



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:43 AM UTC

PDB ID : 1W25 / pdb_00001w25
Title : Response regulator PleD in complex with c-diGMP
Authors : Chan, C.; Schirmer, T.; Jenal, U.
Deposited on : 2004-06-28
Resolution : 2.70 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

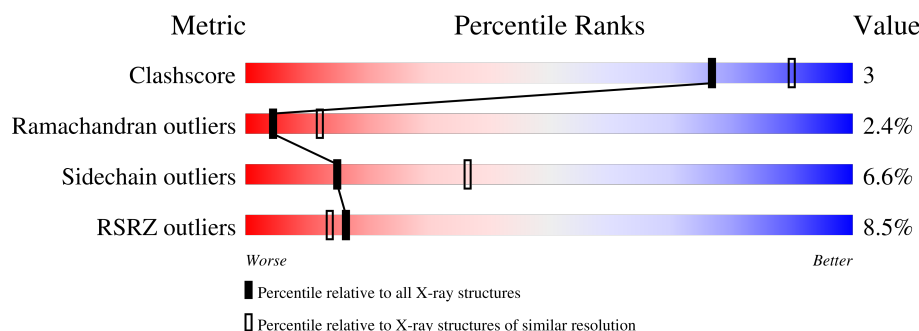
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	459	5% 84% 11% ...
1	B	459	11% 86% 10% ...

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7210 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 STALKED-CELL DIFFERENTIATION CONTROLLING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	164	0	0
			3481	2166	639	661	15			
1	B	454	Total	C	N	O	S	164	0	0
			3481	2166	639	661	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	HIS	-	expression tag	UNP Q9A5I5
A	456	HIS	-	expression tag	UNP Q9A5I5
A	457	HIS	-	expression tag	UNP Q9A5I5
A	458	HIS	-	expression tag	UNP Q9A5I5
A	459	HIS	-	expression tag	UNP Q9A5I5
A	460	HIS	-	expression tag	UNP Q9A5I5
B	455	HIS	-	expression tag	UNP Q9A5I5
B	456	HIS	-	expression tag	UNP Q9A5I5
B	457	HIS	-	expression tag	UNP Q9A5I5
B	458	HIS	-	expression tag	UNP Q9A5I5
B	459	HIS	-	expression tag	UNP Q9A5I5
B	460	HIS	-	expression tag	UNP Q9A5I5

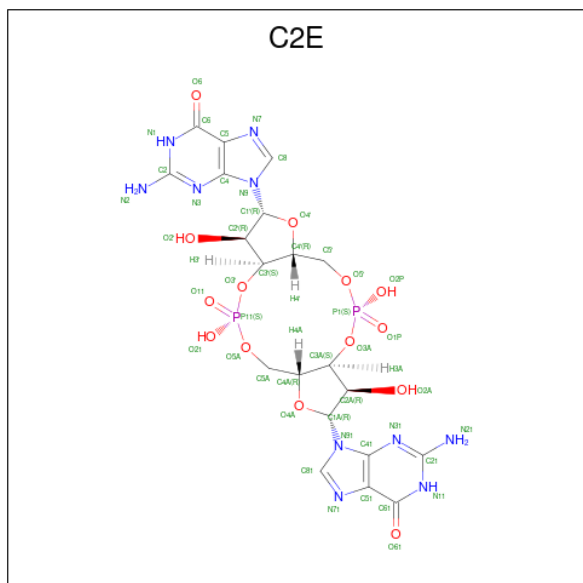
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

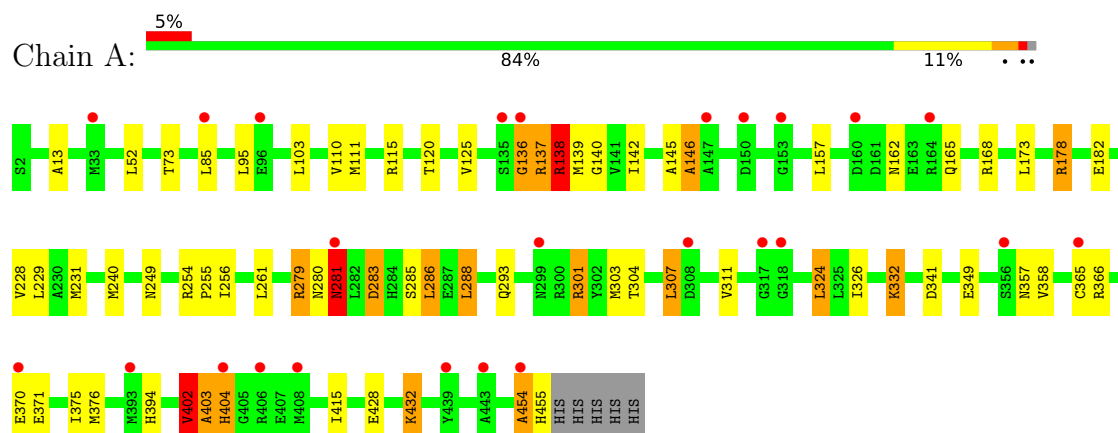
- Molecule 4 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (CCD ID: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).



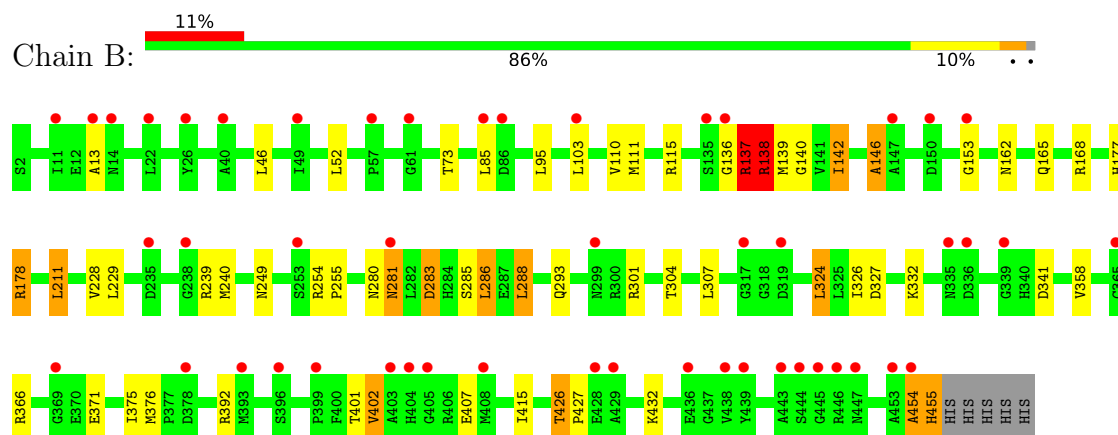
3 Residue-property plots

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: STALKED-CELL DIFFERENTIATION CONTROLLING PROTEIN



• Molecule 1: STALKED-CELL DIFFERENTIATION CONTROLLING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	135.87Å 135.87Å 169.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.70) 98.9 (50.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0001	Depositor
R, R_{free}	0.210 , 0.239 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.5	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	0.91	EDS
Total number of atoms	7210	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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: MG, C2E, ZN

