



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:24 AM UTC

PDB ID : 8V8M / pdb_00008v8m
Title : Switchgrass Chalcone Synthase
Authors : Lewis, J.A.; Kang, C.
Deposited on : 2023-12-05
Resolution : 1.82 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

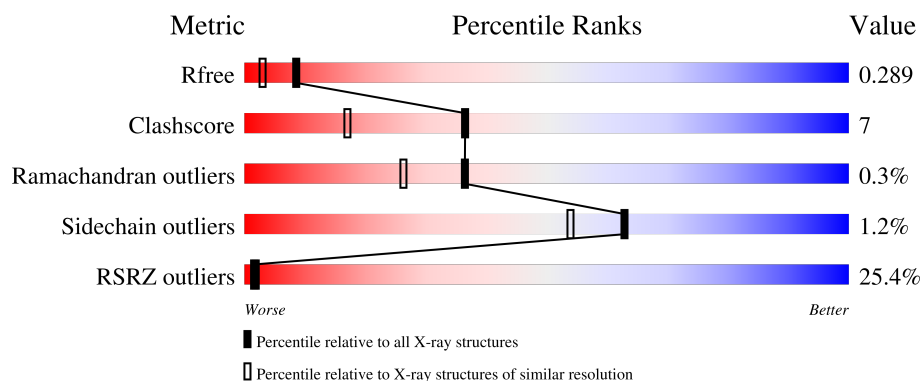
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	402	21% 79% 17% .
1	B	402	28% 78% 18% .
1	C	402	22% 82% 14% .
1	D	402	26% 82% 14% .

2 Entry composition [i](#)

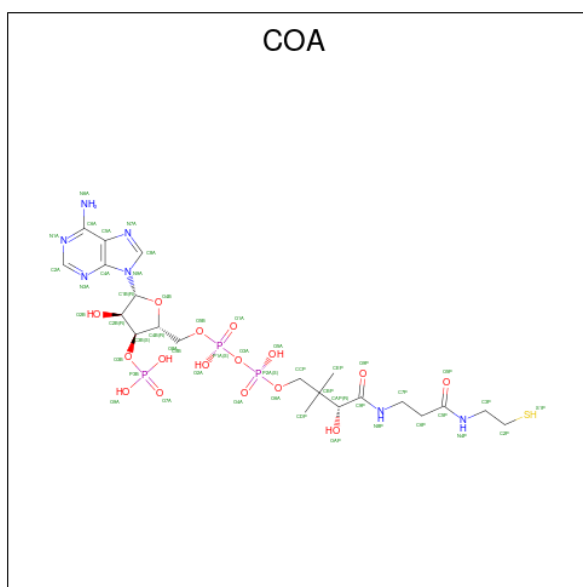
There are 4 unique types of molecules in this entry. The entry contains 12924 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 synthase.

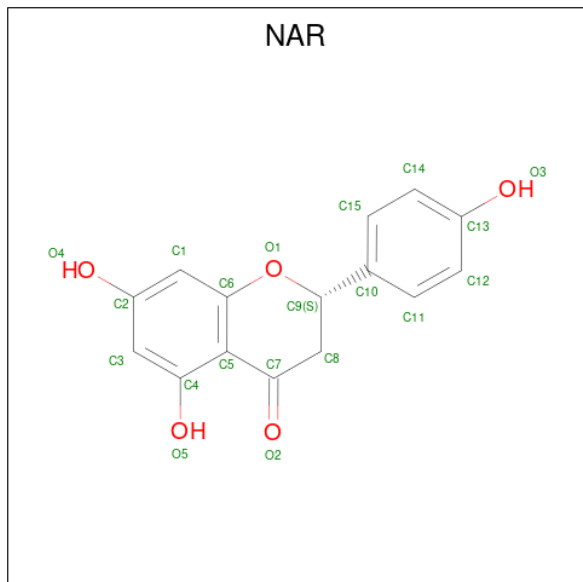
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	1	0
			2970	1872	524	555	19			
1	B	388	Total	C	N	O	S	0	0	0
			2963	1868	523	553	19			
1	C	389	Total	C	N	O	S	0	1	0
			2970	1872	524	555	19			
1	D	388	Total	C	N	O	S	0	0	0
			2963	1867	523	554	19			

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	1
			48	21	7	16	3 1		
2	C	1	Total	C	N	O	P S	0	1
			48	21	7	16	3 1		

- Molecule 3 is NARINGENIN (CCD ID: NAR) (formula: $C_{15}H_{12}O_5$) (labeled as "Ligand of Interest" by depositor).



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

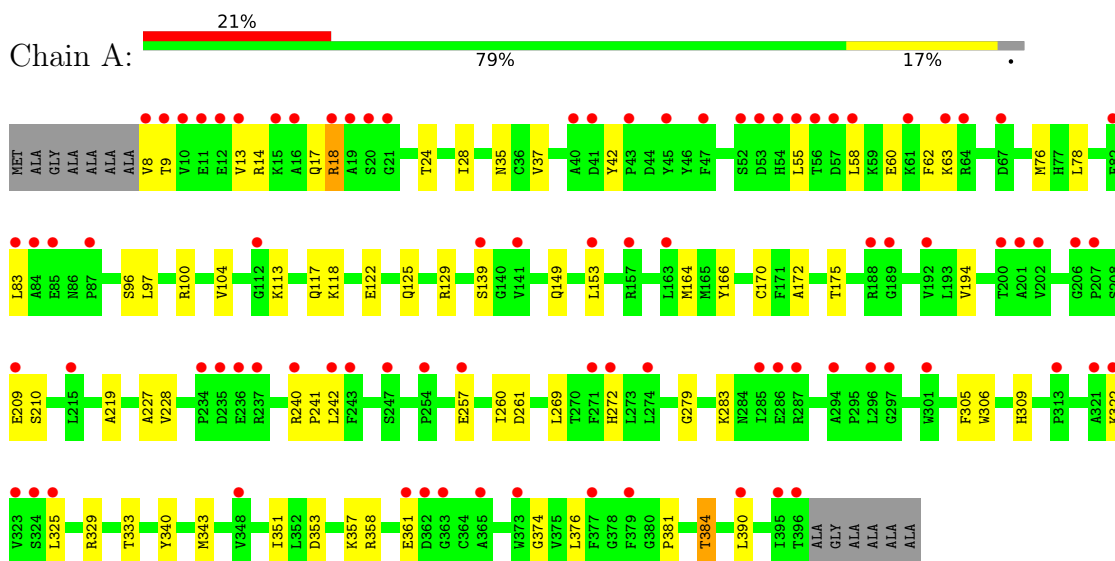
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	229	Total	O	0	0
			229	229		
4	B	247	Total	O	0	0
			247	247		
4	C	214	Total	O	0	0
			214	214		
4	D	232	Total	O	0	0
			232	232		

