Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2026 – 03:53 am BST

PDB ID	:	2WB4 / pdb_00002wb4
Title	:	activated diguanylate cyclase PleD in complex with c-di-GMP
Authors	:	Wassmann, P.; Schirmer, T.
Deposited on	:	2009-02-20
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

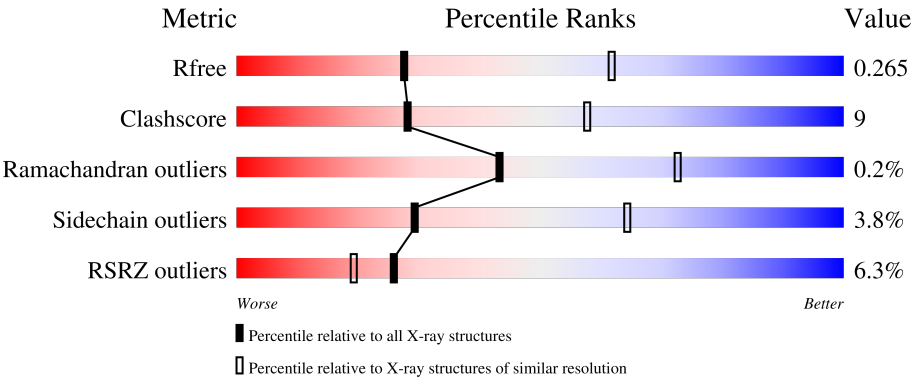
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 <=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	4% 79% 17% ·
1	B	459	8% 75% 19% · ·

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
5	SO4	A	1461	-	-	X	-

2 Entry composition (i)

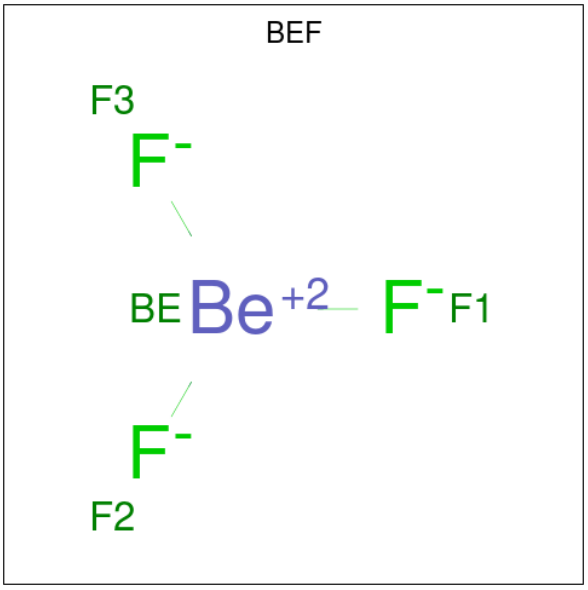
There are 6 unique types of molecules in this entry. The entry contains 7214 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIGUANYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	124	0	0
			3521	2190	651	665	15			
1	B	441	Total	C	N	O	S	78	0	0
			3387	2110	615	648	14			

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).

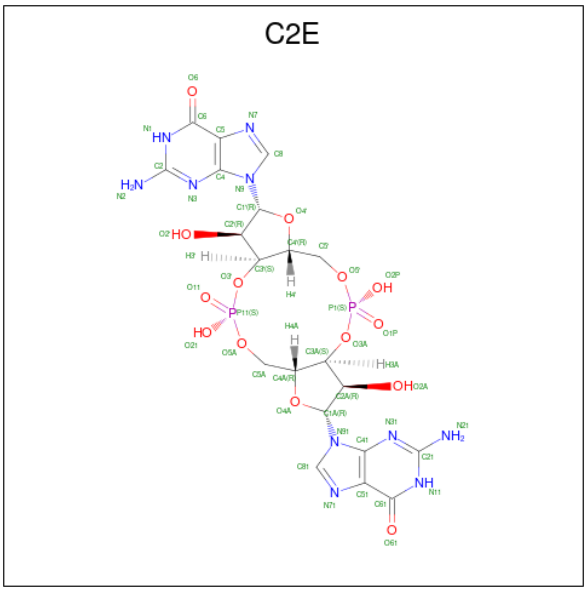


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	Be	F		0	0
			4	1	3			
2	B	1	Total	Be	F		0	0
			4	1	3			

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

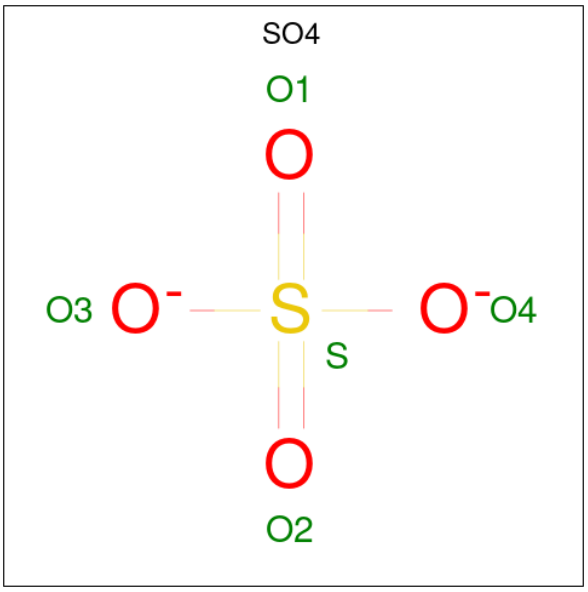
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	2	Total Mg 2 2	0	0

- Molecule 4 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidooctahydro-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: $C_{20}H_{24}N_{10}O_{14}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 46 20 10 14 2	0	0
4	A	1	Total C N O P 46 20 10 14 2	0	0
4	B	1	Total C N O P 46 20 10 14 2	0	0
4	B	1	Total C N O P 46 20 10 14 2	0	0
4	B	1	Total C N O P 46 20 10 14 2	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

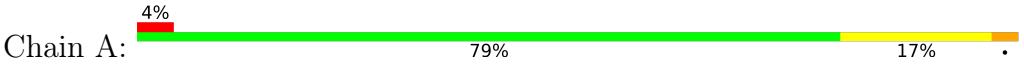
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	25	Total O 25 25	0	0
6	B	25	Total O 25 25	0	0

