291	PRO	C-O	-5.68	1.16	1.23
1	A	40	ALA	C-O	-5.68	1.17	1.24
1	A	75	THR	C-O	-5.67	1.16	1.24
1	A	110	ILE	C-O	-5.67	1.17	1.24
1	A	326	ILE	C-O	-5.66	1.17	1.24
1	A	178	VAL	C-O	-5.65	1.17	1.24
1	A	108	GLN	C-O	-5.65	1.17	1.24
1	A	176	GLU	C-O	-5.64	1.17	1.24
1	A	109	SER	C-O	-5.62	1.17	1.24
1	A	255	LYS	C-O	-5.61	1.17	1.23
1	A	238	VAL	C-O	-5.61	1.17	1.24
1	A	51	SER	C-O	-5.58	1.16	1.23
1	A	57	VAL	C-O	-5.57	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	SER	C-O	-5.57	1.17	1.23
1	A	81	ALA	C-O	-5.56	1.17	1.23
1	A	137	SER	C-O	-5.54	1.16	1.24
1	A	310	ILE	C-O	-5.54	1.17	1.24
1	A	280	PRO	C-O	-5.52	1.17	1.24
1	A	313	PHE	C-O	-5.51	1.16	1.23
1	A	45	LEU	C-O	-5.50	1.17	1.24
1	A	220	LEU	C-O	-5.49	1.17	1.24
1	A	213	ALA	C-O	-5.48	1.17	1.24
1	A	183	PRO	C-O	-5.46	1.16	1.23
1	A	177	PHE	C-O	-5.44	1.17	1.24
1	A	41	ASN	C-O	-5.43	1.17	1.24
1	A	139	ASP	C-O	-5.43	1.16	1.24
1	A	68	LEU	C-O	-5.42	1.17	1.24
1	A	146	SER	C-O	-5.42	1.17	1.23
1	A	156	LYS	C-O	-5.40	1.17	1.24
1	A	116	GLN	C-O	-5.39	1.17	1.24
1	A	89	GLU	C-O	-5.39	1.17	1.24
1	A	295	ASP	C-O	-5.39	1.17	1.24
1	A	286	LEU	C-O	-5.37	1.19	1.24
1	A	174	ALA	C-O	-5.36	1.18	1.24
1	A	290	LYS	C-O	-5.36	1.18	1.24
1	A	232	THR	C-O	-5.36	1.17	1.23
1	A	329	VAL	C-O	-5.35	1.18	1.24
1	A	198	PRO	C-O	-5.34	1.17	1.23
1	A	202	ASP	C-O	-5.32	1.17	1.24
1	A	138	PRO	C-O	-5.32	1.17	1.24
1	A	306	LYS	C-O	-5.30	1.18	1.24
1	A	104	LYS	C-O	-5.29	1.18	1.24
1	A	143	SER	C-O	-5.29	1.17	1.24
1	A	293	SER	C-O	-5.29	1.17	1.24
1	A	59	GLU	C-O	-5.28	1.17	1.24
1	A	118	THR	C-O	-5.27	1.17	1.24