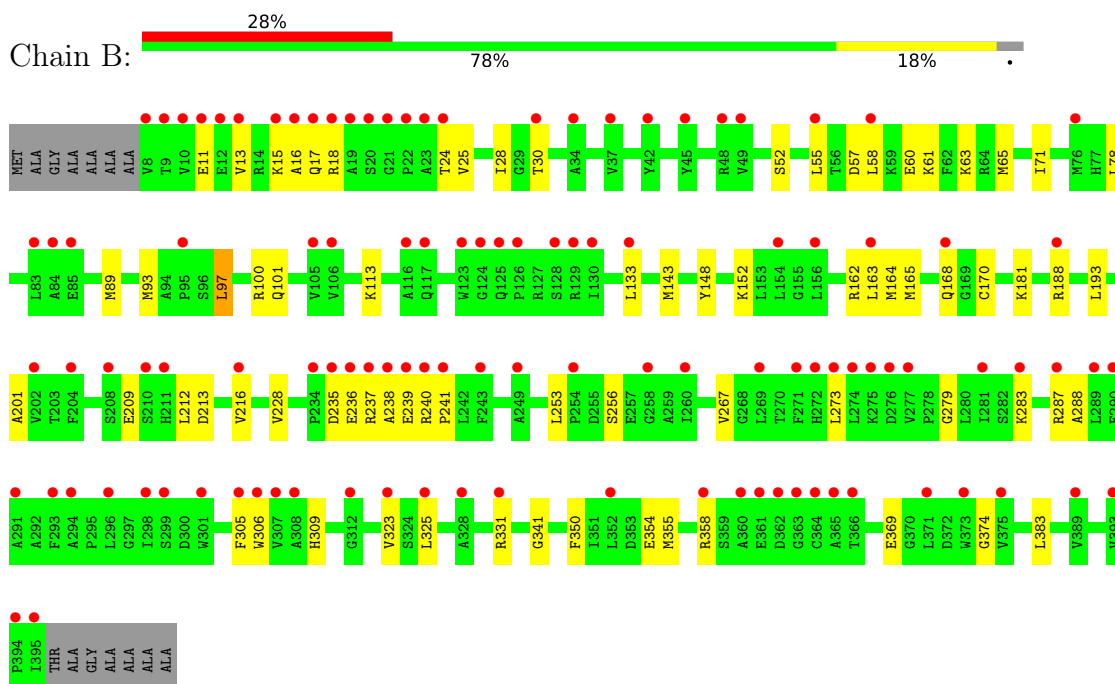
3 Residue-property plots

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

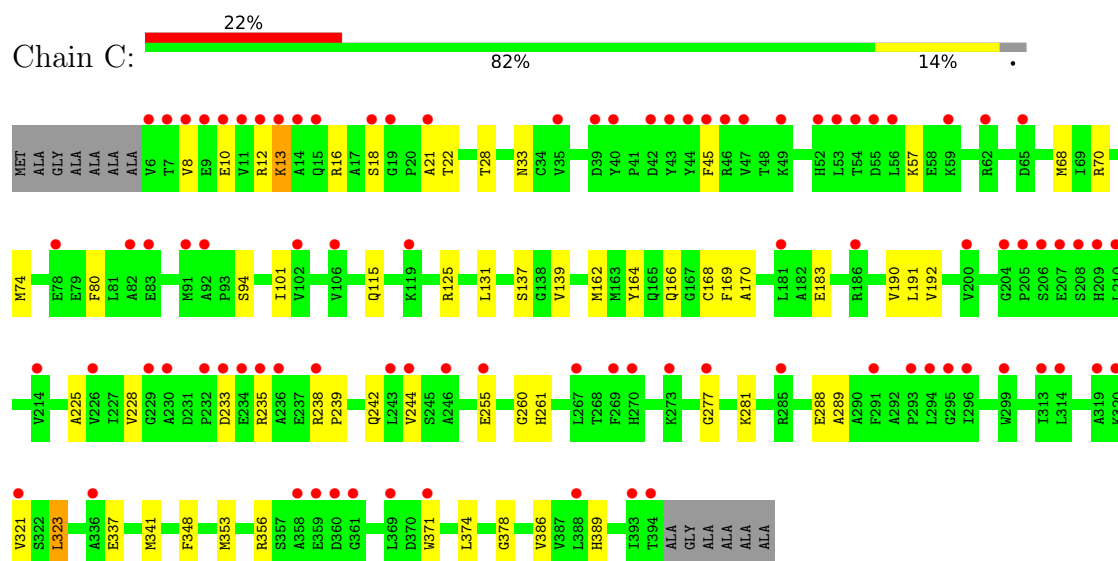
• Molecule 1: Chalcone synthase



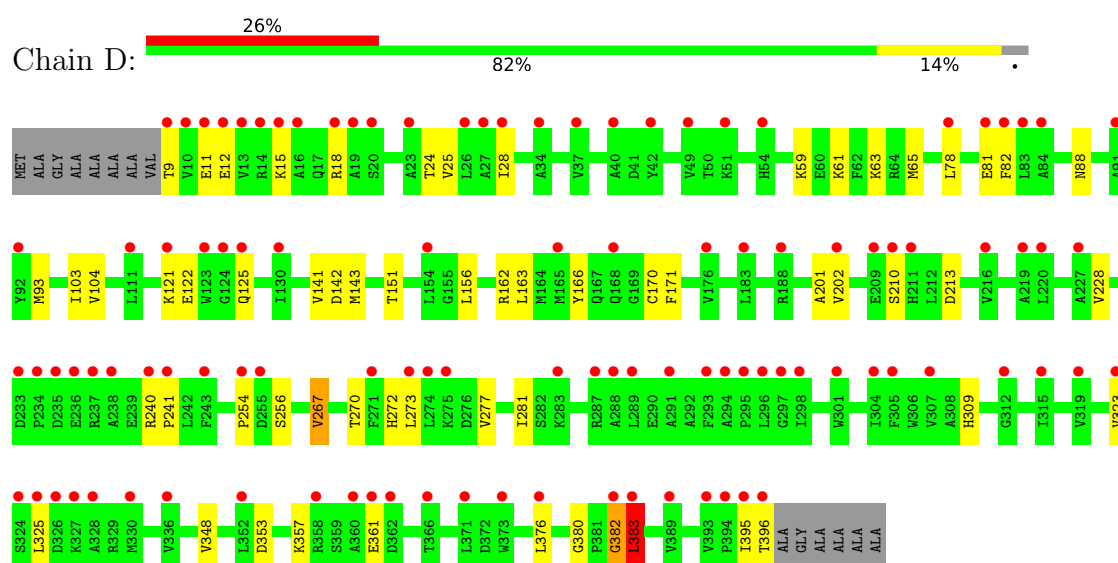
• Molecule 1: Chalcone synthase



● Molecule 1: Chalcone synthase



● Molecule 1: Chalcone synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.05Å 83.08Å 106.45Å 79.43° 76.25° 77.21°	Depositor
Resolution (Å)	48.72 – 1.82 48.72 – 1.82	Depositor EDS
% Data completeness (in resolution range)	71.9 (48.72-1.82) 69.7 (48.72-1.82)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 1.82Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.264 , 0.289 0.264 , 0.289	Depositor DCC
R_{free} test set	1983 reflections (1.35%)	wwPDB-VP
Wilson B-factor (Å ²)	0.7	Xtriage
Anisotropy	3.906	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	12924	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% 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, COA, CSD

