



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 10:08 AM JST

PDB ID : 7VEZ
Title : Crystal structure of Cyclosorus parasiticus chalcone synthase 1 (CpCHS1) complex with naringenin
Authors : Li, J.X.; Cheng, A.X.
Deposited on : 2021-09-10
Resolution : 2.40 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 : 2.23.2
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) : 2.23.2

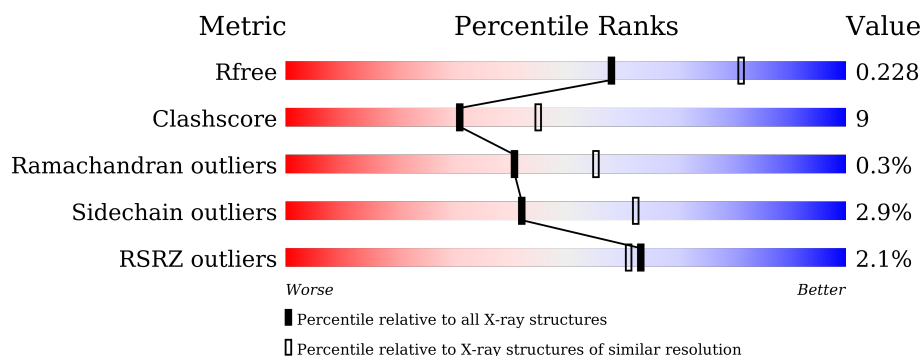
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	404	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	404	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>• •</div> </div> </div>
1	C	404	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>
1	D	404	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

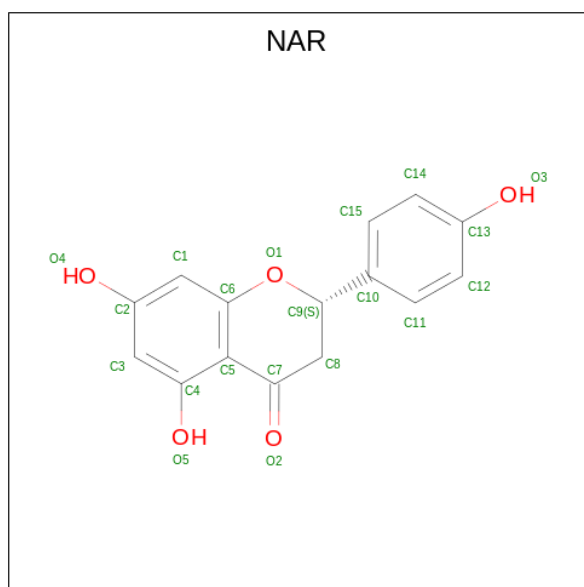
There are 3 unique types of molecules in this entry. The entry contains 12224 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 chalcone synthases 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3010	1919	511	558	22			
1	B	391	Total	C	N	O	S	0	0	0
			3010	1919	511	558	22			
1	C	390	Total	C	N	O	S	0	0	0
			3005	1916	510	557	22			
1	D	392	Total	C	N	O	S	0	0	0
			3014	1921	512	559	22			

- Molecule 2 is NARINGENIN (three-letter code: NAR) (formula: C₁₅H₁₂O₅) (labeled as "Ligand of Interest" by depositor).



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

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

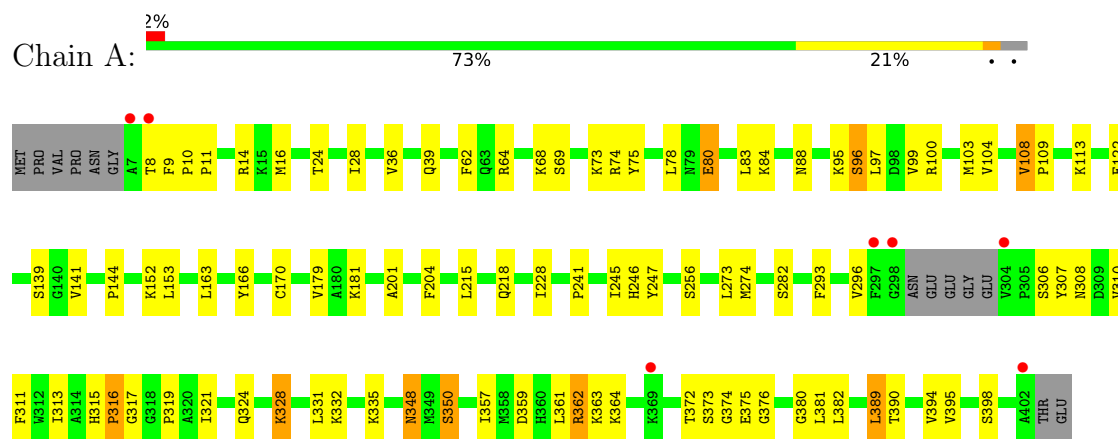
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	16	Total	O	0	0
			16	16		
3	C	22	Total	O	0	0
			22	22		
3	D	34	Total	O	0	0
			34	34		

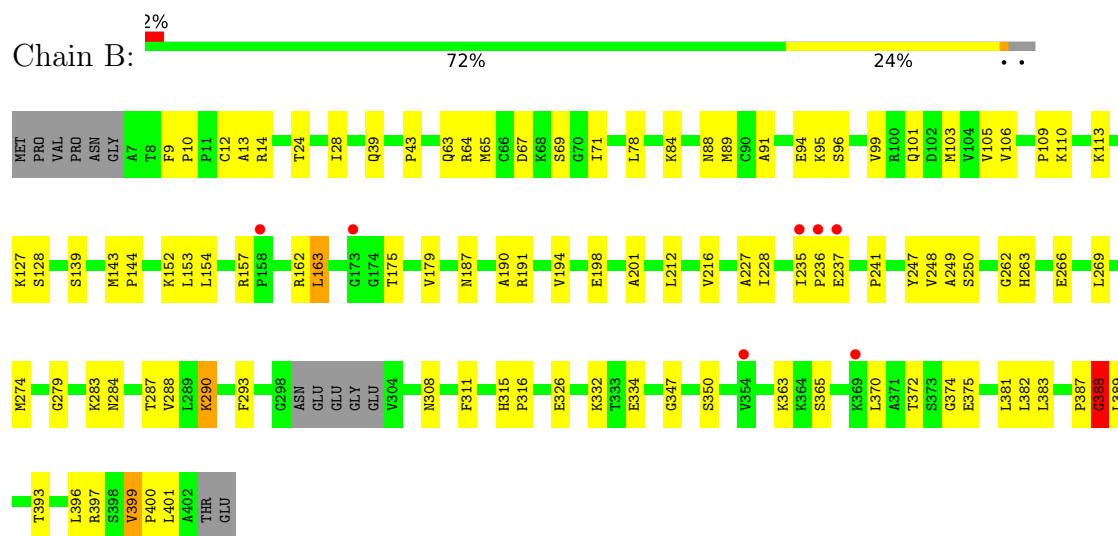
3 Residue-property plots [i](#)

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.

