



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:11 pm BST

PDB ID : 6MS8
Title : Crystal Structure of Chalcone Isomerase from *Medicago Truncatula* Complexed with (2S) Naringenin
Authors : Burke, J.R.; La Clair, J.J.; Philippe, R.N.; Pabis, A.; Jez, J.M.; Cortina, G.; Kaltenbach, M.; Bowman, M.E.; Woods, K.B.; Nelson, A.T.; Tawfik, D.S.; Kamerlin, S.C.L.; Noel, J.P.
Deposited on : 2018-10-16
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

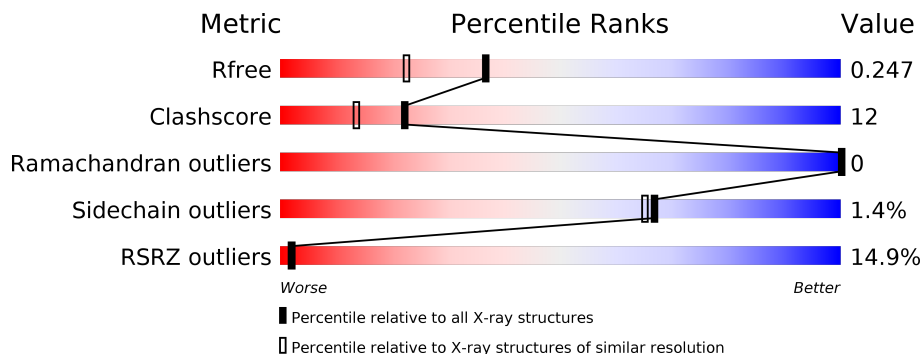
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



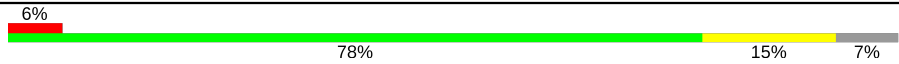

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	224	
1	B	224	
1	C	224	
1	D	224	
1	E	224	
1	F	224	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	224	
1	H	224	

2 Entry composition [i](#)

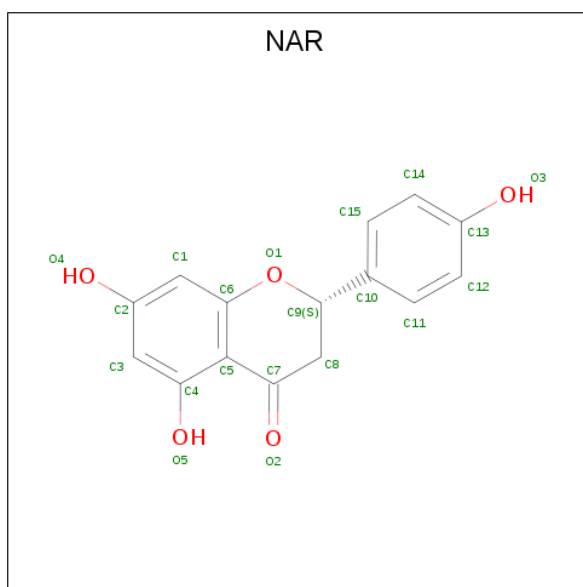
There are 3 unique types of molecules in this entry. The entry contains 26382 atoms, of which 12930 are hydrogens and 0 are deuteriums.

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-flavonone isomerase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	208	3227	1047	1615	258	303	4	0	0	0
1	B	207	3216	1044	1610	257	301	4	0	0	0
1	C	209	3249	1053	1628	260	304	4	0	0	0
1	D	207	3209	1042	1604	257	302	4	0	0	0
1	E	208	3224	1045	1613	258	304	4	0	0	0
1	F	207	3205	1041	1602	256	302	4	0	0	0
1	G	209	3232	1049	1616	259	304	4	0	0	0
1	H	205	3166	1026	1582	254	300	4	0	0	0

- Molecule 2 is NARINGENIN (three-letter code: NAR) (formula: C₁₅H₁₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	32	15	12	5	0	0
2	D	1	32	15	12	5	0	0
2	E	1	32	15	12	5	0	0
2	F	1	32	15	12	5	0	0
2	G	1	32	15	12	5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	71	71	71	0	0
3	B	84	84	84	0	0
3	C	53	53	53	0	0
3	D	57	57	57	0	0
3	E	54	54	54	0	0
3	F	57	57	57	0	0
3	G	61	61	61	0	0

Continued on next page...

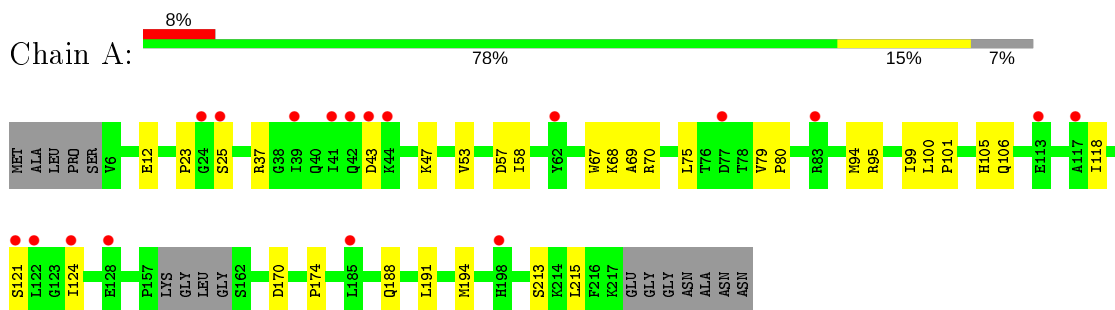
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	57	Total	O	0	0
			57	57		

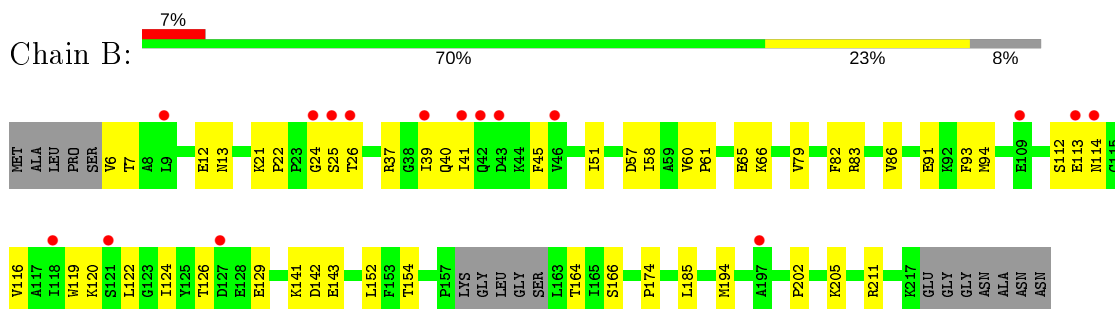
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

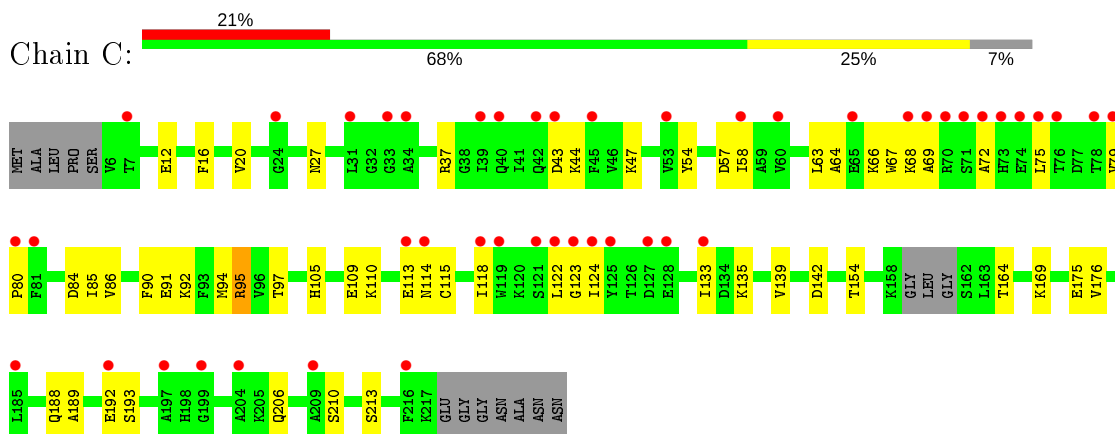
- Molecule 1: Chalcone-flavonone isomerase family protein



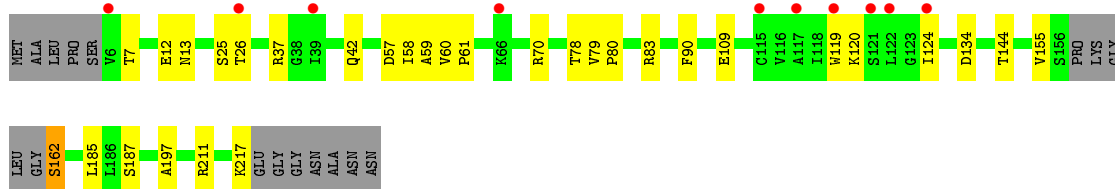
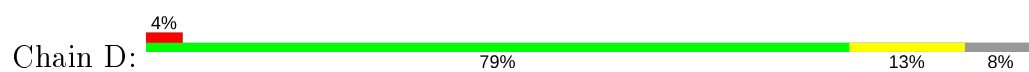
- Molecule 1: Chalcone-flavonone isomerase family protein



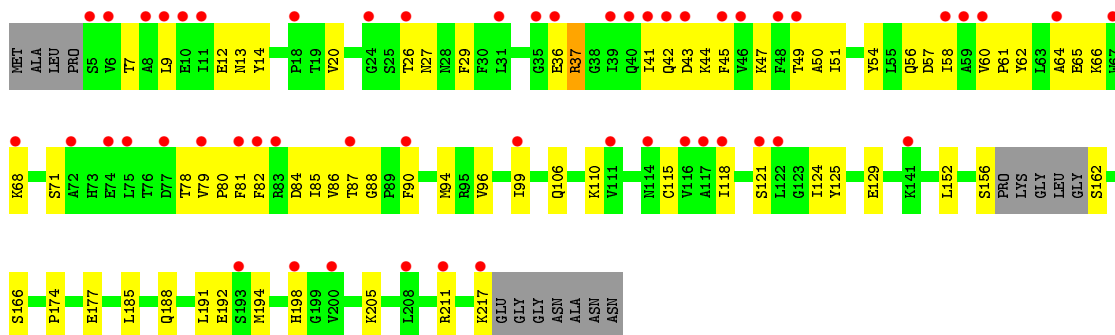
- Molecule 1: Chalcone-flavonone isomerase family protein