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	0.19	0/3020	0.41	0/4095
1	B	0.24	0/3013	0.48	0/4085
1	C	0.19	0/3020	0.40	0/4095
1	D	0.21	0/3013	0.44	2/4085 (0.0%)
All	All	0.21	0/12066	0.43	2/16360 (0.0%)

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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	382	GLY	N-CA-C	-7.76	104.52	115.30
1	D	267	VAL	N-CA-C	-5.27	107.33	112.29

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	382	GLY	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2970	0	2981	53	0
1	B	2963	0	2974	54	0
1	C	2970	0	2981	42	0
1	D	2963	0	2972	34	0
2	A	48	0	3	1	0
2	C	48	0	3	1	0
3	A	40	0	19	0	0
4	A	229	0	0	2	0
4	B	247	0	0	0	0
4	C	214	0	0	2	0
4	D	232	0	0	3	0
All	All	12924	0	11933	172	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (172) 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:240:ARG:O	1:A:240:ARG:NH1	2.12	0.83
1:A:14:ARG:HH21	1:A:17:GLN:HE21	1.34	0.74
1:D:18:ARG:NH2	4:D:501:HOH:O	2.20	0.73
1:C:115:GLN:HE21	1:C:125:ARG:HH22	1.39	0.67
1:C:13:LYS:HA	1:C:13:LYS:HE2	1.76	0.67
1:A:358:ARG:NH2	4:A:603:HOH:O	2.26	0.66
1:A:376:LEU:HB2	1:A:390:LEU:HD21	1.78	0.64
1:B:148:TYR:CZ	1:B:152:LYS:HD2	2.32	0.63
1:B:89:MET:HE3	1:B:100:ARG:HG2	1.80	0.63
1:B:93:MET:HE3	1:B:267:VAL:HG21	1.80	0.62
1:C:255:GLU:H	1:C:255:GLU:CD	2.08	0.61
1:A:261:ASP:HB2	1:A:272:HIS:HB2	1.83	0.61
1:B:24:THR:HG21	1:B:241:PRO:HB3	1.82	0.61
1:D:213:ASP:HB2	1:D:273:LEU:HD12	1.83	0.59
1:D:256:SER:HB2	1:D:383:LEU:HB2	1.84	0.58
1:D:125:GLN:NE2	4:D:504:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:VAL:HG13	1:C:323:LEU:HD13	1.85	0.58
1:A:24:THR:HG21	1:A:241:PRO:HB3	1.85	0.58
1:C:12:ARG:NH1	4:C:606:HOH:O	2.36	0.58
1:C:22:THR:HG21	1:C:239:PRO:HB3	1.85	0.57
1:A:122:GLU:OE2	1:A:240:ARG:NH2	2.37	0.57
1:B:323:VAL:HG23	1:B:325:LEU:HG	1.87	0.57
1:A:381:PRO:O	1:A:384:THR:HG23	2.05	0.57
1:A:17:GLN:HE22	1:B:181:LYS:HZ1	1.53	0.57
1:A:257:GLU:HG2	1:B:148:TYR:OH	2.05	0.57
1:C:168:CSD:OD2	2:C:501[B]:COA:S1P	2.62	0.56
1:B:354:GLU:OE2	1:B:358:ARG:NH2	2.39	0.56
1:C:261:HIS:HD2	1:D:142:ASP:OD1	1.88	0.56
1:A:58:LEU:HD22	1:A:209:GLU:HG3	1.88	0.56
1:B:13:VAL:O	1:B:17:GLN:HB2	2.07	0.55
1:A:333:THR:HA	1:A:351:ILE:HG12	1.89	0.55
1:A:118:LYS:HA	1:A:118:LYS:HE3	1.89	0.54
1:D:121:LYS:HD2	1:D:122:GLU:N	2.22	0.54
1:A:306:TRP:CE2	1:A:325:LEU:HD11	2.42	0.54
1:C:260:GLY:HA3	1:D:143:MET:HE3	1.89	0.54
1:C:8:VAL:HG12	1:C:10:GLU:H	1.73	0.54
1:D:11:GLU:O	1:D:15:LYS:HD3	2.07	0.54
1:C:169:PHE:HD2	1:C:378:GLY:HA3	1.72	0.53
1:A:240:ARG:NH1	1:A:242:LEU:HG	2.23	0.53
1:B:15:LYS:N	1:B:15:LYS:HD2	2.23	0.53
1:B:61:LYS:O	1:B:65:MET:HG3	2.07	0.53
1:B:52:SER:HB3	1:B:55:LEU:HD23	1.91	0.53
1:C:277:GLY:O	1:C:281:LYS:HG3	2.09	0.53
1:B:28:ILE:HG12	1:B:228:VAL:HG22	1.90	0.53
1:C:115:GLN:HE21	1:C:125:ARG:NH2	2.06	0.52
1:B:253:LEU:HD12	1:B:383:LEU:HD13	1.92	0.52
1:C:233:ASP:OD2	1:C:235:ARG:HB2	2.10	0.52
1:A:240:ARG:HH12	1:A:242:LEU:HG	1.73	0.52
1:B:212:LEU:O	1:B:216:VAL:HG23	2.10	0.52
1:C:162:MET:HE2	1:C:164:TYR:CE1	2.45	0.52
1:A:17:GLN:HE22	1:B:181:LYS:NZ	2.07	0.51
1:A:164:MET:HE2	1:A:166:TYR:CE1	2.45	0.51
1:A:322:LYS:HA	1:A:322:LYS:HE2	1.92	0.51
1:D:151:THR:HG23	1:D:156:LEU:HB2	1.93	0.51
1:B:30:THR:HB	1:B:350:PHE:CZ	2.46	0.51
1:A:357:LYS:O	1:A:361:GLU:HG3	2.10	0.50
2:A:501[A]:COA:S1P	4:A:646:HOH:O	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLY:O	1:B:283:LYS:HB2	2.11	0.50
1:A:8:VAL:HG13	1:A:9:THR:HG23	1.94	0.50
1:C:16:ARG:HE	1:D:18:ARG:HH21	1.60	0.50
1:B:164:MET:HE3	1:B:165:MET:N	2.27	0.50
1:A:18:ARG:HE	1:B:18:ARG:HH21	1.60	0.49
1:A:35:ASN:HB3	1:A:76:MET:O	2.13	0.49
1:B:97:LEU:HD22	1:B:101:GLN:HG2	1.94	0.49
1:B:162:ARG:O	1:B:163:LEU:HD23	2.13	0.49
1:B:235:ASP:OD1	1:B:238:ALA:HB3	2.12	0.49
1:C:12:ARG:NE	1:C:12:ARG:HA	2.26	0.49
1:D:25:VAL:HG13	1:D:228:VAL:HG13	1.93	0.49
1:D:11:GLU:HB3	1:D:15:LYS:HE2	1.94	0.49
1:D:81:GLU:H	1:D:81:GLU:CD	2.20	0.49
1:D:323:VAL:HG23	1:D:325:LEU:HG	1.93	0.49
1:B:60:GLU:HA	1:B:63:LYS:HD2	1.94	0.49
1:D:9:THR:OG1	1:D:12:GLU:HG3	2.12	0.49
1:D:104:VAL:HG11	1:D:202:VAL:HG23	1.95	0.49
1:D:171:PHE:HD2	1:D:380:GLY:HA3	1.78	0.49
1:C:8:VAL:HG12	1:C:10:GLU:N	2.27	0.48
1:C:16:ARG:HB2	4:D:501:HOH:O	2.11	0.48
1:C:166:GLN:HB3	1:C:170:ALA:HB2	1.95	0.48
1:A:194:VAL:HB	1:A:228:VAL:HG22	1.96	0.48
1:D:28:ILE:HG21	1:D:353:ASP:HB2	1.94	0.48
1:D:61:LYS:O	1:D:65:MET:HG3	2.14	0.48
1:B:235:ASP:OD1	1:B:239:GLU:HG3	2.13	0.47
1:D:277:VAL:O	1:D:281:ILE:HG13	2.14	0.47
1:D:82:PHE:CZ	1:D:103:ILE:HD11	2.49	0.47
1:A:164:MET:HB3	1:B:168:GLN:HE22	1.80	0.47
1:B:170:CSD:HB2	1:B:309:HIS:NE2	2.29	0.47
1:C:244:VAL:HG21	1:C:371:TRP:HZ3	1.79	0.47
1:B:71:ILE:HG12	1:B:341:GLY:HA2	1.96	0.47
1:A:55:LEU:HD22	1:A:209:GLU:OE2	2.14	0.47
1:C:70:ARG:NH2	1:C:337:GLU:OE1	2.47	0.47
1:C:190:VAL:HG13	1:C:228:VAL:HB	1.96	0.47
1:A:78:LEU:HD13	1:A:83:LEU:HD21	1.96	0.47