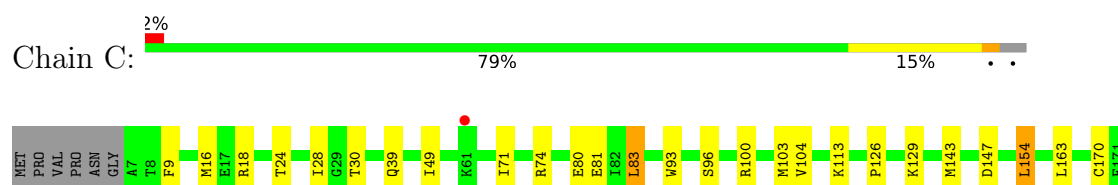
• Molecule 1: chalcone synthases 1

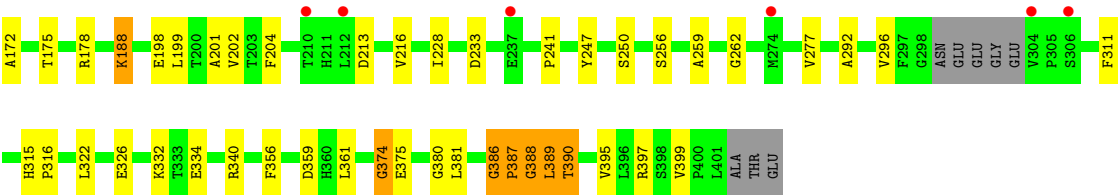


• Molecule 1: chalcone synthases 1

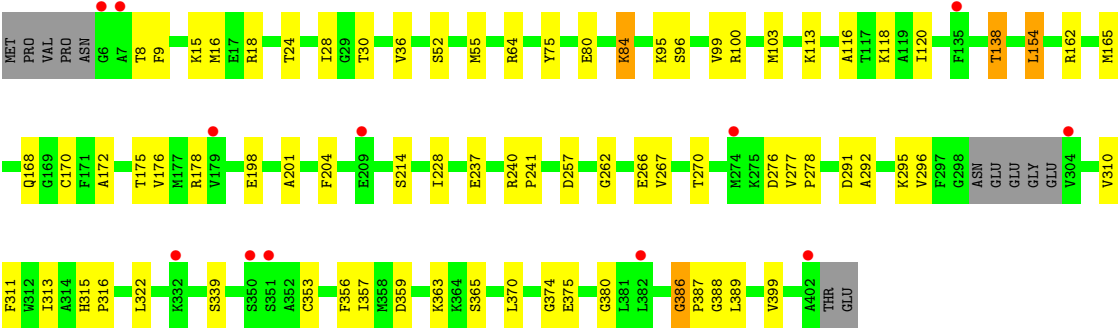
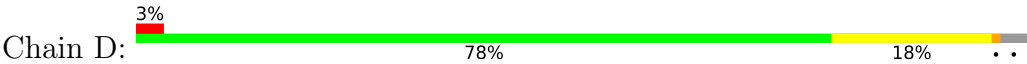


• Molecule 1: chalcone synthases 1





● Molecule 1: chalcone synthases 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.26Å 82.29Å 134.31Å 90.00° 98.94° 90.00°	Depositor
Resolution (Å)	30.43 – 2.40 32.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	66.7 (30.43-2.40) 90.4 (32.47-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.180 , 0.230 0.181 , 0.228	Depositor DCC
R_{free} test set	2000 reflections (3.43%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12224	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.67	0/3076	0.64	1/4168 (0.0%)
1	B	0.71	0/3076	0.67	3/4168 (0.1%)
1	C	0.61	0/3071	0.71	3/4161 (0.1%)
1	D	0.65	0/3080	0.67	4/4173 (0.1%)
All	All	0.66	0/12303	0.67	11/16670 (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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	386	GLY	C-N-CD	-20.25	76.06	120.60
1	D	386	GLY	C-N-CD	-11.82	94.60	120.60
1	A	96	SER	CB-CA-C	7.38	124.12	110.10
1	D	388	GLY	N-CA-C	6.19	128.57	113.10
1	D	237	GLU	CB-CA-C	-6.09	98.22	110.40
1	B	387	PRO	N-CA-C	5.87	127.36	112.10
1	C	388	GLY	N-CA-C	5.57	127.03	113.10
1	D	237	GLU	N-CA-C	5.55	125.98	111.00
1	C	374	GLY	N-CA-C	5.53	126.92	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	GLY	N-CA-C	5.45	126.71	113.10
1	B	399	VAL	C-N-CD	-5.06	109.47	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	388	GLY	Peptide
1	C	386	GLY	Peptide
1	D	386	GLY	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	3010	0	3024	63	0
1	B	3010	0	3024	75	0
1	C	3005	0	3019	54	0
1	D	3014	0	3027	51	0
2	A	20	0	9	2	0
2	B	20	0	9	0	0
2	C	20	0	9	1	0
2	D	20	0	9	0	0
3	A	33	0	0	2	0
3	B	16	0	0	3	0
3	C	22	0	0	2	0
3	D	34	0	0	2	0
All	All	12224	0	12130	221	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 9.