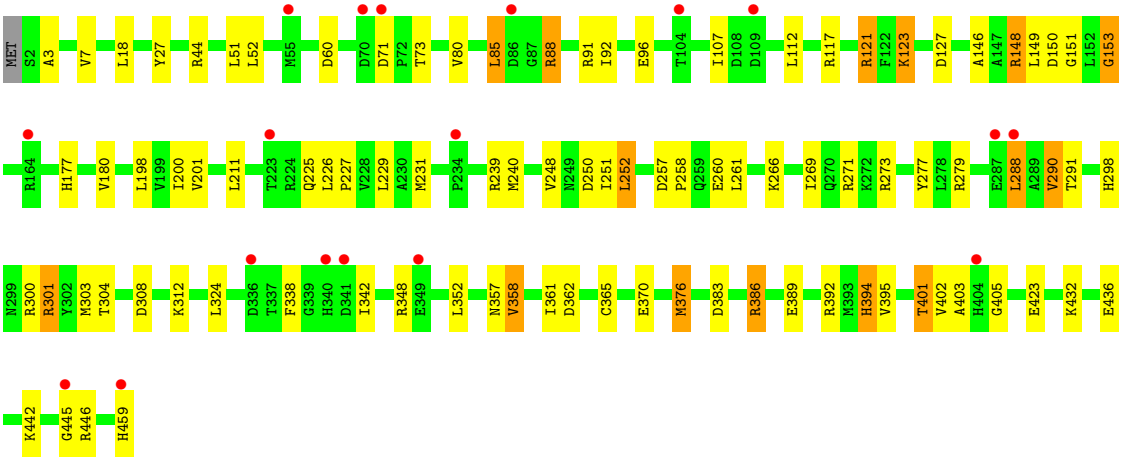
3 Residue-property plots (i)

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

• Molecule 1: DIGUANYLATE CYCLASE

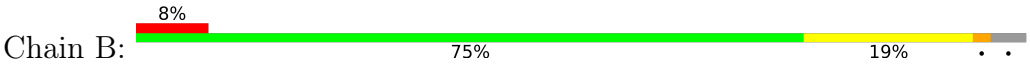
Chain A:

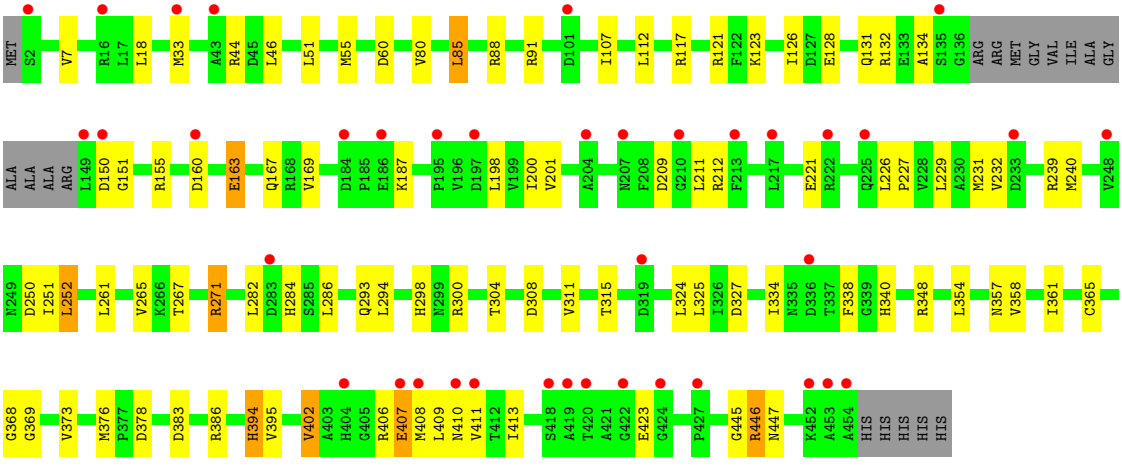




• Molecule 1: DIGUANYLATE CYCLASE

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	123.56Å 127.43Å 88.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 2.80 60.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (60.00-2.80) 94.5 (60.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.41 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.239 , 0.268 0.239 , 0.265	Depositor DCC
R_{free} test set	2170 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 29.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	7214	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, C2E, MG, BEF

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	0.98	7/3569 (0.2%)	1.18	29/4825 (0.6%)
1	B	0.99	10/3429 (0.3%)	1.13	27/4636 (0.6%)
All	All	0.98	17/6998 (0.2%)	1.15	56/9461 (0.6%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	ARG	CZ-NH1	-8.58	1.20	1.32
1	B	88	ARG	CZ-NH1	-8.56	1.20	1.32
1	B	88	ARG	CZ-NH2	-8.40	1.22	1.33
1	A	88	ARG	CZ-NH2	-7.11	1.24	1.33
1	B	160	ASP	CG-OD1	-7.03	1.11	1.25
1	A	85	LEU	CG-CD2	-6.88	1.29	1.52
1	B	293	GLN	CD-NE2	-6.45	1.19	1.33
1	B	394	HIS	N-CA	-6.12	1.39	1.46
1	A	394	HIS	CB-CG	-6.09	1.41	1.50
1	B	327	ASP	CG-OD1	6.00	1.36	1.25
1	B	293	GLN	CD-OE1	-5.77	1.12	1.23
1	A	394	HIS	CA-CB	-5.57	1.44	1.53
1	B	308	ASP	CG-OD2	5.34	1.35	1.25
1	B	46	LEU	N-CA	5.30	1.50	1.46
1	A	308	ASP	CG-OD1	5.22	1.35	1.25
1	B	85	LEU	CG-CD1	-5.05	1.35	1.52
1	A	376	MET	C-O	-5.03	1.19	1.24

