



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:31 PM UTC

PDB ID : 1OYN / pdb_00001oyn
Title : Crystal structure of PDE4D2 in complex with (R,S)-rolipram
Authors : Huai, Q.; Wang, H.; Sun, Y.; Kim, H.Y.; Liu, Y.; Ke, H.
Deposited on : 2003-04-05
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

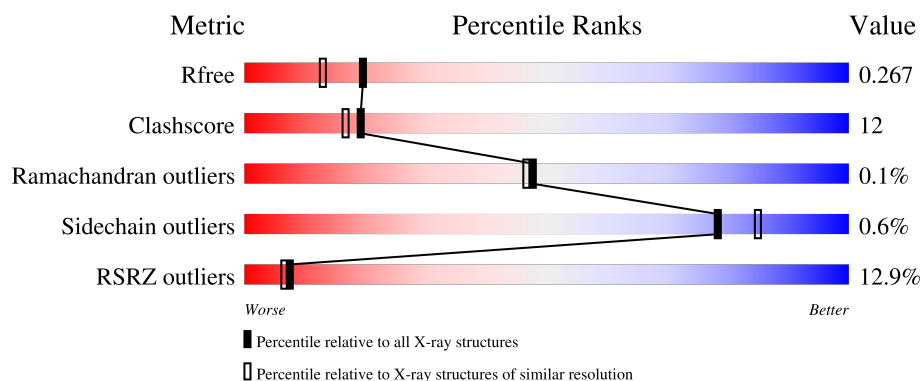
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	360	9% 71% 21% • 7%
1	B	360	18% 61% 29% • 9%
1	C	360	12% 65% 25% • 9%
1	D	360	9% 73% 19% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ROL	A	503[A]	X	-	-	-
3	ROL	B	505[A]	X	-	-	-
3	ROL	C	507[A]	X	-	-	-
3	ROL	D	509[A]	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11043 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.

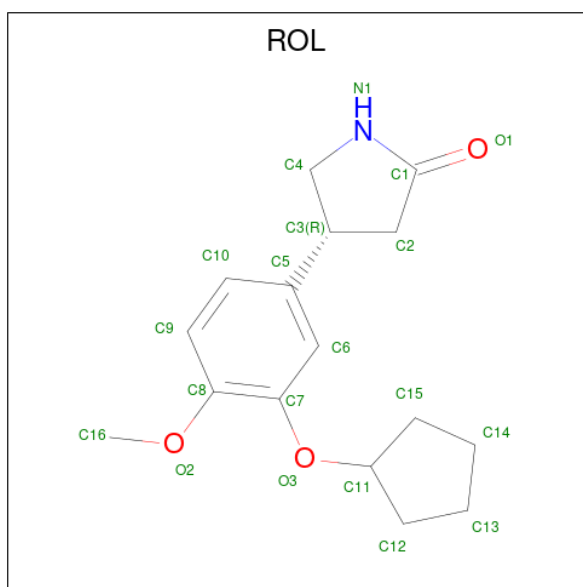
- Molecule 1 is a protein called cAMP-specific phosphodiesterase PDE4D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			
1	B	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	C	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	D	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is ROLIPRAM (CCD ID: ROL) (formula: C₁₆H₂₁NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			40	32	2	6		
3	B	1	Total	C	N	O	0	1
			40	32	2	6		
3	C	1	Total	C	N	O	0	1
			40	32	2	6		
3	D	1	Total	C	N	O	0	1
			40	32	2	6		

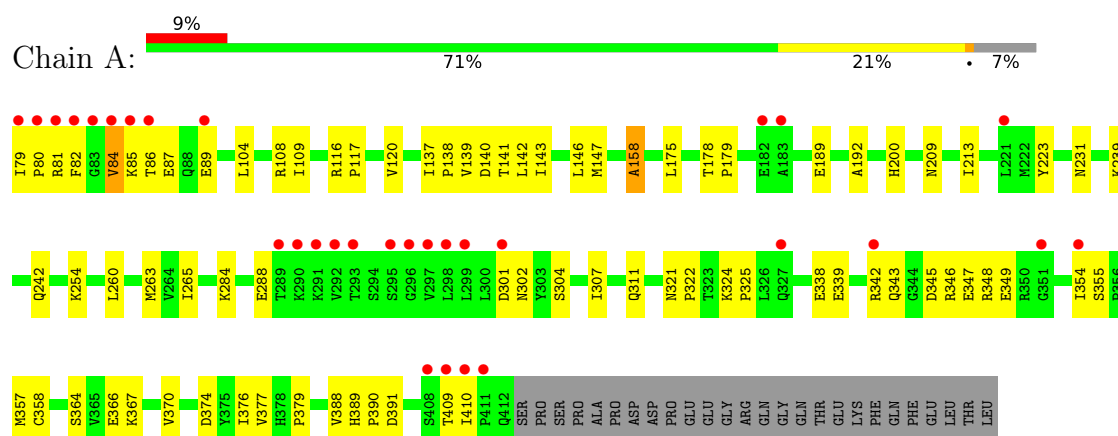
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	30	Total	O	0	0
			30	30		
4	C	33	Total	O	0	0
			33	33		
4	D	49	Total	O	0	0
			49	49		

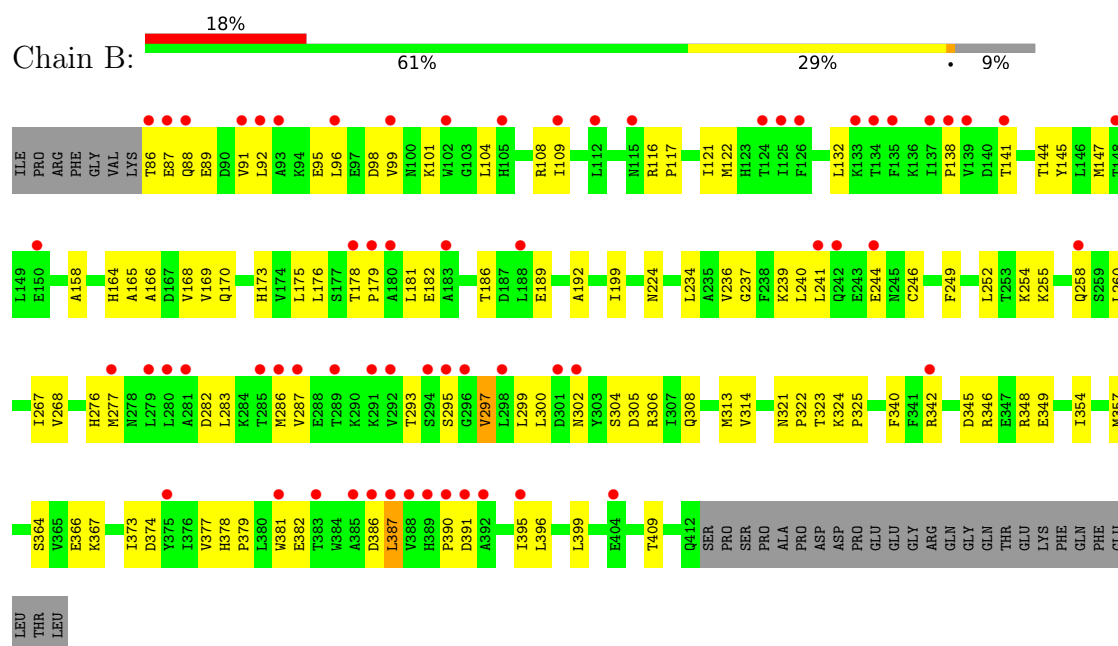
3 Residue-property plots

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: cAMP-specific phosphodiesterase PDE4D2

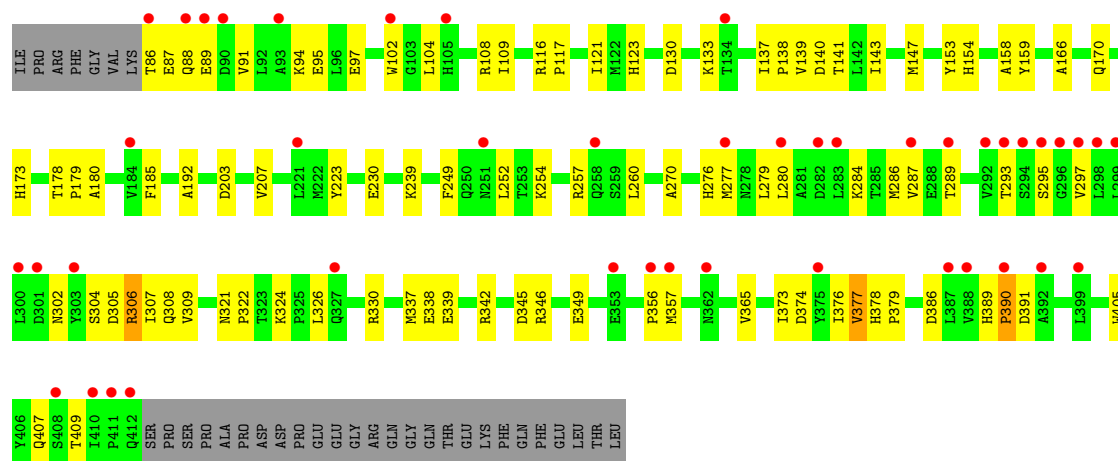


• Molecule 1: cAMP-specific phosphodiesterase PDE4D2

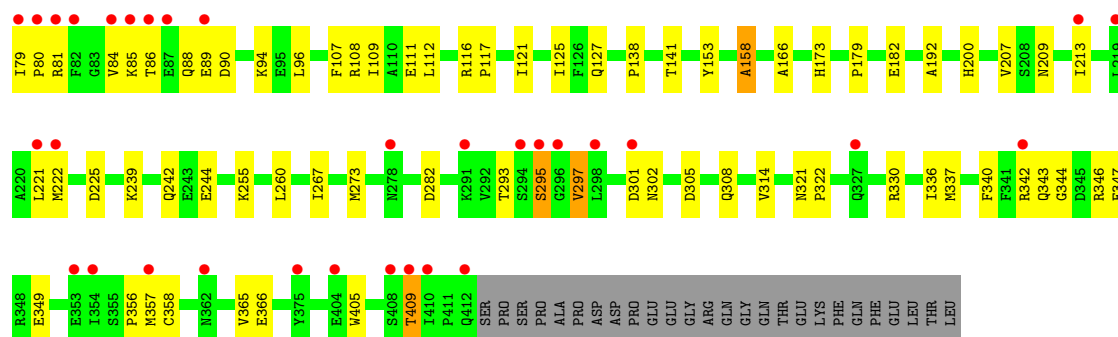


• Molecule 1: cAMP-specific phosphodiesterase PDE4D2





• Molecule 1: cAMP-specific phosphodiesterase PDE4D2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.78Å 111.53Å 160.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.00 91.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	74.2 (99.00-2.00) 74.7 (91.50-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.266 0.234 , 0.267	Depositor DCC
R_{free} test set	9500 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11043	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: ZN, ROL