All (221) 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:B:95:LYS:NZ	1:B:266:GLU:OE2	1.73	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:PRO:HG3	1:C:387:PRO:O	1.05	1.19
1:B:144:PRO:CG	1:C:387:PRO:O	2.00	1.09
1:B:248:VAL:H	1:C:16:MET:HE1	1.28	0.98
1:B:162:ARG:HH22	1:C:390:THR:HG21	1.30	0.96
1:C:100:ARG:NH1	1:C:204:PHE:O	1.98	0.95
1:C:96:SER:OG	1:C:100:ARG:NH2	2.03	0.92
1:C:147:ASP:OD1	3:C:601:HOH:O	1.88	0.92
1:A:100:ARG:NH1	1:A:204:PHE:O	2.04	0.91
1:A:144:PRO:HG3	1:D:387:PRO:O	1.72	0.89
1:B:400:PRO:HD3	1:C:9:PHE:CE2	2.12	0.84
1:C:103:MET:HE3	1:C:201:ALA:HB1	1.58	0.84
1:D:16:MET:O	3:D:601:HOH:O	1.96	0.83
1:D:95:LYS:NZ	1:D:266:GLU:OE2	2.13	0.80
1:B:162:ARG:O	1:C:178:ARG:NH2	2.14	0.80
1:B:326:GLU:OE1	3:B:601:HOH:O	2.01	0.78
1:B:39:GLN:OE1	3:B:602:HOH:O	2.03	0.74
1:B:113:LYS:NZ	1:B:153:LEU:O	2.20	0.74
1:C:311:PHE:HB3	1:C:374:GLY:O	1.89	0.71
1:A:324:GLN:O	1:A:328:LYS:HG2	1.91	0.71
1:B:374:GLY:O	1:B:375:GLU:HB2	1.90	0.70
1:C:361:LEU:HD11	1:C:375:GLU:HG3	1.73	0.70
1:D:80:GLU:HG2	1:D:84:LYS:HZ2	1.56	0.70
1:B:248:VAL:N	1:C:16:MET:HE1	2.06	0.70
1:A:122:GLU:OE2	1:A:362:ARG:NH2	2.27	0.68
1:D:80:GLU:HG2	1:D:84:LYS:NZ	2.09	0.68
1:D:374:GLY:O	1:D:375:GLU:HB2	1.95	0.66
1:A:104:VAL:O	1:A:108:VAL:HG13	1.96	0.66
1:C:126:PRO:HG2	1:C:129:LYS:HG3	1.79	0.64
1:B:162:ARG:HH22	1:C:390:THR:CG2	2.06	0.64
1:B:293:PHE:HE1	1:B:381:LEU:HD21	1.63	0.63
1:D:100:ARG:NH1	1:D:204:PHE:O	2.32	0.63
1:C:256:SER:HB2	1:C:389:LEU:HB2	1.81	0.62
1:A:390:THR:OG1	1:D:162:ARG:NH2	2.32	0.62
1:B:91:ALA:HB3	1:B:94:GLU:HG3	1.80	0.62
1:B:365:SER:HA	1:B:370:LEU:HD12	1.81	0.62
1:A:317:GLY:HA3	1:A:321:ILE:HD12	1.82	0.61
1:D:165:MET:HE1	1:D:176:VAL:HG12	1.83	0.61
1:B:163:LEU:HD21	1:C:163:LEU:HD21	1.82	0.60
1:B:311:PHE:HB3	1:B:374:GLY:O	2.00	0.60
1:A:246:HIS:HB3	1:D:15:LYS:HG3	1.83	0.60
1:B:332:LYS:NZ	1:B:334:GLU:OE2	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ILE:HG12	1:B:347:GLY:HA2	1.84	0.60
1:A:80:GLU:OE1	1:A:84:LYS:NZ	2.36	0.59
1:D:365:SER:HA	1:D:370:LEU:HD12	1.85	0.58
1:C:188:LYS:NZ	1:C:233:ASP:OD2	2.37	0.58
1:C:39:GLN:OE1	1:C:74:ARG:NH1	2.35	0.57
1:A:8:THR:HG22	1:A:9:PHE:O	2.04	0.57
1:D:80:GLU:CG	1:D:84:LYS:HZ2	2.17	0.57
1:B:99:VAL:O	1:B:103:MET:HG3	2.04	0.57
1:D:28:ILE:HG12	1:D:228:ILE:HG22	1.87	0.57
1:D:113:LYS:HG3	1:D:154:LEU:HD13	1.86	0.57
1:A:324:GLN:HB3	1:A:328:LYS:HE3	1.87	0.57
1:A:359:ASP:OD1	1:A:362:ARG:NH1	2.36	0.57
1:B:9:PHE:HB3	1:B:10:PRO:HD2	1.87	0.56
1:D:100:ARG:NH2	1:D:267:VAL:O	2.38	0.56
1:B:28:ILE:HG12	1:B:228:ILE:HG22	1.88	0.56
1:B:248:VAL:HG22	1:C:16:MET:HE3	1.87	0.56
1:A:69:SER:O	1:A:319:PRO:HG3	2.07	0.55
1:C:170:CYS:SG	3:C:613:HOH:O	2.40	0.55
1:C:113:LYS:HG3	1:C:154:LEU:HD13	1.89	0.55
1:D:80:GLU:CB	1:D:84:LYS:HZ2	2.19	0.55
1:A:108:VAL:HG22	1:A:109:PRO:HD3	1.88	0.55
1:A:28:ILE:HG12	1:A:228:ILE:HG22	1.89	0.55
1:A:362:ARG:HG2	1:A:363:LYS:N	2.22	0.54
1:B:279:GLY:O	1:B:283:LYS:HG2	2.08	0.54
1:C:28:ILE:HG21	1:C:359:ASP:HB2	1.88	0.54
1:A:311:PHE:HB3	1:A:374:GLY:O	2.08	0.54
1:B:212:LEU:O	1:B:216:VAL:HG23	2.07	0.54
1:D:96:SER:OG	1:D:100:ARG:NH2	2.41	0.54
1:A:24:THR:HG21	1:A:241:PRO:HB3	1.90	0.54
1:D:168:GLN:HB3	1:D:172:ALA:HB2	1.89	0.54
1:A:293:PHE:HE1	1:A:381:LEU:HD21	1.74	0.53
1:B:383:LEU:HD22	1:B:393:THR:HG22	1.91	0.52
1:B:198:GLU:HG3	1:B:350:SER:HB3	1.92	0.52
1:C:30:THR:HB	1:C:356:PHE:CZ	2.44	0.52
1:A:152:LYS:NZ	3:A:601:HOH:O	2.15	0.52
1:D:291:ASP:O	1:D:295:LYS:HG2	2.10	0.52
1:D:311:PHE:HB3	1:D:374:GLY:O	2.10	0.52
1:A:296:VAL:HG13	1:D:15:LYS:HD2	1.90	0.52
1:C:24:THR:HG21	1:C:241:PRO:HB3	1.90	0.52
1:B:106:VAL:O	1:B:109:PRO:HD2	2.10	0.51
1:D:165:MET:CE	1:D:176:VAL:HG12	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ASN:ND2	1:A:350:SER:H	2.09	0.51
1:B:103:MET:HE3	1:B:201:ALA:HB1	1.92	0.51
1:C:71:ILE:HG21	1:C:74:ARG:HD2	1.91	0.51
2:A:501:NAR:O5	2:A:501:NAR:O2	2.26	0.51
1:B:69:SER:HB2	1:B:71:ILE:HD12	1.92	0.51
1:A:382:LEU:HB3	1:A:394:VAL:HB	1.93	0.50
1:A:96:SER:O	1:A:99:VAL:HG22	2.12	0.50
1:B:247:TYR:HA	1:C:16:MET:CE	2.41	0.50
1:B:106:VAL:O	1:B:110:LYS:HG3	2.11	0.50
1:D:241:PRO:HB2	1:D:399:VAL:HG11	1.93	0.50
1:B:67:ASP:OD2	3:B:603:HOH:O	2.20	0.50
1:A:282:SER:HB2	1:A:328:LYS:HG3	1.93	0.50
1:B:382:LEU:HB2	1:B:396:LEU:HD11	1.94	0.50
1:A:141:VAL:HG12	1:A:166:TYR:CG	2.47	0.49
1:C:374:GLY:O	1:C:375:GLU:HB2	2.11	0.49
1:B:308:ASN:HB3	1:B:332:LYS:HD3	1.94	0.49
1:C:213:ASP:O	1:C:216:VAL:HG12	2.12	0.49
1:A:256:SER:HB2	1:A:389:LEU:HB2	1.94	0.49
1:C:316:PRO:HB3	1:C:322:LEU:HD11	1.94	0.49
1:C:326:GLU:OE1	1:C:340:ARG:NH2	2.42	0.49
1:A:64:ARG:HE	1:A:64:ARG:HA	1.76	0.49
1:D:24:THR:HG21	1:D:241:PRO:HB3	1.93	0.49
1:C:332:LYS:HD3	1:C:334:GLU:OE1	2.13	0.49
1:D:170:CYS:HB3	1:D:315:HIS:NE2	2.28	0.49
1:A:310:VAL:HB	1:A:380:GLY:HA2	1.94	0.48
1:D:353:CYS:O	1:D:357:ILE:HG13	2.13	0.48
1:B:43:PRO:HG2	1:B:63:GLN:OE1	2.14	0.48
1:D:316:PRO:HB3	1:D:322:LEU:HD11	1.96	0.48
1:B:78:LEU:HD21	1:B:103:MET:HE1	1.95	0.48
1:B:65:MET:CE	1:B:216:VAL:HG22	2.43	0.48
1:D:313:ILE:HG23	1:D:357:ILE:HB	1.95	0.48