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	1.36	11/3525 (0.3%)	1.65	24/4765 (0.5%)
1	B	1.23	11/3525 (0.3%)	1.64	20/4765 (0.4%)
All	All	1.30	22/7050 (0.3%)	1.64	44/9530 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	4
All	All	0	12

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	GLY	C-N	-47.54	0.67	1.33
1	B	281	ASN	C-N	-41.27	0.71	1.33
1	A	281	ASN	C-N	-38.34	0.80	1.33
1	B	301	ARG	CD-NE	-33.74	0.99	1.46
1	A	454	ALA	C-N	-25.09	0.98	1.33
1	A	301	ARG	CD-NE	-22.01	1.15	1.46
1	B	136	GLY	C-N	-21.93	1.02	1.33
1	B	281	ASN	CB-CG	-16.07	1.11	1.52
1	A	283	ASP	C-N	13.22	1.51	1.33
1	B	283	ASP	C-N	13.19	1.51	1.33
1	B	332	LYS	CE-NZ	-11.51	1.14	1.49
1	A	332	LYS	CE-NZ	-8.67	1.23	1.49
1	B	288	LEU	C-N	-6.96	1.24	1.33
1	B	146	ALA	C-N	6.73	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	ALA	C-N	-6.59	1.25	1.33
1	B	454	ALA	C-N	-6.58	1.24	1.33
1	A	288	LEU	C-N	-6.14	1.24	1.33
1	A	279	ARG	CG-CD	-5.80	1.35	1.52
1	A	455	HIS	CB-CG	5.50	1.57	1.50
1	A	432	LYS	CG-CD	-5.49	1.35	1.52
1	B	455	HIS	CB-CG	5.44	1.57	1.50
1	B	137	ARG	CA-C	-5.07	1.46	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASN	O-C-N	-64.59	36.68	122.59
1	B	281	ASN	O-C-N	-62.87	38.97	122.59
1	A	454	ALA	O-C-N	-54.57	47.37	122.68
1	B	454	ALA	O-C-N	-36.97	73.42	122.59
1	B	281	ASN	CA-C-N	-27.76	81.68	122.77
1	B	281	ASN	C-N-CA	-27.76	81.68	122.77
1	B	288	LEU	CA-C-N	22.43	153.13	121.05
1	B	288	LEU	C-N-CA	22.43	153.13	121.05
1	A	281	ASN	CA-CB-CG	-20.37	92.23	112.60
1	A	281	ASN	CB-CG-ND2	-15.65	92.93	116.40
1	B	136	GLY	O-C-N	15.24	138.01	122.93
1	B	146	ALA	CA-C-N	-13.63	100.94	121.26
1	B	146	ALA	C-N-CA	-13.63	100.94	121.26
1	A	146	ALA	CA-C-N	-12.36	102.84	121.26
1	A	146	ALA	C-N-CA	-12.36	102.84	121.26
1	B	293	GLN	OE1-CD-NE2	-9.47	113.13	122.60
1	B	332	LYS	CD-CE-NZ	9.29	141.62	111.90
1	A	293	GLN	OE1-CD-NE2	-9.24	113.36	122.60
1	A	146	ALA	O-C-N	8.83	134.34	122.59
1	A	138	ARG	CA-C-N	-8.64	106.78	122.50
1	A	138	ARG	C-N-CA	-8.64	106.78	122.50
1	A	332	LYS	CD-CE-NZ	8.39	138.76	111.90
1	A	288	LEU	O-C-N	8.19	131.49	122.15
1	B	138	ARG	CA-C-N	-8.18	105.95	121.81
1	B	138	ARG	C-N-CA	-8.18	105.95	121.81
1	A	402	VAL	CA-CB-CG2	8.14	124.24	110.40
1	B	137	ARG	N-CA-C	-7.35	95.14	110.80
1	B	146	ALA	O-C-N	6.97	131.86	122.59
1	A	293	GLN	CG-CD-NE2	6.77	126.55	116.40
1	A	136	GLY	CA-C-N	6.74	134.41	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	GLY	C-N-CA	6.74	134.41	121.54
1	A	145	ALA	O-C-N	6.52	130.85	123.42
1	A	301	ARG	CD-NE-CZ	-6.45	115.37	124.40
1	B	288	LEU	O-C-N	-6.44	115.08	122.03
1	B	293	GLN	CG-CD-NE2	6.31	125.86	116.40
1	A	145	ALA	CA-C-O	6.26	127.77	120.14
1	B	455	HIS	CA-CB-CG	6.21	120.01	113.80
1	A	281	ASN	CB-CG-OD1	6.19	133.17	120.80
1	A	137	ARG	N-CA-CB	6.14	120.86	110.49
1	A	432	LYS	CB-CG-CD	6.06	125.24	111.30
1	B	301	ARG	CG-CD-NE	5.99	125.17	112.00
1	A	402	VAL	CA-CB-CG1	5.84	120.34	110.40
1	A	455	HIS	CA-CB-CG	5.50	119.30	113.80
1	B	288	LEU	CB-CA-C	-5.21	102.88	110.95