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	0.43	0/2760	0.87	6/3749 (0.2%)
1	B	0.37	0/2701	0.86	2/3670 (0.1%)
1	C	0.39	0/2701	0.84	6/3670 (0.2%)
1	D	0.43	0/2760	0.91	8/3749 (0.2%)
All	All	0.41	0/10922	0.87	22/14838 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	88	GLN	N-CA-C	-8.53	103.38	112.93
1	D	295	SER	N-CA-C	-7.58	100.75	110.53
1	D	153	TYR	N-CA-C	-7.39	98.58	110.32
1	D	158	ALA	N-CA-C	6.80	118.69	111.28
1	A	158	ALA	N-CA-C	6.04	117.87	111.28
1	A	137	ILE	CA-C-N	-5.97	113.79	119.76
1	A	137	ILE	C-N-CA	-5.97	113.79	119.76
1	A	377	VAL	N-CA-C	5.95	116.14	110.42
1	B	387	LEU	N-CA-C	-5.86	107.94	114.62
1	D	297	VAL	N-CA-C	5.86	117.80	108.89
1	C	374	ASP	N-CA-C	5.84	117.65	111.28
1	C	153	TYR	N-CA-C	-5.78	100.25	109.96
1	A	200	HIS	N-CA-C	5.73	119.79	112.34
1	D	200	HIS	N-CA-C	5.70	119.75	112.34
1	D	81	ARG	N-CA-C	5.64	117.88	111.11
1	D	301	ASP	N-CA-C	5.58	119.93	113.18
1	C	377	VAL	N-CA-C	5.48	115.62	110.30
1	A	85	LYS	N-CA-C	5.10	117.28	110.35
1	C	158	ALA	N-CA-C	5.08	116.51	111.07
1	B	374	ASP	N-CA-C	5.06	116.48	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	THR	CA-C-N	5.05	124.49	119.24
1	C	178	THR	C-N-CA	5.05	124.49	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2704	0	2664	60	0
1	B	2647	0	2599	82	0
1	C	2647	0	2599	63	0
1	D	2704	0	2664	54	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	40	0	42	3	0
3	B	40	0	42	4	0
3	C	40	0	42	3	0
3	D	40	0	42	5	0
4	A	61	0	0	0	0
4	B	30	0	0	0	0
4	C	33	0	0	1	0
4	D	49	0	0	1	0
All	All	11043	0	10694	253	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 12.