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	GLY	N-CA-C	-13.65	97.78	111.56
1	A	301	ARG	CG-CD-NE	12.97	140.53	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	ARG	NE-CZ-NH1	-12.78	108.72	121.50
1	A	91	ARG	NE-CZ-NH2	12.44	130.39	119.20
1	B	163	GLU	CB-CG-CD	11.78	132.63	112.60
1	A	44	ARG	NE-CZ-NH1	-11.57	109.93	121.50
1	B	117	ARG	NE-CZ-NH2	11.51	129.56	119.20
1	A	44	ARG	NE-CZ-NH2	11.49	129.54	119.20
1	A	121	ARG	NE-CZ-NH1	-10.98	110.52	121.50
1	B	44	ARG	NE-CZ-NH2	-10.79	109.49	119.20
1	A	121	ARG	NE-CZ-NH2	10.78	128.90	119.20
1	B	121	ARG	NE-CZ-NH2	-10.74	109.54	119.20
1	B	155	ARG	CG-CD-NE	10.36	134.80	112.00
1	B	117	ARG	NE-CZ-NH1	-10.35	111.15	121.50
1	A	117	ARG	NE-CZ-NH2	-9.93	110.26	119.20
1	A	117	ARG	CD-NE-CZ	9.11	137.15	124.40
1	B	44	ARG	CD-NE-CZ	8.91	136.87	124.40
1	B	44	ARG	NE-CZ-NH1	8.74	130.24	121.50
1	B	121	ARG	CD-NE-CZ	8.62	136.46	124.40
1	B	121	ARG	NE-CZ-NH1	8.61	130.11	121.50
1	A	394	HIS	CB-CA-C	-8.57	94.77	110.63
1	B	117	ARG	CD-NE-CZ	8.50	136.30	124.40
1	A	121	ARG	CD-NE-CZ	8.40	136.16	124.40
1	A	91	ARG	CD-NE-CZ	8.34	136.08	124.40
1	A	44	ARG	CD-NE-CZ	8.24	135.93	124.40
1	A	88	ARG	NH1-CZ-NH2	-8.20	108.64	119.30
1	B	88	ARG	NH1-CZ-NH2	-7.80	109.16	119.30
1	A	394	HIS	N-CA-C	7.79	120.66	111.71
1	B	378	ASP	CA-CB-CG	7.75	120.35	112.60
1	A	117	ARG	NE-CZ-NH1	7.74	129.24	121.50
1	B	91	ARG	NE-CZ-NH2	-7.35	112.58	119.20
1	A	266	LYS	CG-CD-CE	-7.09	95.00	111.30
1	B	394	HIS	N-CA-C	6.92	118.82	111.28
1	B	187	LYS	CB-CG-CD	6.39	126.00	111.30
1	B	88	ARG	NE-CZ-NH2	6.25	124.83	119.20
1	B	410	ASN	CA-CB-CG	6.19	118.79	112.60
1	B	411	VAL	CB-CA-C	-6.08	104.66	111.23
1	B	407	GLU	N-CA-CB	-5.96	100.43	110.49
1	B	91	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	A	423	GLU	CA-CB-CG	5.74	125.59	114.10
1	B	411	VAL	N-CA-C	5.74	116.64	107.98
1	A	88	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	260	GLU	N-CA-C	-5.64	105.13	111.28
1	A	96	GLU	CB-CG-CD	-5.58	103.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	394	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	A	88	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	B	91	ARG	CD-NE-CZ	5.48	132.07	124.40
1	A	52	LEU	N-CA-C	5.44	117.29	108.26
1	B	271	ARG	CD-NE-CZ	-5.41	116.82	124.40
1	A	225	GLN	CA-CB-CG	5.36	124.81	114.10
1	A	308	ASP	CB-CG-OD1	5.34	130.68	118.40
1	B	284	HIS	CA-CB-CG	5.32	119.11	113.80
1	B	33	MET	CB-CG-SD	5.31	128.63	112.70
1	A	312	LYS	CG-CD-CE	5.25	123.38	111.30
1	A	153	GLY	N-CA-C	-5.20	102.35	112.02
1	B	327	ASP	CB-CG-OD2	5.08	130.09	118.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3521	0	3581	68	0
1	B	3387	0	3451	56	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	92	0	44	1	0
4	B	138	0	66	1	0
5	A	10	0	0	3	0
5	B	5	0	0	0	0
6	A	25	0	0	3	0
6	B	25	0	0	1	0
All	All	7214	0	7142	124	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (124) 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:324:LEU:HD13	1:A:376:MET:CE	1.73	1.17
1:A:324:LEU:CD1	1:A:376:MET:HE1	1.81	1.10
1:A:288:LEU:HD11	1:A:291:THR:OG1	1.53	1.06
1:B:324:LEU:HD13	1:B:376:MET:CE	1.89	1.01
1:A:324:LEU:HD13	1:A:376:MET:HE1	1.04	1.01
1:B:324:LEU:HD13	1:B:376:MET:HE1	1.41	1.00
1:A:240:MET:HE3	1:A:251:ILE:HG21	1.43	1.00
1:B:357:ASN:ND2	1:B:394:HIS:CE1	2.30	1.00
1:B:357:ASN:ND2	1:B:394:HIS:HE1	1.60	0.98
1:B:357:ASN:HD21	1:B:394:HIS:HE1	1.09	0.95
1:B:240:MET:HE3	1:B:251:ILE:HG21	1.55	0.89
1:B:324:LEU:CD1	1:B:376:MET:HE1	2.05	0.85
1:B:357:ASN:HD21	1:B:394:HIS:CE1	1.96	0.80
1:A:240:MET:CE	1:A:251:ILE:HG21	2.12	0.79
1:B:200:ILE:HG22	1:B:231:MET:HE2	1.67	0.75
1:B:357:ASN:CG	1:B:394:HIS:CE1	2.68	0.72
1:A:107:ILE:HD13	1:A:112:LEU:HD22	1.71	0.71
1:B:324:LEU:HD13	1:B:376:MET:HE2	1.72	0.70
4:B:507:C2E:H8	4:B:507:C2E:O5'	1.90	0.69
1:B:107:ILE:HD13	1:B:112:LEU:HD22	1.77	0.67
1:B:402:VAL:O	1:B:406:ARG:NH1	2.28	0.66
1:A:342:ILE:HG23	1:A:402:VAL:CG1	2.26	0.66
1:A:200:ILE:HG22	1:A:231:MET:HE2	1.77	0.65
1:A:288:LEU:CD1	1:A:291:THR:OG1	2.39	0.65
1:A:401:THR:O	1:A:402:VAL:HG23	1.97	0.65
4:A:505:C2E:O21	6:A:2024:HOH:O	2.13	0.64
1:A:370:GLU:OE1	6:A:2015:HOH:O	2.15	0.64
1:B:240:MET:CE	1:B:251:ILE:HG21	2.28	0.63
1:B:338:PHE:HZ	1:B:408:MET:HB2	1.65	0.61
1:A:107:ILE:CD1	1:A:112:LEU:HD22	2.30	0.61
1:A:148:ARG:HB3	1:B:340:HIS:CD2	2.36	0.61