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	GLY	Mainchain
1	A	281	ASN	Sidechain,Peptide,Mainchain
1	A	288	LEU	Peptide
1	A	301	ARG	Sidechain
1	A	454	ALA	Peptide,Mainchain
1	B	281	ASN	Mainchain
1	B	288	LEU	Mainchain
1	B	454	ALA	Peptide,Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3481	0	3548	23	3
1	B	3481	0	3548	17	6
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	138	0	66	1	0
4	B	92	0	44	1	0
5	A	7	0	0	1	0
5	B	8	0	0	1	0
All	All	7210	0	7206	40	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (40) 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:165:GLN:HE22	1:B:254:ARG:HD2	1.56	0.71
1:B:73:THR:HG21	5:B:2004:HOH:O	1.92	0.69
1:B:228:VAL:H	1:B:249:ASN:HD22	1.41	0.68
1:B:162:ASN:C	1:B:162:ASN:HD22	2.01	0.66
1:A:324:LEU:HD13	1:A:376:MET:HE1	1.80	0.61
1:A:231:MET:SD	1:A:256:ILE:HD11	2.41	0.60
1:A:111:MET:CE	1:A:115:ARG:HH22	2.16	0.58
1:B:111:MET:CE	1:B:115:ARG:HH22	2.17	0.56
1:B:426:THR:HG22	1:B:427:PRO:HD2	1.88	0.55
1:B:228:VAL:H	1:B:249:ASN:ND2	2.05	0.55
1:A:324:LEU:HD13	1:A:376:MET:CE	2.37	0.54
1:A:73:THR:HG21	5:A:2002:HOH:O	2.07	0.54
1:A:162:ASN:C	1:A:162:ASN:HD22	2.18	0.52
1:B:110:VAL:HG11	1:B:240:MET:HE3	1.92	0.52
1:B:162:ASN:C	1:B:162:ASN:ND2	2.68	0.51
1:B:178:ARG:NH2	4:B:503:C2E:N7	2.60	0.50
1:A:403:ALA:O	1:A:404:HIS:C	2.56	0.49
1:B:324:LEU:HD13	1:B:376:MET:HE1	1.95	0.48
1:A:157:LEU:HD11	1:A:182:GLU:HG3	1.95	0.48
1:A:178:ARG:NH2	4:A:503:C2E:N7	2.62	0.47
1:B:324:LEU:HD13	1:B:376:MET:CE	2.44	0.47
1:A:173:LEU:HD21	1:A:261:LEU:HG	1.96	0.47
1:B:326:ILE:HD13	1:B:415:ILE:HG23	1.97	0.46
1:A:307:LEU:HD22	1:A:311:VAL:HG23	1.97	0.46
1:A:326:ILE:HD13	1:A:415:ILE:HG23	1.99	0.44
1:A:254:ARG:HA	1:A:255:PRO:C	2.42	0.44
1:A:428:GLU:OE1	1:A:428:GLU:N	2.50	0.44
1:A:228:VAL:H	1:A:249:ASN:HD22	1.66	0.43
1:A:332:LYS:HE3	1:A:370:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLY:O	1:B:177:HIS:ND1	2.47	0.42
1:A:111:MET:HE3	1:A:115:ARG:HH22	1.84	0.42
1:A:402:VAL:HB	1:A:403:ALA:H	1.58	0.42
1:A:110:VAL:HG11	1:A:240:MET:HE3	2.02	0.42
1:A:303:MET:HB2	1:A:365:CYS:SG	2.60	0.42
1:B:254:ARG:HA	1:B:255:PRO:C	2.45	0.41
1:B:46:LEU:HD21	1:B:73:THR:HG22	2.02	0.41
1:A:165:GLN:HE22	1:A:254:ARG:HD2	1.84	0.41
1:A:231:MET:SD	1:A:256:ILE:CD1	3.06	0.41
1:B:211:LEU:HD22	1:B:239:ARG:CZ	2.51	0.41
1:A:357:ASN:HD21	1:A:394:HIS:CE1	2.39	0.41

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ARG:NH2	1:B:341:ASP:OD2[8_666]	0.63	1.57
1:A:138:ARG:NH2	1:A:341:ASP:OD2[8_666]	1.12	1.08
1:B:138:ARG:NH2	1:B:341:ASP:CG[8_666]	1.59	0.61
1:B:137:ARG:NH1	1:B:407:GLU:CG[8_666]	1.67	0.53
1:A:138:ARG:NH2	1:A:341:ASP:CG[8_666]	1.89	0.31
1:B:138:ARG:CZ	1:B:341:ASP:OD2[8_666]	1.95	0.25
1:A:138:ARG:CZ	1:A:341:ASP:OD2[8_666]	1.98	0.22
1:B:137:ARG:NH1	1:B:407:GLU:CD[8_666]	2.00	0.20
1:B:137:ARG:NH1	1:B:407:GLU:OE2[8_666]	2.18	0.02

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	452/459 (98%)	428 (95%)	11 (2%)	13 (3%)	3 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	452/459 (98%)	430 (95%)	13 (3%)	9 (2%)	6	16
All	All	904/918 (98%)	858 (95%)	24 (3%)	22 (2%)	4	12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ALA
1	A	281	ASN
1	A	286	LEU
1	A	403	ALA
1	B	146	ALA
1	B	286	LEU
1	A	13	ALA
1	A	137	ARG
1	A	140	GLY
1	A	142	ILE
1	A	402	VAL
1	B	13	ALA
1	B	140	GLY
1	B	142	ILE
1	A	280	ASN
1	A	283	ASP
1	A	404	HIS
1	B	137	ARG
1	B	283	ASP
1	A	285	SER
1	B	285	SER
1	B	402	VAL

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	369/374 (99%)	347 (94%)	22 (6%)	17	41
1	B	369/374 (99%)	342 (93%)	27 (7%)	13	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	738/748 (99%)	689 (93%)	49 (7%)	15	36

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	85	LEU
1	A	95	LEU
1	A	103	LEU
1	A	120	THR
1	A	125	VAL
1	A	138	ARG
1	A	139	MET
1	A	168	ARG
1	A	178	ARG
1	A	229	LEU
1	A	279	ARG
1	A	286	LEU
1	A	304	THR
1	A	307	LEU
1	A	324	LEU
1	A	349	GLU
1	A	358	VAL
1	A	366	ARG
1	A	371	GLU
1	A	375	ILE
1	A	432	LYS
1	B	52	LEU
1	B	85	LEU
1	B	95	LEU
1	B	103	LEU
1	B	138	ARG
1	B	139	MET
1	B	142	ILE
1	B	168	ARG
1	B	178	ARG
1	B	211	LEU
1	B	229	LEU
1	B	280	ASN
1	B	286	LEU
1	B	304	THR
1	B	307	LEU

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Mol	Chain	Res	Type
1	B	324	LEU
1	B	327	ASP
1	B	358	VAL
1	B	366	ARG
1	B	371	GLU
1	B	375	ILE
1	B	392	ARG
1	B	401	THR
1	B	402	VAL
1	B	426	THR
1	B	432	LYS
1	B	455	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	93	GLN
1	A	162	ASN
1	A	165	GLN
1	A	249	ASN
1	A	298	HIS
1	A	306	GLN
1	A	357	ASN
1	A	394	HIS
1	B	93	GLN
1	B	162	ASN
1	B	165	GLN
1	B	249	ASN
1	B	298	HIS
1	B	357	ASN
1	B	394	HIS
1	B	440	GLN

5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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
4	C2E	A	505	-	52,52,52	1.19	7 (13%)	78,82,82	1.81	13 (16%)
4	C2E	B	503	-	52,52,52	1.20	7 (13%)	78,82,82	1.78	12 (15%)
4	C2E	A	503	-	52,52,52	1.16	5 (9%)	78,82,82	1.81	13 (16%)
4	C2E	B	505	-	52,52,52	1.18	8 (15%)	78,82,82	1.80	13 (16%)
4	C2E	A	501	-	52,52,52	1.19	6 (11%)	78,82,82	1.84	12 (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
4	C2E	A	505	-	-	0/30/62/62	0/6/7/7
4	C2E	B	503	-	-	0/30/62/62	0/6/7/7
4	C2E	A	503	-	-	0/30/62/62	0/6/7/7
4	C2E	B	505	-	-	0/30/62/62	0/6/7/7
4	C2E	A	501	-	-	1/30/62/62	0/6/7/7