All (253) 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:254:LYS:O	1:B:258:GLN:HG3	1.80	0.81
1:A:143:ILE:HG22	1:A:147:MET:HE2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ASP:HB3	1:B:308:GLN:NE2	2.01	0.75
1:B:366:GLU:HG2	1:B:409:THR:HG22	1.70	0.73
1:C:88:GLN:NE2	1:C:89:GLU:HB2	2.02	0.73
1:B:255:LYS:HD2	1:B:255:LYS:N	2.01	0.73
1:C:337:MET:HE2	1:C:365:VAL:HG22	1.71	0.72
1:B:132:LEU:H	1:B:132:LEU:HD12	1.54	0.71
1:D:179:PRO:O	1:D:182:GLU:HG2	1.90	0.71
1:D:207:VAL:HG11	1:D:346:ARG:HH21	1.55	0.71
1:D:79:ILE:N	1:D:80:PRO:HD2	2.05	0.70
1:C:293:THR:HG23	1:C:295:SER:H	1.55	0.70
1:B:182:GLU:O	1:B:297:VAL:HG11	1.91	0.70
1:A:86:THR:HG22	1:A:87:GLU:N	2.07	0.69
1:B:293:THR:HG22	1:B:299:LEU:HD13	1.74	0.69
1:C:321:ASN:HB2	1:C:322:PRO:HD3	1.75	0.69
1:B:121:ILE:HD12	1:B:166:ALA:HB1	1.73	0.68
1:B:295:SER:HB2	1:B:297:VAL:HG23	1.74	0.68
1:C:357:MET:SD	3:C:507[A]:ROL:H131	2.34	0.68
1:D:79:ILE:N	1:D:80:PRO:CD	2.57	0.68
1:C:287:VAL:HG11	1:C:386:ASP:HB3	1.76	0.67
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.30	0.67
1:C:357:MET:SD	3:C:507[B]:ROL:H131	2.34	0.67
1:D:337:MET:HE2	1:D:365:VAL:HG22	1.77	0.67
1:D:207:VAL:CG1	1:D:346:ARG:HH21	2.08	0.67
1:A:79:ILE:N	1:A:80:PRO:HD2	2.10	0.67
1:A:254:LYS:HE2	1:D:244:GLU:CD	2.21	0.66
1:A:242:GLN:OE1	1:D:242:GLN:OE1	2.14	0.66
1:D:366:GLU:HG2	1:D:409:THR:HB	1.77	0.66
1:D:158:ALA:HB2	1:D:342:ARG:HH22	1.61	0.65
1:C:254:LYS:HG3	1:C:257:ARG:NH2	2.10	0.65
1:A:80:PRO:HA	1:A:89:GLU:OE2	1.97	0.65
1:A:307:ILE:O	1:A:311:GLN:HG3	1.97	0.65
1:A:357:MET:SD	3:A:503[B]:ROL:H131	2.38	0.64
1:D:321:ASN:HB2	1:D:322:PRO:HD3	1.79	0.63
1:B:236:VAL:O	1:B:240:LEU:HG	2.00	0.62
1:C:192:ALA:HB2	1:C:260:LEU:HD12	1.81	0.62
1:A:81:ARG:O	1:A:82:PHE:HB2	1.99	0.62
1:A:366:GLU:O	1:A:370:VAL:HG23	1.99	0.61
1:A:86:THR:HG22	1:A:87:GLU:H	1.66	0.61
1:D:127:GLN:HE21	1:D:127:GLN:HA	1.66	0.61
1:A:179:PRO:HD2	1:A:391:ASP:OD2	2.00	0.60
1:B:87:GLU:HG3	1:B:88:GLN:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:SD	3:A:503[A]:ROL:H131	2.42	0.60
1:B:302:ASN:OD1	1:B:304:SER:HB3	2.02	0.59
1:A:239:LYS:NZ	1:D:239:LYS:NZ	2.51	0.59
1:B:192:ALA:HB2	1:B:260:LEU:HD12	1.85	0.59
1:B:132:LEU:HD12	1:B:132:LEU:N	2.18	0.58
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.84	0.58
1:B:108:ARG:HG2	1:B:108:ARG:HH11	1.66	0.58
1:A:345:ASP:O	1:A:349:GLU:HG3	2.04	0.58
1:B:138:PRO:HG2	1:B:141:THR:HB	1.86	0.58
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.67	0.58
1:D:282:ASP:HB3	1:D:308:GLN:NE2	2.19	0.57
1:A:239:LYS:NZ	1:D:239:LYS:HZ3	2.01	0.57
1:D:108:ARG:HG2	1:D:108:ARG:HH11	1.68	0.57
1:A:158:ALA:H	1:A:342:ARG:HH12	1.52	0.57
1:B:249:PHE:HA	1:B:252:LEU:HD13	1.87	0.57
1:D:79:ILE:N	1:D:79:ILE:HD12	2.19	0.57
1:C:302:ASN:OD1	1:C:304:SER:HB3	2.04	0.57
1:C:326:LEU:HD21	1:C:405:TRP:CE2	2.40	0.57
1:B:170:GLN:O	1:B:173:HIS:HB3	2.05	0.57
1:C:94:LYS:O	1:C:97:GLU:HB2	2.04	0.56
1:B:321:ASN:HB2	1:B:322:PRO:HD3	1.87	0.56
1:B:179:PRO:HD2	1:B:391:ASP:CG	2.30	0.56
1:B:255:LYS:HD2	1:B:255:LYS:H	1.67	0.56
1:B:96:LEU:O	1:B:99:VAL:HG23	2.06	0.56
1:D:207:VAL:HG11	1:D:346:ARG:NH2	2.20	0.56
1:C:345:ASP:O	1:C:349:GLU:HG3	2.07	0.55
1:A:284:LYS:O	1:A:288:GLU:HG3	2.07	0.54
1:A:388:VAL:O	1:A:391:ASP:HB2	2.07	0.54
1:C:179:PRO:HD2	1:C:391:ASP:OD2	2.06	0.54
1:C:376:ILE:C	1:C:379:PRO:HD2	2.32	0.54
1:C:87:GLU:O	1:C:91:VAL:HG23	2.07	0.54
1:B:378:HIS:HB3	1:B:379:PRO:HD3	1.88	0.54
1:B:244:GLU:HG3	1:C:254:LYS:NZ	2.21	0.54
1:B:287:VAL:HG22	1:B:387:LEU:HD13	1.89	0.54
1:B:175:LEU:O	1:B:178:THR:HG22	2.08	0.54
1:A:343:GLN:O	1:A:347:GLU:HG3	2.08	0.54
1:B:234:LEU:HD21	1:B:268:VAL:HB	1.90	0.54
1:A:79:ILE:N	1:A:80:PRO:CD	2.70	0.54
1:A:138:PRO:HG2	1:A:141:THR:OG1	2.08	0.54
1:C:276:HIS:HD2	1:C:277:MET:HE2	1.73	0.54
1:B:286:MET:HE2	1:B:305:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:PHE:O	1:D:111:GLU:HG3	2.08	0.53
1:B:98:ASP:OD1	1:B:101:LYS:HD2	2.08	0.53
1:C:154:HIS:HE1	1:C:203:ASP:OD1	1.91	0.53
1:B:178:THR:CG2	1:B:181:LEU:HD12	2.39	0.53
1:C:249:PHE:HA	1:C:252:LEU:HD13	1.90	0.52
1:D:213:ILE:HG23	1:D:225:ASP:OD1	2.10	0.52
1:C:286:MET:HE2	1:C:305:ASP:OD1	2.10	0.52
1:C:223:TYR:HE1	1:D:222:MET:O	1.92	0.52
1:C:373:ILE:HA	1:C:377:VAL:HB	1.91	0.52
1:A:348:ARG:HH11	1:A:354:ILE:CD1	2.22	0.52
1:D:221:LEU:HD12	1:D:221:LEU:O	2.09	0.52
1:C:121:ILE:HD12	1:C:166:ALA:HB1	1.92	0.52
1:B:122:MET:SD	1:B:169:VAL:HG11	2.50	0.51
1:B:186:THR:OG1	1:B:189:GLU:HG3	2.09	0.51
1:A:370:VAL:HG21	1:A:410:ILE:HD11	1.92	0.51
1:C:254:LYS:HG3	1:C:257:ARG:HH21	1.74	0.51
1:D:84:VAL:HG12	1:D:85:LYS:N	2.25	0.51
1:D:90:ASP:O	1:D:94:LYS:HG3	2.10	0.51
1:B:286:MET:HE1	1:B:308:GLN:HB3	1.92	0.51
1:C:180:ALA:O	1:C:297:VAL:HG13	2.10	0.51
1:D:127:GLN:HA	1:D:127:GLN:NE2	2.26	0.51
1:A:81:ARG:O	1:A:81:ARG:HG3	2.10	0.51
1:D:302:ASN:ND2	1:D:305:ASP:OD2	2.41	0.51
1:C:280:LEU:O	1:C:284:LYS:HG3	2.11	0.50
1:C:302:ASN:H	1:C:302:ASN:ND2	2.10	0.50
1:A:86:THR:CG2	1:A:87:GLU:N	2.75	0.50
1:C:130:ASP:OD2	1:C:133:LYS:HD3	2.11	0.50
1:D:209:ASN:O	1:D:213:ILE:HG13	2.12	0.50
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.94	0.50
1:B:86:THR:HA	1:B:89:GLU:CB	2.41	0.50
1:B:91:VAL:O	1:B:95:GLU:HG2	2.11	0.50
1:C:102:TRP:NE1	1:C:324:LYS:HD3	2.27	0.50
1:D:343:GLN:O	1:D:347:GLU:HG3	2.11	0.50
1:C:185:PHE:HD1	1:C:306:ARG:HH12	1.57	0.50
1:B:108:ARG:HG2	1:B:108:ARG:NH1	2.27	0.49
1:C:302:ASN:H	1:C:302:ASN:HD22	1.60	0.49
1:B:179:PRO:C	1:B:181:LEU:H	2.20	0.49
1:D:84:VAL:HG12	1:D:85:LYS:H	1.77	0.49
1:B:158:ALA:H	1:B:342:ARG:NH2	2.10	0.49
1:B:366:GLU:HG2	1:B:409:THR:CG2	2.41	0.49
1:C:143:ILE:O	1:C:147:MET:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:GLU:O	1:B:386:ASP:HB2	2.12	0.49
1:C:289:THR:O	1:C:289:THR:HG22	2.13	0.49
1:A:116:ARG:O	1:A:120:VAL:HG22	2.13	0.48
1:B:409:THR:HG22	1:B:409:THR:O	2.12	0.48
1:A:209:ASN:O	1:A:213:ILE:HG13	2.13	0.48
1:D:125:ILE:HD13	1:D:173:HIS:HB2	1.94	0.48
1:C:123:HIS:HE1	1:C:139:VAL:HG23	1.79	0.48
1:C:207:VAL:CG1	1:C:346:ARG:NH2	2.77	0.48
1:C:139:VAL:HG13	1:C:140:ASP:N	2.28	0.48
1:B:276:HIS:HD2	1:B:277:MET:HE2	1.77	0.48
1:C:104:LEU:HD11	1:C:109:ILE:HD11	1.95	0.48
1:D:273:MET:HG3	3:D:509[B]:ROL:O1	2.13	0.47
1:A:324:LYS:O	1:A:325:PRO:C	2.56	0.47
1:B:86:THR:HA	1:B:89:GLU:HB3	1.96	0.47
1:D:182:GLU:HG3	1:D:297:VAL:HG11	1.96	0.47
1:B:138:PRO:HG2	1:B:141:THR:CB	2.43	0.47
1:B:164:HIS:O	1:B:168:VAL:HG23	2.14	0.47
1:C:88:GLN:HE22	1:C:89:GLU:HB2	1.78	0.47
1:C:407:GLN:C	1:C:409:THR:H	2.23	0.47
1:D:330:ARG:HD3	1:D:405:TRP:CH2	2.49	0.47
1:D:344:GLY:HA3	1:D:358:CYS:O	2.14	0.47
1:B:323:THR:HB	1:B:395:ILE:HG23	1.96	0.47
3:D:509[A]:ROL:H61	3:D:509[A]:ROL:H111	1.71	0.47
1:A:376:ILE:C	1:A:379:PRO:HD2	2.40	0.47
1:D:340:PHE:CE2	3:D:509[A]:ROL:H151	2.50	0.47
1:B:345:ASP:OD1	1:B:348:ARG:NH2	2.48	0.47
1:D:79:ILE:O	1:D:79:ILE:HG22	2.14	0.47
1:B:283:LEU:O	1:B:287:VAL:HG23	2.15	0.47
1:B:357:MET:SD	3:B:505[B]:ROL:H131	2.55	0.47
1:D:138:PRO:HG2	1:D:141:THR:OG1	2.15	0.47
1:A:139:VAL:HG13	1:A:140:ASP:N	2.30	0.47
1:B:132:LEU:H	1:B:132:LEU:CD1	2.24	0.47
1:C:104:LEU:HD22	1:C:170:GLN:HG3	1.96	0.47
1:B:340:PHE:CE2	3:B:505[A]:ROL:H151	2.50	0.46
1:D:337:MET:CE	1:D:365:VAL:HG22	2.45	0.46
1:B:104:LEU:HD21	1:B:109:ILE:CD1	2.44	0.46
1:B:396:LEU:O	1:B:396:LEU:HD23	2.15	0.46
1:D:192:ALA:HB2	1:D:260:LEU:HD12	1.96	0.46
1:C:295:SER:C	1:C:297:VAL:H	2.24	0.46
1:B:282:ASP:HB3	1:B:308:GLN:HE22	1.75	0.46
1:B:345:ASP:O	1:B:349:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ARG:N	1:B:117:PRO:CD	2.79	0.46
1:A:355:SER:O	1:A:358:CYS:HB2	2.16	0.46
1:A:82:PHE:C	1:A:84:VAL:H	2.24	0.46
1:B:92:LEU:C	1:B:92:LEU:HD23	2.41	0.46
1:A:158:ALA:H	1:A:342:ARG:NH1	2.14	0.46
1:A:175:LEU:O	1:A:178:THR:HG22	2.16	0.45
1:A:348:ARG:NH1	1:A:354:ILE:HD13	2.31	0.45
1:C:305:ASP:O	1:C:309:VAL:HG23	2.16	0.45
1:B:366:GLU:H	1:B:366:GLU:CD	2.24	0.45
1:D:293:THR:O	1:D:295:SER:O	2.34	0.45
1:B:283:LEU:HD11	1:B:387:LEU:HD22	1.99	0.45
1:A:189:GLU:HG2	1:A:263:MET:SD	2.57	0.45
1:A:254:LYS:HE2	1:D:244:GLU:OE1	2.16	0.45
1:C:307:ILE:HG23	1:C:308:GLN:N	2.32	0.45
1:C:138:PRO:HG2	1:C:141:THR:HB	1.99	0.44
3:C:507[B]:ROL:H21	3:C:507[B]:ROL:H61	1.64	0.44
1:A:82:PHE:O	1:A:84:VAL:HG23	2.17	0.44
1:B:199:ILE:HD12	1:B:237:GLY:HA3	2.00	0.44
1:B:302:ASN:O	1:B:306:ARG:HG3	2.18	0.44
1:C:116:ARG:N	1:C:117:PRO:CD	2.80	0.44
1:D:127:GLN:HE21	1:D:127:GLN:CA	2.28	0.44
1:D:116:ARG:N	1:D:117:PRO:CD	2.80	0.44
1:A:366:GLU:HG2	1:A:409:THR:HG22	2.00	0.44
1:C:95:GLU:OE2	1:C:108:ARG:HD2	2.18	0.44
1:A:364:SER:HB3	1:A:367:LYS:HD2	2.00	0.44
1:A:242:GLN:OE1	1:D:242:GLN:CD	2.60	0.43
1:D:96:LEU:HD23	1:D:109:ILE:HD13	1.98	0.43
1:D:267:ILE:HG21	1:D:314:VAL:HG21	2.00	0.43
1:A:339:GLU:HA	1:A:342:ARG:HD2	2.00	0.43
1:B:239:LYS:NZ	1:C:239:LYS:NZ	2.66	0.43
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.99	0.43
1:C:293:THR:C	1:C:295:SER:H	2.27	0.43
1:A:86:THR:CG2	1:A:87:GLU:H	2.29	0.43
1:A:338:GLU:OE2	1:A:342:ARG:NH2	2.52	0.43
1:B:346:ARG:HD2	4:D:517:HOH:O	2.18	0.43
1:B:178:THR:HG22	1:B:181:LEU:HD12	2.00	0.43
1:C:137:ILE:O	1:C:138:PRO:C	2.60	0.43
1:D:108:ARG:O	1:D:112:LEU:HG	2.18	0.43
1:A:370:VAL:HG12	1:A:374:ASP:OD2	2.20	0.42
1:D:86:THR:O	1:D:89:GLU:HB2	2.19	0.42
1:C:154:HIS:HD2	4:C:529:HOH:O	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:PRO:O	1:C:357:MET:HB2	2.18	0.42
1:D:336:ILE:HG21	3:D:509[B]:ROL:H162	2.01	0.42
1:C:170:GLN:O	1:C:173:HIS:HB3	2.19	0.42
1:C:293:THR:HG22	1:C:297:VAL:O	2.20	0.42
1:D:121:ILE:HD12	1:D:166:ALA:HB1	2.01	0.42
1:D:356:PRO:O	1:D:357:MET:HB2	2.19	0.42
1:B:324:LYS:O	1:B:325:PRO:C	2.63	0.42
1:B:144:THR:HG22	1:B:246:CYS:SG	2.60	0.42
1:C:86:THR:OG1	1:C:88:GLN:HG3	2.19	0.42
1:B:249:PHE:CZ	1:B:260:LEU:HD21	2.55	0.42
1:A:223:TYR:CE1	1:A:231:ASN:HB3	2.54	0.41
1:C:326:LEU:HD21	1:C:405:TRP:CD2	2.55	0.41
1:B:147:MET:HE1	1:D:349:GLU:HB3	2.01	0.41
1:C:338:GLU:OE2	1:C:342:ARG:CZ	2.68	0.41
1:D:357:MET:SD	3:D:509[B]:ROL:H141	2.60	0.41
1:B:178:THR:O	1:B:178:THR:HG23	2.20	0.41
1:B:249:PHE:CA	1:B:252:LEU:HD13	2.48	0.41
1:B:364:SER:HB3	1:B:367:LYS:HB3	2.02	0.41
1:A:142:LEU:O	1:A:146:LEU:HG	2.21	0.41
1:A:108:ARG:HG2	1:A:108:ARG:NH1	2.32	0.41
1:A:389:HIS:CE1	1:A:390:PRO:HB3	2.56	0.41
1:B:145:TYR:CD1	1:B:241:LEU:HD23	2.55	0.41
1:B:176:LEU:HD23	1:B:313:MET:HE1	2.03	0.41
1:B:322:PRO:HB2	1:B:399:LEU:CD1	2.51	0.41
1:B:381:TRP:CZ3	1:B:395:ILE:HG21	2.55	0.41
3:B:505[A]:ROL:H41	3:B:505[A]:ROL:H61	1.79	0.41
1:A:302:ASN:OD1	1:A:304:SER:HB3	2.20	0.41
3:A:503[B]:ROL:H61	3:A:503[B]:ROL:H21	1.72	0.41
1:B:300:LEU:HB3	1:B:306:ARG:HG2	2.03	0.41
3:B:505[B]:ROL:H61	3:B:505[B]:ROL:H111	1.69	0.41
1:C:378:HIS:N	1:C:379:PRO:CD	2.83	0.41
1:A:192:ALA:HB2	1:A:260:LEU:HD12	2.02	0.41
1:A:265:ILE:HD13	1:B:224:ASN:O	2.21	0.41
1:C:389:HIS:CE1	1:C:390:PRO:HB3	2.56	0.41
1:A:116:ARG:N	1:A:117:PRO:CD	2.83	0.41
1:C:159:TYR:HB3	1:C:339:GLU:OE1	2.21	0.41
1:C:230:GLU:CD	1:C:230:GLU:H	2.29	0.41
1:D:108:ARG:HG2	1:D:108:ARG:NH1	2.34	0.41
1:A:346:ARG:HA	1:A:349:GLU:OE1	2.21	0.41
1:B:267:ILE:HG21	1:B:314:VAL:HG21	2.02	0.41
1:A:348:ARG:HH11	1:A:354:ILE:HD11	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:HA	1:B:89:GLU:HB2	2.03	0.40
1:B:348:ARG:HH11	1:B:354:ILE:CD1	2.35	0.40
1:B:373:ILE:HA	1:B:377:VAL:HB	2.02	0.40
1:A:178:THR:OG1	1:A:391:ASP:OD2	2.39	0.40
1:B:165:ALA:O	1:B:169:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/360 (92%)	313 (94%)	18 (5%)	1 (0%)	36	35
1	B	325/360 (90%)	303 (93%)	22 (7%)	0	100	100
1	C	325/360 (90%)	308 (95%)	17 (5%)	0	100	100
1	D	332/360 (92%)	316 (95%)	16 (5%)	0	100	100
All	All	1314/1440 (91%)	1240 (94%)	73 (6%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	ASP