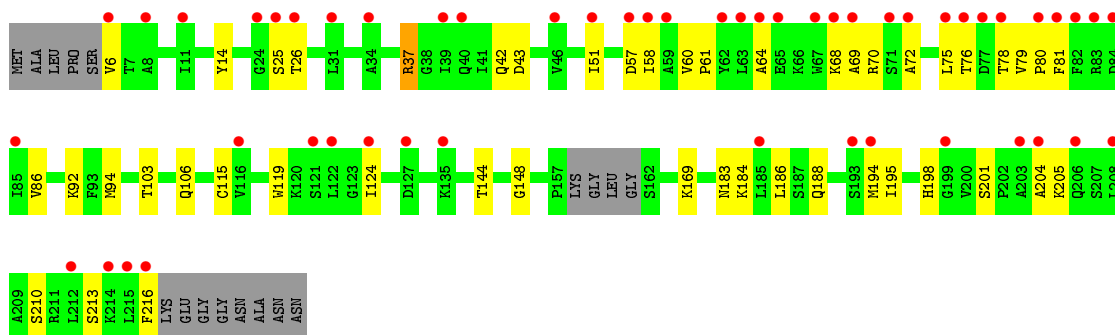
- Molecule 1: Chalcone-flavonone isomerase family protein



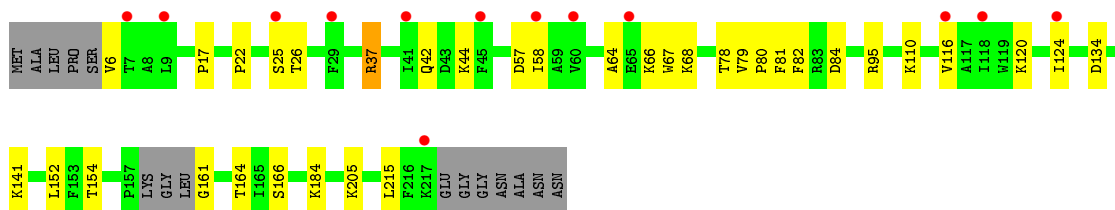
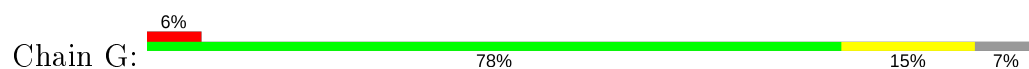
- Molecule 1: Chalcone-flavonone isomerase family protein



- Molecule 1: Chalcone-flavonone isomerase family protein

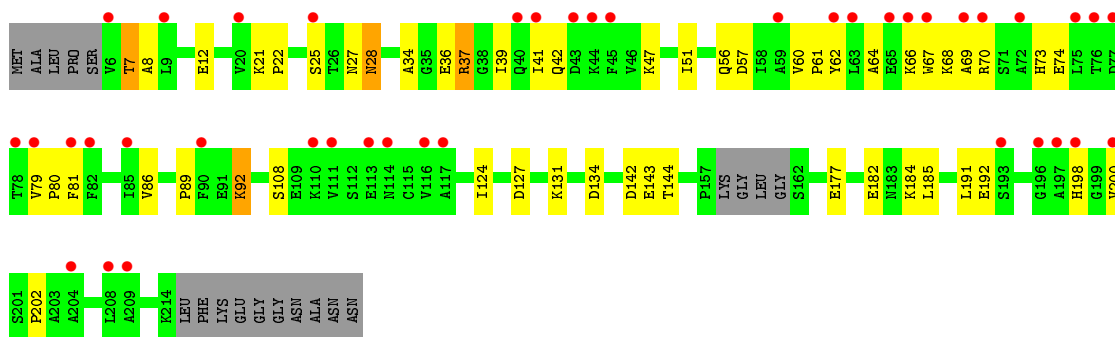


- Molecule 1: Chalcone-flavonone isomerase family protein



- Molecule 1: Chalcone-flavonone isomerase family protein

Chain H:  18% 68% 21% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	85.09Å 85.09Å 221.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.35 – 1.90 61.35 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (61.35-1.90) 98.2 (61.35-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 1.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.241 0.234 , 0.247	Depositor DCC
R_{free} test set	2021 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.059 for -h,-k,l 0.458 for h,-h-k,-l 0.058 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26382	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.50% 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	0.35	0/1650	0.56	0/2237
1	B	0.36	0/1644	0.61	0/2229
1	C	0.32	0/1659	0.57	1/2248 (0.0%)
1	D	0.34	0/1642	0.55	0/2225
1	E	0.35	0/1648	0.60	0/2233
1	F	0.32	0/1641	0.55	0/2226
1	G	0.33	0/1654	0.57	1/2242 (0.0%)
1	H	0.39	0/1621	0.58	0/2199
All	All	0.34	0/13159	0.57	2/17839 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	134	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	95	ARG	NE-CZ-NH1	5.05	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1612	1615	1626	21	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1606	1610	1621	44	2
1	C	1621	1628	1639	46	0
1	D	1605	1604	1619	34	2
1	E	1611	1613	1624	53	1
1	F	1603	1602	1613	36	0
1	G	1616	1616	1629	31	1
1	H	1584	1582	1592	46	2
2	A	20	12	9	0	0
2	D	20	12	10	0	0
2	E	20	12	9	2	0
2	F	20	12	10	1	0
2	G	20	12	11	0	0
3	A	71	0	0	5	1
3	B	84	0	0	11	1
3	C	53	0	0	8	0
3	D	57	0	0	9	1
3	E	54	0	0	12	2
3	F	57	0	0	7	1
3	G	61	0	0	10	0
3	H	57	0	0	10	1
All	All	13452	12930	13012	305	8

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 12.