1:B:170:CSD:HB2	1:B:309:HIS:CE1	2.50	0.47
1:B:25:VAL:HG13	1:B:228:VAL:HG13	1.97	0.47
1:B:256:SER:HB2	1:B:383:LEU:HB2	1.96	0.47
1:B:287:ARG:NH2	1:B:288:ALA:HB2	2.30	0.47
1:A:18:ARG:HE	1:B:18:ARG:NH2	2.12	0.47
1:A:28:ILE:HG12	1:A:228:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:GLU:HG3	1:C:289:ALA:N	2.28	0.47
1:A:170:CSD:HB2	1:A:309:HIS:CE1	2.50	0.46
1:A:240:ARG:HG2	1:A:240:ARG:HH11	1.80	0.46
1:D:170:CSD:HB2	1:D:309:HIS:NE2	2.31	0.46
1:C:80:PHE:CZ	1:C:101:ILE:HD11	2.50	0.46
1:B:16:ALA:C	1:B:188:ARG:HH12	2.22	0.46
1:C:238:ARG:NE	4:C:620:HOH:O	2.49	0.46
1:A:37:VAL:HG11	1:A:42:TYR:CD1	2.50	0.45
1:D:78:LEU:HD11	1:D:201:ALA:HA	1.97	0.45
1:D:348:VAL:HB	1:D:376:LEU:HD11	1.98	0.45
1:B:165:MET:HE3	1:B:168:GLN:NE2	2.32	0.45
1:D:162:ARG:O	1:D:163:LEU:HD23	2.17	0.45
1:A:100:ARG:O	1:A:104:VAL:HG22	2.16	0.45
1:A:353:ASP:O	1:A:357:LYS:HG3	2.17	0.45
1:C:139:VAL:HA	1:C:164:TYR:CE1	2.52	0.45
1:D:141:VAL:HA	1:D:166:TYR:CE1	2.52	0.45
1:A:97:LEU:HD22	1:B:97:LEU:HD12	1.99	0.45
1:B:113:LYS:HB3	1:B:113:LYS:HE3	1.67	0.44
1:D:24:THR:HG21	1:D:241:PRO:HB3	1.98	0.44
1:A:260:ILE:HB	1:A:381:PRO:HA	1.99	0.44
1:A:194:VAL:O	1:A:227:ALA:HA	2.18	0.44
1:A:149:GLN:O	1:A:153:LEU:HD13	2.18	0.44
1:C:192:VAL:O	1:C:225:ALA:HA	2.18	0.44
1:A:125:GLN:HE21	1:A:129:ARG:HH11	1.65	0.44
1:B:331:ARG:NE	1:B:331:ARG:HA	2.32	0.44
1:B:355:MET:HE2	1:B:369:GLU:CD	2.42	0.44
1:A:60:GLU:OE2	1:A:63:LYS:HE3	2.18	0.43
1:C:242:GLN:HB2	1:C:389:HIS:HB3	2.00	0.43
1:D:93:MET:SD	1:D:267:VAL:HG21	2.58	0.43
1:A:113:LYS:HE2	1:A:117:GLN:OE1	2.17	0.43
1:B:253:LEU:O	1:B:256:SER:OG	2.31	0.43
1:C:353:MET:HE2	1:C:353:MET:HB2	1.91	0.43
1:B:213:ASP:HB2	1:B:273:LEU:HD12	2.00	0.43
1:D:240:ARG:HH11	1:D:240:ARG:HG3	1.82	0.43
1:C:244:VAL:HG21	1:C:371:TRP:CZ3	2.53	0.43
1:B:78:LEU:HD11	1:B:201:ALA:HA	2.01	0.43
1:B:287:ARG:HH22	1:B:288:ALA:HB2	1.82	0.43
1:A:9:THR:O	1:A:13:VAL:HG23	2.18	0.42
1:A:257:GLU:OE1	1:B:152:LYS:HE3	2.20	0.42
1:B:57:ASP:O	1:B:61:LYS:HG3	2.19	0.42
1:C:45:PHE:CG	1:C:57:LYS:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:MET:HE3	1:B:165:MET:H	1.83	0.42
1:C:68:MET:HE3	1:C:68:MET:HA	2.02	0.42
1:A:62:PHE:CE1	1:A:219:ALA:HB2	2.55	0.42
1:A:340:TYR:HB3	1:A:343:MET:SD	2.60	0.42
1:C:33:ASN:HB3	1:C:74:MET:O	2.21	0.41
1:B:11:GLU:O	1:B:15:LYS:HD3	2.20	0.41
1:C:341:MET:HE1	1:C:348:PHE:CD2	2.55	0.41
1:C:21:ALA:HB2	1:C:183:GLU:HG3	2.01	0.41
1:C:28:THR:HB	1:C:348:PHE:CZ	2.55	0.41
1:A:305:PHE:CE2	1:A:374:GLY:HA3	2.56	0.41
1:C:341:MET:HE1	1:C:348:PHE:CG	2.56	0.41
1:A:325:LEU:HD22	1:A:329:ARG:HG3	2.02	0.41
1:A:172:ALA:HA	1:A:175:THR:OG1	2.20	0.41
1:B:58:LEU:HD22	1:B:209:GLU:HG2	2.01	0.41
1:C:374:LEU:HB3	1:C:386:VAL:HB	2.03	0.41
1:D:357:LYS:O	1:D:361:GLU:HG3	2.21	0.41
1:C:162:MET:HE2	1:C:164:TYR:CZ	2.55	0.41
1:D:11:GLU:CD	1:D:11:GLU:H	2.29	0.41
1:D:270:THR:OG1	1:D:272:HIS:HE1	2.04	0.41
1:A:125:GLN:NE2	1:A:129:ARG:HH11	2.19	0.41
1:A:279:GLY:O	1:A:283:LYS:HB2	2.21	0.41
1:B:306:TRP:CE2	1:B:325:LEU:HD11	2.55	0.41
1:C:131:LEU:HD13	1:C:191:LEU:HD23	2.02	0.41
1:B:133:LEU:HD13	1:B:193:LEU:HD23	2.03	0.40
1:B:16:ALA:O	1:B:188:ARG:NH1	2.42	0.40
1:A:14:ARG:HH21	1:A:17:GLN:HB3	1.87	0.40
1:A:269:LEU:HD11	1:B:143:MET:HE2	2.03	0.40
1:B:16:ALA:C	1:B:188:ARG:NH1	2.80	0.40
1:C:356:ARG:HD3	1:C:356:ARG:HA	1.85	0.40
1:D:88:ASN:HD22	1:D:88:ASN:HA	1.62	0.40
1:D:59:LYS:C	1:D:63:LYS:HZ2	2.29	0.40
1:A:164:MET:HE2	1:A:166:TYR:CZ	2.57	0.40
1:B:305:PHE:CE2	1:B:374:GLY:HA3	2.57	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	386/402 (96%)	374 (97%)	10 (3%)	2 (0%)	24	14
1	B	385/402 (96%)	371 (96%)	14 (4%)	0	100	100
1	C	386/402 (96%)	376 (97%)	9 (2%)	1 (0%)	36	26
1	D	385/402 (96%)	368 (96%)	15 (4%)	2 (0%)	24	14
All	All	1542/1608 (96%)	1489 (97%)	48 (3%)	5 (0%)	36	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	94	SER
1	A	18	ARG
1	A	96	SER
1	D	383	LEU
1	D	254	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	314/315 (100%)	311 (99%)	3 (1%)	68	60
1	B	313/315 (99%)	309 (99%)	4 (1%)	61	50
1	C	314/315 (100%)	310 (99%)	4 (1%)	61	50
1	D	313/315 (99%)	309 (99%)	4 (1%)	61	50
All	All	1254/1260 (100%)	1239 (99%)	15 (1%)	63	54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	SER
1	A	210	SER
1	A	384	THR
1	B	97	LEU
1	B	236	GLU
1	B	237	ARG
1	B	240	ARG
1	C	13	LYS
1	C	18	SER
1	C	137	SER
1	C	323	LEU
1	D	210	SER
1	D	383	LEU
1	D	395	ILE
1	D	396	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	38	HIS
1	A	125	GLN
1	A	161	ASN
1	A	167	GLN
1	A	244	GLN
1	A	318	GLN
1	B	117	GLN
1	B	168	GLN
1	C	115	GLN
1	C	185	ASN
1	C	261	HIS
1	D	54	HIS
1	D	86	ASN
1	D	88	ASN
1	D	117	GLN
1	D	167	GLN
1	D	272	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSD	A	170	1	4,7,8	0.84	0	1,8,10	0.88	0
1	CSD	B	170	1	4,7,8	0.99	0	1,8,10	1.27	0
1	CSD	D	170	1	4,7,8	1.01	0	1,8,10	0.21	0
1	CSD	C	168	1	4,7,8	0.86	0	1,8,10	0.09	0