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	305/328 (93%)	304 (100%)	1 (0%)	86	91
1	B	299/328 (91%)	297 (99%)	2 (1%)	76	82
1	C	299/328 (91%)	297 (99%)	2 (1%)	76	82
1	D	305/328 (93%)	303 (99%)	2 (1%)	76	82
All	All	1208/1312 (92%)	1201 (99%)	7 (1%)	78	85

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	VAL
1	B	297	VAL
1	B	390	PRO
1	C	306	ARG
1	C	390	PRO
1	D	255	LYS
1	D	409	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	245	ASN
1	A	250	GLN
1	A	258	GLN
1	A	308	GLN
1	A	362	ASN
1	B	127	GLN
1	B	210	GLN
1	B	245	ASN
1	B	250	GLN
1	B	308	GLN
1	B	407	GLN
1	C	88	GLN
1	C	154	HIS
1	C	210	GLN
1	C	245	ASN
1	C	362	ASN
1	C	407	GLN
1	D	123	HIS
1	D	127	GLN

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Mol	Chain	Res	Type
1	D	210	GLN
1	D	245	ASN
1	D	258	GLN
1	D	308	GLN
1	D	312	ASN
1	D	389	HIS
1	D	407	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	ROL	A	503[A]	-	22,22,22	0.58	0	30,30,30	1.71	8 (26%)
3	ROL	B	505[B]	-	22,22,22	0.54	0	30,30,30	1.57	6 (20%)
3	ROL	D	509[A]	-	22,22,22	0.55	0	30,30,30	1.59	6 (20%)
3	ROL	C	507[B]	-	22,22,22	0.52	0	30,30,30	1.80	7 (23%)
3	ROL	A	503[B]	-	22,22,22	0.54	0	30,30,30	1.82	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ROL	D	509[B]	-	22,22,22	0.56	0	30,30,30	1.62	6 (20%)
3	ROL	B	505[A]	-	22,22,22	0.60	0	30,30,30	1.49	5 (16%)
3	ROL	C	507[A]	-	22,22,22	0.55	0	30,30,30	1.69	8 (26%)

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	ROL	A	503[A]	-	1/1/3/4	5/10/26/26	0/3/3/3
3	ROL	B	505[B]	-	-	4/10/26/26	0/3/3/3
3	ROL	D	509[A]	-	1/1/3/4	4/10/26/26	0/3/3/3
3	ROL	C	507[B]	-	-	5/10/26/26	0/3/3/3
3	ROL	A	503[B]	-	-	4/10/26/26	0/3/3/3
3	ROL	D	509[B]	-	-	4/10/26/26	0/3/3/3
3	ROL	B	505[A]	-	1/1/3/4	4/10/26/26	0/3/3/3
3	ROL	C	507[A]	-	1/1/3/4	7/10/26/26	0/3/3/3

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	507[B]	ROL	C16-O2-C8	-5.19	109.89	117.51
3	A	503[B]	ROL	C16-O2-C8	-5.19	109.90	117.51
3	A	503[A]	ROL	C16-O2-C8	-4.32	111.18	117.51
3	C	507[A]	ROL	C16-O2-C8	-4.13	111.46	117.51
3	D	509[B]	ROL	C16-O2-C8	-4.06	111.56	117.51
3	D	509[A]	ROL	C16-O2-C8	-3.78	111.97	117.51
3	C	507[A]	ROL	C3-C2-C1	3.62	109.69	104.96
3	B	505[A]	ROL	C3-C2-C1	3.62	109.68	104.96
3	A	503[B]	ROL	C3-C2-C1	3.61	109.67	104.96
3	D	509[A]	ROL	C3-C2-C1	3.60	109.66	104.96
3	A	503[A]	ROL	C3-C2-C1	3.59	109.65	104.96
3	B	505[B]	ROL	C3-C2-C1	3.59	109.65	104.96
3	B	505[B]	ROL	C16-O2-C8	-3.57	112.28	117.51
3	C	507[B]	ROL	C3-C2-C1	3.55	109.60	104.96
3	D	509[B]	ROL	C3-C2-C1	3.55	109.59	104.96
3	D	509[A]	ROL	C4-N1-C1	3.30	117.33	114.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	505[B]	ROL	C4-N1-C1	3.26	117.29	114.13
3	A	503[B]	ROL	C4-N1-C1	3.26	117.29	114.13
3	C	507[B]	ROL	C4-N1-C1	3.25	117.28	114.13
3	B	505[A]	ROL	C4-N1-C1	3.24	117.28	114.13
3	D	509[B]	ROL	C4-N1-C1	3.24	117.28	114.13
3	C	507[A]	ROL	C4-N1-C1	3.23	117.26	114.13
3	B	505[A]	ROL	C16-O2-C8	-3.19	112.83	117.51
3	C	507[B]	ROL	O2-C8-C7	3.18	119.72	115.40
3	A	503[B]	ROL	O2-C8-C7	3.18	119.71	115.40
3	A	503[A]	ROL	C4-N1-C1	3.18	117.21	114.13
3	A	503[A]	ROL	O2-C8-C7	2.89	119.33	115.40
3	C	507[A]	ROL	O2-C8-C7	2.83	119.25	115.40
3	A	503[A]	ROL	C2-C3-C5	-2.75	109.63	115.29
3	B	505[B]	ROL	C2-C1-N1	-2.70	106.10	108.68
3	D	509[A]	ROL	C2-C1-N1	-2.67	106.14	108.68
3	D	509[B]	ROL	O2-C8-C7	2.67	119.02	115.40
3	B	505[A]	ROL	C2-C1-N1	-2.65	106.15	108.68
3	C	507[B]	ROL	C2-C1-N1	-2.63	106.18	108.68
3	C	507[B]	ROL	C7-O3-C11	-2.63	111.71	120.14
3	C	507[A]	ROL	C2-C1-N1	-2.62	106.19	108.68
3	A	503[B]	ROL	C2-C1-N1	-2.61	106.19	108.68
3	D	509[A]	ROL	O2-C8-C7	2.55	118.87	115.40
3	A	503[A]	ROL	C2-C1-N1	-2.54	106.26	108.68
3	D	509[B]	ROL	C2-C1-N1	-2.52	106.28	108.68
3	A	503[B]	ROL	C7-O3-C11	-2.51	112.07	120.14
3	C	507[A]	ROL	C2-C3-C5	-2.49	110.17	115.29
3	C	507[A]	ROL	C7-O3-C11	-2.44	112.30	120.14
3	C	507[B]	ROL	O2-C8-C9	-2.41	120.23	124.30
3	B	505[A]	ROL	C2-C3-C5	-2.40	110.35	115.29
3	A	503[A]	ROL	C7-O3-C11	-2.38	112.49	120.14
3	B	505[B]	ROL	O2-C8-C7	2.37	118.61	115.40
3	A	503[B]	ROL	O2-C8-C9	-2.36	120.33	124.30
3	D	509[B]	ROL	C2-C3-C5	-2.35	110.46	115.29
3	A	503[B]	ROL	C2-C3-C5	-2.25	110.66	115.29
3	D	509[A]	ROL	C2-C3-C5	-2.24	110.69	115.29
3	B	505[B]	ROL	C7-O3-C11	-2.21	113.05	120.14
3	A	503[A]	ROL	O2-C8-C9	-2.07	120.80	124.30
3	C	507[A]	ROL	O2-C8-C9	-2.01	120.91	124.30

All (4) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
3	A	503[A]	ROL	C3
3	B	505[A]	ROL	C3
3	C	507[A]	ROL	C3
3	D	509[A]	ROL	C3