All (305) 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:E:36:GLU:OE1	1:E:47:LYS:HE3	1.49	1.11
1:E:12:GLU:OE1	1:E:47:LYS:NZ	1.90	1.05
1:C:95:ARG:NH1	1:C:97:THR:OG1	2.04	0.90
1:E:71:SER:OG	3:E:402:HOH:O	1.94	0.85
1:B:65:GLU:OE2	3:B:301:HOH:O	1.97	0.83
1:B:25:SER:OG	1:B:91:GLU:OE1	1.96	0.82
1:C:66:LYS:O	3:C:301:HOH:O	1.98	0.81
1:H:202:PRO:O	3:H:301:HOH:O	1.98	0.81
1:F:76:THR:O	3:F:401:HOH:O	1.98	0.81
1:H:86:VAL:HG11	1:H:192:GLU:HG2	1.63	0.80
1:H:108:SER:OG	3:H:302:HOH:O	1.99	0.79
1:D:119:TRP:HE1	1:D:185:LEU:HD11	1.45	0.79
1:G:78:THR:C	3:G:401:HOH:O	2.21	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:VAL:HG23	1:H:61:PRO:HD3	1.65	0.79
1:B:185:LEU:HD22	3:B:304:HOH:O	1.83	0.79
1:D:109:GLU:OE2	3:D:401:HOH:O	2.01	0.78
1:G:78:THR:O	3:G:401:HOH:O	2.03	0.77
1:F:169:LYS:NZ	3:F:403:HOH:O	2.18	0.76
1:A:101:PRO:HB2	1:C:176:VAL:HG11	1.68	0.74
1:B:119:TRP:NE1	3:B:304:HOH:O	2.21	0.73
1:B:45:PHE:O	3:B:302:HOH:O	2.06	0.73
1:F:205:LYS:NZ	3:F:404:HOH:O	2.23	0.72
1:E:94:MET:SD	1:E:194:MET:SD	2.87	0.72
1:D:217:LYS:O	3:D:402:HOH:O	2.07	0.71
1:A:170:ASP:OD2	3:A:401:HOH:O	2.08	0.70
1:G:141:LYS:O	3:G:402:HOH:O	2.10	0.70
1:A:215:LEU:O	3:A:402:HOH:O	2.10	0.69
1:B:60:VAL:HG22	1:B:61:PRO:HD3	1.75	0.69
1:H:60:VAL:HG23	1:H:61:PRO:CD	2.22	0.68
1:H:42:GLN:N	3:H:307:HOH:O	2.27	0.68
1:G:42:GLN:NE2	1:H:185:LEU:HD13	2.09	0.68
1:B:129:GLU:OE2	1:B:185:LEU:HD12	1.94	0.67
1:F:194:MET:HG3	1:F:195:ILE:HG23	1.77	0.67
1:A:188:GLN:NE2	3:A:403:HOH:O	2.14	0.67
1:E:217:LYS:O	3:E:404:HOH:O	2.13	0.66
1:B:143:GLU:OE2	3:B:303:HOH:O	2.12	0.66
1:C:86:VAL:O	1:C:92:LYS:NZ	2.25	0.66
1:A:67:TRP:O	3:A:404:HOH:O	2.14	0.66
1:E:86:VAL:HG11	1:E:192:GLU:HG2	1.78	0.65
1:E:13:ASN:ND2	3:E:409:HOH:O	2.30	0.65
1:E:156:SER:O	3:E:406:HOH:O	2.15	0.65
1:C:142:ASP:OD2	3:C:302:HOH:O	2.13	0.64
1:H:60:VAL:O	1:H:64:ALA:N	2.29	0.64
1:G:68:LYS:N	3:G:406:HOH:O	2.30	0.64
1:E:129:GLU:OE2	3:E:405:HOH:O	2.15	0.64
1:E:115:CYS:SG	3:E:451:HOH:O	2.56	0.62
1:E:51:ILE:HG23	1:E:94:MET:HE1	1.82	0.60
1:B:141:LYS:NZ	3:B:310:HOH:O	2.32	0.60
1:D:119:TRP:HE1	1:D:185:LEU:CD1	2.14	0.60
1:B:205:LYS:NZ	3:B:307:HOH:O	2.35	0.60
1:B:24:GLY:N	3:B:308:HOH:O	2.29	0.60
1:H:36:GLU:HG2	3:H:322:HOH:O	2.01	0.60
1:F:198:HIS:HB2	3:F:451:HOH:O	2.02	0.59
1:H:39:ILE:CD1	1:H:41:ILE:HG13	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:SER:CB	1:B:91:GLU:OE1	2.50	0.59
1:D:79:VAL:HG23	3:D:447:HOH:O	2.02	0.59
1:E:7:THR:O	1:E:211:ARG:NH2	2.32	0.59
1:E:26:THR:OG1	3:E:403:HOH:O	2.02	0.58
1:B:185:LEU:HB3	3:B:304:HOH:O	2.03	0.58
1:E:110:LYS:HG3	2:E:301:NAR:C15	2.32	0.58
1:F:60:VAL:HG13	1:F:61:PRO:HD3	1.85	0.58
1:D:119:TRP:NE1	1:D:185:LEU:HD11	2.18	0.58
1:E:60:VAL:HG23	1:E:61:PRO:HD3	1.85	0.58
1:H:198:HIS:CD2	3:H:309:HOH:O	2.55	0.58
1:A:53:VAL:HG22	1:A:94:MET:HE3	1.86	0.58
1:B:51:ILE:HD13	1:B:194:MET:SD	2.44	0.58
1:C:85:ILE:O	1:C:92:LYS:HE2	2.04	0.57
1:E:106:GLN:NE2	3:E:410:HOH:O	2.31	0.57
1:C:72:ALA:HB1	1:C:210:SER:HA	1.86	0.57
1:C:123:GLY:HA2	3:C:315:HOH:O	2.04	0.57
1:G:42:GLN:HE21	1:H:185:LEU:HD13	1.68	0.57
1:G:120:LYS:NZ	3:G:409:HOH:O	2.37	0.57
1:E:51:ILE:HG23	1:E:94:MET:CE	2.34	0.57
1:G:37:ARG:HH22	1:G:110:LYS:HZ3	1.51	0.57
1:G:57:ASP:OD1	1:G:58:ILE:N	2.36	0.57
1:G:79:VAL:HG13	1:G:80:PRO:HD3	1.86	0.57
1:D:60:VAL:HG12	1:D:61:PRO:HD3	1.86	0.57
1:E:57:ASP:OD1	1:E:58:ILE:N	2.38	0.56
1:F:169:LYS:NZ	3:F:402:HOH:O	2.04	0.56
1:H:62:TYR:OH	1:H:66:LYS:NZ	2.38	0.56
1:E:49:THR:HG21	1:E:96:VAL:HG13	1.88	0.56
1:B:124:ILE:O	1:B:124:ILE:HG22	2.05	0.55
1:C:68:LYS:O	1:C:69:ALA:HB3	2.06	0.55
1:B:26:THR:HG22	1:B:26:THR:O	2.05	0.55
1:F:57:ASP:O	1:F:60:VAL:HG12	2.07	0.55
1:E:49:THR:HG21	1:E:96:VAL:CG1	2.37	0.55
1:B:124:ILE:N	1:B:124:ILE:HD12	2.22	0.55
1:C:95:ARG:HG2	1:C:95:ARG:HH11	1.72	0.55
1:H:74:GLU:N	1:H:74:GLU:OE1	2.39	0.55
1:C:105:HIS:NE2	1:C:109:GLU:OE2	2.33	0.55
1:H:134:ASP:OD2	3:H:303:HOH:O	2.18	0.55
1:H:79:VAL:HG12	1:H:80:PRO:HD3	1.89	0.55
1:D:155:VAL:HG12	3:D:405:HOH:O	2.07	0.54
1:H:70:ARG:HH11	1:H:70:ARG:HG3	1.72	0.54
1:C:115:CYS:HB2	1:C:189:ALA:HB1	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:HG3	1:B:142:ASP:N	2.23	0.54
1:E:20:VAL:HG22	1:E:54:TYR:CD2	2.42	0.54
1:H:68:LYS:O	1:H:69:ALA:HB3	2.08	0.54
1:G:25:SER:OG	1:G:26:THR:N	2.37	0.54
1:E:129:GLU:HG2	1:E:185:LEU:HD23	1.90	0.53
1:D:134:ASP:O	3:D:403:HOH:O	2.18	0.53
1:E:64:ALA:O	1:E:68:LYS:HB2	2.08	0.53
1:D:26:THR:O	1:D:26:THR:HG22	2.09	0.53
1:G:124:ILE:O	1:G:124:ILE:HG22	2.09	0.53
1:F:25:SER:O	1:F:26:THR:OG1	2.18	0.53
1:D:124:ILE:HG22	1:D:124:ILE:O	2.09	0.53
1:H:143:GLU:OE1	3:H:304:HOH:O	2.18	0.53
1:C:188:GLN:NE2	3:C:308:HOH:O	2.38	0.52
1:H:37:ARG:HD3	1:H:200:VAL:HB	1.91	0.52
1:A:23:PRO:HG3	1:A:174:PRO:O	2.10	0.52
1:D:57:ASP:OD1	1:D:58:ILE:N	2.42	0.52
1:B:112:SER:O	1:B:116:VAL:HG13	2.10	0.52
1:C:12:GLU:OE2	1:C:47:LYS:NZ	2.40	0.52
1:G:81:PHE:N	3:G:401:HOH:O	1.93	0.52
1:E:26:THR:HG22	3:E:408:HOH:O	2.09	0.52
1:F:183:ASN:OD1	1:F:186:LEU:N	2.35	0.52
1:H:124:ILE:O	1:H:124:ILE:HG22	2.10	0.51
1:E:62:TYR:OH	1:E:66:LYS:NZ	2.42	0.51
1:E:44:LYS:HG2	1:E:45:PHE:N	2.25	0.51
1:H:7:THR:HG22	1:H:8:ALA:O	2.10	0.51
1:H:25:SER:O	1:H:27:ASN:N	2.38	0.51
1:F:64:ALA:O	1:F:68:LYS:HB2	2.11	0.51
1:G:80:PRO:N	3:G:401:HOH:O	2.43	0.51
1:D:60:VAL:HG12	1:D:61:PRO:CD	2.41	0.51
1:C:43:ASP:O	1:C:44:LYS:HD2	2.11	0.50
1:H:28:ASN:N	1:H:28:ASN:OD1	2.43	0.50
1:E:124:ILE:HG22	1:E:124:ILE:O	2.11	0.50
1:F:72:ALA:CB	1:F:210:SER:HA	2.41	0.50
1:B:113:GLU:O	1:B:116:VAL:HG22	2.12	0.50
1:B:119:TRP:CD1	3:B:304:HOH:O	2.62	0.50
1:C:27:ASN:ND2	1:C:91:GLU:OE2	2.39	0.50
1:H:21:LYS:O	3:H:305:HOH:O	2.20	0.50
1:F:115:CYS:HB3	1:F:119:TRP:CZ2	2.46	0.50
1:E:37:ARG:NH2	2:E:301:NAR:O1	2.36	0.50
1:A:95:ARG:NH2	3:A:407:HOH:O	2.45	0.50
1:A:94:MET:SD	1:A:191:LEU:HD13	2.53	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:VAL:O	1:E:64:ALA:N	2.42	0.49
1:B:116:VAL:O	1:B:120:LYS:N	2.42	0.49
1:F:184:LYS:NZ	1:F:188:GLN:OE1	2.39	0.49
1:G:95:ARG:NH2	3:G:411:HOH:O	2.46	0.49
1:B:40:GLN:OE1	1:B:45:PHE:HB2	2.13	0.49
1:E:51:ILE:CG2	1:E:94:MET:HE1	2.43	0.49
1:F:57:ASP:OD1	1:F:58:ILE:N	2.41	0.48
1:F:75:LEU:HD12	1:F:213:SER:OG	2.13	0.48
1:F:78:THR:OG1	1:F:81:PHE:HB3	2.14	0.48
1:B:202:PRO:HA	1:B:205:LYS:HE3	1.95	0.48
1:A:105:HIS:CE1	1:A:106:GLN:HG3	2.49	0.48
1:E:79:VAL:N	1:E:80:PRO:CD	2.77	0.48
1:F:94:MET:SD	1:F:194:MET:HG2	2.53	0.48
1:H:86:VAL:O	1:H:92:LYS:HE2	2.13	0.48
1:C:115:CYS:CB	1:C:189:ALA:HB1	2.43	0.48
1:D:79:VAL:CG1	1:D:80:PRO:HD3	2.44	0.48