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	C2E	C5-C4	3.26	1.47	1.38
4	B	503	C2E	C51-C41	3.21	1.47	1.38
4	A	501	C2E	C5-C4	3.11	1.47	1.38
4	A	505	C2E	C5-C4	3.06	1.47	1.38
4	A	501	C2E	C51-C41	3.06	1.47	1.38
4	A	503	C2E	C6-N1	-3.01	1.33	1.38
4	B	505	C2E	C51-C41	3.00	1.47	1.38
4	A	505	C2E	C51-C41	2.99	1.46	1.38
4	A	503	C2E	C5-C4	2.92	1.46	1.38
4	A	503	C2E	C51-C41	2.92	1.46	1.38
4	B	503	C2E	C6-N1	-2.90	1.33	1.38
4	B	503	C2E	C5-C4	2.85	1.46	1.38
4	A	501	C2E	C61-N11	-2.75	1.33	1.38
4	A	505	C2E	C6-N1	-2.73	1.33	1.38
4	B	505	C2E	C61-N11	-2.70	1.33	1.38
4	A	505	C2E	C61-N11	-2.70	1.33	1.38
4	B	503	C2E	C5-N7	-2.56	1.33	1.39
4	B	503	C2E	C61-N11	-2.55	1.34	1.38
4	A	501	C2E	C6-N1	-2.47	1.34	1.38
4	B	505	C2E	C51-N71	-2.45	1.34	1.39
4	A	503	C2E	C61-N11	-2.43	1.34	1.38
4	A	505	C2E	C5-N7	-2.40	1.34	1.39
4	A	503	C2E	C5-N7	-2.39	1.34	1.39
4	A	501	C2E	C51-N71	-2.33	1.34	1.39
4	B	505	C2E	C41-N91	-2.32	1.32	1.38
4	B	505	C2E	C5-N7	-2.32	1.34	1.39
4	B	503	C2E	C41-N91	-2.30	1.32	1.38
4	A	501	C2E	C5-N7	-2.28	1.34	1.39
4	B	503	C2E	C51-N71	-2.25	1.34	1.39
4	A	505	C2E	C51-N71	-2.20	1.34	1.39
4	B	505	C2E	C4-N9	-2.16	1.32	1.38
4	B	505	C2E	C6-N1	-2.15	1.34	1.38
4	A	505	C2E	C41-N91	-2.11	1.32	1.38

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	C2E	C5-C4-N3	-6.27	118.42	128.39
4	A	501	C2E	C5-C4-N3	-6.23	118.48	128.39
4	B	503	C2E	C5-C4-N3	-6.17	118.57	128.39
4	A	501	C2E	C51-C41-N31	-6.08	118.71	128.39
4	B	505	C2E	C5-C4-N3	-6.02	118.81	128.39
4	A	505	C2E	C5-C4-N3	-5.90	119.00	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	C2E	C51-C41-N31	-5.40	119.80	128.39
4	B	505	C2E	C51-C41-N31	-5.37	119.84	128.39
4	B	505	C2E	C2-N3-C4	5.36	121.53	112.30
4	B	503	C2E	C51-C41-N31	-5.22	120.08	128.39
4	A	503	C2E	C51-C41-N31	-5.19	120.12	128.39
4	A	501	C2E	C2-N3-C4	5.14	121.15	112.30
4	A	503	C2E	C2-N3-C4	5.05	120.99	112.30
4	B	503	C2E	C2-N3-C4	4.97	120.86	112.30
4	A	505	C2E	C2-N3-C4	4.93	120.80	112.30
4	A	501	C2E	C21-N31-C41	4.80	120.56	112.30
4	A	505	C2E	C21-N31-C41	4.62	120.25	112.30
4	A	503	C2E	N9-C4-N3	4.59	135.13	125.95
4	A	503	C2E	C21-N31-C41	4.52	120.09	112.30
4	B	503	C2E	N9-C4-N3	4.48	134.91	125.95
4	B	505	C2E	C21-N31-C41	4.43	119.93	112.30
4	A	501	C2E	N9-C4-N3	4.43	134.81	125.95
4	A	501	C2E	N91-C41-N31	4.30	134.56	125.95
4	B	503	C2E	C21-N31-C41	4.28	119.67	112.30
4	A	505	C2E	N9-C4-N3	4.19	134.33	125.95
4	B	505	C2E	N9-C4-N3	4.15	134.26	125.95
4	B	503	C2E	C61-C51-N71	3.87	137.33	130.29
4	A	503	C2E	C61-C51-N71	3.84	137.28	130.29
4	A	505	C2E	C61-C51-N71	3.73	137.09	130.29
4	A	503	C2E	N91-C41-N31	3.72	133.38	125.95
4	B	505	C2E	N91-C41-N31	3.64	133.24	125.95
4	A	505	C2E	N91-C41-N31	3.53	133.02	125.95
4	B	505	C2E	C61-C51-N71	3.50	136.66	130.29
4	B	503	C2E	N91-C41-N31	3.44	132.83	125.95
4	A	503	C2E	C6-C5-N7	3.41	136.49	130.29
4	A	501	C2E	C6-C5-N7	3.41	136.49	130.29
4	A	505	C2E	C6-C5-N7	3.35	136.38	130.29
4	A	501	C2E	C61-C51-N71	3.21	136.13	130.29
4	B	503	C2E	C6-C5-N7	3.20	136.12	130.29
4	B	505	C2E	C6-C5-N7	3.16	136.04	130.29
4	A	505	C2E	C3'-C2'-C1'	3.01	106.52	99.89
4	A	505	C2E	C41-C51-N71	-2.92	106.05	110.67
4	B	503	C2E	C41-C51-N71	-2.91	106.06	110.67
4	A	503	C2E	C4-C5-N7	-2.78	106.27	110.67
4	B	503	C2E	C4-C5-N7	-2.75	106.31	110.67
4	A	501	C2E	C3'-C2'-C1'	2.74	105.93	99.89
4	A	501	C2E	C4-C5-N7	-2.74	106.33	110.67
4	B	505	C2E	C3'-C2'-C1'	2.73	105.90	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	505	C2E	C41-C51-N71	-2.70	106.40	110.67
4	A	501	C2E	C41-C51-N71	-2.67	106.45	110.67
4	A	503	C2E	C41-C51-N71	-2.65	106.47	110.67
4	A	501	C2E	C3A-C2A-C1A	2.59	105.59	99.89
4	B	505	C2E	O6-C6-C5	-2.57	119.76	126.53
4	A	505	C2E	C4-C5-N7	-2.56	106.62	110.67
4	A	505	C2E	C3A-C2A-C1A	2.38	105.13	99.89
4	B	505	C2E	C3A-C2A-C1A	2.38	105.12	99.89
4	B	503	C2E	C3A-C2A-C1A	2.25	104.85	99.89
4	A	503	C2E	C8-N7-C5	2.25	108.26	104.26
4	B	505	C2E	C4-C5-N7	-2.23	107.14	110.67
4	B	503	C2E	C8-N7-C5	2.21	108.20	104.26
4	A	503	C2E	C3A-C2A-C1A	2.18	104.68	99.89
4	A	505	C2E	C2A-C3A-C4A	-2.14	99.50	103.24
4	A	503	C2E	C3'-C2'-C1'	2.00	104.30	99.89

There are no chirality outliers.