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503[A]	ROL	C15-C11-O3-C7
3	A	503[A]	ROL	C12-C11-O3-C7
3	A	503[B]	ROL	C15-C11-O3-C7
3	A	503[B]	ROL	C12-C11-O3-C7
3	B	505[A]	ROL	C15-C11-O3-C7
3	B	505[A]	ROL	C12-C11-O3-C7
3	B	505[B]	ROL	C15-C11-O3-C7
3	B	505[B]	ROL	C12-C11-O3-C7
3	C	507[A]	ROL	C15-C11-O3-C7
3	C	507[A]	ROL	C12-C11-O3-C7
3	C	507[B]	ROL	C15-C11-O3-C7
3	C	507[B]	ROL	C12-C11-O3-C7
3	D	509[A]	ROL	C15-C11-O3-C7
3	D	509[A]	ROL	C12-C11-O3-C7
3	D	509[B]	ROL	C15-C11-O3-C7
3	D	509[B]	ROL	C12-C11-O3-C7
3	C	507[B]	ROL	C7-C8-O2-C16
3	A	503[B]	ROL	C7-C8-O2-C16
3	A	503[A]	ROL	C7-C8-O2-C16
3	C	507[A]	ROL	C7-C8-O2-C16
3	D	509[B]	ROL	C7-C8-O2-C16
3	A	503[B]	ROL	C9-C8-O2-C16
3	C	507[B]	ROL	C9-C8-O2-C16
3	A	503[A]	ROL	C9-C8-O2-C16
3	D	509[A]	ROL	C7-C8-O2-C16
3	C	507[A]	ROL	C9-C8-O2-C16
3	D	509[B]	ROL	C9-C8-O2-C16
3	D	509[A]	ROL	C9-C8-O2-C16
3	B	505[B]	ROL	C7-C8-O2-C16
3	C	507[A]	ROL	C8-C7-O3-C11
3	B	505[B]	ROL	C9-C8-O2-C16
3	C	507[B]	ROL	C6-C7-O3-C11
3	B	505[A]	ROL	C2-C3-C5-C10

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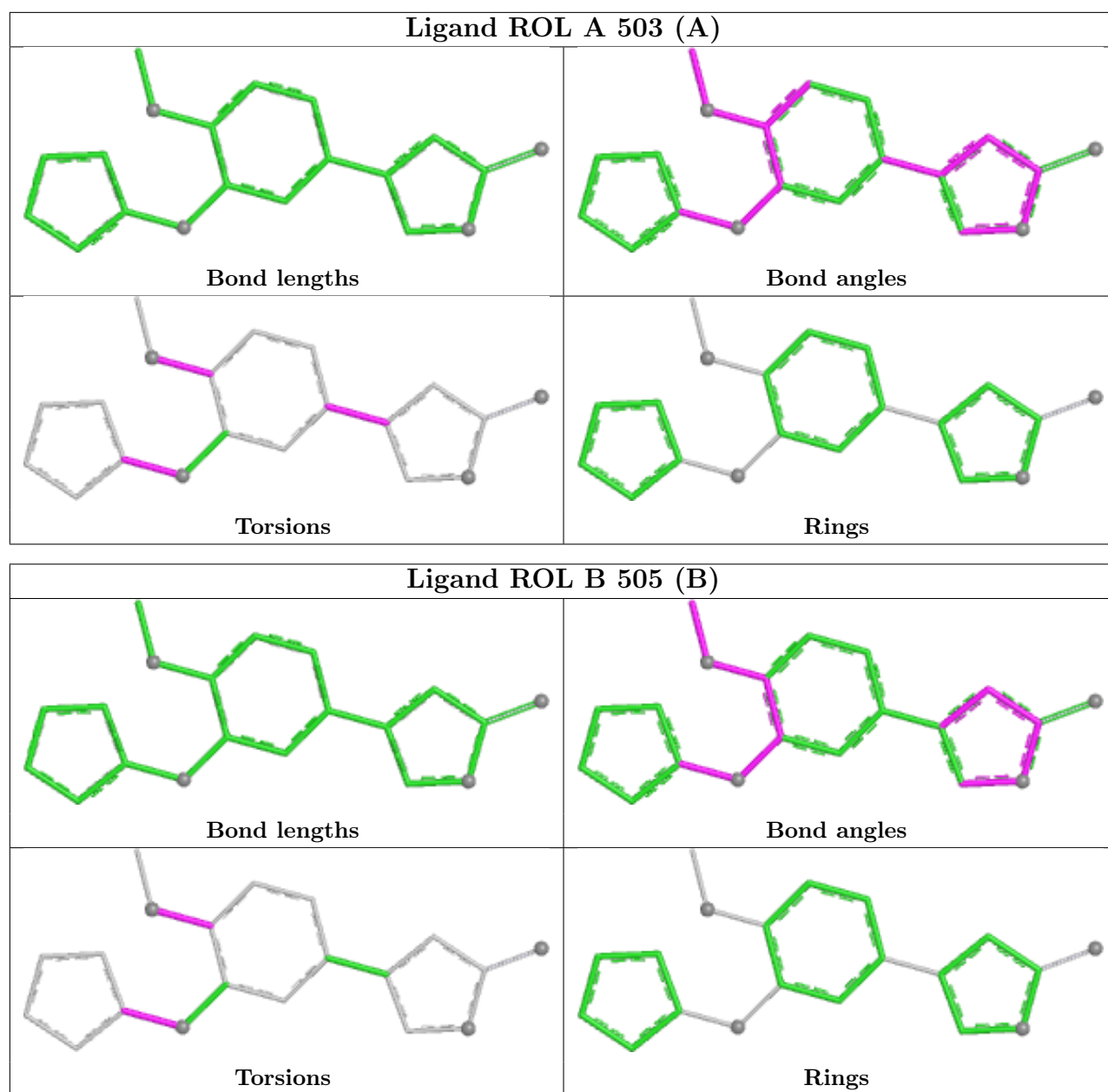
Mol	Chain	Res	Type	Atoms
3	C	507[A]	ROL	C2-C3-C5-C10
3	C	507[A]	ROL	C2-C3-C5-C6
3	A	503[A]	ROL	C2-C3-C5-C6
3	B	505[A]	ROL	C2-C3-C5-C6

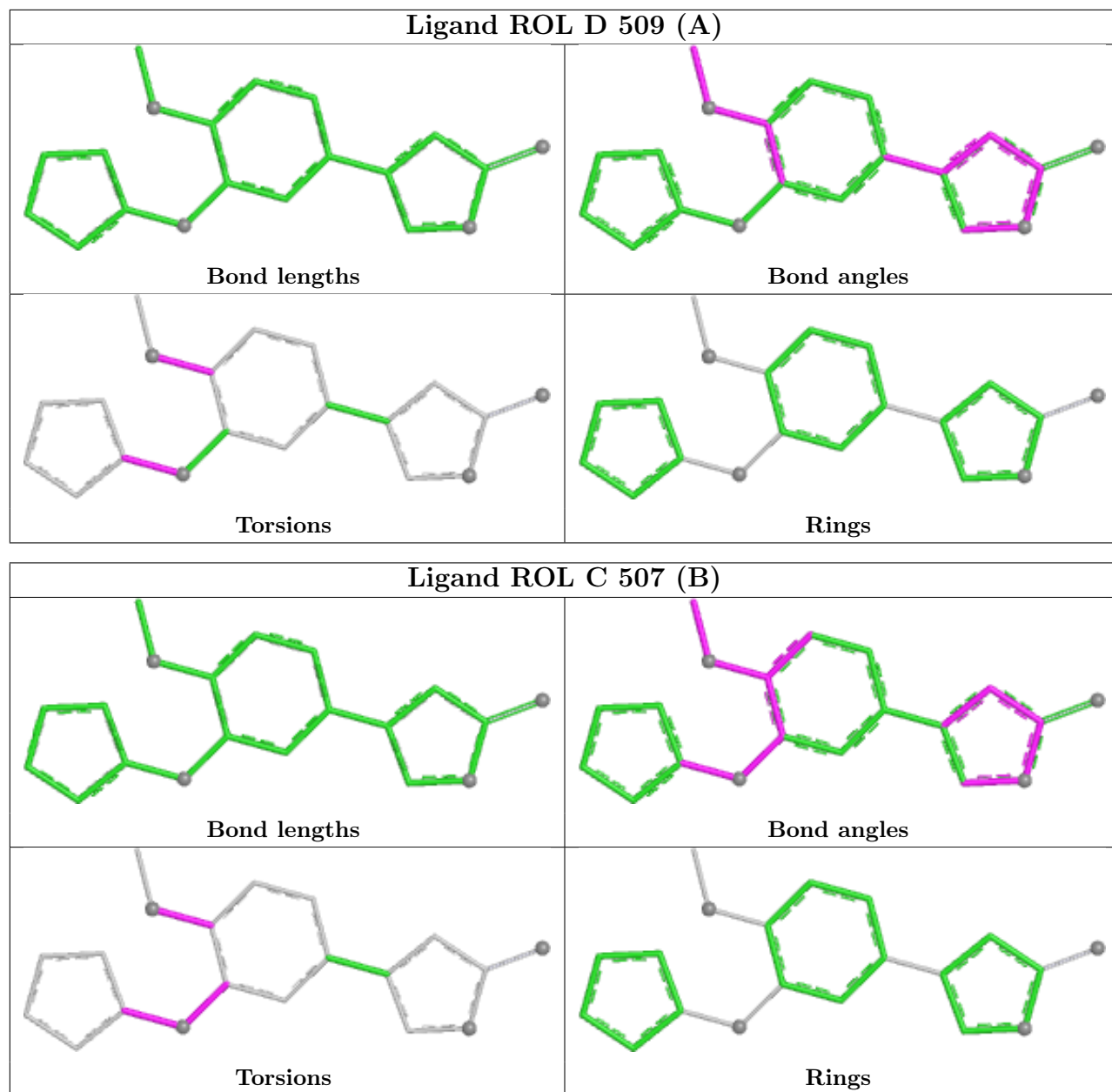
There are no ring outliers.