1:F:124:ILE:O	1:F:124:ILE:HG22	2.14	0.48
1:A:118:ILE:O	1:A:121:SER:HB3	2.13	0.48
1:D:120:LYS:NZ	3:D:412:HOH:O	2.46	0.48
1:D:185:LEU:O	1:D:185:LEU:HD12	2.13	0.47
1:D:119:TRP:CE2	1:D:185:LEU:HG	2.48	0.47
1:F:194:MET:SD	1:F:201:SER:HB3	2.53	0.47
1:H:27:ASN:ND2	3:H:310:HOH:O	2.46	0.47
1:C:79:VAL:N	1:C:80:PRO:CD	2.77	0.47
1:G:116:VAL:O	1:G:120:LYS:N	2.32	0.47
1:H:79:VAL:N	1:H:80:PRO:CD	2.77	0.47
1:D:119:TRP:CZ2	1:D:185:LEU:HG	2.49	0.47
1:C:64:ALA:O	1:C:68:LYS:HB2	2.14	0.47
1:G:161:GLY:HA3	1:G:184:LYS:HE3	1.96	0.47
1:G:44:LYS:HD2	1:H:184:LYS:NZ	2.30	0.47
1:A:124:ILE:O	1:A:124:ILE:HG22	2.14	0.47
1:C:64:ALA:O	1:C:68:LYS:CB	2.62	0.47
1:D:144:THR:OG1	1:H:177:GLU:OE1	2.25	0.47
1:F:70:ARG:HB2	1:F:75:LEU:HD21	1.96	0.47
1:C:175:GLU:HG2	3:C:342:HOH:O	2.14	0.47
1:C:20:VAL:HG13	1:C:54:TYR:CE2	2.51	0.46
1:F:72:ALA:HB1	1:F:210:SER:HA	1.97	0.46
1:C:206:GLN:NE2	3:C:307:HOH:O	2.32	0.46
1:G:37:ARG:NH2	1:G:110:LYS:HZ3	2.13	0.46
1:C:114:ASN:HD22	1:C:193:SER:HB2	1.81	0.46
1:H:86:VAL:HG22	1:H:191:LEU:HG	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:VAL:HG13	1:F:61:PRO:CD	2.45	0.46
1:E:152:LEU:CD1	1:E:174:PRO:HD2	2.46	0.46
1:G:6:VAL:N	3:G:414:HOH:O	2.48	0.46
1:H:62:TYR:C	1:H:62:TYR:CD1	2.89	0.46
1:E:27:ASN:O	1:E:29:PHE:CD1	2.69	0.46
1:E:65:GLU:HG3	3:E:417:HOH:O	2.15	0.46
1:F:194:MET:HE3	1:F:204:ALA:HB3	1.98	0.46
1:C:67:TRP:NE1	1:C:84:ASP:OD2	2.40	0.46
1:C:57:ASP:OD1	1:C:58:ILE:N	2.49	0.45
1:H:22:PRO:O	1:H:25:SER:HB3	2.16	0.45
1:E:60:VAL:HG23	1:E:61:PRO:CD	2.47	0.45
1:C:86:VAL:HG11	1:C:192:GLU:HB3	1.98	0.45
1:D:155:VAL:C	3:D:405:HOH:O	2.54	0.45
1:E:50:ALA:HB2	1:E:99:ILE:HD11	1.98	0.45
1:F:79:VAL:N	1:F:80:PRO:CD	2.79	0.45
1:G:64:ALA:O	1:G:68:LYS:HB2	2.17	0.45
1:H:67:TRP:CD1	1:H:81:PHE:HD1	2.35	0.45
1:C:124:ILE:O	1:C:124:ILE:HG22	2.17	0.45
1:F:42:GLN:HG2	1:F:43:ASP:H	1.81	0.45
1:B:58:ILE:O	1:B:61:PRO:HD2	2.16	0.45
1:E:118:ILE:O	1:E:121:SER:HB3	2.16	0.45
1:A:43:ASP:O	1:A:43:ASP:OD1	2.35	0.45
1:E:198:HIS:NE2	3:E:407:HOH:O	2.15	0.45
1:H:28:ASN:ND2	1:H:57:ASP:HB2	2.32	0.45
1:A:68:LYS:O	1:A:69:ALA:HB3	2.16	0.45
1:B:141:LYS:CD	3:B:310:HOH:O	2.65	0.45
1:C:110:LYS:O	1:C:113:GLU:HG2	2.16	0.45
1:E:14:TYR:CE2	1:E:99:ILE:HD12	2.52	0.45
1:A:47:LYS:O	1:A:100:LEU:HD13	2.18	0.44
1:C:122:LEU:HB3	1:C:124:ILE:HD12	2.00	0.44
1:A:94:MET:CE	1:A:194:MET:SD	3.05	0.44
1:B:39:ILE:HG12	1:B:41:ILE:HG13	2.00	0.44
1:H:21:LYS:O	1:H:21:LYS:HG3	2.18	0.44
1:D:59:ALA:HB2	1:D:90:PHE:CG	2.53	0.44
1:C:72:ALA:CB	1:C:210:SER:HA	2.46	0.44
1:C:58:ILE:HD11	1:C:90:PHE:HB3	2.00	0.44
1:D:58:ILE:CD1	1:D:90:PHE:HB3	2.47	0.44
1:A:79:VAL:N	1:A:80:PRO:CD	2.79	0.44
1:E:41:ILE:HG22	1:E:42:GLN:N	2.32	0.44
1:H:67:TRP:CG	1:H:81:PHE:HD1	2.35	0.44
1:D:162:SER:O	1:D:187:SER:OG	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ALA:HA	3:D:427:HOH:O	2.17	0.44
1:D:60:VAL:CG1	1:D:61:PRO:HD3	2.48	0.44
1:E:56:GLN:HG2	1:E:57:ASP:OD1	2.18	0.44
1:H:127:ASP:O	1:H:131:LYS:HG3	2.18	0.44
1:H:67:TRP:CE2	1:H:81:PHE:HA	2.53	0.43
1:C:115:CYS:SG	1:C:133:ILE:HD11	2.59	0.43
1:C:16:PHE:CE2	1:C:95:ARG:NH1	2.86	0.43
1:E:49:THR:HG22	1:E:50:ALA:N	2.33	0.43
1:G:116:VAL:O	1:G:120:LYS:HB2	2.17	0.43
1:B:152:LEU:HB2	1:B:166:SER:HB2	2.01	0.43
1:E:42:GLN:O	1:E:43:ASP:HB3	2.18	0.43
1:E:68:LYS:O	1:E:68:LYS:HG2	2.18	0.43
1:G:67:TRP:NE1	1:G:84:ASP:OD2	2.48	0.43
1:G:17:PRO:HD2	1:G:95:ARG:HH22	1.84	0.43
1:D:58:ILE:HD11	1:D:90:PHE:HB3	2.00	0.43
1:E:9:LEU:HD11	3:E:441:HOH:O	2.19	0.43
1:B:79:VAL:O	1:B:83:ARG:HG2	2.19	0.43
1:E:85:ILE:HA	1:E:90:PHE:HZ	1.84	0.43
1:F:25:SER:OG	1:F:26:THR:N	2.52	0.43
1:G:22:PRO:HB2	1:G:25:SER:HB3	2.00	0.43
1:B:57:ASP:OD1	1:B:58:ILE:N	2.51	0.43
1:E:82:PHE:CE2	1:E:205:LYS:HE2	2.54	0.43
1:H:62:TYR:CE2	1:H:89:PRO:CG	3.02	0.43
1:C:135:LYS:O	1:C:139:VAL:HG23	2.19	0.42
1:A:94:MET:SD	1:A:194:MET:SD	3.17	0.42
1:A:12:GLU:HG2	1:A:99:ILE:HD13	2.01	0.42
1:C:115:CYS:HA	1:C:118:ILE:HD12	2.01	0.42
1:C:66:LYS:CG	3:C:301:HOH:O	2.67	0.42
1:B:13:ASN:HB3	1:E:125:TYR:O	2.18	0.42
1:D:83:ARG:HD3	3:D:411:HOH:O	2.19	0.42
1:F:37:ARG:NH2	2:F:301:NAR:O1	2.46	0.42
1:D:42:GLN:HG3	1:D:42:GLN:O	2.20	0.42
1:F:68:LYS:O	1:F:69:ALA:HB3	2.19	0.42
1:F:86:VAL:O	1:F:92:LYS:NZ	2.40	0.42
1:F:213:SER:O	1:F:216:PHE:HB2	2.19	0.42
1:F:51:ILE:HG21	1:F:194:MET:SD	2.59	0.42
1:H:34:ALA:HA	1:H:51:ILE:O	2.20	0.42
1:B:152:LEU:CD1	1:B:174:PRO:HD2	2.49	0.42
1:C:79:VAL:N	1:C:80:PRO:HD2	2.35	0.42
1:F:103:THR:OG1	1:F:106:GLN:HG3	2.19	0.42
1:E:87:THR:HG22	1:E:188:GLN:OE1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:THR:HB	1:B:129:GLU:OE1	2.19	0.42
1:B:154:THR:HB	1:B:164:THR:HB	2.01	0.42
1:F:6:VAL:N	3:F:411:HOH:O	2.53	0.42
1:E:84:ASP:O	1:E:88:GLY:N	2.53	0.41
1:H:56:GLN:HG2	1:H:57:ASP:N	2.35	0.41
1:B:6:VAL:HG12	1:B:7:THR:H	1.84	0.41
1:C:79:VAL:H	1:C:80:PRO:CD	2.33	0.41
1:G:78:THR:HG22	3:G:401:HOH:O	2.20	0.41
1:H:12:GLU:OE2	1:H:47:LYS:NZ	2.37	0.41
1:B:94:MET:SD	1:B:194:MET:HG3	2.60	0.41
1:G:161:GLY:N	1:G:184:LYS:HZ1	2.18	0.41
1:C:95:ARG:HG2	1:C:95:ARG:NH1	2.36	0.41
1:F:144:THR:O	3:F:403:HOH:O	2.22	0.41
1:G:154:THR:HB	1:G:164:THR:HB	2.02	0.41
1:B:6:VAL:HG12	1:B:211:ARG:NH2	2.36	0.41
1:B:82:PHE:O	1:B:86:VAL:HG23	2.20	0.41
1:C:63:LEU:HD11	1:C:90:PHE:CZ	2.56	0.41
1:E:78:THR:HG22	1:E:81:PHE:H	1.84	0.41
1:B:122:LEU:HB2	1:B:124:ILE:HD13	2.02	0.41
1:D:25:SER:O	1:D:26:THR:HB	2.21	0.41
1:F:14:TYR:CE1	1:F:148:GLY:HA2	2.56	0.41
1:G:152:LEU:HB2	1:G:166:SER:HB2	2.02	0.41
1:H:36:GLU:CG	3:H:322:HOH:O	2.65	0.41
1:B:22:PRO:HB3	1:B:93:PHE:CD1	2.56	0.41
1:C:113:GLU:HG3	1:C:114:ASN:N	2.36	0.41
1:D:7:THR:HB	1:D:211:ARG:HH12	1.86	0.41
1:C:66:LYS:HG2	3:C:301:HOH:O	2.20	0.41
1:G:25:SER:C	1:G:26:THR:HG23	2.42	0.41
1:A:75:LEU:HD12	1:A:213:SER:HB3	2.02	0.41
1:C:189:ALA:HA	1:C:192:GLU:HG2	2.03	0.40
1:G:82:PHE:CE2	1:G:205:LYS:HE2	2.55	0.40
1:H:62:TYR:CZ	1:H:89:PRO:HD2	2.56	0.40
1:A:57:ASP:OD1	1:A:58:ILE:N	2.54	0.40
1:D:12:GLU:O	1:D:13:ASN:HB2	2.22	0.40
1:E:86:VAL:HG22	1:E:191:LEU:HG	2.03	0.40
1:B:122:LEU:O	1:B:124:ILE:HD12	2.21	0.40
1:B:141:LYS:CG	1:B:142:ASP:N	2.83	0.40
1:D:60:VAL:CG1	1:D:61:PRO:CD	3.00	0.40
1:D:78:THR:HG22	1:D:80:PRO:HD2	2.04	0.40
1:D:79:VAL:HG12	1:D:80:PRO:HD3	2.04	0.40
1:C:154:THR:HB	1:C:164:THR:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:LEU:HB2	1:E:166:SER:HB2	2.03	0.40
1:B:124:ILE:CG2	1:B:124:ILE:O	2.70	0.40
1:B:12:GLU:O	1:B:13:ASN:HB2	2.22	0.40
1:C:75:LEU:HD12	1:C:213:SER:OG	2.21	0.40
1:H:25:SER:C	1:H:27:ASN:H	2.23	0.40