All (1) torsion outliers are listed below:

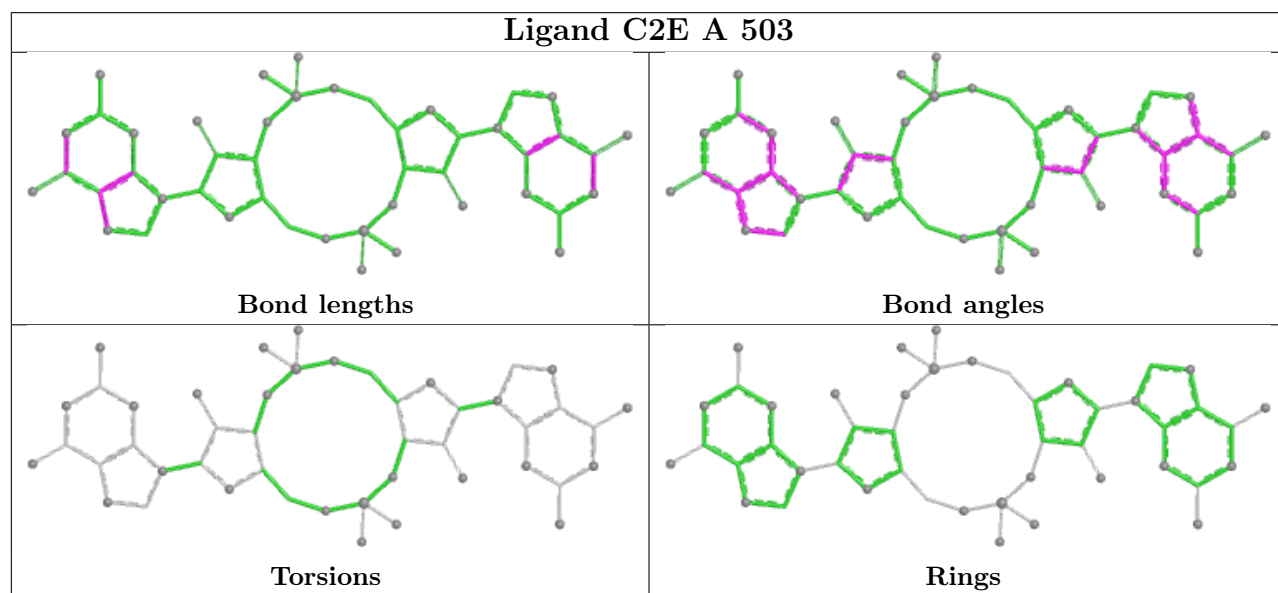
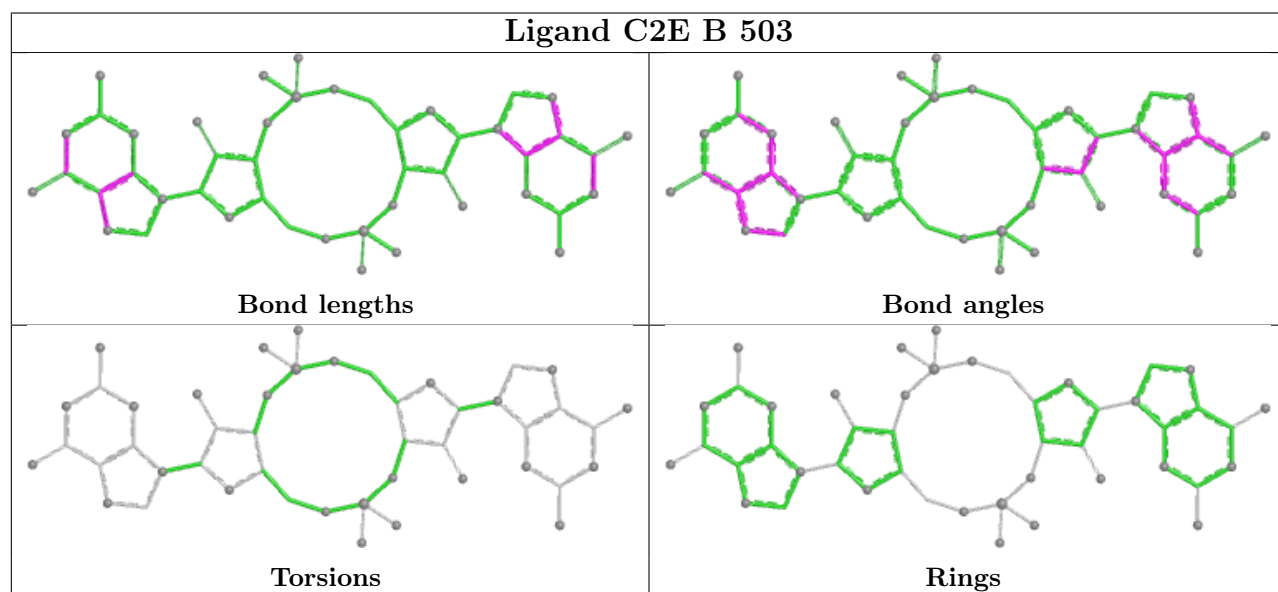
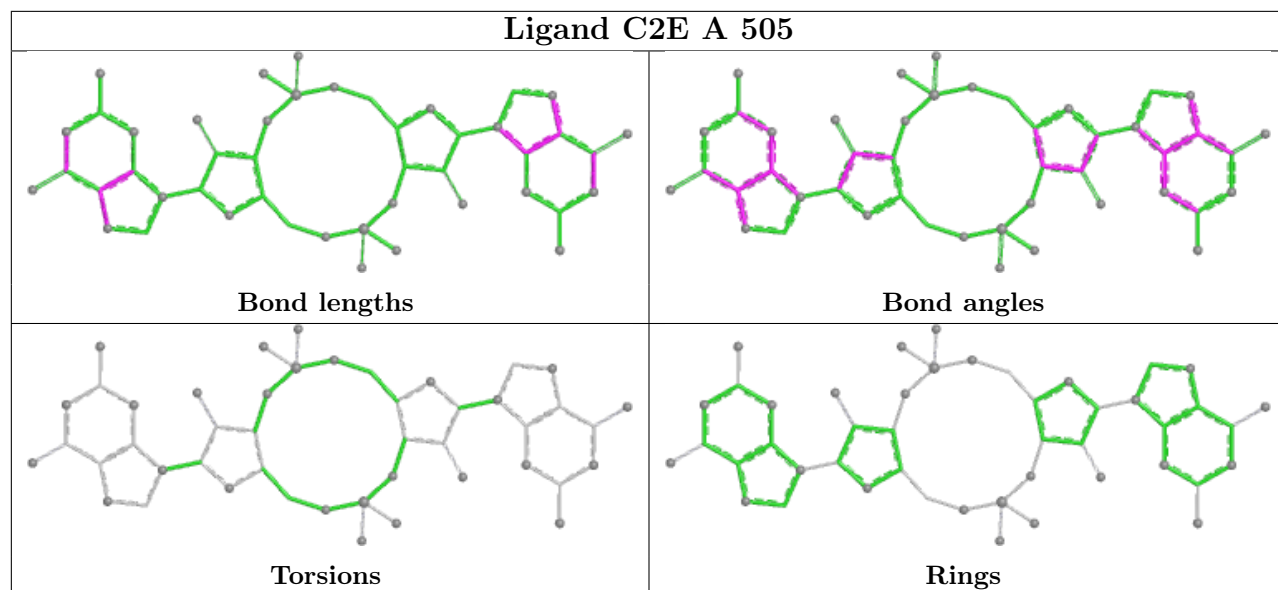
Mol	Chain	Res	Type	Atoms
4	A	501	C2E	C5A-O5A-P11-O11