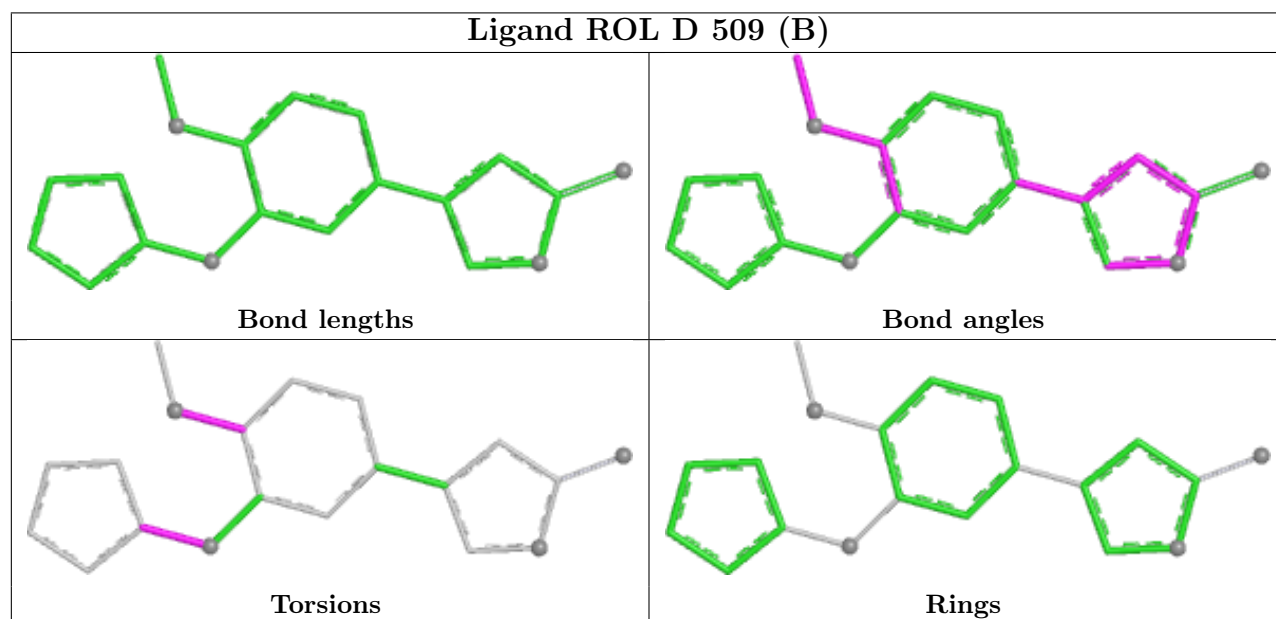
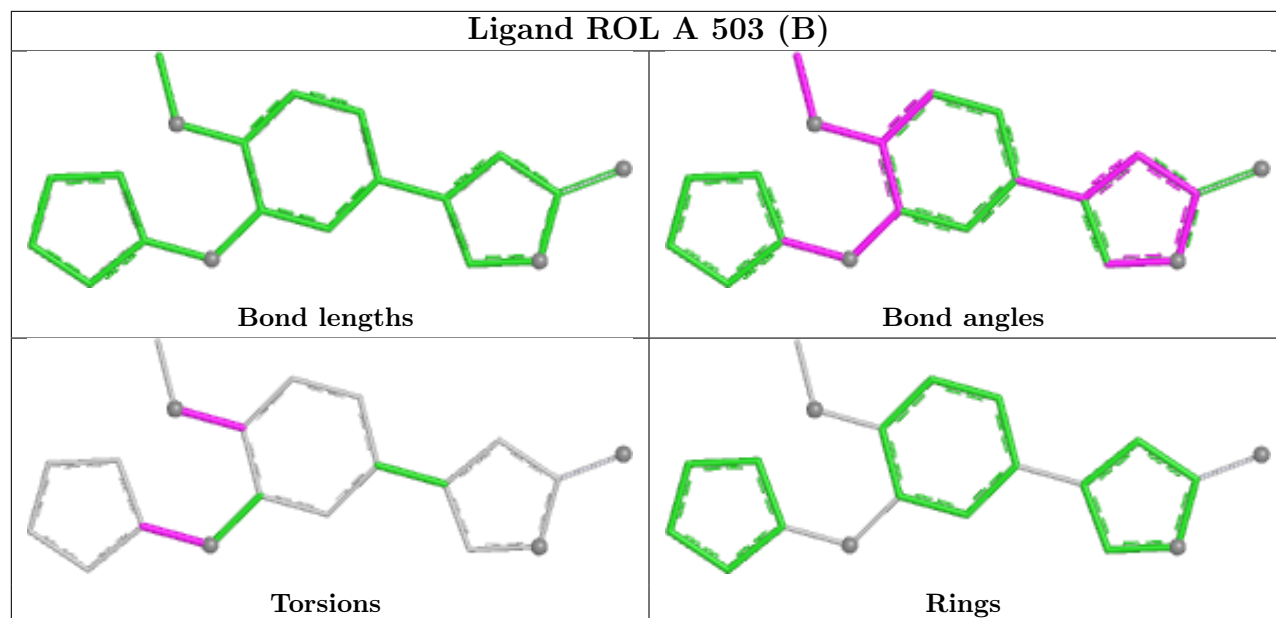
8 monomers are involved in 15 short contacts:

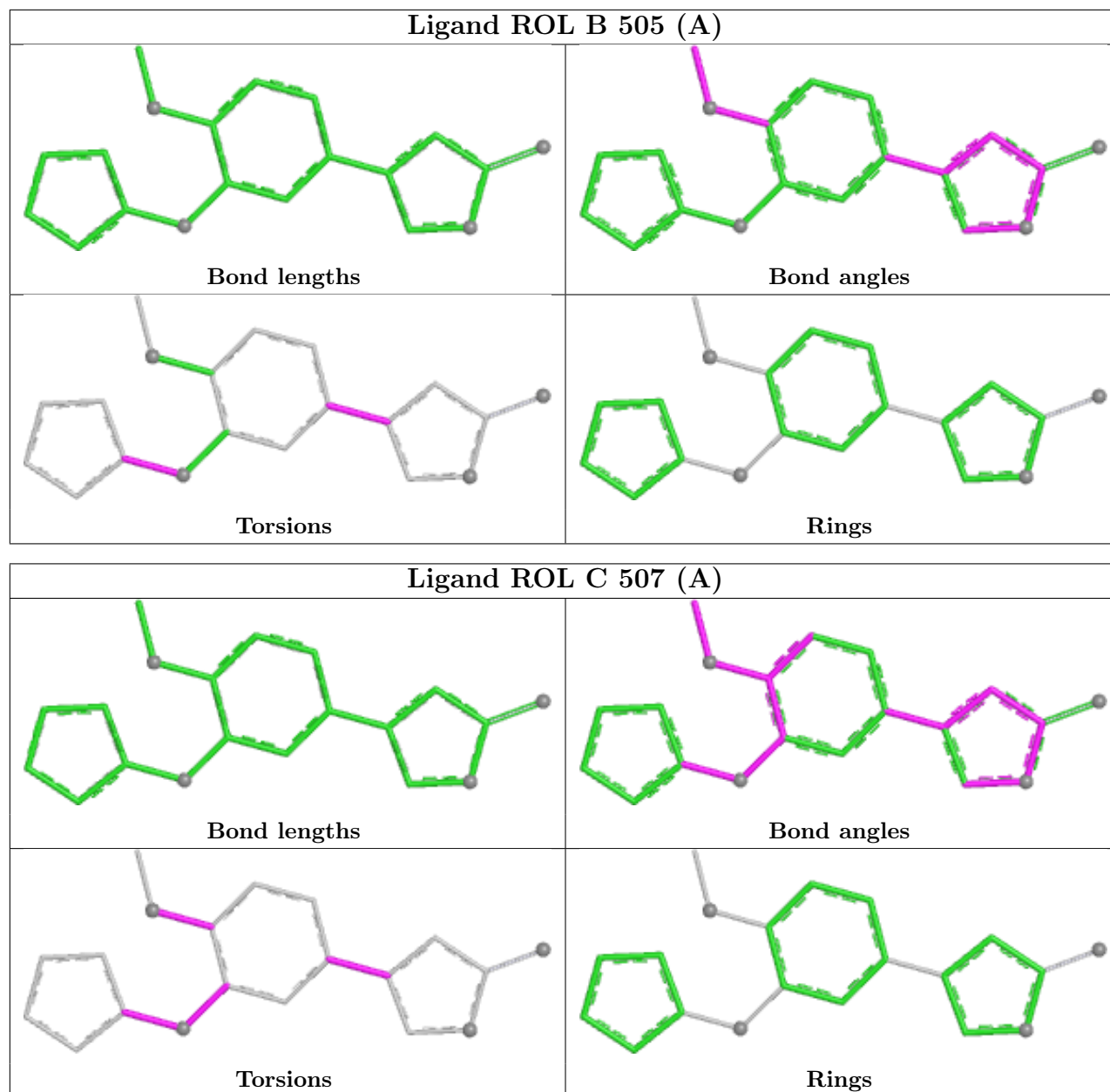
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503[A]	ROL	1	0
3	B	505[B]	ROL	2	0
3	D	509[A]	ROL	2	0
3	C	507[B]	ROL	2	0
3	A	503[B]	ROL	2	0
3	D	509[B]	ROL	3	0
3	B	505[A]	ROL	2	0
3	C	507[A]	ROL	1	0