All (8) 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)
3:E:454:HOH:O	3:H:355:HOH:O[1_665]	2.01	0.19
3:D:410:HOH:O	3:F:410:HOH:O[1_455]	2.01	0.19
1:B:21:LYS:HZ1	1:D:109:GLU:OE2[1_665]	1.49	0.11
3:A:411:HOH:O	3:B:358:HOH:O[2_754]	2.11	0.09
1:E:177:GLU:OE1	1:H:144:THR:HG1[1_665]	1.57	0.03
1:D:70:ARG:HH22	1:G:66:LYS:O[3_665]	1.58	0.02
1:H:142:ASP:OD1	3:E:403:HOH:O[1_445]	2.18	0.02
1:A:70:ARG:HH22	1:B:66:LYS:O[2_754]	1.60	0.00

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	204/224 (91%)	199 (98%)	5 (2%)	0	100	100
1	B	203/224 (91%)	198 (98%)	5 (2%)	0	100	100
1	C	205/224 (92%)	199 (97%)	6 (3%)	0	100	100
1	D	203/224 (91%)	196 (97%)	7 (3%)	0	100	100
1	E	204/224 (91%)	200 (98%)	4 (2%)	0	100	100
1	F	203/224 (91%)	193 (95%)	10 (5%)	0	100	100
1	G	205/224 (92%)	195 (95%)	10 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	201/224 (90%)	195 (97%)	6 (3%)	0	100	100
All	All	1628/1792 (91%)	1575 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	178/188 (95%)	176 (99%)	2 (1%)	73	73
1	B	177/188 (94%)	175 (99%)	2 (1%)	73	73
1	C	179/188 (95%)	176 (98%)	3 (2%)	60	57
1	D	177/188 (94%)	175 (99%)	2 (1%)	73	73
1	E	178/188 (95%)	176 (99%)	2 (1%)	73	73
1	F	177/188 (94%)	176 (99%)	1 (1%)	86	87
1	G	178/188 (95%)	176 (99%)	2 (1%)	73	73
1	H	175/188 (93%)	169 (97%)	6 (3%)	37	28
All	All	1419/1504 (94%)	1399 (99%)	20 (1%)	67	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	37	ARG
1	B	37	ARG
1	B	114	ASN
1	C	37	ARG
1	C	94	MET
1	C	169	LYS
1	D	37	ARG
1	D	162	SER
1	E	37	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	162	SER
1	F	37	ARG
1	G	37	ARG
1	G	215	LEU
1	H	7	THR
1	H	28	ASN
1	H	37	ARG
1	H	73	HIS
1	H	92	LYS
1	H	182	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	114	ASN
1	E	42	GLN
1	G	42	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	F	301	-	22,22,22	1.41	2 (9%)	32,32,32	1.39	4 (12%)
2	NAR	E	301	-	22,22,22	1.29	2 (9%)	32,32,32	1.40	2 (6%)
2	NAR	D	301	-	22,22,22	1.42	2 (9%)	32,32,32	1.35	6 (18%)
2	NAR	A	301	-	22,22,22	1.37	2 (9%)	32,32,32	1.38	4 (12%)
2	NAR	G	301	-	22,22,22	1.89	3 (13%)	32,32,32	1.99	5 (15%)

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	F	301	-	-	3/4/16/16	0/3/3/3
2	NAR	E	301	-	-	0/4/16/16	0/3/3/3
2	NAR	D	301	-	-	4/4/16/16	0/3/3/3
2	NAR	A	301	-	-	4/4/16/16	0/3/3/3
2	NAR	G	301	-	-	4/4/16/16	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	NAR	C5-C4	5.47	1.50	1.41
2	G	301	NAR	C5-C6	5.39	1.50	1.40
2	D	301	NAR	C5-C4	4.49	1.48	1.41
2	F	301	NAR	C5-C4	4.46	1.48	1.41
2	A	301	NAR	C5-C6	4.06	1.47	1.40
2	A	301	NAR	C5-C4	4.01	1.47	1.41
2	D	301	NAR	C5-C6	3.94	1.47	1.40
2	F	301	NAR	C5-C6	3.91	1.47	1.40
2	E	301	NAR	C5-C4	3.84	1.47	1.41
2	E	301	NAR	C5-C6	3.61	1.47	1.40
2	G	301	NAR	C3-C2	2.52	1.42	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	NAR	C3-C4-C5	-6.18	113.75	120.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	NAR	C4-C3-C2	5.67	124.83	119.70
2	E	301	NAR	O1-C6-C5	-4.69	116.72	121.56
2	E	301	NAR	O1-C6-C1	4.44	123.37	116.38
2	G	301	NAR	C6-C5-C7	-4.26	116.46	120.33
2	F	301	NAR	O1-C6-C1	4.22	123.03	116.38
2	A	301	NAR	O1-C6-C1	3.98	122.65	116.38
2	F	301	NAR	O1-C6-C5	-3.90	117.54	121.56
2	D	301	NAR	O1-C6-C1	3.51	121.91	116.38
2	A	301	NAR	O1-C6-C5	-3.47	117.99	121.56
2	D	301	NAR	O1-C6-C5	-3.30	118.16	121.56
2	A	301	NAR	C3-C2-C1	2.49	123.86	120.43
2	G	301	NAR	C4-C5-C6	2.32	119.71	117.35
2	D	301	NAR	C3-C4-C5	-2.29	118.28	120.93
2	D	301	NAR	C6-C5-C7	-2.27	118.27	120.33
2	F	301	NAR	C6-C5-C7	-2.25	118.29	120.33
2	A	301	NAR	C3-C4-C5	-2.18	118.40	120.93
2	D	301	NAR	C6-O1-C9	2.18	119.16	115.50
2	G	301	NAR	C4-C5-C7	2.13	123.80	120.81
2	F	301	NAR	C3-C4-C5	-2.01	118.59	120.93
2	D	301	NAR	C4-C5-C7	2.00	123.62	120.81

There are no chirality outliers.

All (15) torsion outliers are listed below:

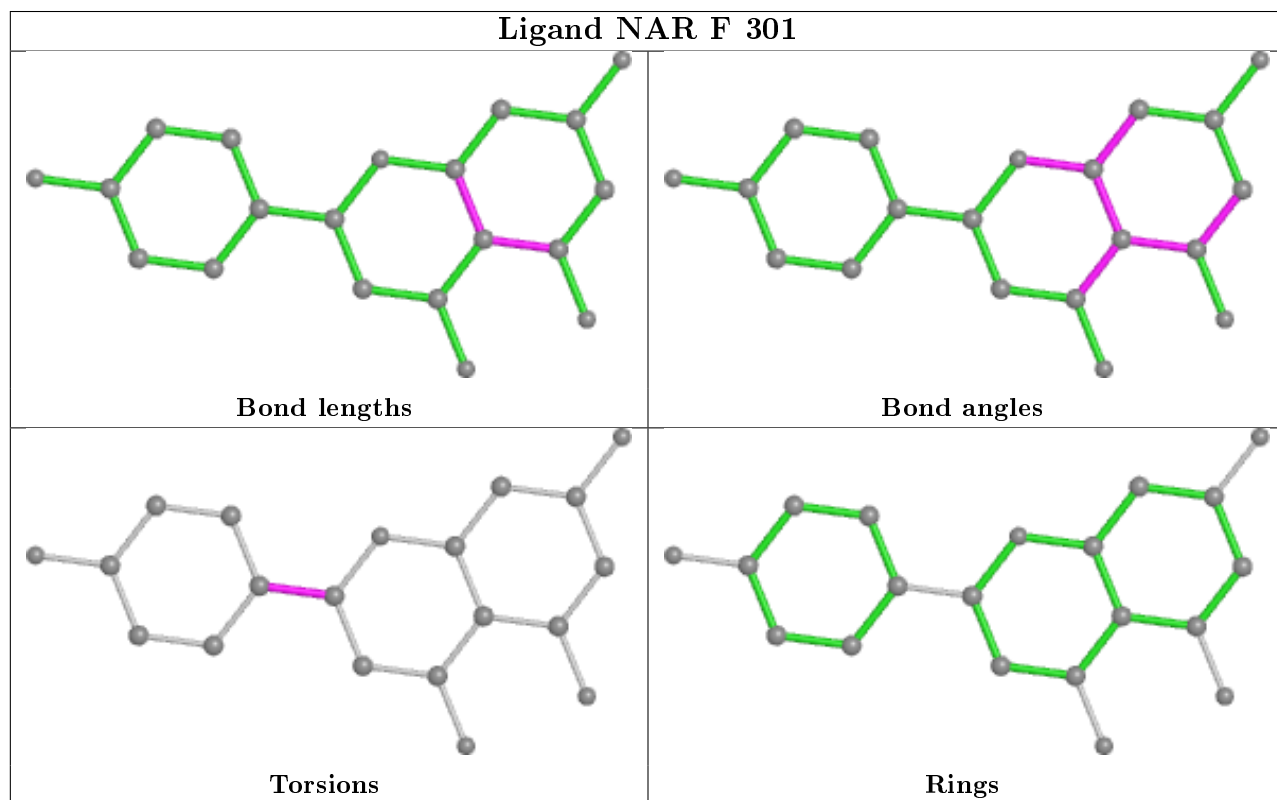
Mol	Chain	Res	Type	Atoms
2	D	301	NAR	C11-C10-C9-O1
2	D	301	NAR	C15-C10-C9-O1
2	G	301	NAR	C15-C10-C9-O1
2	D	301	NAR	C11-C10-C9-C8
2	A	301	NAR	C11-C10-C9-C8
2	A	301	NAR	C11-C10-C9-O1
2	A	301	NAR	C15-C10-C9-O1
2	G	301	NAR	C11-C10-C9-O1
2	A	301	NAR	C15-C10-C9-C8
2	D	301	NAR	C15-C10-C9-C8
2	G	301	NAR	C11-C10-C9-C8
2	G	301	NAR	C15-C10-C9-C8
2	F	301	NAR	C15-C10-C9-O1
2	F	301	NAR	C11-C10-C9-O1
2	F	301	NAR	C11-C10-C9-C8

