



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:46 AM UTC

PDB ID : 1CGK / pdb_00001cgk
Title : CHALCONE SYNTHASE FROM ALFALFA COMPLEXED WITH NARIN-
GENIN
Authors : Ferrer, J.-L.; Jez, J.; Bowman, M.E.; Dixon, R.; Noel, J.P.
Deposited on : 1999-03-25
Resolution : 1.84 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

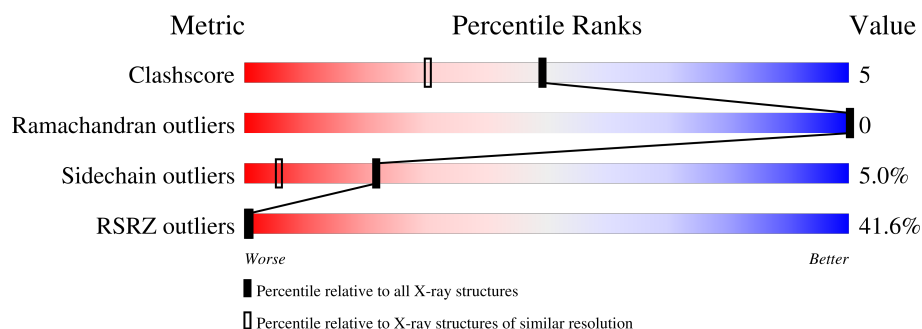
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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))
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	389	

2 Entry composition [i](#)

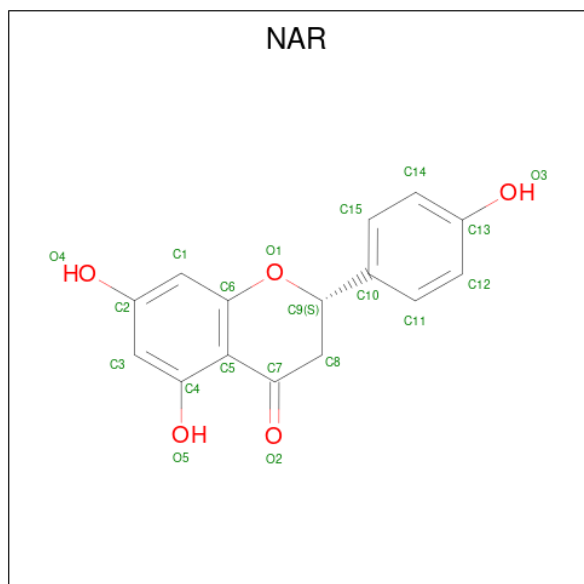
There are 3 unique types of molecules in this entry. The entry contains 3484 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (CHALCONE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	15	0
			3104	1964	525	596	19			

- Molecule 2 is NARINGENIN (CCD ID: NAR) (formula: C₁₅H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	15	5		