1:B:101:GLN:O	1:B:105:VAL:HG12	2.14	0.47
1:B:383:LEU:CD2	1:B:393:THR:HG22	2.44	0.47
1:A:97:LEU:O	1:A:97:LEU:HG	2.14	0.47
1:B:128:SER:O	1:B:157:ARG:HD2	2.15	0.47
1:A:163:LEU:HD23	1:A:179:VAL:HG11	1.97	0.47
1:D:8:THR:HG22	1:D:9:PHE:O	2.14	0.47
1:B:175:THR:O	1:B:179:VAL:HG23	2.15	0.47
1:A:373:SER:OG	1:A:398:SER:HB2	2.14	0.47
1:A:218:GLN:NE2	3:A:606:HOH:O	2.38	0.46
1:A:28:ILE:HG21	1:A:359:ASP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASN:OD1	1:A:332:LYS:HG2	2.15	0.46
1:A:78:LEU:HD11	1:A:201:ALA:HA	1.97	0.46
1:B:24:THR:HG21	1:B:241:PRO:HB3	1.96	0.46
1:B:290:LYS:HA	1:B:290:LYS:HD3	1.37	0.46
1:B:389:LEU:HD23	1:B:389:LEU:C	2.36	0.46
1:D:138:THR:HG23	1:D:198:GLU:OE2	2.16	0.46
1:A:313:ILE:HG23	1:A:357:ILE:HB	1.97	0.45
1:A:68:LYS:HA	1:A:68:LYS:HD3	1.69	0.45
1:B:372:THR:HA	1:B:399:VAL:O	2.17	0.45
1:B:187:ASN:HB2	1:B:190:ALA:HB2	1.98	0.45
1:A:103:MET:HE1	1:A:201:ALA:HB1	1.99	0.45
1:B:113:LYS:NZ	1:B:153:LEU:C	2.70	0.45
1:A:331:LEU:HB3	1:A:335:LYS:HG3	1.98	0.45
1:A:348:ASN:HD22	1:A:350:SER:H	1.63	0.45
1:C:388:GLY:H	1:C:390:THR:HG23	1.81	0.45
1:A:372:THR:H	1:A:376:GLY:HA2	1.82	0.45
1:B:88:ASN:OD1	1:B:88:ASN:N	2.50	0.45
1:A:348:ASN:HD22	1:A:348:ASN:C	2.20	0.45
1:B:103:MET:CE	1:B:201:ALA:HB1	2.47	0.45
1:B:143:MET:HE2	1:C:262:GLY:HA3	1.99	0.44
1:D:165:MET:HB3	1:D:168:GLN:HE21	1.82	0.44
1:D:30:THR:O	1:D:118:LYS:NZ	2.35	0.44
1:A:14:ARG:HG3	1:A:16:MET:O	2.16	0.44
1:A:36:VAL:HG22	1:A:75:TYR:CE1	2.52	0.44
1:A:282:SER:HB2	1:A:328:LYS:CG	2.46	0.44
1:D:18:ARG:NH1	3:D:606:HOH:O	2.32	0.44
1:A:88:ASN:OD1	1:A:88:ASN:N	2.48	0.44
1:A:170:CYS:SG	2:A:501:NAR:H11	2.58	0.44
1:A:361:LEU:HD11	1:A:375:GLU:HG3	1.99	0.44
1:B:127:LYS:HE3	1:B:154:LEU:O	2.18	0.44
1:B:400:PRO:HD3	1:C:9:PHE:CD2	2.50	0.44
1:D:310:VAL:HB	1:D:380:GLY:HA2	1.99	0.44
1:D:277:VAL:HG13	1:D:389:LEU:HD11	2.00	0.43
1:B:113:LYS:HE3	1:B:154:LEU:HD23	2.00	0.43
1:B:249:ALA:HB3	1:B:393:THR:OG1	2.19	0.43
1:C:83:LEU:HD12	1:C:83:LEU:HA	1.86	0.43
1:A:73:LYS:HE2	1:A:75:TYR:OH	2.18	0.43
1:C:104:VAL:HG11	1:C:202:VAL:HG13	1.99	0.43
1:B:113:LYS:HZ2	1:B:153:LEU:C	2.22	0.43
2:C:501:NAR:O2	2:C:501:NAR:O5	2.34	0.43
1:D:165:MET:HB3	1:D:168:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ALA:CB	1:B:94:GLU:HG3	2.49	0.42
1:B:143:MET:CE	1:C:262:GLY:HA3	2.49	0.42
1:B:194:VAL:O	1:B:227:ALA:HA	2.19	0.42
1:D:99:VAL:O	1:D:103:MET:HG3	2.19	0.42
1:D:240:ARG:HA	1:D:241:PRO:HD2	1.96	0.42
1:D:339:SER:HA	1:D:357:ILE:HD13	2.00	0.42
1:A:122:GLU:CD	1:A:362:ARG:HH22	2.22	0.42
1:B:263:HIS:O	1:B:269:LEU:HD12	2.19	0.42
1:D:36:VAL:HG22	1:D:75:TYR:CE2	2.53	0.42
1:B:247:TYR:HA	1:C:16:MET:HE1	2.01	0.42
1:B:284:ASN:O	1:B:288:VAL:HG23	2.20	0.42
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.67	0.42
1:C:198:GLU:O	1:C:199:LEU:HD23	2.19	0.42
1:D:175:THR:HG23	1:D:178:ARG:NH2	2.33	0.42
1:B:248:VAL:HG22	1:C:16:MET:CE	2.50	0.42
1:C:49:ILE:HD12	1:C:49:ILE:HA	1.83	0.42
1:B:10:PRO:O	1:C:397:ARG:NH2	2.51	0.42
1:A:144:PRO:CG	1:D:387:PRO:O	2.57	0.42
1:A:181:LYS:HD2	1:A:245:ILE:HG22	2.01	0.42
1:C:28:ILE:HG12	1:C:228:ILE:HG22	2.01	0.42
1:D:52:SER:HB3	1:D:55:MET:HG3	2.00	0.42
1:B:315:HIS:HA	1:B:316:PRO:HD3	1.70	0.42
1:D:262:GLY:HA2	1:D:270:THR:O	2.19	0.42
1:A:39:GLN:OE1	1:A:74:ARG:NH2	2.53	0.41
1:C:259:ALA:HB1	1:C:277:VAL:HG22	2.01	0.41
1:D:103:MET:HE1	1:D:201:ALA:HB1	2.02	0.41
1:A:113:LYS:HD2	1:A:153:LEU:HB3	2.02	0.41
1:A:273:LEU:C	1:A:274:MET:HG3	2.40	0.41
1:A:311:PHE:CD2	1:A:374:GLY:HA3	2.55	0.41
1:D:276:ASP:OD1	1:D:278:PRO:HD2	2.21	0.41
1:D:359:ASP:OD1	1:D:363:LYS:HE3	2.19	0.41
1:B:13:ALA:O	1:B:14:ARG:C	2.59	0.41
1:B:190:ALA:O	1:B:191:ARG:NH1	2.54	0.41
1:C:170:CYS:HB3	1:C:315:HIS:NE2	2.35	0.41
1:C:172:ALA:HA	1:C:175:THR:OG1	2.20	0.41
1:D:116:ALA:O	1:D:120:ILE:HG13	2.20	0.41
1:B:247:TYR:HA	1:C:16:MET:HE2	2.03	0.41
1:C:311:PHE:CE1	1:C:380:GLY:HA3	2.56	0.41
1:D:30:THR:HB	1:D:356:PHE:CZ	2.56	0.41
1:D:96:SER:O	1:D:100:ARG:HG3	2.20	0.41
1:A:62:PHE:CD1	1:A:215:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LYS:O	1:B:84:LYS:HG2	2.20	0.41
1:B:89:MET:HB3	1:B:89:MET:HE2	1.94	0.41
1:C:80:GLU:HG2	1:C:81:GLU:OE1	2.21	0.41
1:C:241:PRO:O	1:C:399:VAL:HG21	2.20	0.41
1:A:10:PRO:HA	1:A:11:PRO:HD3	1.89	0.41
1:A:99:VAL:O	1:A:103:MET:HG3	2.21	0.41
1:A:315:HIS:HA	1:A:316:PRO:HD3	1.58	0.41
1:D:292:ALA:O	1:D:296:VAL:HG13	2.21	0.41
1:B:43:PRO:HG2	1:B:63:GLN:CD	2.41	0.40
1:A:306:SER:OG	1:A:307:TYR:N	2.54	0.40
1:B:262:GLY:HA3	1:C:143:MET:HE3	2.03	0.40
1:C:247:TYR:HB3	1:C:395:VAL:HB	2.04	0.40
1:A:247:TYR:HB3	1:A:395:VAL:HB	2.04	0.40
1:B:235:ILE:HA	1:B:236:PRO:HD3	1.91	0.40
1:C:292:ALA:O	1:C:296:VAL:HG23	2.21	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	387/404 (96%)	375 (97%)	11 (3%)	1 (0%)	41	55
1	B	387/404 (96%)	366 (95%)	19 (5%)	2 (0%)	29	41
1	C	386/404 (96%)	370 (96%)	15 (4%)	1 (0%)	41	55
1	D	388/404 (96%)	376 (97%)	12 (3%)	0	100	100
All	All	1548/1616 (96%)	1487 (96%)	57 (4%)	4 (0%)	41	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	388	GLY
1	C	387	PRO
1	B	96	SER
1	A	316	PRO