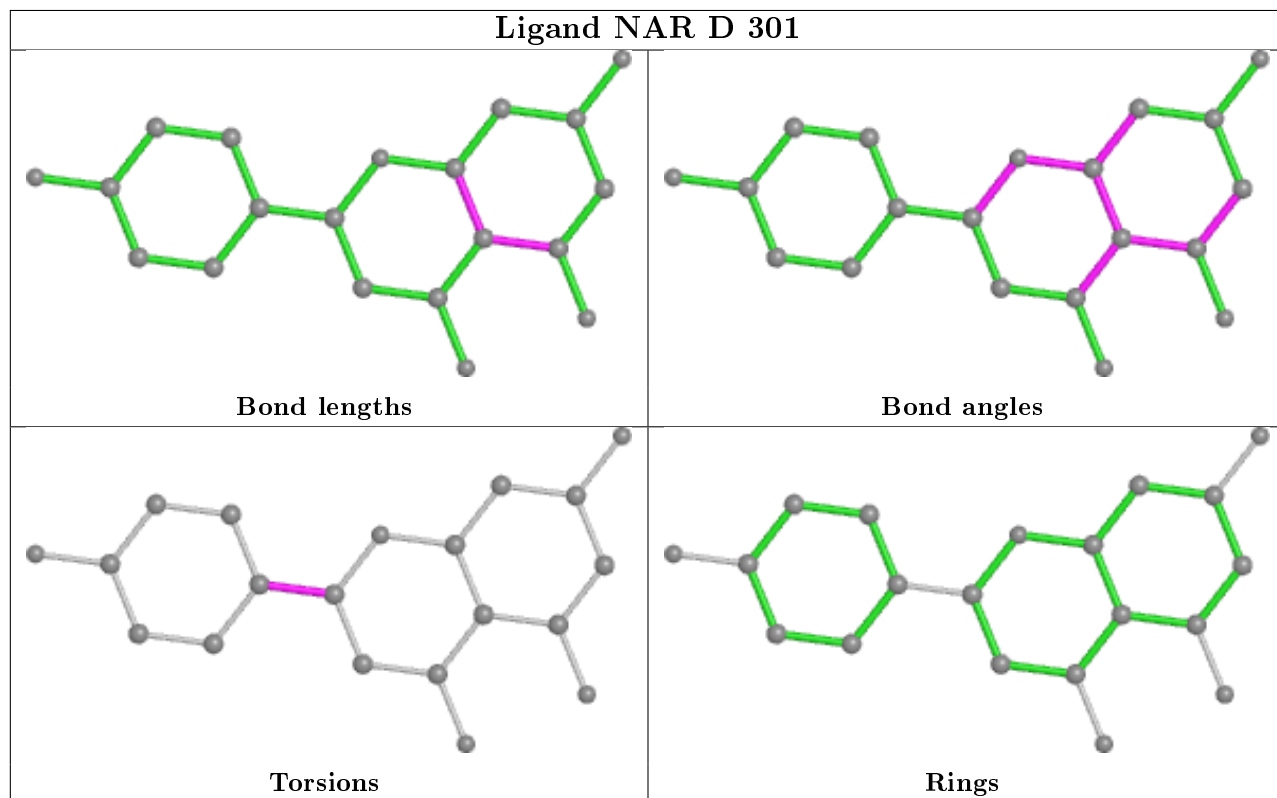
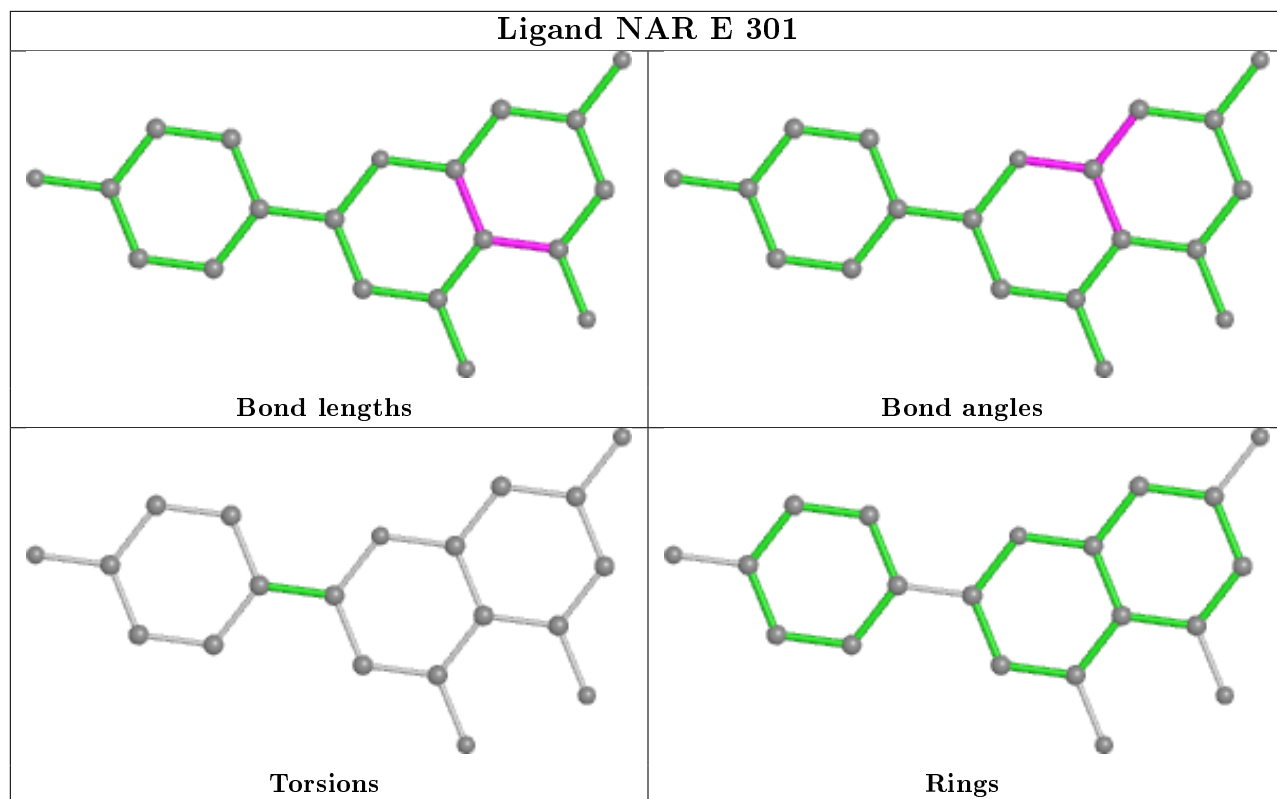
There are no ring outliers.

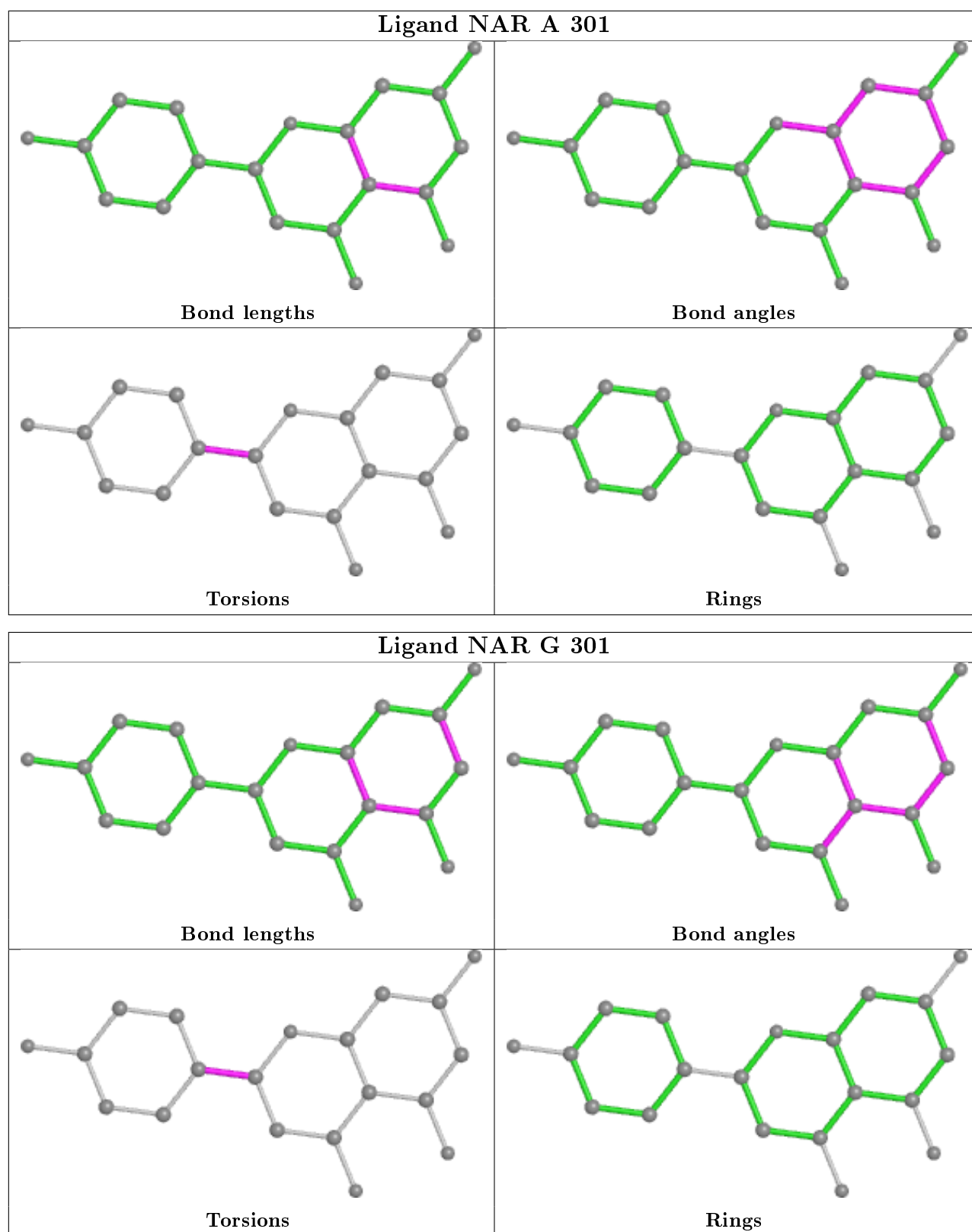
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	NAR	1	0
2	E	301	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