1	A	141	VAL	C-O	-5.27	1.18	1.24
1	A	262	SER	C-O	-5.25	1.18	1.23
1	A	8	SER	C-O	-5.25	1.17	1.23
1	A	37	GLU	C-O	-5.25	1.17	1.24
1	A	317	ASP	C-O	-5.24	1.16	1.23
1	A	248	ALA	C-O	-5.22	1.17	1.24
1	A	73	GLU	C-O	-5.21	1.17	1.24
1	A	237	ASP	C-O	-5.20	1.17	1.23
1	A	304	ASP	C-O	-5.20	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	VAL	C-O	-5.20	1.18	1.24
1	A	263	ASN	C-O	-5.17	1.17	1.24
1	A	171	GLU	C-O	-5.17	1.18	1.24
1	A	235	PHE	C-O	-5.17	1.17	1.23
1	A	20	ALA	C-O	-5.17	1.18	1.24
1	A	239	ARG	C-O	-5.16	1.18	1.24
1	A	259	LEU	C-O	-5.15	1.18	1.24
1	A	11	THR	C-O	-5.14	1.17	1.24
1	A	77	PHE	C-O	-5.13	1.18	1.24
1	A	211	HIS	C-O	-5.12	1.18	1.24
1	A	276	ARG	C-O	-5.12	1.18	1.24
1	A	119	ARG	C-O	-5.11	1.17	1.23
1	A	215	MET	C-O	-5.11	1.18	1.24
1	A	190	VAL	C-O	-5.09	1.18	1.24
1	A	27	TYR	C-O	-5.07	1.17	1.23
1	A	188	SER	C-O	-5.06	1.17	1.23
1	A	67	ALA	C-O	-5.06	1.18	1.24
1	A	228	VAL	C-O	-5.06	1.18	1.25
1	A	328	GLN	C-O	-5.04	1.18	1.24
1	A	307	THR	C-O	-5.03	1.18	1.24
1	A	257	GLU	C-O	-5.03	1.18	1.23
1	A	318	PHE	C-O	-5.02	1.18	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLY	N-CA-C	13.17	128.42	112.49
1	A	118	THR	N-CA-C	7.89	119.96	111.36
1	A	278	ASN	N-CA-C	6.78	119.69	111.82
1	A	180	GLN	N-CA-C	6.28	118.21	111.36
1	A	117	ILE	CA-C-N	5.95	128.74	120.29
1	A	117	ILE	C-N-CA	5.95	128.74	120.29
1	A	169	PHE	N-CA-C	5.70	117.57	111.36
1	A	212	SER	N-CA-C	5.63	117.09	111.07
1	A	250	GLU	N-CA-C	5.48	117.34	111.36
1	A	100	ILE	N-CA-C	5.23	115.34	110.42
1	A	130	SER	N-CA-C	5.18	115.37	108.38
1	A	46	TYR	N-CA-C	5.12	119.67	113.38