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
1	CSD	A	170	1	-	1/2/6/8	-
1	CSD	B	170	1	-	1/2/6/8	-
1	CSD	D	170	1	-	1/2/6/8	-
1	CSD	C	168	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	170	CSD	CA-CB-SG-OD1
1	B	170	CSD	CA-CB-SG-OD1
1	C	168	CSD	CA-CB-SG-OD1

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Mol	Chain	Res	Type	Atoms
1	D	170	CSD	CA-CB-SG-OD1

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	170	CSD	1	0
1	B	170	CSD	2	0
1	D	170	CSD	1	0
1	C	168	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
3	NAR	A	502	-	22,22,22	0.67	1 (4%)	32,32,32	0.49	0
3	NAR	A	503	-	22,22,22	0.74	1 (4%)	32,32,32	0.53	0

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
3	NAR	A	502	-	-	0/4/16/16	0/3/3/3
3	NAR	A	503	-	-	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)
3	A	503	NAR	O1-C6	-2.70	1.34	1.38
3	A	502	NAR	O1-C6	-2.46	1.34	1.38

There are no bond angle outliers.

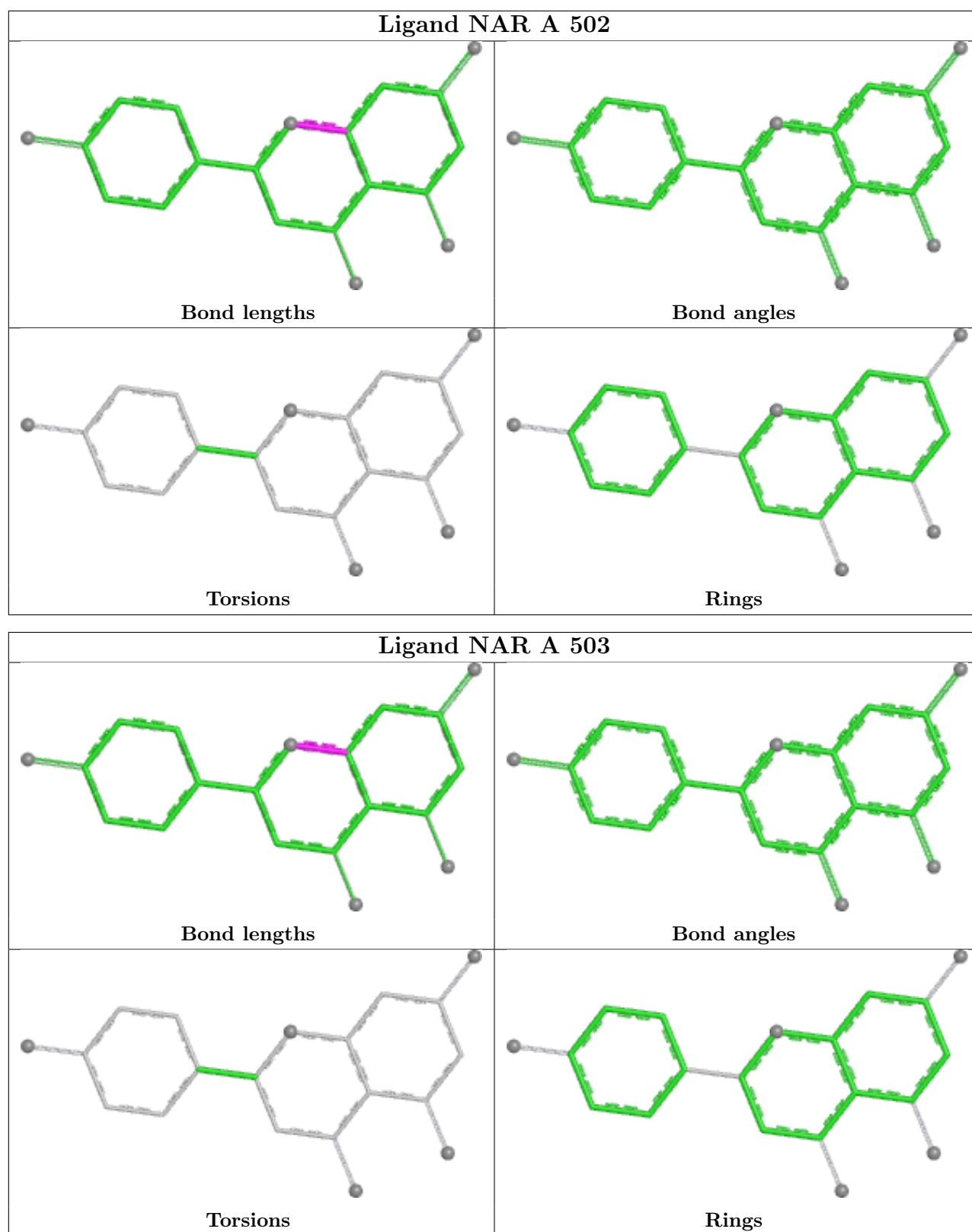
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	388/402 (96%)	1.48	86 (22%) 2 2	3, 11, 26, 42	0
1	B	387/402 (96%)	1.70	111 (28%) 1 1	4, 13, 26, 60	0
1	C	388/402 (96%)	1.51	90 (23%) 2 2	4, 10, 27, 49	0
1	D	387/402 (96%)	1.67	106 (27%) 1 1	4, 13, 24, 67	0
All	All	1550/1608 (96%)	1.59	393 (25%) 1 2	3, 12, 26, 67	0