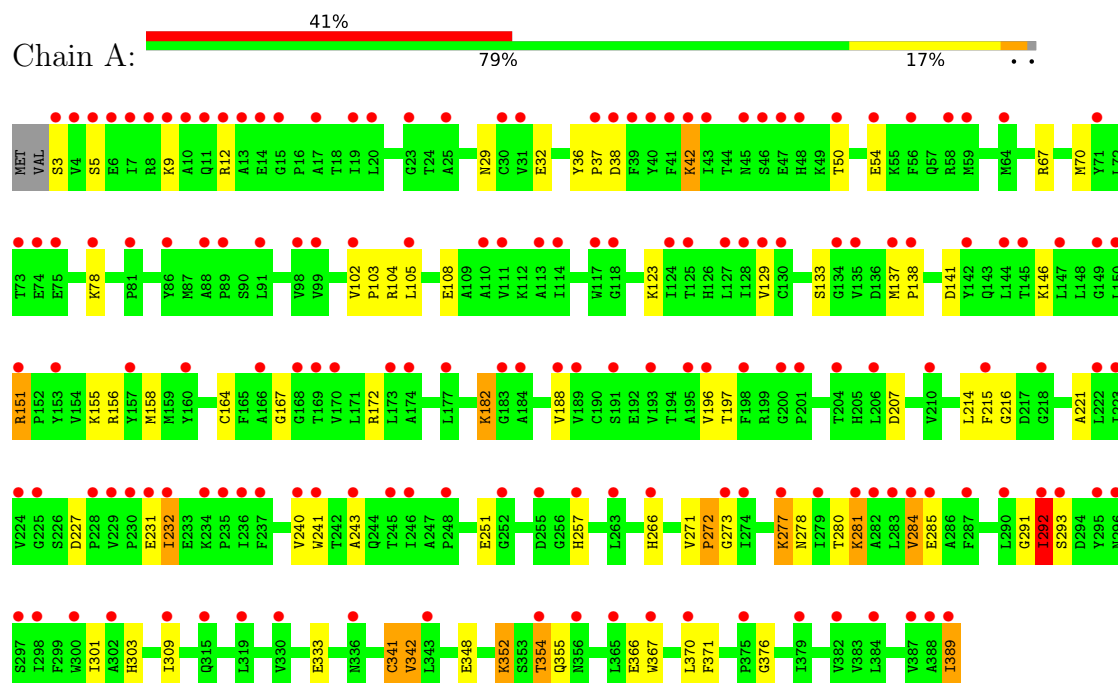
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	360	Total	O	0	0
			360	360		

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 (CHALCONE SYNTHASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	97.92Å 97.92Å 65.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.50 – 1.84 84.50 – 1.85	Depositor EDS
% Data completeness (in resolution range)	85.5 (84.50-1.84) 86.6 (84.50-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.16 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.225 0.303 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3484	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: NAR

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	0.78	0/3161	1.54	33/4275 (0.8%)

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	4

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	CD-NE-CZ	16.51	147.51	124.40
1	A	342	VAL	N-CA-CB	-11.85	94.43	110.54
1	A	232	ILE	N-CA-C	-11.61	101.58	111.56
1	A	376	GLY	O-C-N	-11.40	107.87	122.70
1	A	137	MET	CA-C-O	-10.98	109.32	119.86
1	A	137	MET	O-C-N	9.34	130.34	121.38
1	A	342	VAL	CB-CA-C	8.46	123.55	112.14
1	A	389	ILE	CA-CB-CG2	7.45	123.17	110.50
1	A	138	PRO	N-CA-CB	7.44	110.79	102.60
1	A	371	PHE	CA-C-N	-7.33	116.97	122.33
1	A	371	PHE	C-N-CA	-7.33	116.97	122.33
1	A	292	ILE	CA-CB-CG2	6.45	121.46	110.50
1	A	272	PRO	CA-C-N	6.32	126.95	120.00
1	A	272	PRO	C-N-CA	6.32	126.95	120.00
1	A	172	ARG	CA-C-O	6.29	127.22	120.55
1	A	342	VAL	CA-CB-CG1	6.21	120.95	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	389	ILE	CB-CA-C	5.98	123.56	111.60
1	A	303	HIS	CA-CB-CG	-5.97	107.83	113.80
1	A	291	GLY	CA-C-N	-5.93	115.83	123.19
1	A	291	GLY	C-N-CA	-5.93	115.83	123.19
1	A	227	ASP	CA-C-O	5.81	124.95	120.48
1	A	366	GLU	N-CA-C	5.63	118.27	111.40
1	A	167	GLY	N-CA-C	-5.60	106.01	112.73
1	A	156	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	A	341	CYS	N-CA-C	5.46	117.66	111.11
1	A	38	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	12	ARG	NE-CZ-NH1	-5.40	116.10	121.50
1	A	231	GLU	CB-CG-CD	-5.39	103.44	112.60
1	A	67	ARG	NE-CZ-NH1	5.33	126.83	121.50
1	A	105	LEU	CA-C-O	5.13	125.85	120.42
1	A	214	LEU	N-CA-C	5.07	119.60	113.41
1	A	278	ASN	CB-CG-ND2	5.07	124.01	116.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32[B]	GLU	Mainchain
1	A	333[B]	GLU	Mainchain
1	A	354[B]	THR	Mainchain
1	A	42[B]	LYS	Mainchain