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	208/224 (92%)	0.73	18 (8%) 10 11	18, 42, 74, 102	0
1	B	207/224 (92%)	0.72	16 (7%) 13 15	17, 41, 73, 106	0
1	C	209/224 (93%)	1.32	46 (22%) 0 0	22, 56, 87, 113	0
1	D	207/224 (92%)	0.70	10 (4%) 30 33	22, 43, 67, 89	0
1	E	208/224 (92%)	1.40	52 (25%) 0 0	25, 57, 87, 105	0
1	F	207/224 (92%)	1.30	52 (25%) 0 0	22, 58, 89, 104	0
1	G	209/224 (93%)	0.75	13 (6%) 20 23	22, 45, 71, 85	0
1	H	205/224 (91%)	1.23	41 (20%) 1 1	28, 58, 84, 107	0
All	All	1660/1792 (92%)	1.02	248 (14%) 2 2	17, 49, 83, 113	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	41	ILE	8.6
1	C	122	LEU	7.5
1	F	75	LEU	6.7
1	C	69	ALA	6.7
1	B	41	ILE	6.6
1	E	122	LEU	5.8
1	C	123	GLY	5.4
1	C	58	ILE	5.3
1	C	60	VAL	5.0
1	C	121	SER	5.0
1	F	216	PHE	4.9
1	H	116	VAL	4.8
1	F	34	ALA	4.8
1	F	122	LEU	4.6
1	H	25	SER	4.5
1	F	212	LEU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	113	GLU	4.3
1	E	116	VAL	4.3
1	H	45	PHE	4.2
1	H	43	ASP	4.2
1	E	39	ILE	4.2
1	H	67	TRP	4.1
1	C	79	VAL	4.1
1	C	7	THR	4.0
1	E	68	LYS	4.0
1	G	65	GLU	4.0
1	B	43	ASP	4.0
1	H	198	HIS	4.0
1	B	121	SER	3.9
1	B	25	SER	3.9
1	C	118	ILE	3.9
1	A	42	GLN	3.9
1	F	194	MET	3.9
1	E	83	ARG	3.8
1	F	84	ASP	3.8
1	E	42	GLN	3.8
1	H	77	ASP	3.8
1	E	77	ASP	3.8
1	E	121	SER	3.6
1	E	9	LEU	3.5
1	E	46	VAL	3.5
1	F	71	SER	3.5
1	H	85	ILE	3.5
1	H	41	ILE	3.5
1	E	117	ALA	3.5
1	E	90	PHE	3.5
1	E	200	VAL	3.4
1	F	185	LEU	3.4
1	H	69	ALA	3.4
1	C	75	LEU	3.4
1	C	127	ASP	3.4
1	A	44	LYS	3.4
1	C	24	GLY	3.4
1	F	62	TYR	3.4
1	C	72	ALA	3.4
1	A	62	TYR	3.4
1	C	119	TRP	3.3
1	E	198	HIS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	71	SER	3.3
1	C	185	LEU	3.3
1	H	62	TYR	3.3
1	H	79	VAL	3.3
1	E	208	LEU	3.3
1	E	75	LEU	3.3
1	H	72	ALA	3.3
1	C	209	ALA	3.2
1	E	87	THR	3.2
1	A	41	ILE	3.2
1	C	125	TYR	3.2
1	E	45	PHE	3.2
1	C	80	PRO	3.1
1	H	59	ALA	3.1
1	F	39	ILE	3.1
1	F	59	ALA	3.1
1	H	209	ALA	3.1
1	H	9	LEU	3.1
1	G	124	ILE	3.1
1	H	66	LYS	3.1
1	H	63	LEU	3.0
1	F	8	ALA	3.0
1	F	72	ALA	3.0
1	G	45	PHE	3.0
1	F	26	THR	3.0
1	B	127	ASP	3.0
1	F	76	THR	3.0
1	D	117	ALA	3.0
1	F	51	ILE	3.0
1	F	24	GLY	3.0
1	A	121	SER	3.0
1	E	26	THR	2.9
1	E	81	PHE	2.9
1	E	59	ALA	2.9
1	F	69	ALA	2.9
1	H	65	GLU	2.9
1	F	204	ALA	2.9
1	E	72	ALA	2.9
1	F	127	ASP	2.9
1	C	76	THR	2.9
1	C	192	GLU	2.9
1	A	117	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	41	ILE	2.8
1	E	67	TRP	2.8
1	G	25	SER	2.8
1	F	80	PRO	2.8
1	D	122	LEU	2.8
1	E	82	PHE	2.8
1	C	65	GLU	2.8
1	A	43	ASP	2.8
1	C	81	PHE	2.8
1	F	193	SER	2.8
1	H	117	ALA	2.7
1	E	35	GLY	2.7
1	H	75	LEU	2.7
1	E	58	ILE	2.7
1	F	64	ALA	2.7
1	A	24	GLY	2.7
1	D	124	ILE	2.7
1	E	5	SER	2.7
1	C	40	GLN	2.7
1	F	116	VAL	2.7
1	H	110	LYS	2.7
1	F	208	LEU	2.7
1	A	77	ASP	2.6
1	H	40	GLN	2.6
1	B	118	ILE	2.6
1	F	83	ARG	2.6
1	E	48	PHE	2.6
1	H	6	VAL	2.6
1	C	199	GLY	2.6
1	F	11	ILE	2.6
1	C	74	GLU	2.6
1	F	57	ASP	2.6
1	F	215	LEU	2.6
1	B	39	ILE	2.6
1	E	79	VAL	2.6
1	B	113	GLU	2.5
1	D	119	TRP	2.5
1	B	46	VAL	2.5
1	H	20	VAL	2.5
1	C	124	ILE	2.5
1	A	25	SER	2.5
1	F	58	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	118	ILE	2.5
1	E	10	GLU	2.5
1	F	65	GLU	2.5
1	C	78	THR	2.5
1	E	8	ALA	2.4
1	E	36	GLU	2.4
1	H	76	THR	2.4
1	C	216	PHE	2.4
1	F	199	GLY	2.4
1	C	204	ALA	2.4
1	H	197	ALA	2.4
1	A	124	ILE	2.4
1	C	70	ARG	2.4
1	D	39	ILE	2.4
1	E	99	ILE	2.4
1	F	85	ILE	2.4
1	G	58	ILE	2.4
1	E	60	VAL	2.4
1	E	111	VAL	2.4
1	F	77	ASP	2.4
1	H	196	GLY	2.4
1	F	40	GLN	2.4
1	C	128	GLU	2.4
1	A	113	GLU	2.4
1	A	122	LEU	2.4
1	H	81	PHE	2.4
1	E	64	ALA	2.4
1	A	83	ARG	2.4
1	E	141	LYS	2.4
1	E	11	ILE	2.4
1	C	43	ASP	2.3
1	H	208	LEU	2.3
1	B	197	ALA	2.3
1	F	81	PHE	2.3
1	H	82	PHE	2.3
1	F	121	SER	2.3
1	E	6	VAL	2.3
1	E	40	GLN	2.3
1	B	109	GLU	2.3
1	D	66	LYS	2.3
1	E	43	ASP	2.3
1	H	90	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	114	ASN	2.3
1	G	60	VAL	2.3
1	F	203	ALA	2.3
1	F	68	LYS	2.3
1	E	49	THR	2.3
1	E	118	ILE	2.3
1	F	46	VAL	2.2
1	G	9	LEU	2.2
1	E	24	GLY	2.2
1	C	68	LYS	2.2
1	G	217	LYS	2.2
1	B	114	ASN	2.2
1	D	121	SER	2.2
1	F	124	ILE	2.2
1	C	33	GLY	2.2
1	F	31	LEU	2.2
1	B	26	THR	2.2
1	B	42	GLN	2.2
1	H	78	THR	2.2
1	C	197	ALA	2.2
1	G	29	PHE	2.2
1	H	204	ALA	2.2
1	F	6	VAL	2.2
1	H	200	VAL	2.2
1	C	133	ILE	2.2
1	E	217	LYS	2.2
1	H	193	SER	2.2
1	F	63	LEU	2.2
1	A	198	HIS	2.2
1	B	24	GLY	2.2
1	C	42	GLN	2.2
1	F	82	PHE	2.1
1	F	25	SER	2.1
1	C	53	VAL	2.1
1	C	73	HIS	2.1
1	G	116	VAL	2.1
1	D	115	CYS	2.1
1	F	78	THR	2.1
1	F	206	GLN	2.1
1	C	39	ILE	2.1
1	B	9	LEU	2.1
1	D	26	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	44	LYS	2.1
1	H	70	ARG	2.1
1	C	31	LEU	2.1
1	E	193	SER	2.1
1	E	74	GLU	2.1
1	F	135	LYS	2.1
1	G	7	THR	2.1
1	A	128	GLU	2.1
1	C	113	GLU	2.1
1	H	114	ASN	2.1
1	A	39	ILE	2.1
1	E	211	ARG	2.0
1	C	34	ALA	2.0
1	A	185	LEU	2.0
1	E	114	ASN	2.0
1	F	214	LYS	2.0
1	D	6	VAL	2.0
1	H	111	VAL	2.0
1	C	45	PHE	2.0
1	E	18	PRO	2.0
1	F	67	TRP	2.0
1	E	31	LEU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