All (393) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	VAL	7.6
1	D	237	ARG	7.5
1	C	394	THR	7.1
1	A	8	VAL	6.9
1	A	396	THR	6.6
1	D	16	ALA	6.2
1	C	14	ALA	6.1
1	D	9	THR	6.0
1	D	10	VAL	5.9
1	B	16	ALA	5.8
1	B	237	ARG	5.7
1	D	13	VAL	5.7
1	B	236	GLU	5.5
1	B	235	ASP	5.5
1	C	7	THR	5.5
1	C	9	GLU	5.5
1	C	235	ARG	5.3
1	A	236	GLU	5.1
1	D	396	THR	5.0
1	C	12	ARG	5.0
1	B	298	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	271	PHE	4.8
1	B	363	GLY	4.8
1	B	238	ALA	4.8
1	A	10	VAL	4.7
1	C	8	VAL	4.7
1	B	234	PRO	4.6
1	A	13	VAL	4.6
1	B	271	PHE	4.5
1	C	270	HIS	4.4
1	B	361	GLU	4.4
1	B	8	VAL	4.3
1	B	362	ASP	4.3
1	B	296	LEU	4.2
1	B	301	TRP	4.2
1	A	237	ARG	4.2
1	D	236	GLU	4.2
1	C	53	LEU	4.2
1	C	11	VAL	4.1
1	A	272	HIS	4.1
1	C	55	ASP	4.1
1	B	10	VAL	4.0
1	B	395	ILE	4.0
1	D	326	ASP	3.9
1	D	15	LYS	3.9
1	D	254	PRO	3.8
1	D	323	VAL	3.8
1	A	58	LEU	3.8
1	D	176	VAL	3.8
1	B	287	ARG	3.8
1	A	395	ILE	3.8
1	A	64	ARG	3.7
1	B	37	VAL	3.7
1	A	296	LEU	3.7
1	B	328	ALA	3.7
1	C	19	GLY	3.7
1	A	235	ASP	3.6
1	D	235	ASP	3.6
1	C	246	ALA	3.6
1	D	395	ILE	3.6
1	D	210	SER	3.6
1	B	393	VAL	3.6
1	C	321	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	275	LYS	3.6
1	C	56	LEU	3.6
1	A	21	GLY	3.5
1	D	324	SER	3.5
1	B	55	LEU	3.5
1	D	12	GLU	3.5
1	C	54	THR	3.5
1	C	234	GLU	3.5
1	C	371	TRP	3.5
1	B	360	ALA	3.5
1	D	327	LYS	3.5
1	A	234	PRO	3.4
1	D	19	ALA	3.4
1	D	383	LEU	3.4
1	D	11	GLU	3.4
1	A	9	THR	3.4
1	A	56	THR	3.4
1	D	240	ARG	3.4
1	D	287	ARG	3.4
1	B	9	THR	3.4
1	D	54	HIS	3.3
1	C	18	SER	3.3
1	B	275	LYS	3.3
1	A	20	SER	3.3
1	C	214	VAL	3.3
1	B	85	GLU	3.3
1	D	188	ARG	3.3
1	B	116	ALA	3.2
1	D	274	LEU	3.2
1	B	11	GLU	3.2
1	A	15	LYS	3.2
1	D	234	PRO	3.2
1	B	274	LEU	3.2
1	C	42	ASP	3.2
1	D	233	ASP	3.2
1	B	188	ARG	3.2
1	D	301	TRP	3.1
1	D	26	LEU	3.1
1	A	54	HIS	3.1
1	C	62	ARG	3.1
1	D	255	ASP	3.1
1	B	15	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	360	ALA	3.1
1	A	12	GLU	3.1
1	A	301	TRP	3.1
1	B	168	GLN	3.1
1	C	52	HIS	3.1
1	A	11	GLU	3.1
1	A	274	LEU	3.0
1	D	373	TRP	3.0
1	C	10	GLU	3.0
1	C	358	ALA	3.0
1	B	240	ARG	3.0
1	C	243	LEU	3.0
1	D	325	LEU	3.0
1	A	45	TYR	3.0
1	C	200	VAL	3.0
1	B	373	TRP	3.0
1	A	61	LYS	3.0
1	C	393	ILE	3.0
1	C	269[A]	PHE	3.0
1	A	363	GLY	3.0
1	D	238	ALA	3.0
1	D	51	LYS	2.9
1	B	308	ALA	2.9
1	B	364	CYS	2.9
1	D	294	ALA	2.9
1	D	328	ALA	2.9
1	A	55	LEU	2.9
1	D	273	LEU	2.9
1	B	129	ARG	2.9
1	B	124	GLY	2.9
1	A	271[A]	PHE	2.9
1	C	83	GLU	2.9
1	B	323	VAL	2.9
1	D	216	VAL	2.9
1	B	283	LYS	2.9
1	B	352	LEU	2.9
1	B	49	VAL	2.8
1	C	92	ALA	2.8
1	D	82	PHE	2.8
1	A	57	ASP	2.8
1	C	65	ASP	2.8
1	B	394	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	336	ALA	2.8
1	D	291	ALA	2.8
1	C	285	ARG	2.8
1	D	14	ARG	2.8
1	D	319	VAL	2.8
1	B	84	ALA	2.8
1	C	45	PHE	2.8
1	C	46	ARG	2.8
1	B	273	LEU	2.8
1	D	352	LEU	2.8
1	B	299	SER	2.7
1	A	18	ARG	2.7
1	A	84	ALA	2.7
1	C	273	LYS	2.7
1	C	207	GLU	2.7
1	D	298	ILE	2.7
1	B	358	ARG	2.7
1	A	63	LYS	2.7
1	A	85	GLU	2.7
1	A	83	LEU	2.7
1	C	293	PRO	2.7
1	C	255	GLU	2.7
1	B	294	ALA	2.7
1	C	82	ALA	2.7
1	C	230	ALA	2.7
1	D	34	ALA	2.7
1	D	371	LEU	2.7
1	C	313	ILE	2.7
1	D	211	HIS	2.7
1	A	287	ARG	2.6
1	B	366	THR	2.6
1	C	59	LYS	2.6
1	A	325	LEU	2.6
1	D	49	VAL	2.6
1	B	125	GLN	2.6
1	C	40	TYR	2.6
1	B	293	PHE	2.6
1	B	269	LEU	2.6
1	D	289	LEU	2.6
1	B	331	ARG	2.6
1	D	358	ARG	2.6
1	A	294	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	202	VAL	2.6
1	A	207	PRO	2.6
1	D	123	TRP	2.6
1	B	18	ARG	2.6
1	B	325	LEU	2.6