1:A:342:ILE:HG23	1:A:402:VAL:HG13	1.83	0.60
1:A:151:GLY:HA2	1:A:269:ILE:HG22	1.83	0.60
1:A:401:THR:HG23	1:A:405:GLY:HA2	1.84	0.60
1:B:445:GLY:O	1:B:446:ARG:HB2	2.01	0.59
1:A:153:GLY:O	1:A:177:HIS:ND1	2.34	0.58
1:B:211:LEU:HD12	1:B:239:ARG:NH1	2.19	0.58
1:A:300:ARG:O	1:A:304:THR:HG23	2.03	0.58
1:A:342:ILE:CG2	1:A:402:VAL:HG11	2.35	0.57
1:A:446:ARG:NH1	5:A:1461:SO4:O2	2.38	0.57
1:A:146:ALA:HB2	1:A:277:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:ILE:O	1:B:447:ASN:HA	2.06	0.56
1:A:229:LEU:CD1	1:A:250:ASP:HB3	2.36	0.55
1:A:211:LEU:HD12	1:A:239:ARG:NH1	2.22	0.55
1:A:121:ARG:NH2	5:A:1460:SO4:O2	2.38	0.55
1:B:107:ILE:CD1	1:B:112:LEU:HD22	2.36	0.54
1:B:55:MET:SD	1:B:85:LEU:HD21	2.48	0.54
1:B:126:ILE:HD11	1:B:271:ARG:HE	1.71	0.54
1:B:200:ILE:CG2	1:B:231:MET:HE2	2.36	0.54
1:B:229:LEU:CD1	1:B:250:ASP:HB3	2.38	0.53
1:B:315:THR:HB	1:B:423:GLU:HA	1.91	0.53
1:A:88:ARG:HH11	1:A:92:ILE:HD11	1.73	0.53
1:A:389:GLU:OE2	1:A:392:ARG:NH1	2.43	0.52
1:B:338:PHE:CZ	1:B:408:MET:HB2	2.44	0.52
1:B:294:LEU:HD12	1:B:348:ARG:HH21	1.75	0.51
1:A:298:HIS:O	1:A:365:CYS:HB2	2.11	0.50
1:A:291:THR:HG23	6:A:2010:HOH:O	2.11	0.50
1:A:240:MET:HE3	1:A:251:ILE:CG2	2.30	0.50
1:A:229:LEU:HD12	1:A:250:ASP:O	2.12	0.49
1:A:402:VAL:CG1	1:A:403:ALA:N	2.75	0.49
1:B:325:LEU:HD13	1:B:373:VAL:HG22	1.95	0.49
1:A:383:ASP:OD1	1:A:386:ARG:NH2	2.39	0.49
1:A:123:LYS:O	1:A:127:ASP:CB	2.61	0.49
1:A:402:VAL:HG12	1:A:403:ALA:N	2.27	0.49
1:B:126:ILE:HD11	1:B:271:ARG:NE	2.27	0.49
1:A:226:LEU:HD12	1:A:227:PRO:HD2	1.95	0.49
1:A:401:THR:C	1:A:402:VAL:HG23	2.37	0.49
1:A:342:ILE:HG23	1:A:402:VAL:HG11	1.92	0.48
1:B:338:PHE:HZ	1:B:408:MET:CB	2.25	0.48
1:B:354:LEU:O	1:B:358:VAL:HG22	2.14	0.47
1:A:432:LYS:O	1:A:436:GLU:HG2	2.14	0.47
1:B:232:VAL:CG2	1:B:251:ILE:HG23	2.44	0.47
1:B:298:HIS:O	1:B:365:CYS:HB2	2.15	0.47
1:A:348:ARG:O	1:A:352:LEU:CD1	2.62	0.47
1:A:348:ARG:O	1:A:352:LEU:HD13	2.15	0.47
1:B:163:GLU:O	1:B:167:GLN:HG2	2.14	0.47
1:B:383:ASP:OD1	1:B:386:ARG:NH2	2.41	0.46
1:A:290:VAL:O	1:A:290:VAL:CG1	2.64	0.46
1:A:342:ILE:CG2	1:A:402:VAL:CG1	2.91	0.46
1:B:334:ILE:HG12	1:B:409:LEU:HD21	1.98	0.46
1:A:442:LYS:NZ	5:A:1461:SO4:O1	2.36	0.46
1:B:232:VAL:HG22	1:B:251:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ARG:C	1:B:408:MET:H	2.25	0.45
1:A:88:ARG:HD2	1:A:257:ASP:OD2	2.16	0.45
1:B:229:LEU:HD12	1:B:250:ASP:O	2.16	0.45
1:A:258:PRO:O	1:A:261:LEU:HB3	2.17	0.45
1:B:7:VAL:HG13	1:B:18:LEU:HD23	1.99	0.45
1:A:146:ALA:O	1:A:149:LEU:HD23	2.17	0.44
1:A:342:ILE:HG21	1:A:402:VAL:HG11	1.99	0.44
1:A:358:VAL:HG13	1:A:362:ASP:OD2	2.17	0.44
1:A:229:LEU:HG	1:A:252:LEU:HD12	1.99	0.44
1:A:401:THR:O	1:A:402:VAL:CG2	2.63	0.44
1:B:51:LEU:HD23	1:B:80:VAL:HB	2.00	0.44
1:A:123:LYS:O	1:A:127:ASP:HB2	2.18	0.44
1:A:279:ARG:NH1	1:B:128:GLU:CD	2.76	0.44
1:A:338:PHE:HB3	1:A:342:ILE:HD12	2.00	0.44
1:A:71:ASP:OD2	1:A:73:THR:HB	2.18	0.44
1:B:7:VAL:CG1	1:B:18:LEU:HD23	2.48	0.44
1:A:229:LEU:HD13	1:A:250:ASP:HB3	1.99	0.43
1:A:7:VAL:HG13	1:A:18:LEU:HD23	2.01	0.43
1:B:229:LEU:HG	1:B:252:LEU:CD1	2.49	0.43
1:B:300:ARG:HD3	6:B:2019:HOH:O	2.19	0.43
1:A:60:ASP:OD1	1:A:60:ASP:C	2.61	0.42
1:B:60:ASP:C	1:B:60:ASP:OD1	2.61	0.42
1:B:169:VAL:HG13	1:B:261:LEU:HD21	2.01	0.42
1:A:200:ILE:CG2	1:A:231:MET:HE2	2.45	0.42
1:B:300:ARG:O	1:B:304:THR:HG23	2.19	0.42
1:B:150:ASP:OD1	1:B:151:GLY:N	2.50	0.42
1:B:229:LEU:HD13	1:B:250:ASP:HB3	2.00	0.42
1:B:209:ASP:HB3	1:B:212:ARG:HB3	2.02	0.41
1:B:226:LEU:HD12	1:B:227:PRO:HD2	2.02	0.41
1:A:7:VAL:CG1	1:A:18:LEU:HD23	2.50	0.41
1:A:149:LEU:HD13	1:A:149:LEU:HA	1.92	0.41
1:A:3:ALA:HB3	1:A:27:TYR:CD1	2.55	0.41
1:B:368:GLY:O	1:B:369:GLY:C	2.64	0.41
1:A:357:ASN:OD1	1:A:394:HIS:CE1	2.74	0.41
1:A:51:LEU:HD23	1:A:80:VAL:HB	2.02	0.41
1:A:149:LEU:HD12	1:A:273:ARG:HB3	2.03	0.41
1:A:303:MET:HG3	1:A:365:CYS:SG	2.60	0.41
1:B:198:LEU:CD2	1:B:265:VAL:HG22	2.50	0.41
1:A:150:ASP:OD2	1:A:150:ASP:C	2.64	0.40
1:B:311:VAL:O	1:B:315:THR:HG23	2.21	0.40
1:B:131:GLN:O	1:B:134:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD12	1:A:227:PRO:O	2.22	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	456/459 (99%)	444 (97%)	12 (3%)	0	100	100
1	B	437/459 (95%)	422 (97%)	13 (3%)	2 (0%)	24	55
All	All	893/918 (97%)	866 (97%)	25 (3%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	446	ARG
1	B	407	GLU