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	2609	0	2613	35	0
2	A	48	25	25	9	0
3	A	228	0	0	5	0
All	All	2885	25	2638	37	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 7.

All (37) 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)
2:A:401:NAP:O1X	3:A:501:HOH:O	1.70	1.09
1:A:66:GLU:OE1	1:A:69:LYS:NZ	1.87	1.06
1:A:219:VAL:CG1	1:A:271:LEU:HD21	1.88	1.02
1:A:182:LYS:NZ	3:A:502:HOH:O	1.81	1.00
1:A:219:VAL:HG11	1:A:271:LEU:HD21	1.62	0.81
1:A:11:THR:OG1	2:A:401:NAP:O3X	2.01	0.77
1:A:87:GLU:HG2	1:A:87:GLU:O	1.90	0.70
1:A:167:LYS:NZ	2:A:401:NAP:O2D	2.17	0.70
1:A:193:VAL:HG21	1:A:234:THR:HG23	1.73	0.69
1:A:219:VAL:CG1	1:A:271:LEU:CD2	2.70	0.68
1:A:193:VAL:HG11	1:A:234:THR:CG2	2.25	0.67
1:A:125:SER:HB2	2:A:401:NAP:H6N	1.78	0.65
1:A:219:VAL:HG11	1:A:271:LEU:CD2	2.26	0.65
1:A:167:LYS:HZ3	2:A:401:NAP:HO2N	1.45	0.58
1:A:275:VAL:HG22	1:A:326:ILE:HD13	1.87	0.56
1:A:151:SER:OG	1:A:154:GLN:HG3	2.08	0.53
1:A:193:VAL:HG11	1:A:234:THR:HG21	1.92	0.52
1:A:84:VAL:HG21	2:A:401:NAP:O2A	2.10	0.51
1:A:216:VAL:O	1:A:219:VAL:HG13	2.10	0.51
1:A:333:GLN:OE1	1:A:333:GLN:HA	2.14	0.48
1:A:127:VAL:HB	1:A:164:PHE:CD2	2.48	0.47
1:A:36:GLU:OE2	1:A:52:TYR:OH	2.28	0.46
1:A:43:LYS:HE3	3:A:507:HOH:O	2.15	0.46
1:A:219:VAL:HG12	1:A:271:LEU:HD21	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:CD1	1:A:106:VAL:HG22	2.51	0.45
1:A:195:ILE:HD12	2:A:401:NAP:N7N	2.32	0.45
1:A:275:VAL:HG22	1:A:326:ILE:CD1	2.48	0.44
1:A:284:ASP:OD1	1:A:285:LYS:HE3	2.18	0.44
1:A:219:VAL:HG11	1:A:271:LEU:CG	2.48	0.43
1:A:167:LYS:NZ	2:A:401:NAP:HO2N	2.11	0.43
1:A:6:PHE:HB2	1:A:74:VAL:HG11	2.00	0.42
2:A:401:NAP:N7N	2:A:401:NAP:O1N	2.53	0.42
1:A:193:VAL:CG2	1:A:234:THR:HG23	2.46	0.41
1:A:9:GLY:HA3	1:A:81:ALA:HB2	2.01	0.41
1:A:22:VAL:HG13	1:A:27:TYR:HB2	2.02	0.41
1:A:51:SER:HB2	3:A:642:HOH:O	2.20	0.41
1:A:243:LYS:NZ	3:A:519:HOH:O	2.53	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	331/334 (99%)	326 (98%)	4 (1%)	1 (0%)	36	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	VAL

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	289/289 (100%)	285 (99%)	4 (1%)	59 60

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	206	LYS
1	A	221	LYS
1	A	235	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	158	HIS

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](#)

1 ligand is 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	NAP	A	401	-	50,52,52	1.16	5 (10%)	71,80,80	1.60	12 (16%)

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	NAP	A	401	-	-	7/35/67/67	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	C5A-C4A	4.62	1.47	1.39
2	A	401	NAP	C5A-C6A	2.71	1.48	1.41
2	A	401	NAP	C8A-N7A	2.39	1.36	1.31
2	A	401	NAP	C5A-N7A	-2.24	1.35	1.39
2	A	401	NAP	O4D-C1D	2.06	1.43	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	C5A-C4A-N3A	-5.83	118.69	126.72
2	A	401	NAP	N3A-C4A-N9A	4.64	135.07	127.17
2	A	401	NAP	C2A-N3A-C4A	3.88	121.32	111.83
2	A	401	NAP	N3A-C2A-N1A	-3.72	122.95	128.58
2	A	401	NAP	C4A-C5A-N7A	-3.58	106.49	110.58
2	A	401	NAP	C4A-N9A-C8A	2.92	108.80	105.74
2	A	401	NAP	C5A-N7A-C8A	2.79	107.84	103.45
2	A	401	NAP	N9A-C8A-N7A	-2.34	110.62	113.94
2	A	401	NAP	C2B-C1B-N9A	-2.24	110.07	113.75
2	A	401	NAP	C6A-C5A-N7A	2.20	136.33	132.09
2	A	401	NAP	C2A-N1A-C6A	2.09	122.16	118.73
2	A	401	NAP	C2B-C3B-C4B	2.01	106.32	101.99

There are no chirality outliers.