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	3104	0	3117	34	4
2	A	20	0	10	2	0
3	A	360	0	0	12	8
All	All	3484	0	3127	34	9

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 (34) 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:301:ILE:HG21	3:A:736:HOH:O	1.69	0.93
1:A:370:LEU:CD1	3:A:736:HOH:O	2.43	0.67
1:A:241:TRP:CH2	1:A:285:GLU:HG2	2.34	0.63
1:A:257:HIS:HB2	3:A:692:HOH:O	2.05	0.57
1:A:348:GLU:OE2	1:A:352:LYS:HD3	2.06	0.55
1:A:102:VAL:HB	1:A:103:PRO:HD3	1.89	0.55
1:A:104:ARG:NH1	1:A:108[A]:GLU:OE2	2.40	0.55
1:A:70:MET:HG2	3:A:727:HOH:O	2.08	0.54
1:A:266:HIS:CE1	3:A:720:HOH:O	2.61	0.53
1:A:50:THR:O	1:A:54:GLU:HG3	2.11	0.50
1:A:370:LEU:HD11	3:A:736:HOH:O	2.06	0.49
1:A:273:GLY:O	1:A:277:LYS:HG3	2.11	0.49
1:A:271:VAL:HB	1:A:272:PRO:HD3	1.94	0.49
1:A:164:CYS:SG	2:A:390:NAR:H11	2.53	0.49
1:A:182:LYS:HD3	3:A:520:HOH:O	2.12	0.49
1:A:292:ILE:HD12	1:A:293:SER:N	2.27	0.48
1:A:215:PHE:CD1	2:A:390:NAR:H111	2.49	0.47
1:A:281:LYS:HB3	3:A:567:HOH:O	2.15	0.46
1:A:151:ARG:HH11	1:A:151:ARG:HD2	1.60	0.45
1:A:36:TYR:N	1:A:37:PRO:CD	2.80	0.45
1:A:240:VAL:HG21	1:A:367:TRP:HZ3	1.83	0.44
1:A:29:ASN:HB3	1:A:70:MET:O	2.17	0.44
1:A:241:TRP:HH2	1:A:285:GLU:HG2	1.82	0.44
1:A:129:VAL:HG21	1:A:141:ASP:HA	2.00	0.44
1:A:280:THR:O	1:A:284:VAL:HG13	2.18	0.44
1:A:309:ILE:HG13	3:A:740:HOH:O	2.18	0.42
1:A:354[B]:THR:O	1:A:355:GLN:C	2.62	0.42
1:A:257:HIS:N	3:A:720:HOH:O	2.52	0.42
1:A:182:LYS:HB3	1:A:182:LYS:HE3	1.75	0.42
1:A:188:VAL:O	1:A:221:ALA:HA	2.19	0.42
1:A:241:TRP:CH2	1:A:243:ALA:HB2	2.55	0.42
1:A:216:GLY:HA2	3:A:727:HOH:O	2.19	0.41
1:A:133:SER:HA	1:A:196:VAL:HG11	2.03	0.41
1:A:197:THR:HG23	3:A:476:HOH:O	2.21	0.40