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	373/374 (100%)	356 (95%)	17 (5%)	24	58
1	B	362/374 (97%)	351 (97%)	11 (3%)	36	72
All	All	735/748 (98%)	707 (96%)	28 (4%)	29	64

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	123	LYS
1	A	148	ARG
1	A	180	VAL
1	A	201	VAL
1	A	248	VAL
1	A	252	LEU
1	A	271	ARG
1	A	288	LEU
1	A	290	VAL
1	A	301	ARG
1	A	358	VAL
1	A	361	ILE
1	A	386	ARG
1	A	395	VAL
1	A	401	THR
1	A	459	HIS
1	B	123	LYS
1	B	132	ARG
1	B	201	VAL
1	B	221	GLU
1	B	252	LEU
1	B	267	THR
1	B	282	LEU
1	B	286	LEU
1	B	361	ILE
1	B	395	VAL
1	B	402	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	93	GLN
1	A	162	ASN
1	A	280	ASN
1	A	394	HIS
1	A	459	HIS
1	B	76	HIS
1	B	93	GLN
1	B	357	ASN

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Mol	Chain	Res	Type
1	B	394	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	1.14	3 (5%)	80,82,82	1.74	19 (23%)
4	C2E	B	505	-	52,52,52	1.24	7 (13%)	80,82,82	1.72	20 (25%)
5	SO4	B	1455	-	4,4,4	0.30	0	6,6,6	0.25	0
2	BEF	B	501	1	0,3,3	-	-	-		
4	C2E	A	503	-	52,52,52	1.20	5 (9%)	80,82,82	1.62	16 (20%)
4	C2E	B	503	-	52,52,52	1.10	5 (9%)	80,82,82	1.83	20 (25%)
2	BEF	A	501	1	0,3,3	-	-	-		
5	SO4	A	1461	-	4,4,4	0.13	0	6,6,6	0.44	0
4	C2E	B	507	3	52,52,52	1.06	5 (9%)	80,82,82	1.77	23 (28%)
5	SO4	A	1460	-	4,4,4	0.30	0	6,6,6	0.83	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
4	C2E	A	505	-	-	0/30/62/62	0/6/7/7
4	C2E	B	505	-	-	1/30/62/62	0/6/7/7
4	C2E	A	503	-	-	3/30/62/62	0/6/7/7
4	C2E	B	503	-	-	0/30/62/62	0/6/7/7
4	C2E	B	507	3	-	0/30/62/62	0/6/7/7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	C2E	C6-N1	-4.05	1.31	1.38
4	A	505	C2E	C61-N11	-3.89	1.31	1.38
4	B	505	C2E	C61-N11	-3.88	1.31	1.38
4	A	503	C2E	C61-N11	-3.42	1.32	1.38
4	B	503	C2E	C6-N1	-2.83	1.33	1.38
4	B	505	C2E	C51-N71	-2.83	1.33	1.39
4	B	505	C2E	C21-N11	-2.66	1.31	1.37
4	A	505	C2E	C6-N1	-2.60	1.34	1.38
4	A	503	C2E	C41-N91	-2.55	1.31	1.38
4	B	507	C2E	C51-N71	-2.51	1.34	1.39
4	B	505	C2E	C6-N1	-2.47	1.34	1.38
4	B	505	C2E	C41-N91	-2.39	1.31	1.38
4	B	503	C2E	C5-N7	-2.39	1.34	1.39
4	B	507	C2E	C5-N7	-2.34	1.34	1.39
4	B	503	C2E	C61-N11	-2.29	1.34	1.38
4	A	505	C2E	C5-N7	-2.28	1.34	1.39
4	B	505	C2E	C5-N7	-2.24	1.34	1.39
4	A	503	C2E	C51-N71	-2.22	1.34	1.39
4	B	505	C2E	C51-C61	-2.16	1.36	1.44
4	B	503	C2E	C21-N31	2.14	1.38	1.33
4	B	507	C2E	C6-N1	-2.12	1.34	1.38
4	B	507	C2E	C4-N9	-2.09	1.32	1.38
4	B	507	C2E	C81-N71	2.06	1.38	1.32
4	B	503	C2E	C4-N9	-2.04	1.32	1.38
4	A	503	C2E	C2-N1	-2.02	1.32	1.37