6.4 Ligands [\(i\)](#)

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

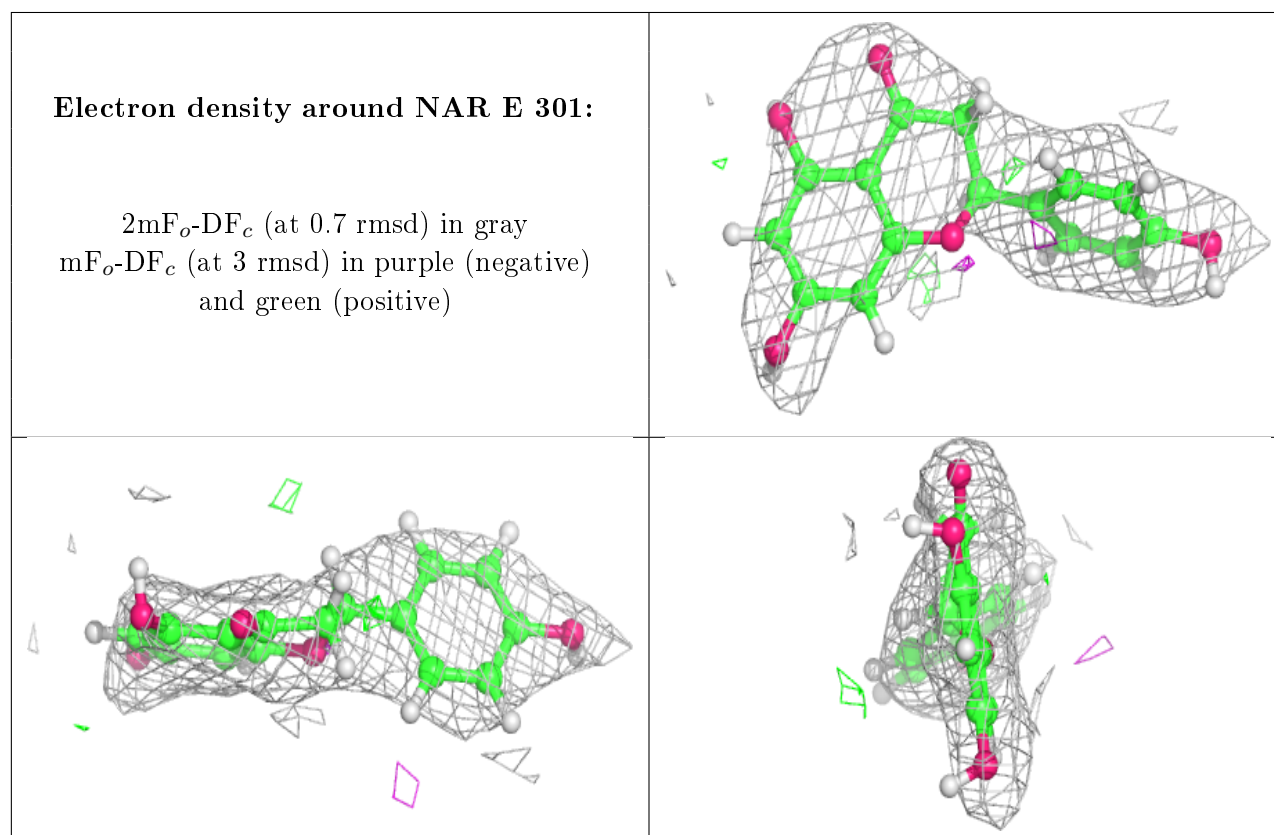
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAR	E	301	20/20	0.78	0.19	55,70,87,93	0

Continued on next page...

Continued from previous page...

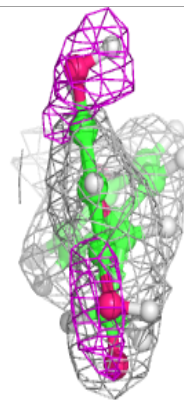
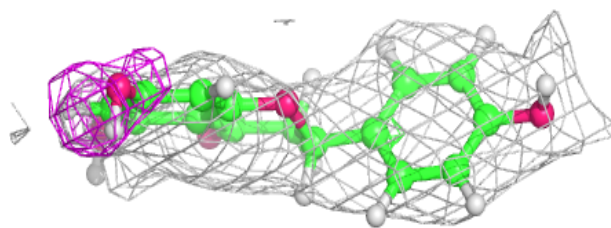
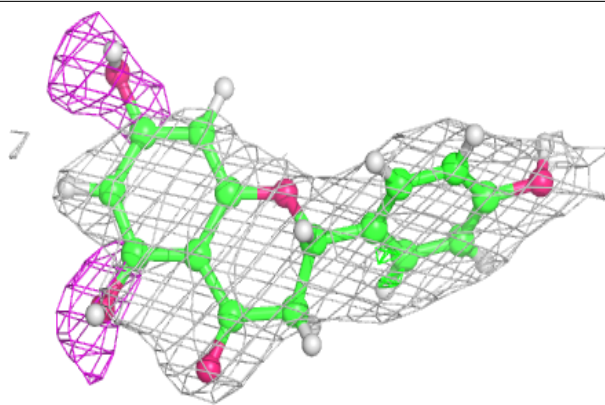
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAR	G	301	20/20	0.78	0.25	36,52,68,74	0
2	NAR	D	301	20/20	0.79	0.20	42,58,75,81	0
2	NAR	A	301	20/20	0.89	0.15	35,57,78,83	0
2	NAR	F	301	20/20	0.89	0.14	47,64,79,88	0

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.

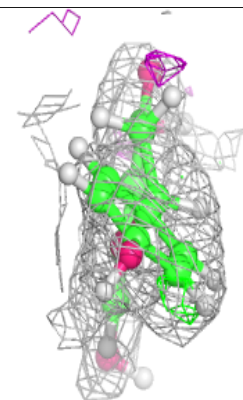
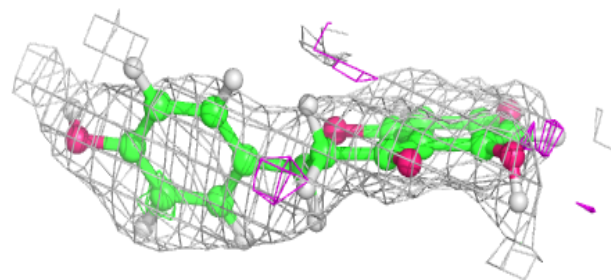
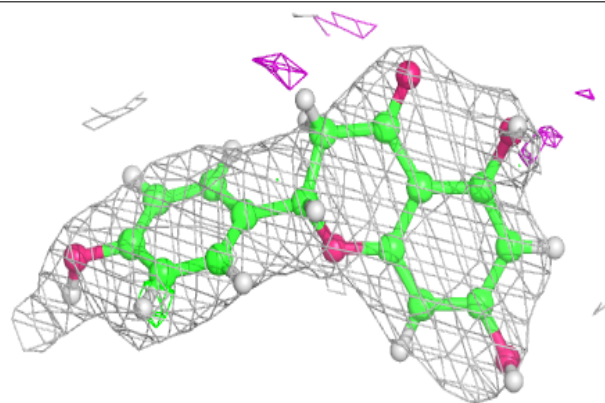


Electron density around NAR G 301:

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

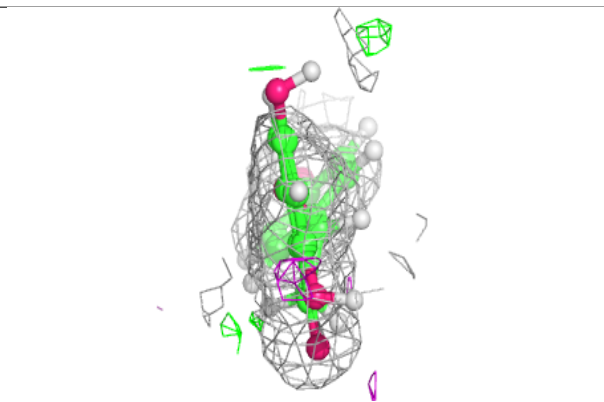
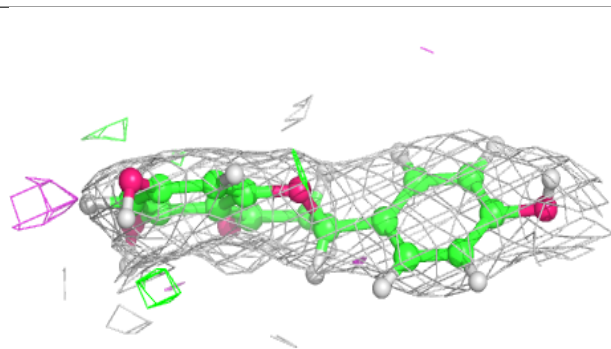
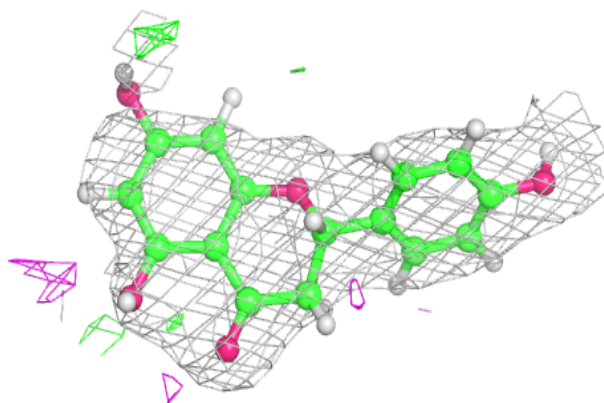
**Electron density around NAR D 301:**

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

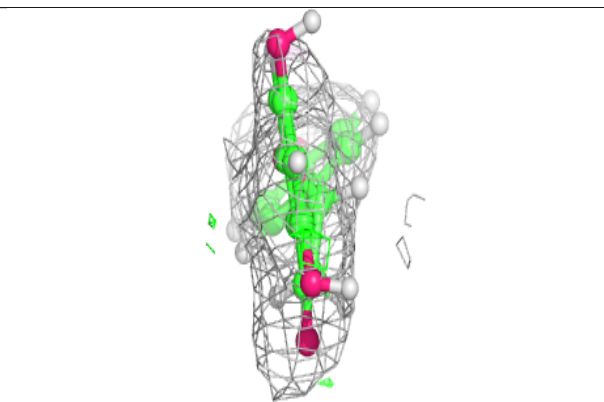
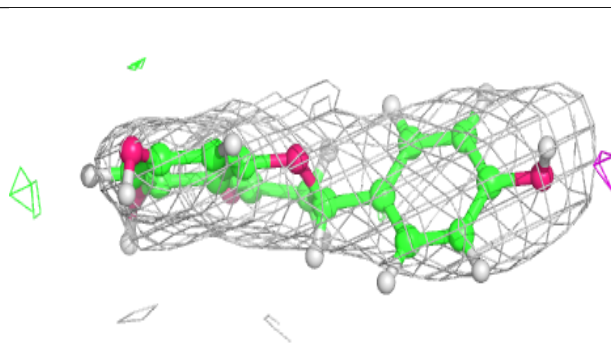
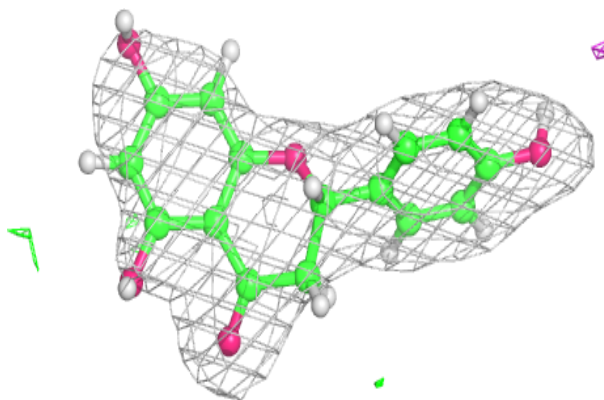


Electron density around NAR A 301:

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

**Electron density around NAR F 301:**

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



6.5 Other polymers

There are no such residues in this entry.