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	334/360 (92%)	0.51	31 (9%) 14 13	20, 33, 73, 92	0
1	B	327/360 (90%)	1.14	64 (19%) 3 3	23, 45, 68, 100	0
1	C	327/360 (90%)	0.86	44 (13%) 7 6	23, 43, 82, 93	0
1	D	334/360 (92%)	0.47	32 (9%) 13 12	20, 33, 65, 77	0
All	All	1322/1440 (91%)	0.74	171 (12%) 7 6	20, 39, 71, 100	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ILE	8.8
1	A	82	PHE	8.8
1	A	298	LEU	6.9
1	B	294	SER	6.6
1	A	296	GLY	6.1
1	D	79	ILE	5.7
1	D	84	VAL	5.6
1	D	296	GLY	4.8
1	B	391	ASP	4.8
1	B	385	ALA	4.7
1	A	80	PRO	4.7
1	B	392	ALA	4.6
1	B	179	PRO	4.6
1	D	86	THR	4.3
1	B	387	LEU	4.2
1	A	81	ARG	4.1
1	D	412	GLN	4.1
1	D	221	LEU	4.1
1	C	298	LEU	4.0
1	A	86	THR	3.8
1	B	298	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	297	VAL	3.8
1	C	411	PRO	3.7
1	A	411	PRO	3.7
1	B	93	ALA	3.6
1	A	293	THR	3.6
1	B	86	THR	3.5
1	C	387	LEU	3.4
1	B	295	SER	3.3
1	C	86	THR	3.3
1	B	281	ALA	3.3
1	A	295	SER	3.2
1	B	296	GLY	3.2
1	B	92	LEU	3.2
1	C	412	GLN	3.2
1	D	295	SER	3.2
1	B	138	PRO	3.2
1	D	342	ARG	3.2
1	A	410	ILE	3.1
1	B	183	ALA	3.1
1	C	299	LEU	3.1
1	B	404	GLU	3.1
1	C	296	GLY	3.1
1	C	289	THR	3.1
1	A	290	LYS	3.1
1	D	213	ILE	3.1
1	A	83	GLY	3.0
1	D	362	ASN	3.0
1	C	258	GLN	3.0
1	B	139	VAL	3.0
1	C	292	VAL	3.0
1	B	277	MET	3.0
1	C	88	GLN	3.0
1	B	388	VAL	3.0
1	C	287	VAL	2.9
1	B	280	LEU	2.9
1	B	287	VAL	2.9
1	A	289	THR	2.9
1	C	293	THR	2.9
1	D	409	THR	2.9
1	C	295	SER	2.9
1	D	80	PRO	2.9
1	B	87	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	300	LEU	2.8
1	A	409	THR	2.8
1	B	291	LYS	2.8
1	B	375	TYR	2.8
1	D	301	ASP	2.8
1	B	102	TRP	2.8
1	C	221	LEU	2.8
1	D	298	LEU	2.8
1	B	141	THR	2.8
1	C	388	VAL	2.8
1	B	285	THR	2.7
1	B	242	GLN	2.7
1	C	353	GLU	2.7
1	D	404	GLU	2.7
1	B	99	VAL	2.7
1	D	375	TYR	2.6
1	D	410	ILE	2.6
1	A	299	LEU	2.6
1	B	279	LEU	2.6
1	C	356	PRO	2.6
1	B	134	THR	2.6
1	A	84	VAL	2.5
1	D	408	SER	2.5
1	C	280	LEU	2.5
1	B	135	PHE	2.5
1	C	102	TRP	2.5
1	B	395	ILE	2.5
1	D	81	ARG	2.5
1	B	289	THR	2.5
1	C	294	SER	2.5
1	B	241	LEU	2.5
1	C	357	MET	2.5
1	B	105	HIS	2.5
1	D	82	PHE	2.5
1	C	327	GLN	2.4
1	A	297	VAL	2.4
1	B	381	TRP	2.4
1	A	408	SER	2.4
1	A	291	LYS	2.4
1	D	353	GLU	2.4
1	C	282	ASP	2.4
1	A	292	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	410	ILE	2.4
1	D	357	MET	2.4
1	D	85	LYS	2.4
1	C	93	ALA	2.4
1	A	221	LEU	2.4
1	B	301	ASP	2.4
1	A	182	GLU	2.3
1	B	88	GLN	2.3
1	B	258	GLN	2.3
1	B	115	ASN	2.3
1	A	85	LYS	2.3
1	B	286	MET	2.3
1	B	342	ARG	2.3
1	D	294	SER	2.3
1	D	222	MET	2.3
1	D	87	GLU	2.3
1	A	301	ASP	2.3
1	B	386	ASP	2.3
1	D	219	LEU	2.3
1	C	184	VAL	2.3
1	B	390	PRO	2.3
1	B	150	GLU	2.2
1	B	126	PHE	2.2
1	C	89	GLU	2.2
1	A	354	ILE	2.2
1	C	251	ASN	2.2
1	B	91	VAL	2.2
1	D	291	LYS	2.2
1	B	244	GLU	2.2
1	C	105	HIS	2.2
1	C	303	TYR	2.2
1	C	301	ASP	2.2
1	C	392	ALA	2.2
1	B	188	LEU	2.2
1	C	399	LEU	2.2
1	A	342	ARG	2.2
1	C	362	ASN	2.2
1	D	354	ILE	2.1
1	A	183	ALA	2.1
1	D	89	GLU	2.1
1	D	327	GLN	2.1
1	B	292	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	389	HIS	2.1
1	B	180	ALA	2.1
1	B	112	LEU	2.1
1	C	283	LEU	2.1
1	B	302	ASN	2.1
1	C	90	ASP	2.1
1	B	148	THR	2.1
1	B	178	THR	2.1
1	C	390	PRO	2.1
1	B	96	LEU	2.1
1	A	89	GLU	2.1
1	A	327	GLN	2.1
1	C	134	THR	2.1
1	B	125	ILE	2.1
1	B	133	LYS	2.1
1	B	137	ILE	2.1
1	C	408	SER	2.1
1	B	124	THR	2.0
1	B	383	THR	2.0
1	A	351	GLY	2.0
1	C	375	TYR	2.0
1	B	109	ILE	2.0
1	C	277	MET	2.0
1	D	278	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

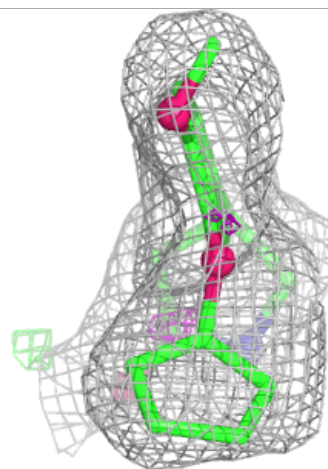
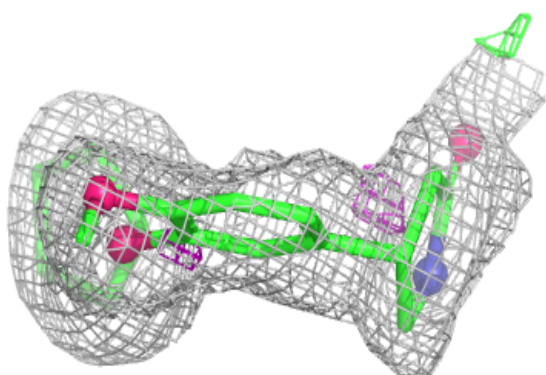
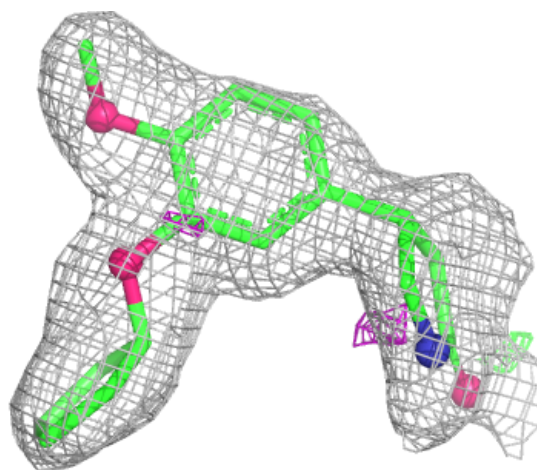
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ROL	A	503[A]	20/20	0.86	0.13	48,48,48,49	20
3	ROL	A	503[B]	20/20	0.86	0.13	49,50,50,51	20
3	ROL	B	505[A]	20/20	0.87	0.16	47,48,49,49	20
3	ROL	B	505[B]	20/20	0.87	0.16	48,49,50,50	20
3	ROL	C	507[A]	20/20	0.89	0.16	52,52,53,53	20
3	ROL	C	507[B]	20/20	0.89	0.16	51,52,52,52	20
3	ROL	D	509[A]	20/20	0.89	0.12	39,41,42,42	20
3	ROL	D	509[B]	20/20	0.89	0.12	45,46,49,50	20
2	ZN	C	506	1/1	0.91	0.24	60,60,60,60	0
2	ZN	B	504	1/1	0.93	0.17	67,67,67,67	0
2	ZN	A	502	1/1	0.94	0.17	56,56,56,56	0
2	ZN	D	508	1/1	0.95	0.23	63,63,63,63	0
2	ZN	B	503	1/1	0.97	0.05	36,36,36,36	0
2	ZN	A	501	1/1	0.98	0.04	33,33,33,33	0
2	ZN	D	507	1/1	0.99	0.03	33,33,33,33	0
2	ZN	C	505	1/1	0.99	0.03	37,37,37,37	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.

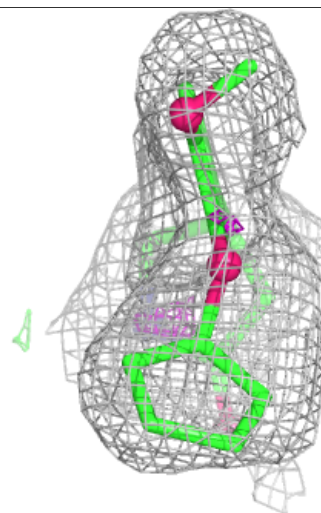
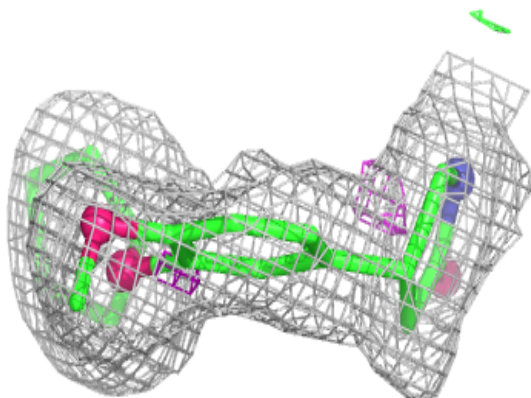
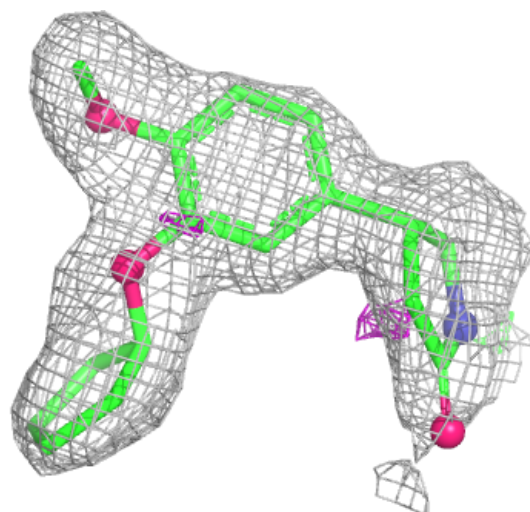
Electron density around ROL A 503 (A):