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	C2E	C5-C4-N3	-5.83	119.01	128.46
4	B	505	C2E	C5-C4-N3	-5.74	119.14	128.46
4	B	503	C2E	C51-C41-N31	-5.53	119.49	128.46
4	B	503	C2E	C5-C4-N3	-5.30	119.87	128.46
4	A	505	C2E	C5-C4-N3	-5.22	120.00	128.46
4	A	505	C2E	C51-C41-N31	-5.02	120.31	128.46
4	B	507	C2E	C5-C4-N3	-4.95	120.43	128.46
4	B	505	C2E	C51-C41-N31	-4.91	120.49	128.46
4	A	503	C2E	C51-C41-N31	-4.83	120.63	128.46
4	B	507	C2E	C51-C41-N31	-4.63	120.95	128.46
4	B	503	C2E	C21-N31-C41	4.11	119.62	112.30
4	B	505	C2E	C2-N3-C4	4.09	119.59	112.30
4	B	507	C2E	C21-N31-C41	4.06	119.53	112.30
4	B	503	C2E	C3'-C2'-C1'	3.99	108.72	99.89
4	A	503	C2E	C2-N3-C4	3.95	119.34	112.30
4	B	503	C2E	C2-N3-C4	3.83	119.12	112.30
4	B	503	C2E	N91-C41-N31	3.81	133.59	125.94
4	A	505	C2E	C21-N31-C41	3.75	118.98	112.30
4	A	505	C2E	C2-N3-C4	3.72	118.93	112.30
4	B	507	C2E	N9-C4-N3	3.57	133.10	125.94
4	A	503	C2E	N9-C4-N3	3.39	132.75	125.94
4	B	503	C2E	C3A-C2A-C1A	3.27	107.14	99.89
4	B	507	C2E	O6-C6-C5	-3.27	117.92	126.60
4	B	507	C2E	C2'-C1'-N9	-3.27	103.95	113.22
4	A	505	C2E	C3A-C2A-C1A	3.21	107.00	99.89
4	B	505	C2E	C2-N1-C6	-3.21	119.25	125.10
4	A	503	C2E	C21-N31-C41	3.19	117.99	112.30
4	A	505	C2E	N9-C4-N3	3.13	132.23	125.94
4	B	505	C2E	C5-C6-N1	3.12	121.12	113.19
4	A	505	C2E	C51-C61-N11	3.10	121.06	113.19
4	B	507	C2E	C2-N3-C4	3.07	117.77	112.30
4	B	503	C2E	N9-C4-N3	3.02	131.99	125.94
4	B	505	C2E	C3'-C2'-C1'	2.99	106.52	99.89
4	B	505	C2E	N9-C4-N3	2.97	131.90	125.94
4	A	505	C2E	C3'-C2'-C1'	2.94	106.39	99.89
4	B	507	C2E	O5A-P11-O11	-2.93	97.61	109.07
4	B	507	C2E	C3A-C2A-C1A	2.92	106.36	99.89
4	B	505	C2E	N91-C41-N31	2.90	131.77	125.94
4	B	503	C2E	C2'-C3'-C4'	-2.88	98.12	103.22
4	A	503	C2E	N91-C41-N31	2.88	131.71	125.94
4	A	505	C2E	C2A-C3A-C4A	-2.84	98.18	103.22
4	B	507	C2E	C2-N1-C6	-2.84	119.92	125.10
4	A	505	C2E	N91-C41-N31	2.79	131.54	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503	C2E	O6-C6-N1	-2.74	114.87	120.12
4	A	505	C2E	C21-N11-C61	-2.73	120.12	125.10
4	B	505	C2E	O5A-C5A-C4A	2.66	118.13	108.99
4	B	505	C2E	O6-C6-C5	-2.65	119.57	126.60
4	B	505	C2E	C21-N31-C41	2.63	116.98	112.30
4	A	503	C2E	C5-C6-N1	2.61	119.83	113.19
4	B	503	C2E	N91-C81-N71	-2.61	108.47	113.39
4	B	507	C2E	P11-O3'-C3'	-2.61	109.91	119.41
4	B	507	C2E	O4A-C1A-N91	2.60	114.31	108.36
4	B	505	C2E	C3A-C2A-C1A	2.56	105.56	99.89
4	B	507	C2E	P1-O3A-C3A	-2.54	110.17	119.41
4	A	503	C2E	P1-O3A-C3A	-2.50	110.30	119.41
4	A	503	C2E	P11-O3'-C3'	-2.50	110.33	119.41
4	B	503	C2E	C51-C61-N11	2.47	119.47	113.19
4	A	503	C2E	C3'-C2'-C1'	2.47	105.36	99.89
4	A	505	C2E	P11-O3'-C3'	-2.45	110.49	119.41
4	B	507	C2E	C3'-C2'-C1'	2.44	105.30	99.89
4	B	503	C2E	C5-C6-N1	2.44	119.39	113.19
4	A	505	C2E	N91-C81-N71	-2.40	108.86	113.39
4	B	505	C2E	P1-O3A-C3A	-2.39	110.72	119.41
4	B	505	C2E	P11-O3'-C3'	-2.38	110.74	119.41
4	A	505	C2E	O6-C6-C5	-2.37	120.32	126.60
4	B	505	C2E	C51-C61-N11	2.34	119.14	113.19
4	B	507	C2E	C5-C6-N1	2.34	119.12	113.19
4	B	503	C2E	C2A-C3A-C4A	-2.33	99.10	103.22
4	B	507	C2E	O61-C61-C51	-2.31	120.46	126.60
4	A	505	C2E	P1-O3A-C3A	-2.29	111.07	119.41
4	A	503	C2E	N9-C8-N7	-2.27	109.11	113.39
4	B	503	C2E	O4'-C1'-N9	2.26	113.53	108.36
4	B	503	C2E	P11-O3'-C3'	-2.25	111.21	119.41
4	B	507	C2E	C51-C61-N11	2.24	118.87	113.19
4	A	505	C2E	C2-N1-C6	-2.24	121.02	125.10
4	B	503	C2E	P1-O3A-C3A	-2.23	111.30	119.41
4	A	505	C2E	C5-C6-N1	2.22	118.83	113.19
4	B	505	C2E	C21-N11-C61	-2.22	121.06	125.10
4	B	503	C2E	C2-N1-C6	-2.19	121.10	125.10
4	B	505	C2E	O61-C61-C51	-2.17	120.83	126.60
4	B	507	C2E	C61-C51-N71	2.17	134.29	130.25
4	B	505	C2E	O4A-C1A-N91	2.16	113.30	108.36
4	A	503	C2E	C4-C5-N7	-2.14	107.33	110.72
4	B	507	C2E	N9-C8-N7	-2.14	109.36	113.39
4	B	507	C2E	O21-P11-O11	2.14	122.83	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	505	C2E	C2A-C1A-N91	-2.13	107.17	113.22
4	B	507	C2E	C21-N11-C61	-2.11	121.26	125.10
4	B	507	C2E	C41-C51-N71	-2.10	107.39	110.72
4	A	503	C2E	C51-C61-N11	2.10	118.51	113.19
4	A	503	C2E	C2'-C3'-C4'	-2.09	99.51	103.22
4	B	503	C2E	O5A-P11-O11	-2.07	100.96	109.07
4	B	507	C2E	C51-C41-N91	2.07	109.39	105.63
4	B	503	C2E	N9-C8-N7	-2.07	109.50	113.39
4	A	505	C2E	N9-C8-N7	-2.04	109.55	113.39
4	B	503	C2E	C4-C5-N7	-2.03	107.50	110.72
4	A	505	C2E	O5'-P1-O1P	-2.01	101.23	109.07
4	B	505	C2E	C4-C5-N7	-2.01	107.55	110.72
4	A	503	C2E	C21-N11-C61	-2.01	121.44	125.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	C2E	C5A-O5A-P11-O11
4	A	503	C2E	O4A-C4A-C5A-O5A
4	A	503	C2E	C3A-C4A-C5A-O5A
4	B	505	C2E	C3'-O3'-P11-O5A

There are no ring outliers.