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	327/338 (97%)	316 (97%)	11 (3%)	37	56
1	B	327/338 (97%)	315 (96%)	12 (4%)	34	53
1	C	327/338 (97%)	318 (97%)	9 (3%)	43	63
1	D	327/338 (97%)	321 (98%)	6 (2%)	59	76
All	All	1308/1352 (97%)	1270 (97%)	38 (3%)	42	62

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	83	LEU
1	A	95	LYS
1	A	108	VAL
1	A	139	SER
1	A	328	LYS
1	A	348	ASN
1	A	350	SER
1	A	362	ARG
1	A	364	LYS
1	A	389	LEU
1	B	12	CYS
1	B	64	ARG
1	B	139	SER
1	B	152	LYS
1	B	163	LEU
1	B	237	GLU
1	B	250	SER

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Mol	Chain	Res	Type
1	B	274	MET
1	B	287	THR
1	B	290	LYS
1	B	363	LYS
1	B	397	ARG
1	C	18	ARG
1	C	83	LEU
1	C	93	TRP
1	C	154	LEU
1	C	188	LYS
1	C	250	SER
1	C	381	LEU
1	C	389	LEU
1	C	390	THR
1	D	64	ARG
1	D	84	LYS
1	D	138	THR
1	D	154	LEU
1	D	214	SER
1	D	257	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	348	ASN
1	A	368	GLN
1	C	167	GLN
1	D	187	ASN
1	D	368	GLN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	NAR	A	501	-	22,22,22	1.94	7 (31%)	32,32,32	2.28	12 (37%)
2	NAR	C	501	-	22,22,22	1.73	6 (27%)	32,32,32	2.45	12 (37%)
2	NAR	B	501	-	22,22,22	1.98	7 (31%)	32,32,32	1.60	7 (21%)
2	NAR	D	501	-	22,22,22	1.84	8 (36%)	32,32,32	2.33	11 (34%)

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	501	-	-	0/4/16/16	0/3/3/3
2	NAR	C	501	-	-	0/4/16/16	0/3/3/3
2	NAR	B	501	-	-	0/4/16/16	0/3/3/3
2	NAR	D	501	-	-	0/4/16/16	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAR	C5-C6	4.44	1.48	1.40
2	C	501	NAR	C5-C4	4.06	1.48	1.41
2	A	501	NAR	C10-C9	-3.91	1.44	1.51
2	D	501	NAR	C5-C6	3.86	1.47	1.40
2	B	501	NAR	O1-C6	-3.71	1.32	1.38
2	A	501	NAR	C5-C4	3.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NAR	O2-C7	-3.27	1.17	1.22
2	D	501	NAR	C5-C4	3.14	1.46	1.41
2	B	501	NAR	C10-C9	-2.99	1.46	1.51
2	D	501	NAR	O2-C7	-2.97	1.17	1.22
2	B	501	NAR	C5-C4	2.96	1.46	1.41
2	C	501	NAR	C5-C6	2.88	1.45	1.40
2	A	501	NAR	C12-C11	-2.82	1.33	1.38
2	C	501	NAR	O2-C7	-2.76	1.17	1.22
2	A	501	NAR	O1-C9	-2.69	1.38	1.44
2	D	501	NAR	O1-C9	-2.42	1.38	1.44
2	D	501	NAR	O1-C6	-2.37	1.34	1.38
2	C	501	NAR	C10-C9	-2.37	1.47	1.51
2	C	501	NAR	O1-C6	-2.35	1.34	1.38
2	A	501	NAR	C5-C6	2.34	1.44	1.40
2	C	501	NAR	O1-C9	-2.26	1.39	1.44
2	D	501	NAR	C15-C14	-2.25	1.34	1.38
2	D	501	NAR	O4-C2	-2.21	1.31	1.37
2	B	501	NAR	O3-C13	-2.19	1.31	1.37
2	A	501	NAR	O3-C13	-2.08	1.32	1.37
2	B	501	NAR	C15-C14	-2.05	1.35	1.38
2	B	501	NAR	O5-C4	-2.03	1.32	1.36
2	D	501	NAR	C15-C10	-2.02	1.35	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	NAR	C4-C5-C6	5.74	123.18	117.35
2	D	501	NAR	C4-C5-C6	5.44	122.88	117.35
2	D	501	NAR	C3-C4-C5	-5.37	114.70	120.93
2	C	501	NAR	O2-C7-C5	-5.13	114.26	122.38
2	C	501	NAR	O1-C6-C1	5.07	124.36	116.38
2	D	501	NAR	O1-C6-C1	4.61	123.64	116.38
2	A	501	NAR	O5-C4-C5	-4.40	112.91	121.14
2	D	501	NAR	O2-C7-C5	-4.34	115.51	122.38
2	A	501	NAR	C4-C5-C6	4.28	121.70	117.35
2	A	501	NAR	O2-C7-C5	-4.22	115.70	122.38
2	A	501	NAR	O2-C7-C8	4.09	126.53	120.79
2	A	501	NAR	O1-C6-C1	4.01	122.70	116.38
2	C	501	NAR	C3-C4-C5	-4.00	116.29	120.93
2	C	501	NAR	C6-C5-C7	-3.64	117.02	120.33
2	A	501	NAR	O5-C4-C3	3.56	129.01	119.46
2	C	501	NAR	C1-C6-C5	-3.34	115.99	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAR	C14-C15-C10	-3.29	117.89	121.20
2	C	501	NAR	O5-C4-C3	3.28	128.24	119.46
2	B	501	NAR	C4-C5-C6	3.22	120.62	117.35
2	B	501	NAR	O2-C7-C8	3.20	125.29	120.79
2	D	501	NAR	C6-C5-C7	-3.18	117.44	120.33
2	B	501	NAR	C3-C4-C5	-3.08	117.35	120.93
2	D	501	NAR	C3-C2-C1	3.04	124.63	120.43
2	C	501	NAR	O5-C4-C5	-3.03	115.46	121.14
2	D	501	NAR	C6-O1-C9	2.99	120.53	115.50
2	A	501	NAR	C15-C10-C11	2.97	122.00	118.29
2	C	501	NAR	O2-C7-C8	2.89	124.85	120.79
2	A	501	NAR	C1-C6-C5	-2.88	116.79	121.86
2	B	501	NAR	C3-C2-C1	2.88	124.41	120.43
2	D	501	NAR	C1-C6-C5	-2.79	116.95	121.86
2	C	501	NAR	C6-O1-C9	2.72	120.08	115.50
2	D	501	NAR	C4-C3-C2	2.64	122.09	119.70
2	A	501	NAR	O4-C2-C1	-2.55	113.22	119.84
2	A	501	NAR	C3-C4-C5	-2.46	118.08	120.93
2	D	501	NAR	O2-C7-C8	2.43	124.21	120.79
2	B	501	NAR	O1-C6-C1	2.33	120.05	116.38
2	B	501	NAR	C1-C6-C5	-2.21	117.96	121.86
2	B	501	NAR	C15-C10-C11	2.16	120.99	118.29
2	C	501	NAR	O4-C2-C1	-2.16	114.22	119.84
2	D	501	NAR	O1-C6-C5	-2.08	119.41	121.56
2	C	501	NAR	C3-C2-C1	2.03	123.23	120.43
2	A	501	NAR	C6-C1-C2	2.01	122.32	119.05

There are no chirality outliers.