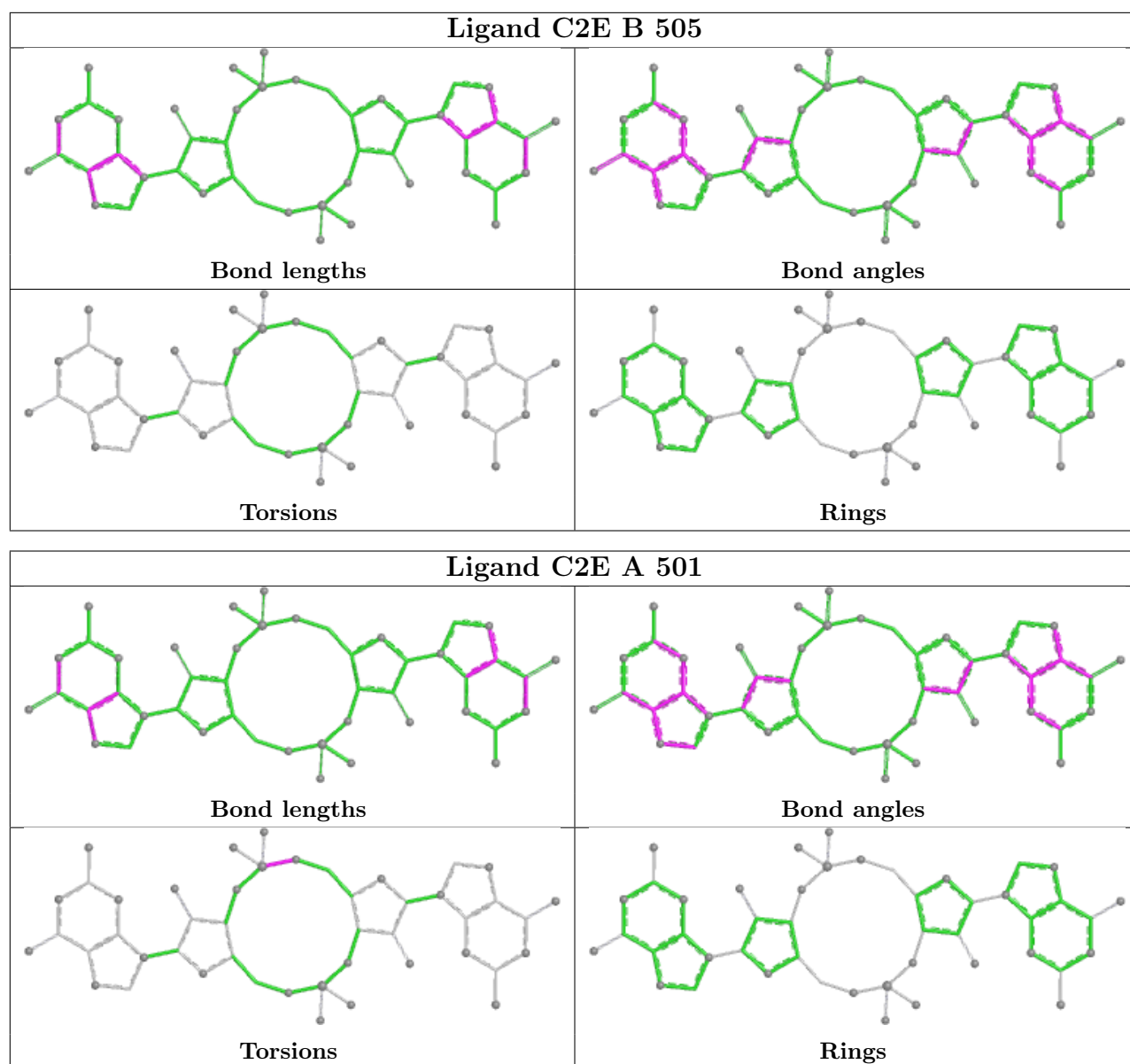
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	503	C2E	1	0
4	A	503	C2E	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	136:GLY	C	137:ARG	N	1.03
1	A	454:ALA	C	455:HIS	N	0.98
1	A	281:ASN	C	282:LEU	N	0.80
1	B	281:ASN	C	282:LEU	N	0.71
1	A	136:GLY	C	137:ARG	N	0.67

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	436/459 (94%)	0.43	25 (5%) 29 26	13, 27, 37, 44	9 (2%)
1	B	436/459 (94%)	0.95	49 (11%) 10 8	13, 27, 36, 44	9 (2%)
All	All	872/918 (94%)	0.69	74 (8%) 16 14	13, 27, 37, 44	18 (2%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	ARG	5.3
1	B	443	ALA	4.5
1	B	365	CYS	4.0
1	B	136	GLY	3.6
1	B	444	SER	3.6
1	B	135	SER	3.5
1	A	439	TYR	3.4
1	A	150	ASP	3.3
1	B	439	TYR	3.2
1	B	299	ASN	3.2
1	B	235	ASP	3.2
1	B	13	ALA	3.2
1	A	281	ASN	3.1
1	B	150	ASP	3.0
1	B	26	TYR	3.0
1	B	86	ASP	3.0
1	B	393	MET	3.0
1	A	160	ASP	2.9
1	B	57	PRO	2.8
1	B	429	ALA	2.8
1	A	408	MET	2.8
1	A	164	ARG	2.8
1	B	447	ASN	2.8
1	A	365	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	438	VAL	2.7
1	B	454	ALA	2.7
1	B	319	ASP	2.7
1	A	443	ALA	2.6
1	A	308	ASP	2.6
1	B	22	LEU	2.6
1	B	153	GLY	2.6
1	B	281	ASN	2.6
1	B	405	GLY	2.6
1	A	85	LEU	2.5
1	A	299	ASN	2.5
1	B	436	GLU	2.5
1	A	136	GLY	2.5
1	A	135	SER	2.4
1	A	404	HIS	2.4
1	A	153	GLY	2.4
1	A	317	GLY	2.4
1	A	454	ALA	2.4
1	B	396	SER	2.4
1	A	96	GLU	2.4
1	B	428	GLU	2.4
1	A	406	ARG	2.4
1	B	408	MET	2.3
1	B	404	HIS	2.2
1	A	393	MET	2.2
1	B	14	ASN	2.2
1	B	335	ASN	2.2
1	B	339	GLY	2.2
1	B	49	ILE	2.2
1	B	369	GLY	2.2
1	B	445	GLY	2.2
1	B	378	ASP	2.2
1	A	356	SER	2.2
1	B	403	ALA	2.1
1	A	318	GLY	2.1
1	B	11	ILE	2.1
1	B	336	ASP	2.1
1	B	253	SER	2.1
1	B	453	ALA	2.1
1	B	238	GLY	2.1
1	A	147	ALA	2.1
1	B	40	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	399	PRO	2.1
1	B	103	LEU	2.1
1	B	317	GLY	2.1
1	A	33	MET	2.1
1	B	147	ALA	2.0
1	B	85	LEU	2.0
1	B	61	GLY	2.0
1	A	370	GLU	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](#)