All (9) 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:A:9[A]:LYS:CG	3:A:693:HOH:O[4_557]	1.82	0.38
1:A:146:LYS:NZ	1:A:251:GLU:OE2[4_557]	1.86	0.34
3:A:668:HOH:O	3:A:715:HOH:O[4_557]	1.99	0.21
3:A:596:HOH:O	3:A:626:HOH:O[4_557]	2.02	0.18
1:A:155:LYS:NZ	3:A:556:HOH:O[4_557]	2.13	0.07
3:A:409:HOH:O	3:A:441:HOH:O[4_557]	2.15	0.05
3:A:462:HOH:O	3:A:474:HOH:O[5_666]	2.15	0.05
3:A:459:HOH:O	3:A:660:HOH:O[4_556]	2.16	0.04
1:A:158:MET:N	3:A:435:HOH:O[4_557]	2.19	0.01

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	400/389 (103%)	389 (97%)	11 (3%)	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	338/325 (104%)	320 (95%)	18 (5%)	20	5

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	5[A]	SER
1	A	5[B]	SER
1	A	42[A]	LYS
1	A	42[B]	LYS
1	A	78	LYS
1	A	123	LYS
1	A	151	ARG
1	A	182	LYS
1	A	232	ILE
1	A	277	LYS
1	A	281	LYS
1	A	284	VAL
1	A	292	ILE
1	A	341	CYS
1	A	342	VAL
1	A	352	LYS
1	A	389	ILE

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

Mol	Chain	Res	Type
1	A	205	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	NAR	A	390	-	22,22,22	1.27	2 (9%)	32,32,32	2.71	16 (50%)

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	NAR	A	390	-	-	0/4/16/16	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	390	NAR	C10-C9	3.48	1.57	1.51
2	A	390	NAR	C12-C11	2.35	1.42	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	390	NAR	C14-C15-C10	-6.73	114.47	121.18
2	A	390	NAR	C4-C5-C6	6.01	123.14	117.41
2	A	390	NAR	C3-C4-C5	-5.34	114.94	120.92
2	A	390	NAR	O1-C6-C1	3.79	122.77	116.29
2	A	390	NAR	O4-C2-C3	-3.76	110.01	119.85
2	A	390	NAR	C3-C2-C1	-3.32	115.93	120.47
2	A	390	NAR	C4-C5-C7	-3.16	116.77	120.92
2	A	390	NAR	C15-C10-C9	-2.95	113.96	120.63
2	A	390	NAR	C11-C10-C9	2.91	127.20	120.63
2	A	390	NAR	C6-C5-C7	-2.89	117.47	120.29
2	A	390	NAR	C11-C12-C13	-2.78	116.93	119.88
2	A	390	NAR	C1-C6-C5	-2.78	116.95	121.79
2	A	390	NAR	O4-C2-C1	2.76	127.08	119.85
2	A	390	NAR	C14-C13-C12	-2.56	115.70	119.77
2	A	390	NAR	C4-C3-C2	2.25	121.75	119.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	390	NAR	C8-C9-C10	-2.00	107.76	114.22

There are no chirality outliers.