There are no torsion outliers.

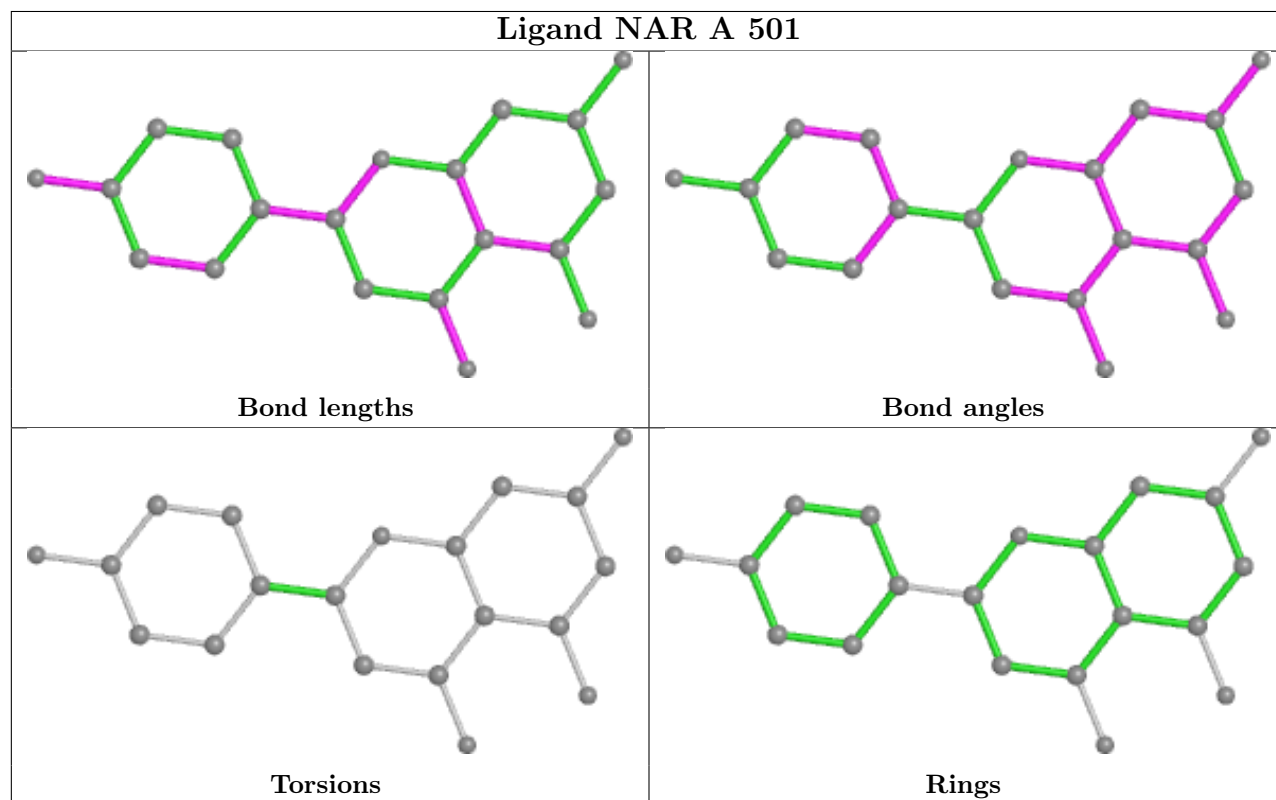
There are no ring outliers.

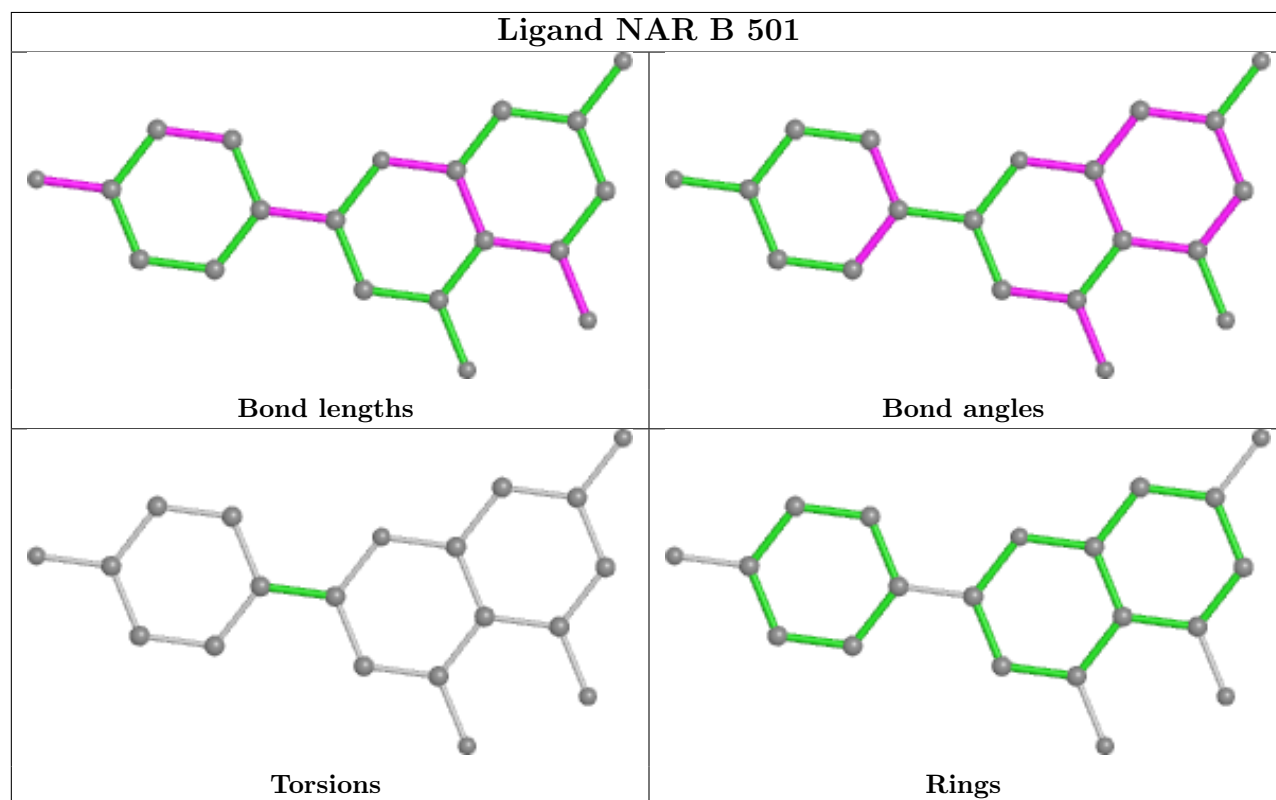
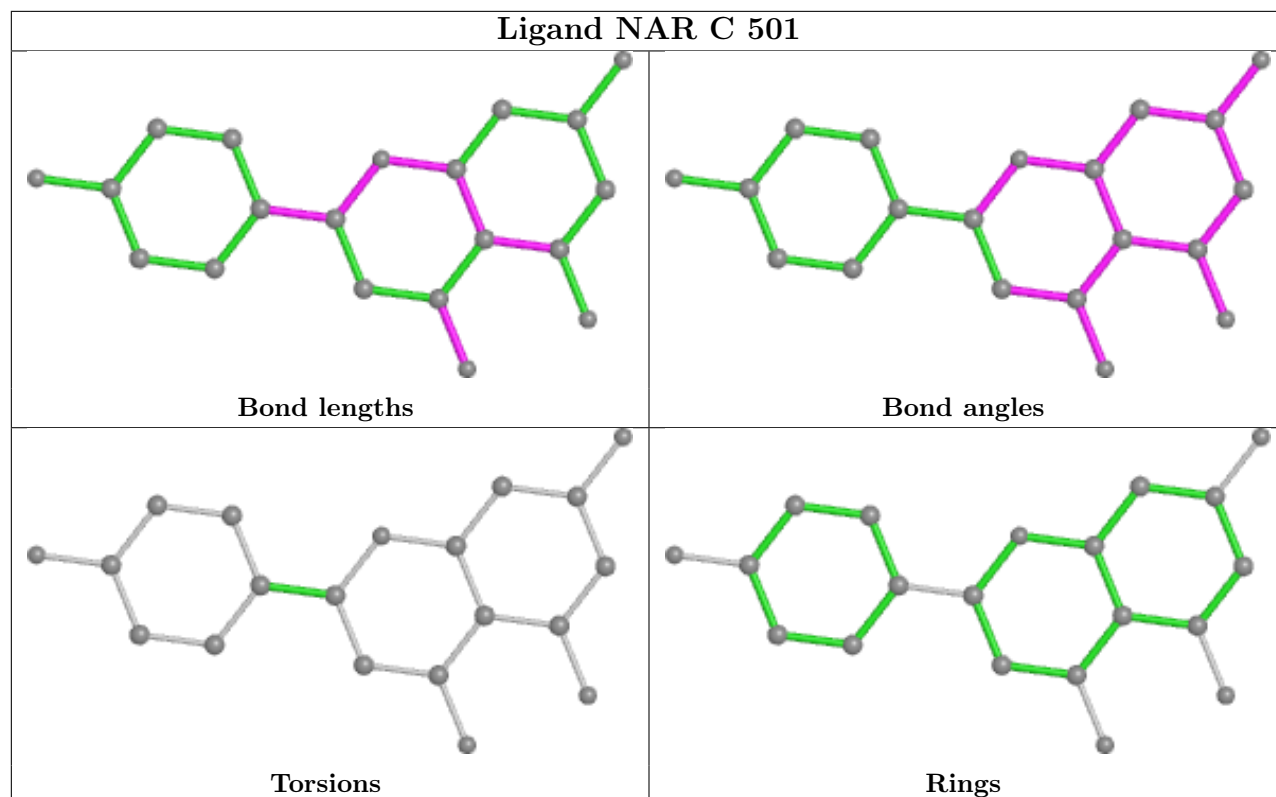
2 monomers are involved in 3 short contacts:

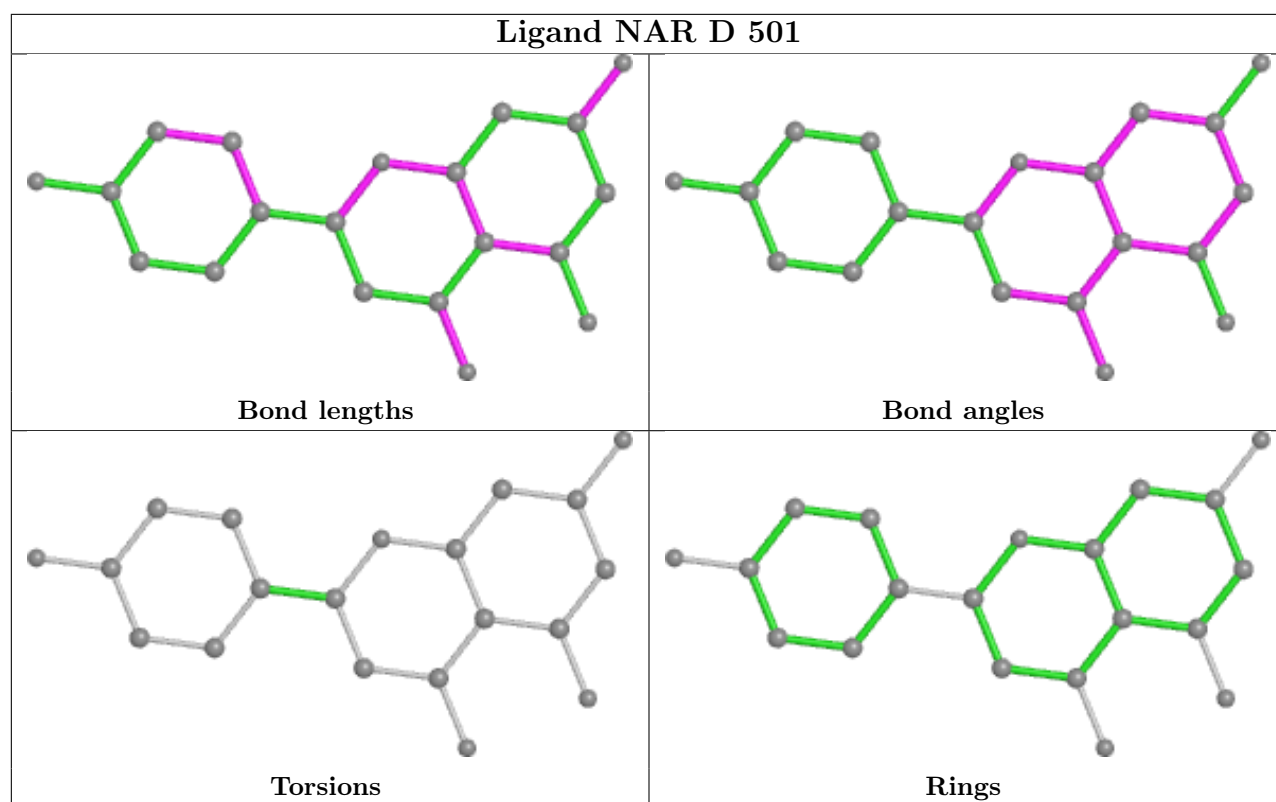
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAR	2	0
2	C	501	NAR	1	0

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	391/404 (96%)	-0.02	7 (1%) 68 66	4, 7, 15, 24	0
1	B	391/404 (96%)	-0.02	7 (1%) 68 66	5, 9, 16, 24	0
1	C	390/404 (96%)	0.03	7 (1%) 68 66	4, 9, 18, 26	0
1	D	392/404 (97%)	0.05	12 (3%) 49 47	4, 7, 15, 25	0
All	All	1564/1616 (96%)	0.01	33 (2%) 63 61	4, 8, 16, 26	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	304	VAL	5.0
1	D	274	MET	3.8
1	A	7	ALA	3.4
1	A	298	GLY	3.3
1	D	6	GLY	3.2
1	D	402	ALA	3.2
1	C	274	MET	3.1
1	C	212	LEU	2.9
1	B	237	GLU	2.9
1	D	135	PHE	2.9
1	B	158	PRO	2.9
1	D	382	LEU	2.8
1	D	179	VAL	2.8
1	B	235	ILE	2.7
1	A	402	ALA	2.7
1	D	304	VAL	2.7
1	D	332	LYS	2.6
1	B	236	PRO	2.5
1	D	351	SER	2.4
1	A	369	LYS	2.4
1	D	209	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	369	LYS	2.3
1	D	350	SER	2.2
1	A	297	PHE	2.2
1	D	7	ALA	2.2
1	A	304	VAL	2.1
1	A	8	THR	2.1
1	C	210	THR	2.1
1	C	237	GLU	2.1
1	B	173	GLY	2.1
1	C	306	SER	2.1
1	B	354	VAL	2.0
1	C	61	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