All (7) torsion outliers are listed below:

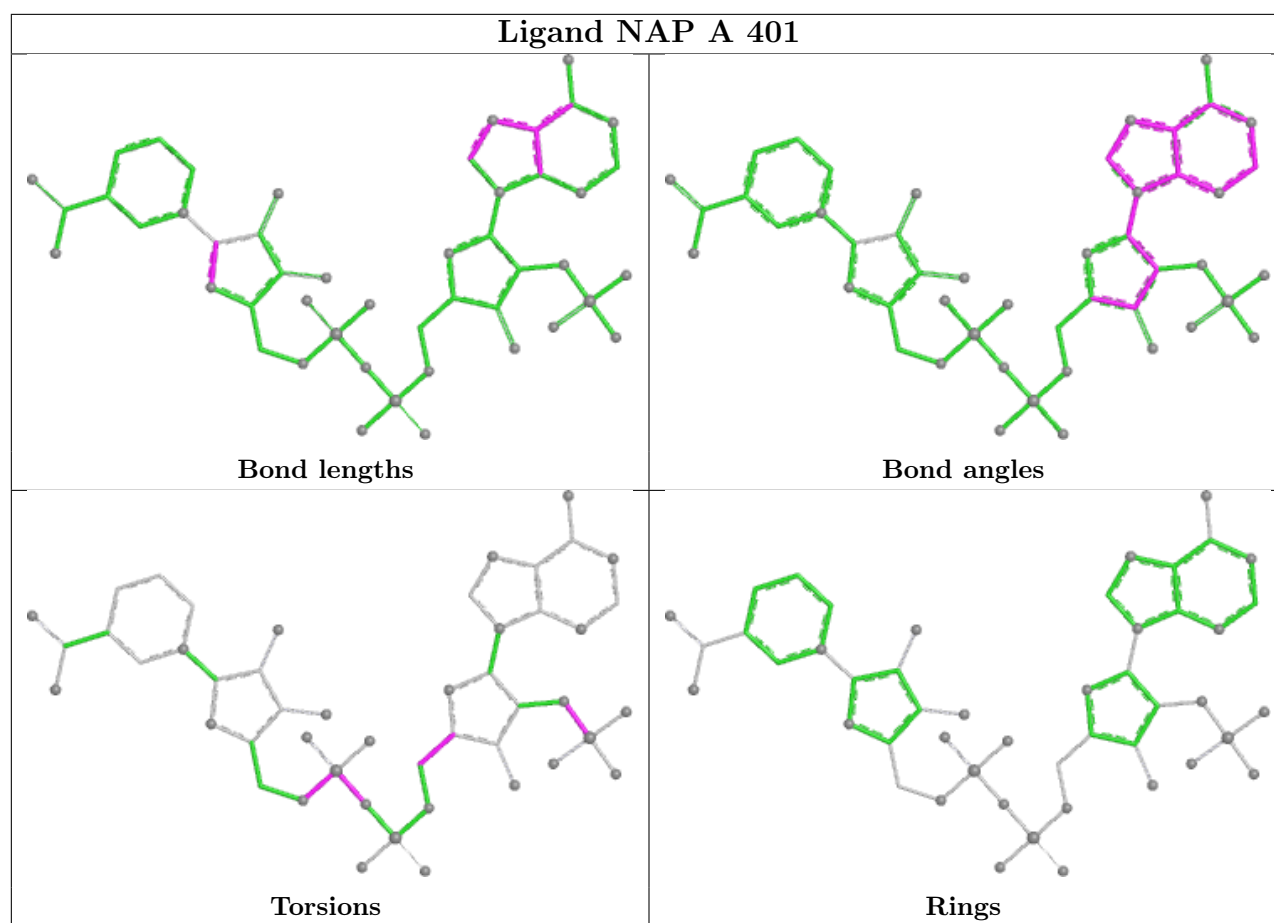
Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C5D-O5D-PN-O3
2	A	401	NAP	C5D-O5D-PN-O2N
2	A	401	NAP	O4B-C4B-C5B-O5B
2	A	401	NAP	C3B-C4B-C5B-O5B
2	A	401	NAP	C5D-O5D-PN-O1N
2	A	401	NAP	PA-O3-PN-O2N
2	A	401	NAP	C2B-O2B-P2B-O1X