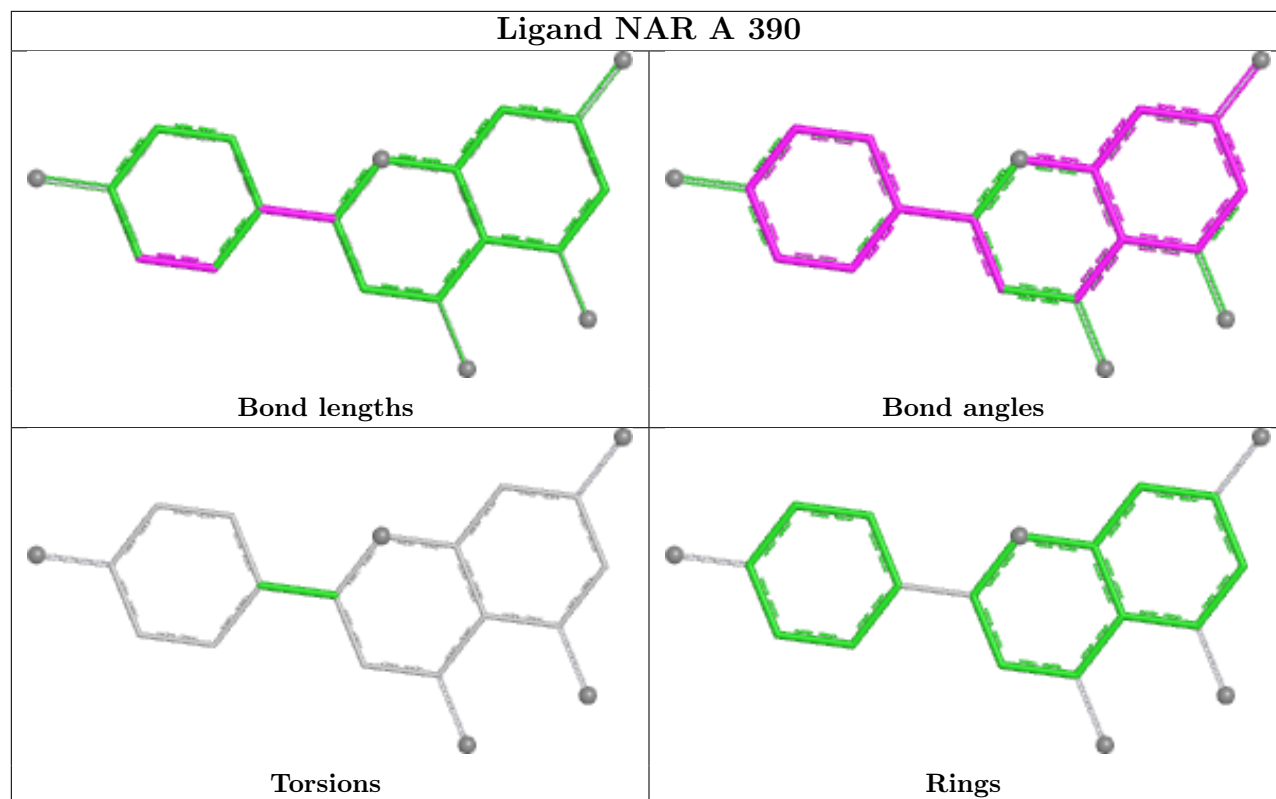
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	390	NAR	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.