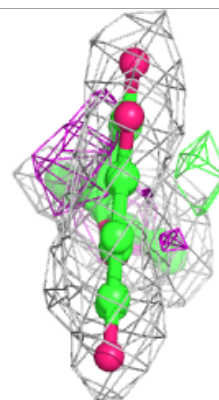
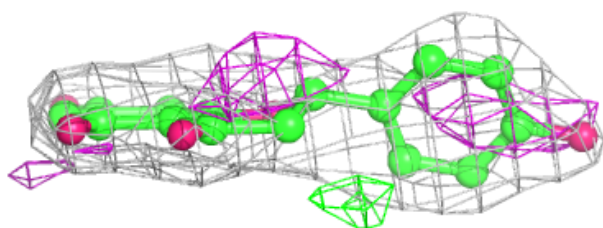
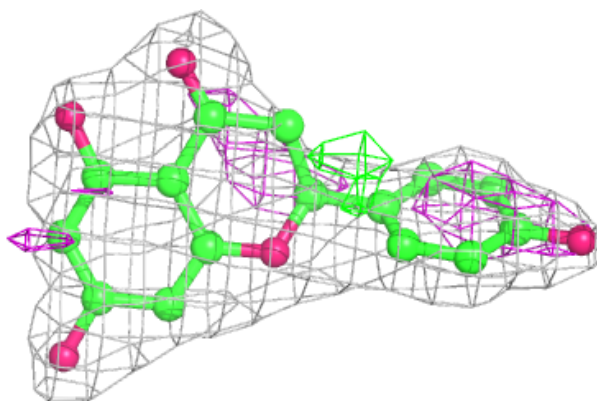
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAR	B	501	20/20	0.87	0.19	4,9,14,15	0
2	NAR	C	501	20/20	0.89	0.16	3,10,12,14	0
2	NAR	A	501	20/20	0.92	0.14	2,8,15,18	0
2	NAR	D	501	20/20	0.94	0.12	4,9,13,17	0

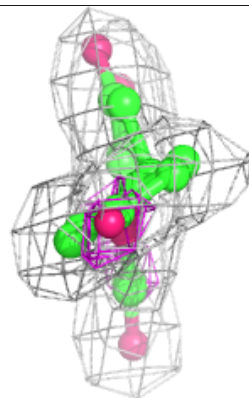
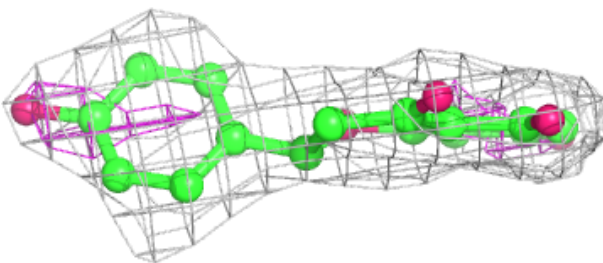
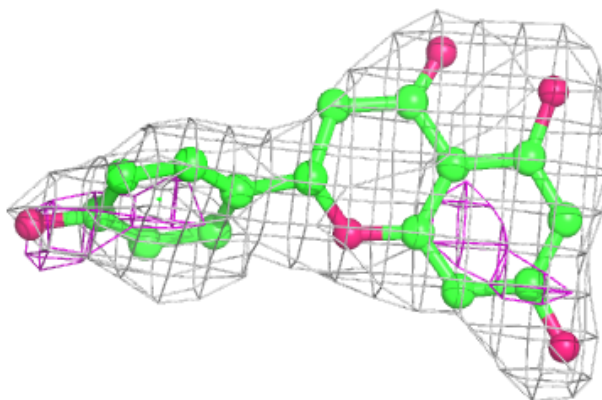
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAR B 501:

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

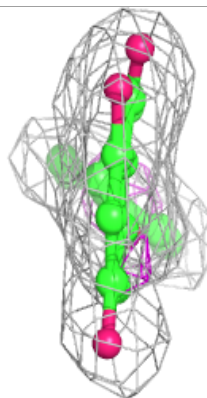
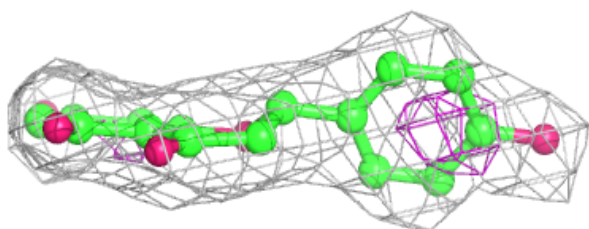
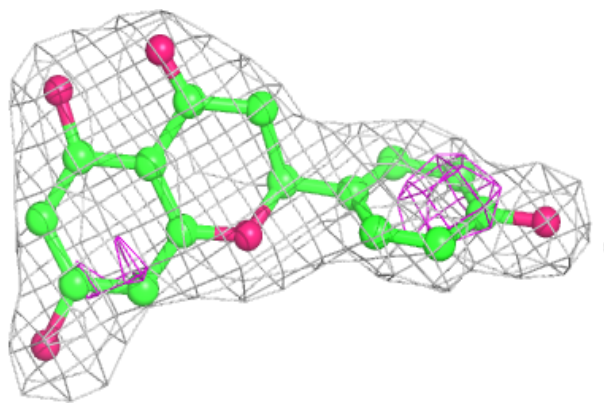
**Electron density around NAR C 501:**

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

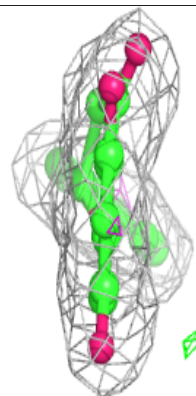
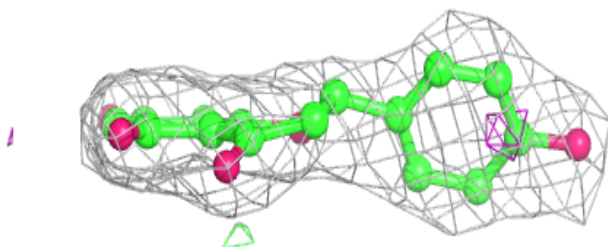
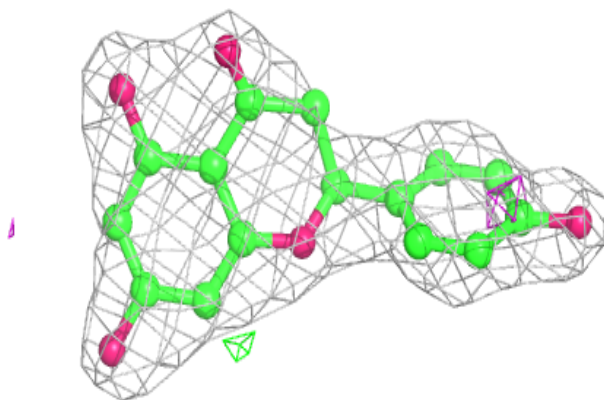


Electron density around NAR A 501:

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

**Electron density around NAR D 501:**

$2mF_o-DF_c$ (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.