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	9	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	333/334 (99%)	-0.01	6 (1%) 67 69	19, 27, 40, 62	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.4
1	A	208	THR	3.7
1	A	209	LEU	3.0
1	A	134	GLU	2.5
1	A	207	GLY	2.4
1	A	211	HIS	2.1

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](#)

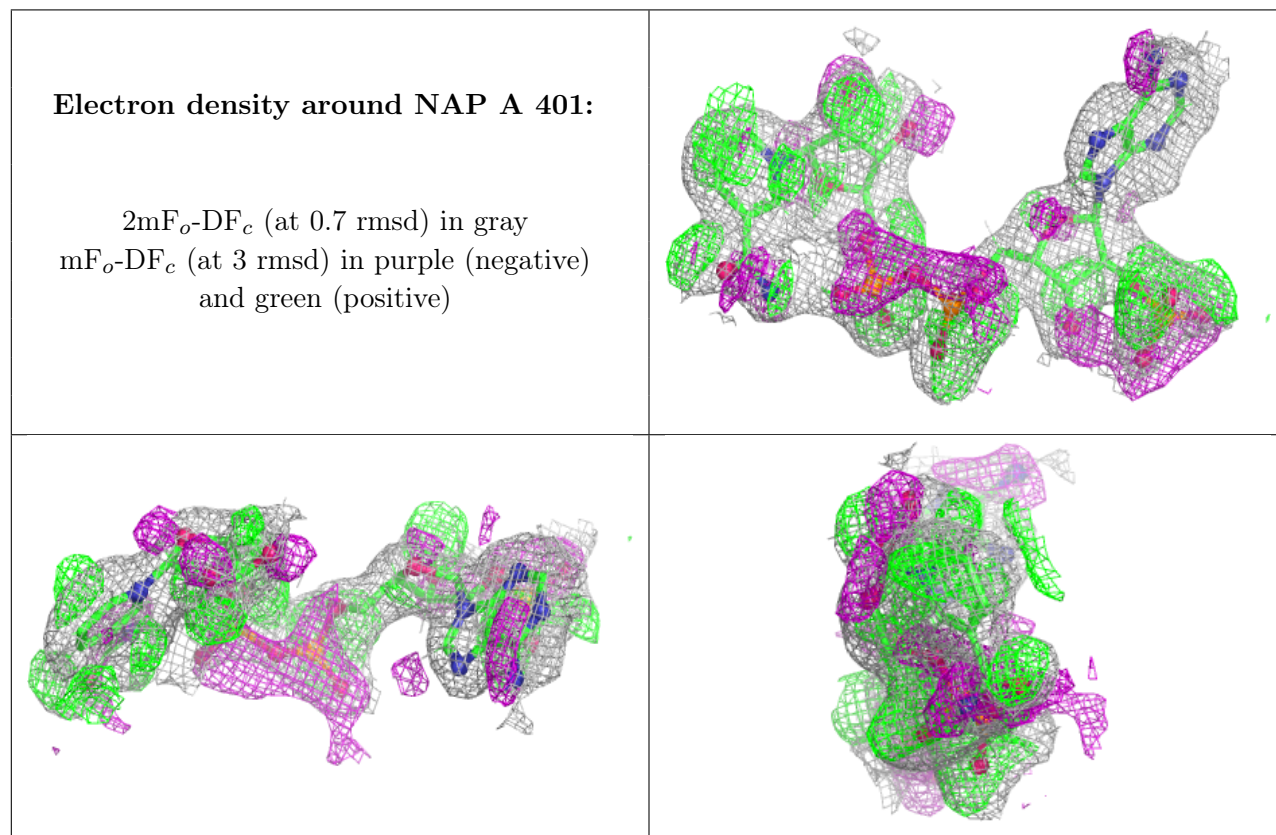
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
2	NAP	A	401	48/48	0.74	0.17	20,28,35,39	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.