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, 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	387/389 (99%)	1.96	161 (41%) 0 1	8, 16, 30, 46	15 (3%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	389	ILE	5.2
1	A	4	VAL	4.6
1	A	252	GLY	4.4
1	A	230	PRO	4.3
1	A	292	ILE	4.3
1	A	232	ILE	4.2
1	A	48	HIS	4.2
1	A	47	GLU	3.9
1	A	3	SER	3.8
1	A	9[A]	LYS	3.8
1	A	13	ALA	3.7
1	A	7	ILE	3.7
1	A	223	ILE	3.7
1	A	42[A]	LYS	3.6
1	A	235	PRO	3.4
1	A	160	TYR	3.3
1	A	118	GLY	3.3
1	A	354[A]	THR	3.3
1	A	375	PRO	3.3
1	A	19	ILE	3.3
1	A	229	VAL	3.3
1	A	284	VAL	3.3
1	A	14[A]	GLU	3.2
1	A	138	PRO	3.2
1	A	290	LEU	3.2
1	A	5[A]	SER	3.2
1	A	117	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	246	ILE	3.2
1	A	234	LYS	3.1
1	A	45	ASN	3.1
1	A	183	GLY	3.1
1	A	189	VAL	3.1
1	A	8	ARG	3.1
1	A	266	HIS	3.1
1	A	38	ASP	3.1
1	A	240	VAL	3.0
1	A	237	PHE	3.0
1	A	184	ALA	3.0
1	A	388	ALA	3.0
1	A	58	ARG	3.0
1	A	144	LEU	3.0
1	A	231	GLU	3.0
1	A	31	VAL	2.9
1	A	241	TRP	2.9
1	A	12	ARG	2.9
1	A	99	VAL	2.9
1	A	153	TYR	2.9
1	A	20	LEU	2.9
1	A	127	LEU	2.9
1	A	225	GLY	2.9
1	A	10	ALA	2.9
1	A	295	TYR	2.8
1	A	41	PHE	2.8
1	A	384	LEU	2.8
1	A	142	TYR	2.8
1	A	37	PRO	2.8
1	A	174	ALA	2.8
1	A	157	TYR	2.7
1	A	15	GLY	2.7
1	A	196	VAL	2.7
1	A	86	TYR	2.7
1	A	204	THR	2.7
1	A	282	ALA	2.7
1	A	39	PHE	2.7
1	A	54	GLU	2.7
1	A	336	ASN	2.7
1	A	201	PRO	2.6
1	A	277	LYS	2.6
1	A	224	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	228	PRO	2.6
1	A	315	GLN	2.6
1	A	46	SER	2.6
1	A	319	LEU	2.6
1	A	370	LEU	2.6
1	A	255[A]	ASP	2.6
1	A	73	THR	2.6
1	A	75	GLU	2.5
1	A	193	VAL	2.5
1	A	173	LEU	2.5
1	A	124	ILE	2.5
1	A	145	THR	2.5
1	A	150	LEU	2.5
1	A	177	LEU	2.5
1	A	198	PHE	2.5
1	A	215	PHE	2.5
1	A	222	LEU	2.5
1	A	98	VAL	2.5
1	A	149	GLY	2.4
1	A	257	HIS	2.4
1	A	283	LEU	2.4
1	A	17	ALA	2.4
1	A	78	LYS	2.4
1	A	129	VAL	2.4
1	A	64	MET	2.4
1	A	105	LEU	2.4
1	A	50	THR	2.4
1	A	210	VAL	2.4
1	A	300	TRP	2.4
1	A	367	TRP	2.4
1	A	356	ASN	2.4
1	A	59	MET	2.4
1	A	245	THR	2.4
1	A	102	VAL	2.4
1	A	43	ILE	2.3
1	A	248	PRO	2.3
1	A	287	PHE	2.3
1	A	309	ILE	2.3
1	A	81	PRO	2.3
1	A	200	GLY	2.3
1	A	137	MET	2.3
1	A	114	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	218	GLY	2.3
1	A	279	ILE	2.3
1	A	293	SER	2.3
1	A	6	GLU	2.3
1	A	281	LYS	2.3
1	A	166	ALA	2.2
1	A	243	ALA	2.2
1	A	151	ARG	2.2
1	A	147	LEU	2.2
1	A	343	LEU	2.2
1	A	56	PHE	2.2
1	A	71	TYR	2.2
1	A	88	ALA	2.2
1	A	296	ASN	2.2
1	A	170	VAL	2.2
1	A	387	VAL	2.2
1	A	91	LEU	2.2
1	A	263	LEU	2.2
1	A	273	GLY	2.2
1	A	89	PRO	2.2
1	A	302	ALA	2.2
1	A	236	ILE	2.1
1	A	379	ILE	2.1
1	A	191	SER	2.1
1	A	206	LEU	2.1
1	A	365	LEU	2.1
1	A	25	ALA	2.1
1	A	113	ALA	2.1
1	A	128	ILE	2.1
1	A	169	THR	2.1
1	A	134	GLY	2.1
1	A	135	VAL	2.1
1	A	382	VAL	2.1
1	A	30	CYS	2.1
1	A	110	ALA	2.1
1	A	40	TYR	2.1
1	A	125	THR	2.1
1	A	23	GLY	2.1
1	A	168	GLY	2.1
1	A	330	VAL	2.1
1	A	130	CYS	2.1
1	A	74	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	274	ILE	2.0
1	A	285	GLU	2.0
1	A	195	ALA	2.0
1	A	297[1]	SER	2.0
1	A	298	ILE	2.0
1	A	11	GLN	2.0
1	A	111	VAL	2.0
1	A	188	VAL	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](#)