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



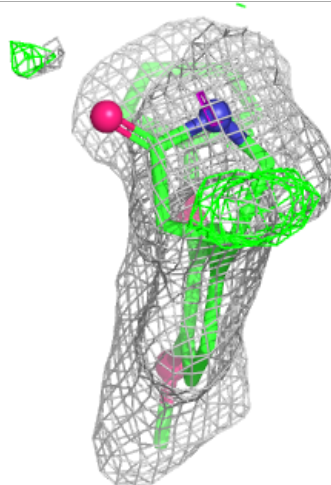
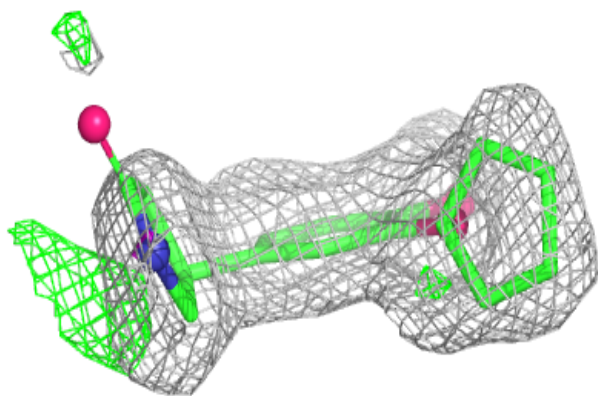
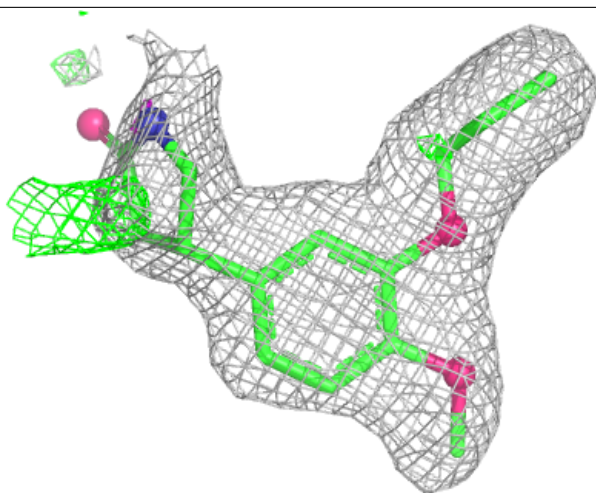
Electron density around ROL A 503 (B):

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



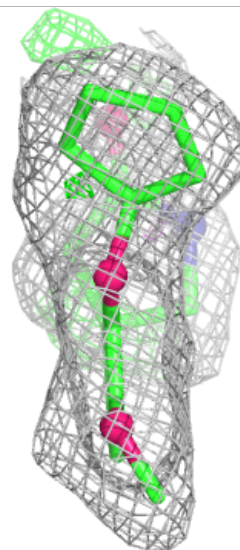
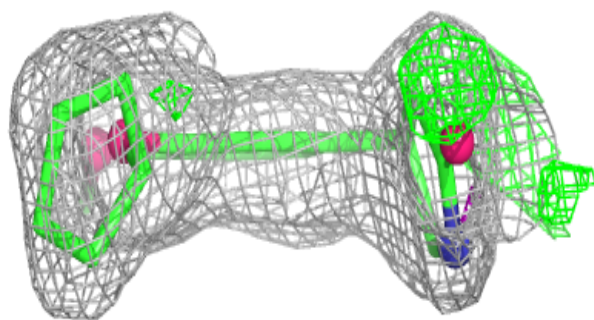
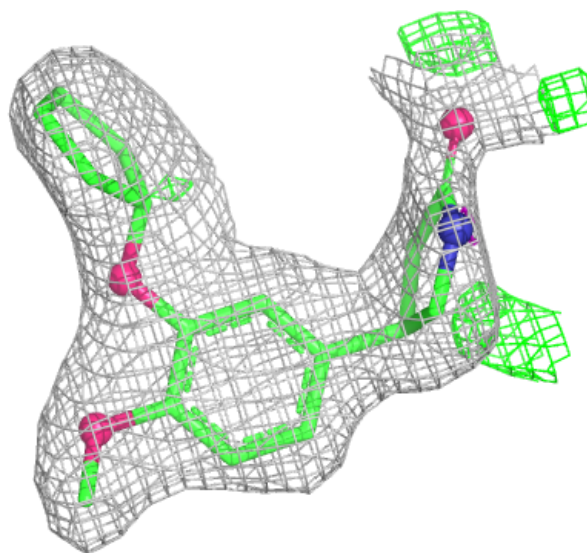
Electron density around ROL B 505 (A):

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



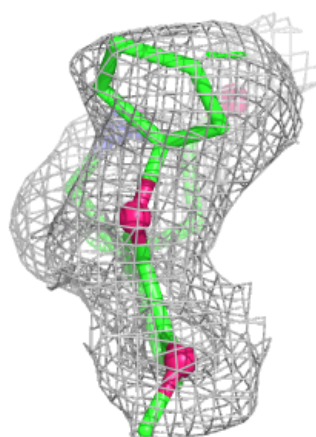
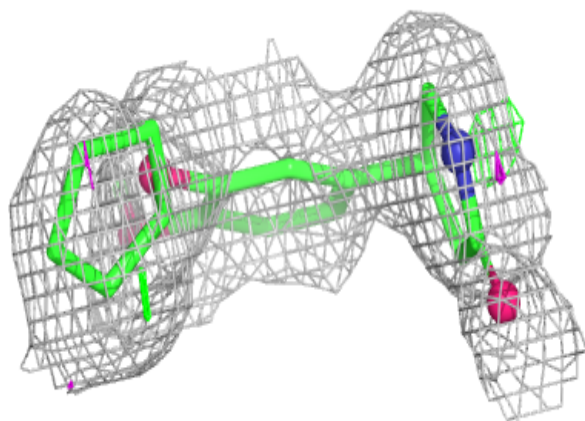
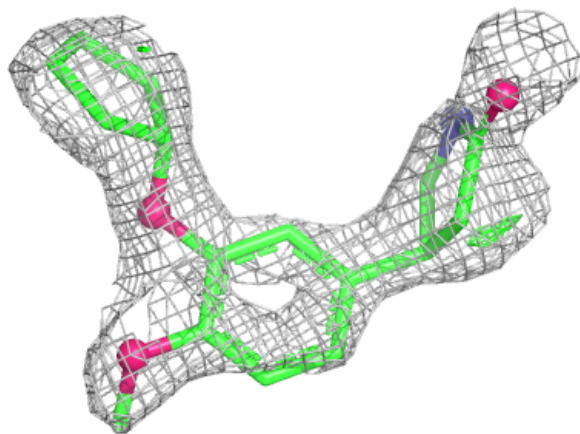
Electron density around ROL B 505 (B):

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



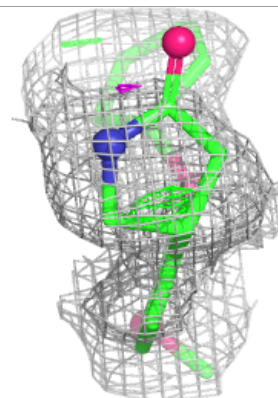
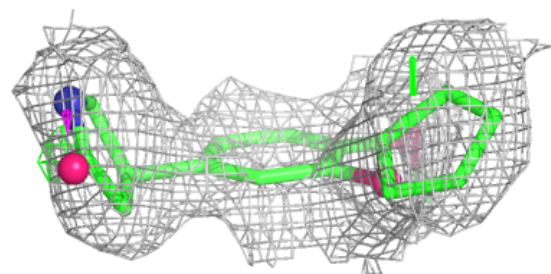
Electron density around ROL C 507 (A):

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

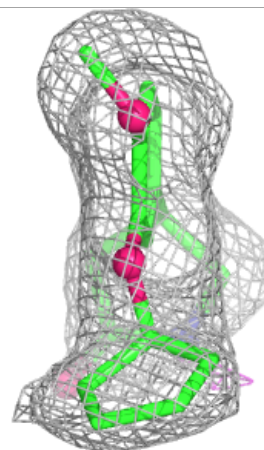
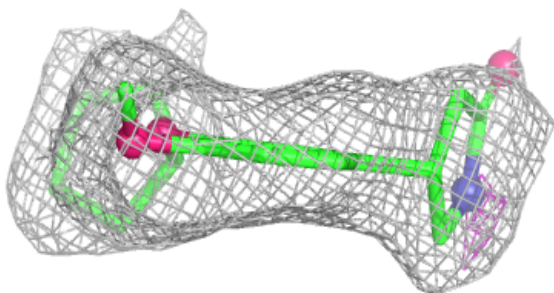
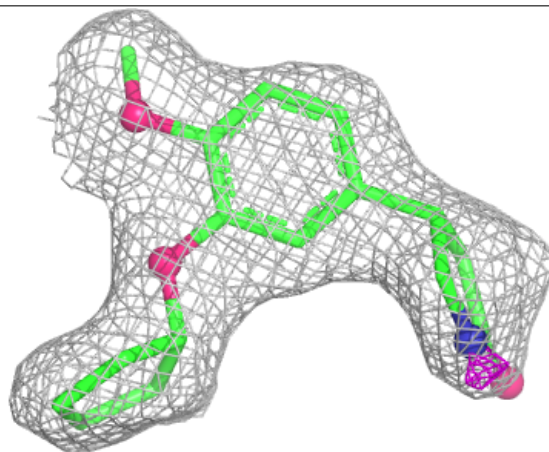


Electron density around ROL C 507 (B):

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

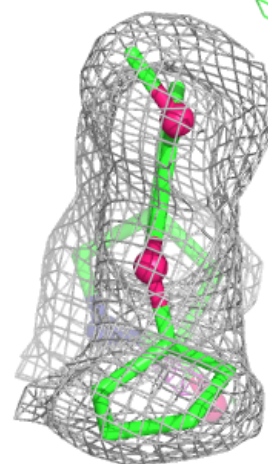
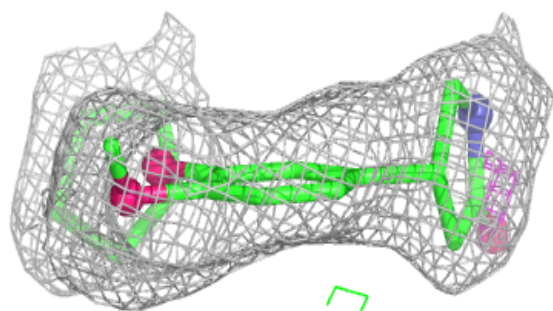
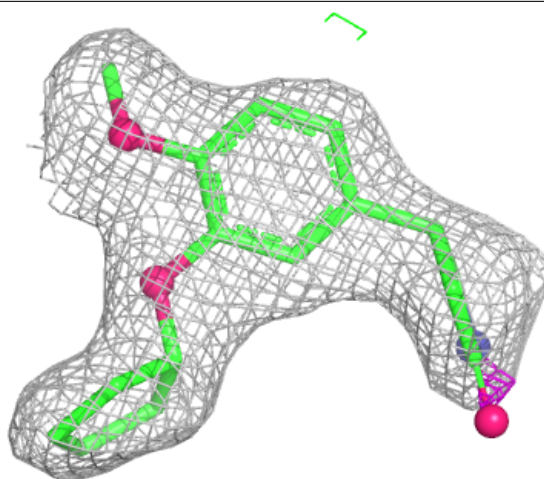
**Electron density around ROL D 509 (A):**

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



Electron density around ROL D 509 (B):

$2mF_o-DF_c$ (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.