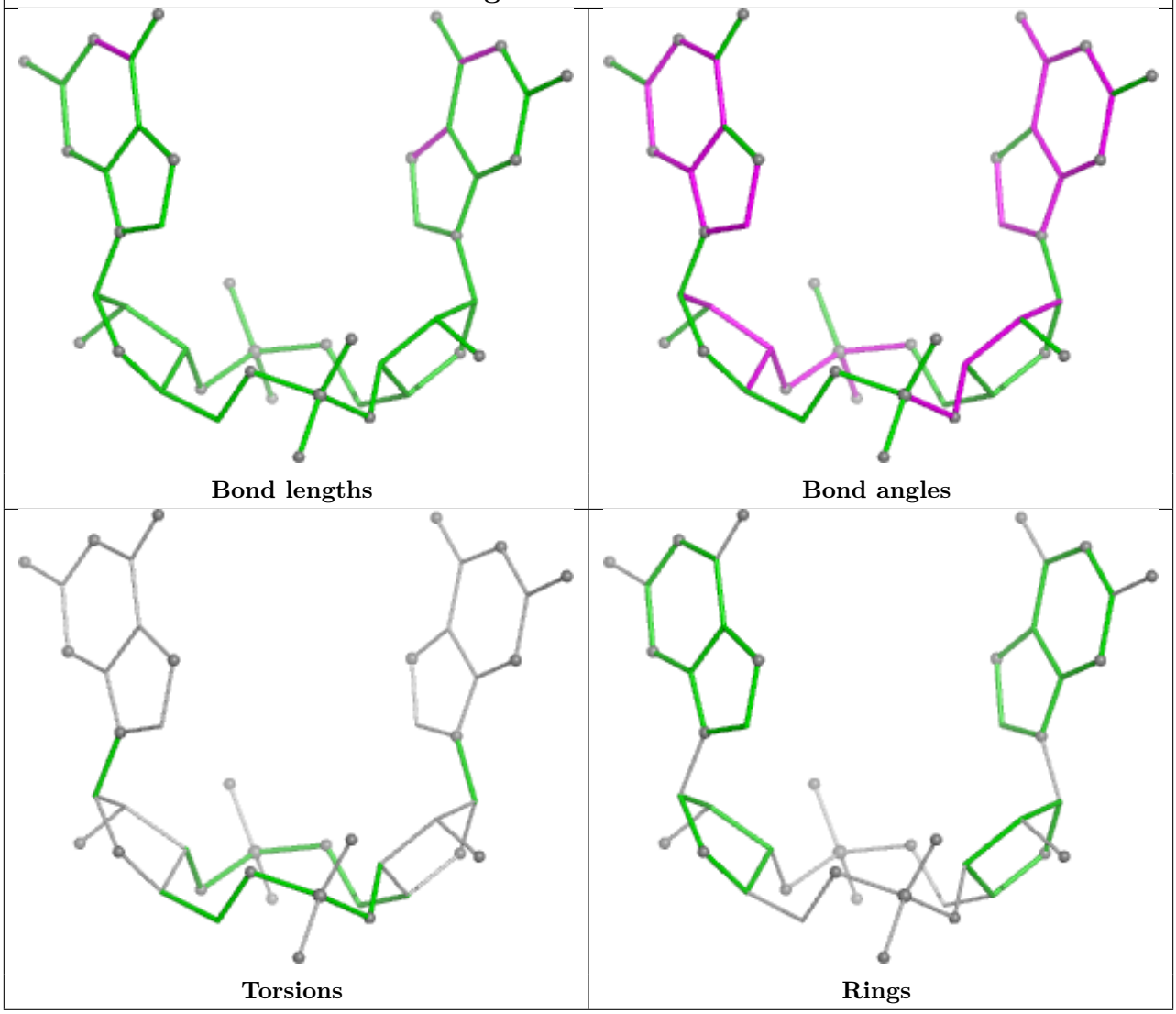
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	505	C2E	1	0
5	A	1461	SO4	2	0
4	B	507	C2E	1	0
5	A	1460	SO4	1	0

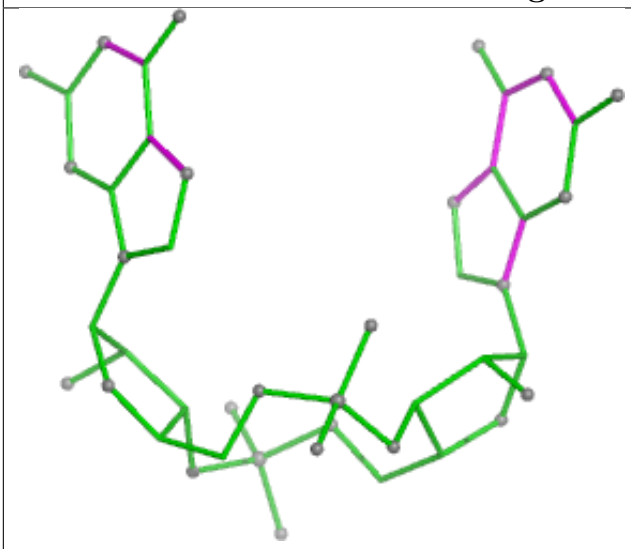
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