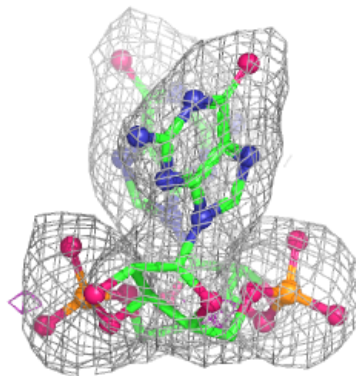
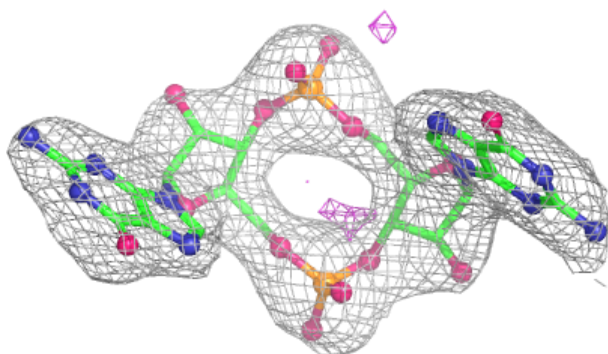
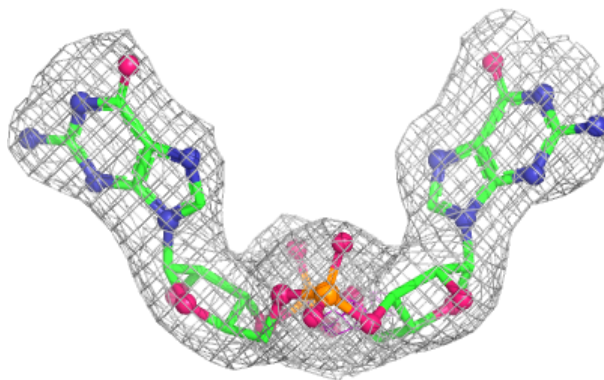
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	B	500	1/1	0.74	0.20	39,39,39,39	0
3	MG	A	500	1/1	0.82	0.13	43,43,43,43	0
4	C2E	A	501	46/46	0.92	0.12	58,61,66,68	0
2	ZN	A	499	1/1	0.93	0.17	86,86,86,86	0
4	C2E	B	503	46/46	0.95	0.09	20,24,25,27	0
4	C2E	A	503	46/46	0.96	0.09	20,24,26,27	0
4	C2E	B	505	46/46	0.96	0.08	13,21,23,24	0
4	C2E	A	505	46/46	0.97	0.07	13,21,23,24	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.

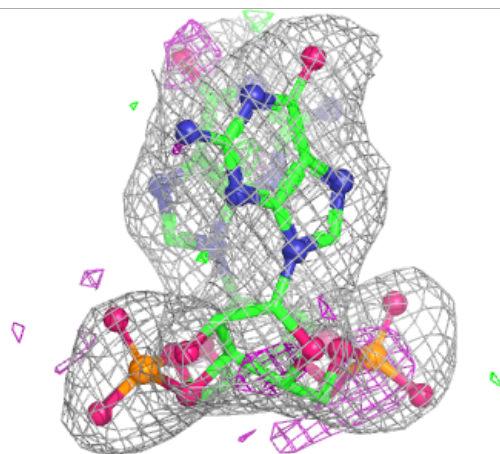
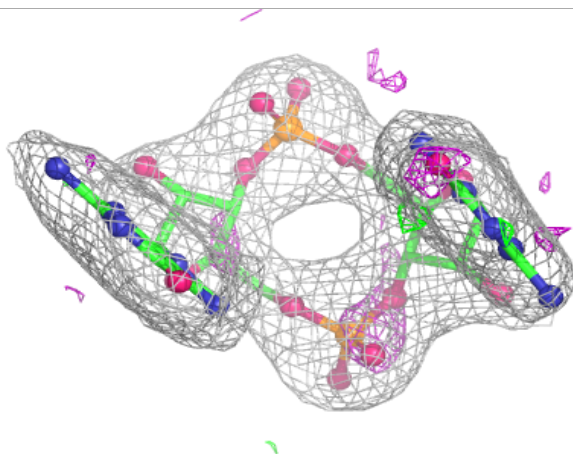
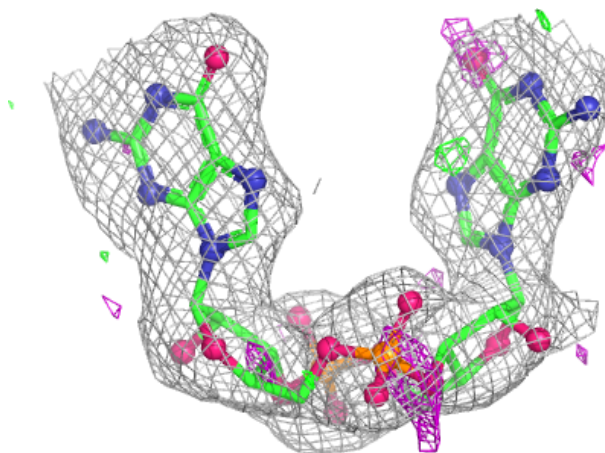
Electron density around C2E A 501:

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



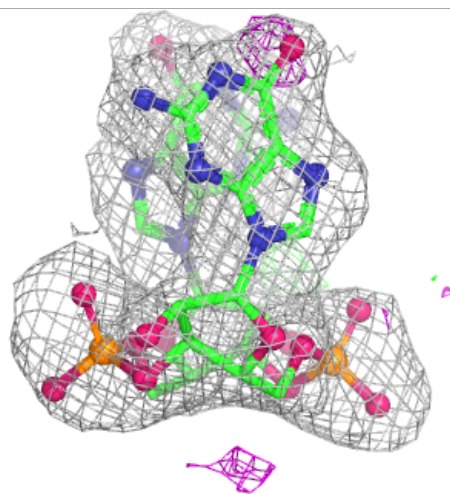
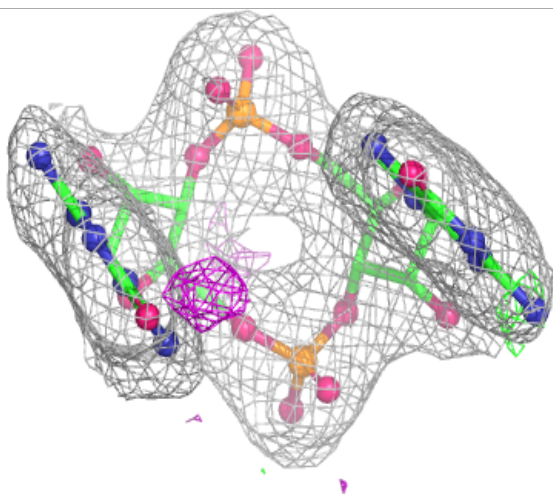
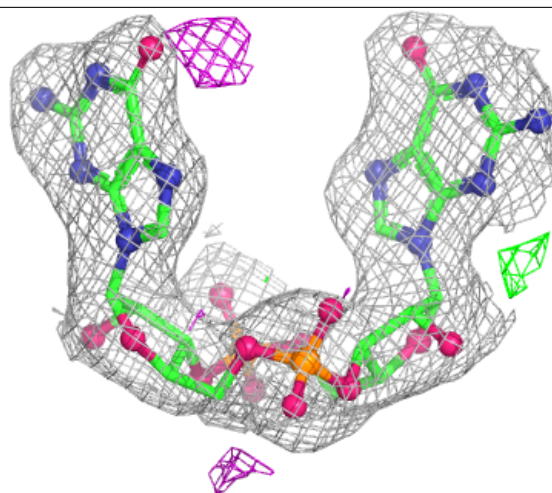
Electron density around C2E B 503:

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



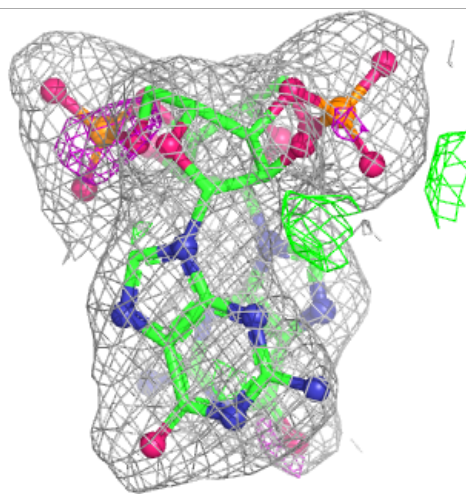
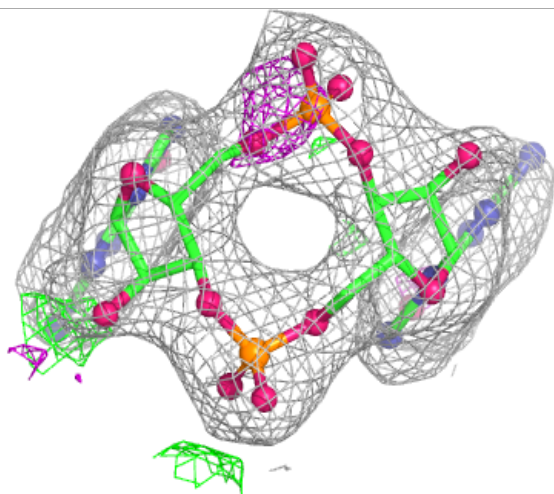
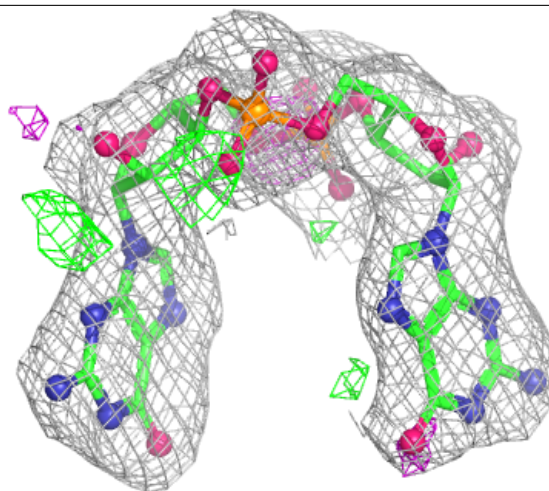
Electron density around C2E A 503:

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



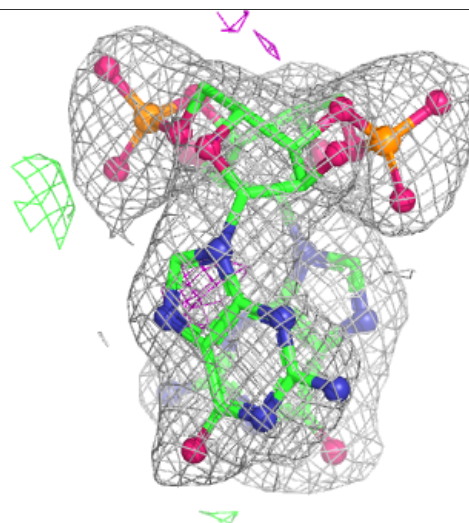
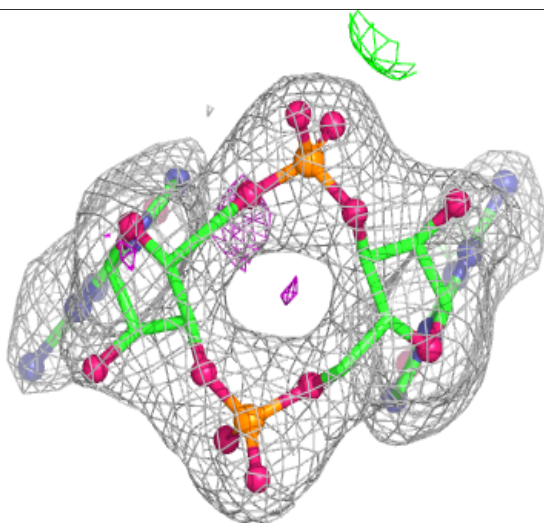
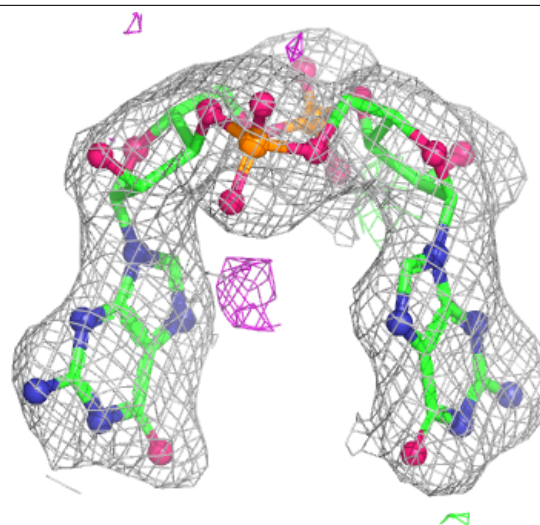
Electron density around C2E B 505:

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



Electron density around C2E A 505:

$2mF_o-DF_c$ (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.