1	D	18	ARG	2.6
1	B	12	GLU	2.6
1	B	312	GLY	2.6
1	B	291	ALA	2.6
1	B	365	ALA	2.6
1	C	47	VAL	2.6
1	A	243	PHE	2.5
1	C	91	MET	2.5
1	B	83	LEU	2.5
1	C	181	LEU	2.5
1	B	123	TRP	2.5
1	B	34	ALA	2.5
1	B	13	VAL	2.5
1	B	95	PRO	2.5
1	B	290	GLU	2.5
1	B	45	TYR	2.5
1	C	43	TYR	2.5
1	B	163	LEU	2.5
1	C	369	LEU	2.5
1	D	165	MET	2.5
1	A	313	PRO	2.5
1	B	22	PRO	2.5
1	B	276	ASP	2.5
1	C	233	ASP	2.5
1	C	360	ASP	2.5
1	D	121	LYS	2.5
1	D	382	GLY	2.5
1	C	209	HIS	2.5
1	D	28	ILE	2.5
1	A	209	GLU	2.5
1	D	361	GLU	2.5
1	A	41	ASP	2.5
1	D	297	GLY	2.4
1	B	243	PHE	2.4
1	D	183	LEU	2.4
1	D	315	ILE	2.4
1	B	30	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	241	PRO	2.4
1	B	277	VAL	2.4
1	D	393	VAL	2.4
1	D	20	SER	2.4
1	A	379	PHE	2.4
1	A	362	ASP	2.4
1	C	244	VAL	2.4
1	B	258	GLY	2.4
1	A	153	LEU	2.4
1	D	92	TYR	2.4
1	A	188	ARG	2.4
1	B	260	ILE	2.4
1	A	16	ALA	2.4
1	A	19	ALA	2.4
1	C	299	TRP	2.4
1	C	320	LYS	2.4
1	B	133	LEU	2.3
1	B	156	LEU	2.3
1	C	238	ARG	2.3
1	D	83	LEU	2.3
1	D	376	LEU	2.3
1	A	82	PHE	2.3
1	A	377	PHE	2.3
1	D	305	PHE	2.3
1	D	227	ALA	2.3
1	C	232	PRO	2.3
1	A	112	GLY	2.3
1	D	81	GLU	2.3
1	A	215	LEU	2.3
1	B	58	LEU	2.3
1	C	294	LEU	2.3
1	D	154	LEU	2.3
1	A	47	PHE	2.3
1	D	42	TYR	2.3
1	A	285	ILE	2.3
1	B	130	ILE	2.3
1	C	296	ILE	2.3
1	D	394	PRO	2.3
1	A	206	GLY	2.3
1	A	192	VAL	2.3
1	A	323	VAL	2.3
1	B	106	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	267	LEU	2.3
1	C	44	TYR	2.3
1	A	322	LYS	2.3
1	D	293	PHE	2.3
1	C	236	ALA	2.3
1	C	229	GLY	2.3
1	A	52	SER	2.3
1	A	324	SER	2.3
1	B	210	SER	2.3
1	C	15	GLN	2.3
1	D	125	GLN	2.3
1	B	375	VAL	2.3
1	B	24	THR	2.3
1	C	210	LEU	2.3
1	D	330	MET	2.3
1	A	373	TRP	2.2
1	A	297	GLY	2.2
1	B	21	GLY	2.2
1	C	277	GLY	2.2
1	C	319	ALA	2.2
1	D	23	ALA	2.2
1	D	209	GLU	2.2
1	D	288	ALA	2.2
1	B	208	SER	2.2
1	A	202	VAL	2.2
1	B	389	VAL	2.2
1	B	76	MET	2.2
1	A	87	PRO	2.2
1	B	19	ALA	2.2
1	C	39	ASP	2.2
1	B	42	TYR	2.2
1	B	211	HIS	2.2
1	C	49	LYS	2.2
1	C	186	ARG	2.2
1	B	202	VAL	2.2
1	C	102	VAL	2.2
1	B	239	GLU	2.2
1	C	78	GLU	2.2
1	D	78	LEU	2.2
1	C	204	GLY	2.2
1	C	206	SER	2.2
1	B	305	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	272	HIS	2.2
1	A	348	VAL	2.2
1	D	336	VAL	2.2
1	D	389	VAL	2.2
1	A	200	THR	2.2
1	A	53	ASP	2.2
1	A	139	SER	2.2
1	B	154	LEU	2.2
1	C	314	LEU	2.2
1	C	361	GLY	2.2
1	D	111	LEU	2.2
1	D	295	PRO	2.2
1	D	283	LYS	2.2
1	A	361	GLU	2.1
1	C	359	GLU	2.1
1	B	306	TRP	2.1
1	B	105	VAL	2.1
1	C	35	VAL	2.1
1	D	307	VAL	2.1
1	B	128	SER	2.1
1	B	126	PRO	2.1
1	D	220	LEU	2.1
1	C	13	LYS	2.1
1	A	365	ALA	2.1
1	B	249	ALA	2.1
1	D	27	ALA	2.1
1	D	219	ALA	2.1
1	B	17	GLN	2.1
1	C	291	PHE	2.1
1	B	281	ILE	2.1
1	D	362	ASP	2.1
1	C	208	SER	2.1
1	A	189	GLY	2.1
1	C	295	GLY	2.1
1	D	312	GLY	2.1
1	A	43	PRO	2.1
1	A	254	PRO	2.1
1	A	390	LEU	2.1
1	B	289	LEU	2.1
1	B	371	LEU	2.1
1	C	205	PRO	2.1
1	D	241	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	168	GLN	2.1
1	D	366	THR	2.1
1	D	124	GLY	2.1
1	B	216	VAL	2.1
1	C	106	VAL	2.1
1	A	163	LEU	2.1
1	A	242	LEU	2.1
1	C	388	LEU	2.1
1	A	40	ALA	2.1
1	A	321	ALA	2.1
1	C	21	ALA	2.1
1	D	40	ALA	2.1
1	D	91	ALA	2.1
1	A	157	ARG	2.1
1	D	130	ILE	2.0
1	D	243	PHE	2.0
1	A	247	SER	2.0
1	B	20	SER	2.0
1	B	307	VAL	2.0
1	C	226	VAL	2.0
1	D	296	LEU	2.0
1	A	201	ALA	2.0
1	B	23	ALA	2.0
1	A	67	ASP	2.0
1	A	240	ARG	2.0
1	B	48	ARG	2.0
1	D	84	ALA	2.0
1	A	257	GLU	2.0
1	A	286	GLU	2.0
1	C	119	LYS	2.0
1	B	204	PHE	2.0
1	D	304	ILE	2.0
1	B	117	GLN	2.0
1	B	254	PRO	2.0
1	A	141	VAL	2.0
1	D	37	VAL	2.0