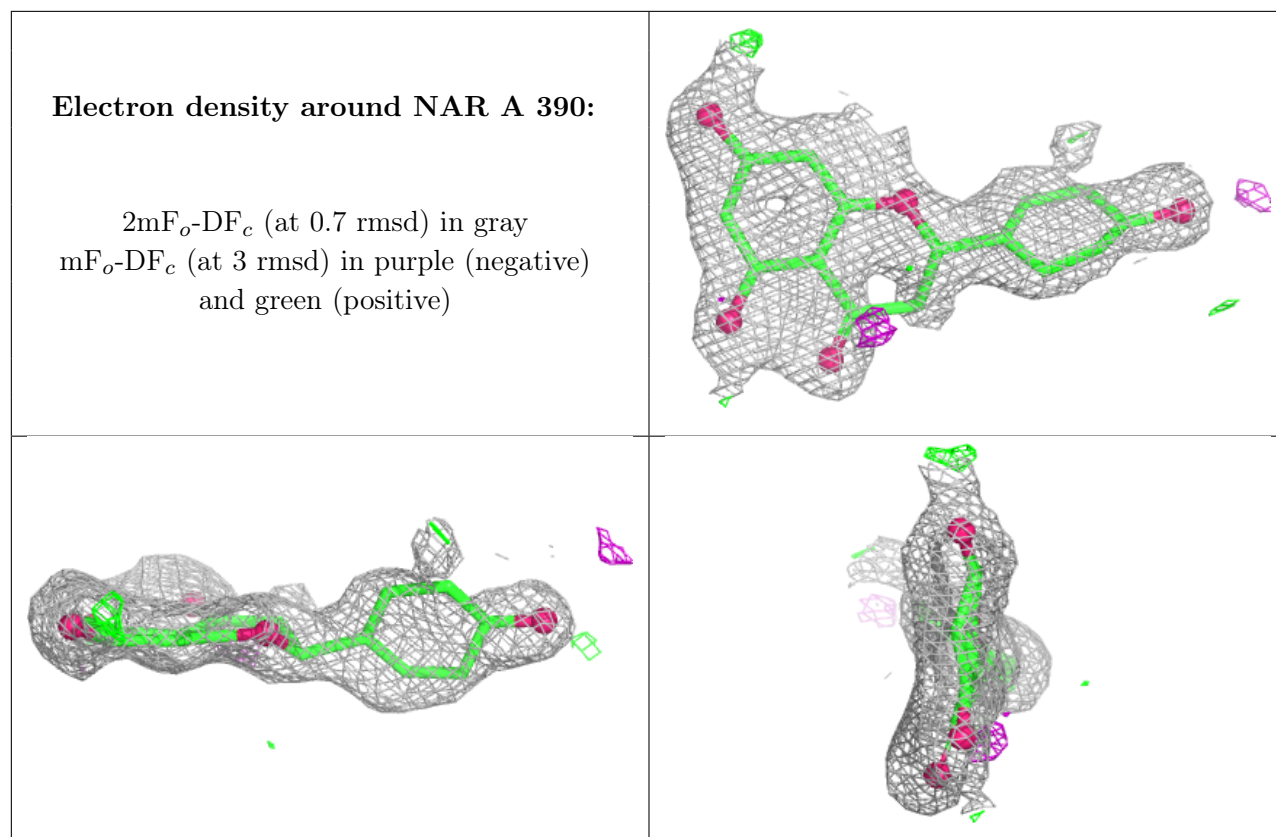
There are no oligosaccharides in this entry.

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	NAR	A	390	20/20	0.72	0.15	28,32,34,34	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 ⓘ

There are no such residues in this entry.