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

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
1	CSD	D	170	8/9	0.83	0.16	9,10,23,23	0
1	CSD	B	170	8/9	0.87	0.15	8,9,20,23	0
1	CSD	A	170	8/9	0.87	0.14	6,10,18,19	0
1	CSD	C	168	8/9	0.88	0.16	6,7,21,22	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

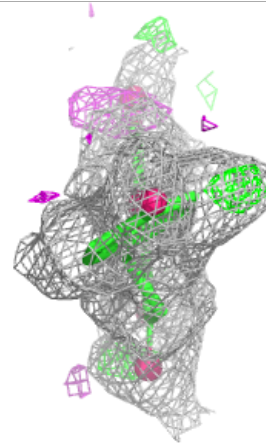
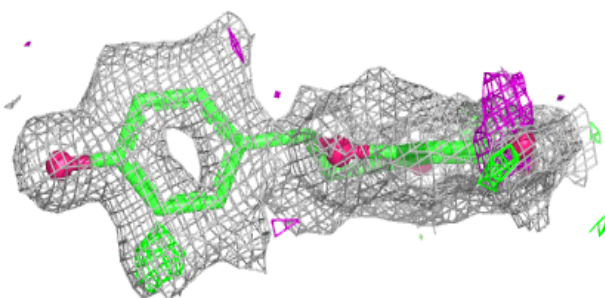
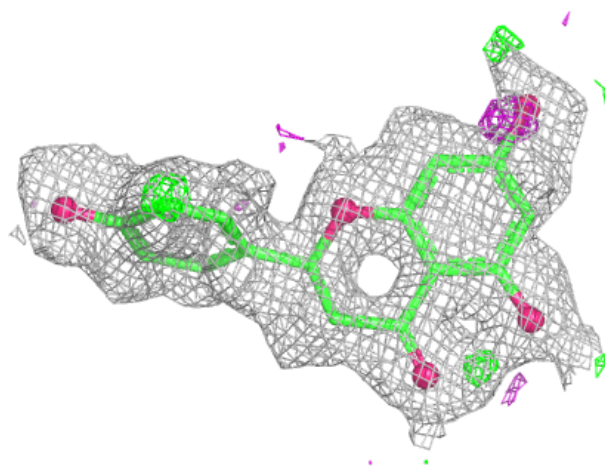
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	COA	C	501[B]	48/48	0.72	0.20	13,29,53,64	0
2	COA	A	501[A]	48/48	0.75	0.19	10,29,50,57	1
3	NAR	A	503	20/20	0.75	0.14	7,9,12,14	0
3	NAR	A	502	20/20	0.79	0.13	6,9,11,12	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.

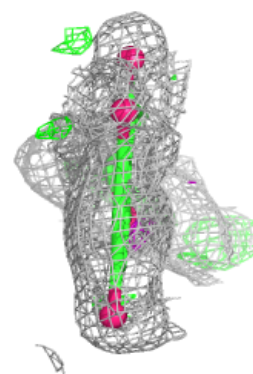
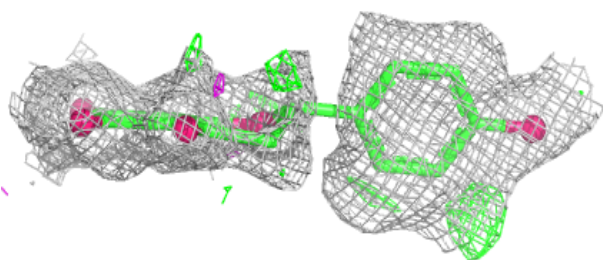
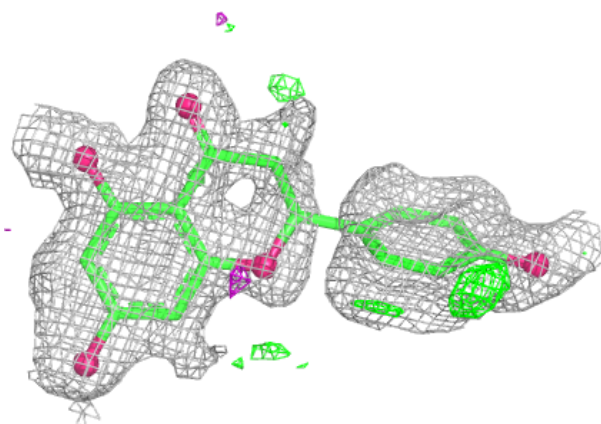
Electron density around NAR A 503:

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



Electron density around NAR A 502:

$2mF_o - DF_c$ (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.