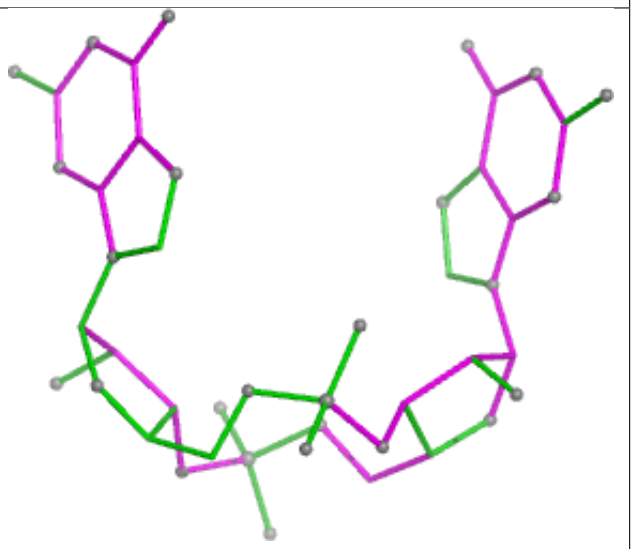
Ligand C2E A 505



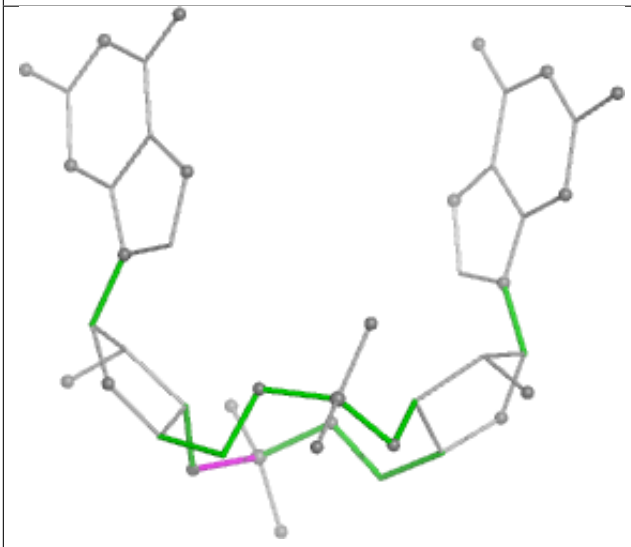
Ligand C2E B 505



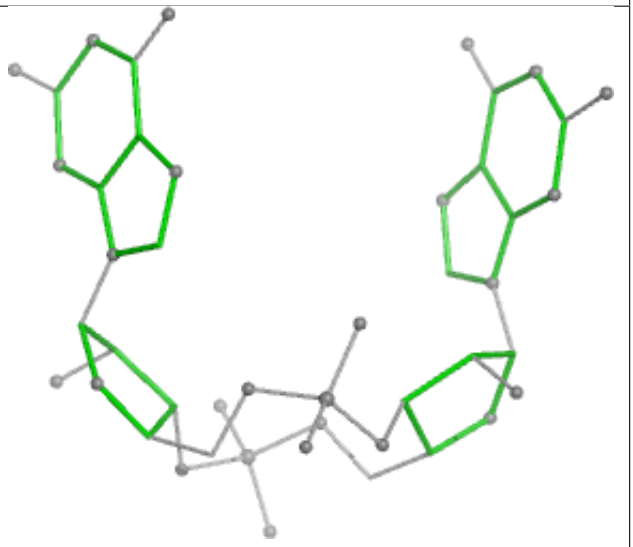
Bond lengths



Bond angles

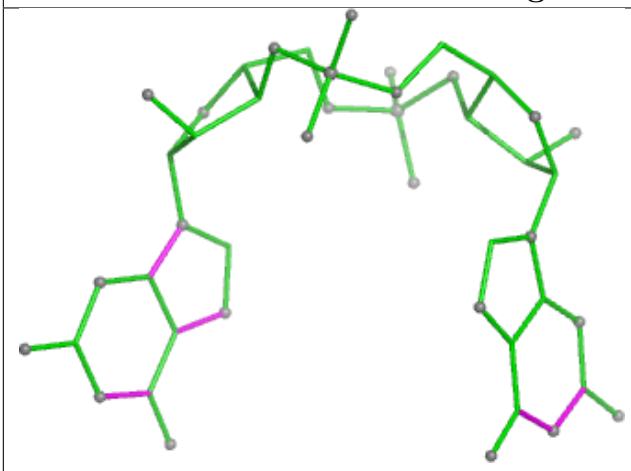


Torsions

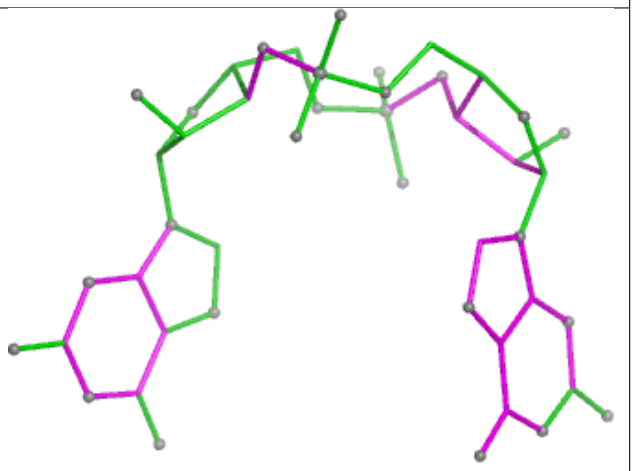


Rings

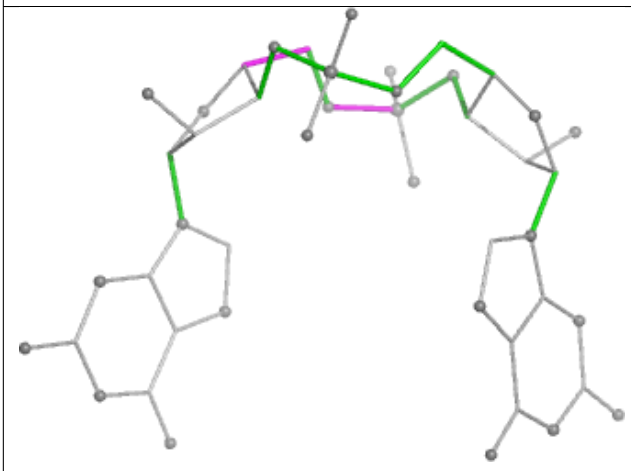
Ligand C2E A 503



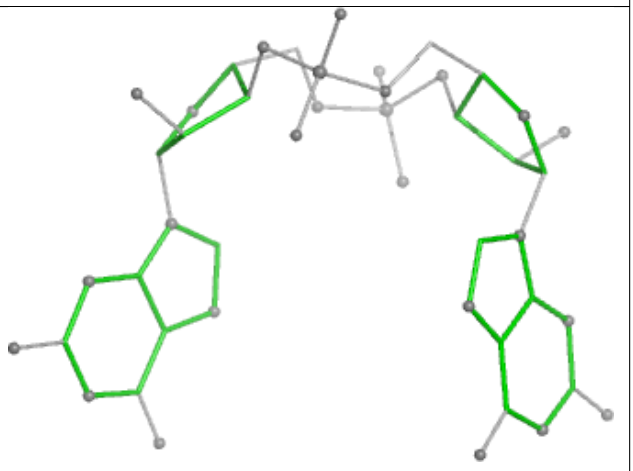
Bond lengths



Bond angles

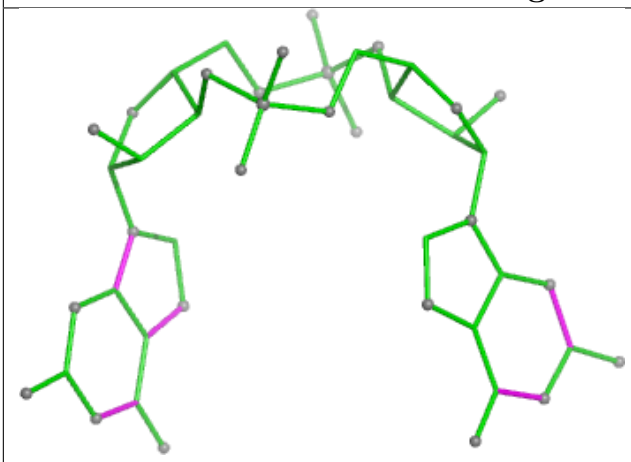


Torsions

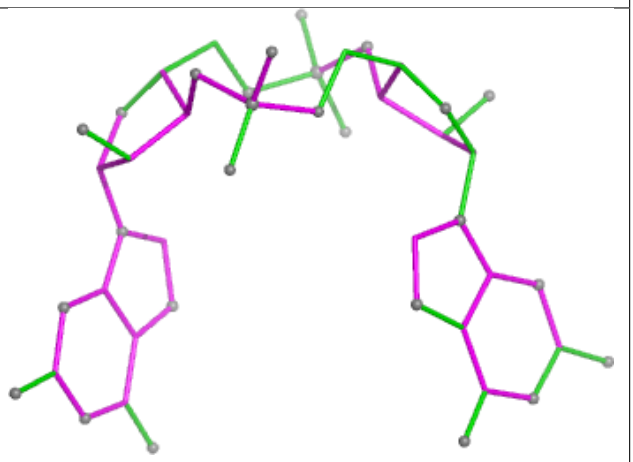


Rings

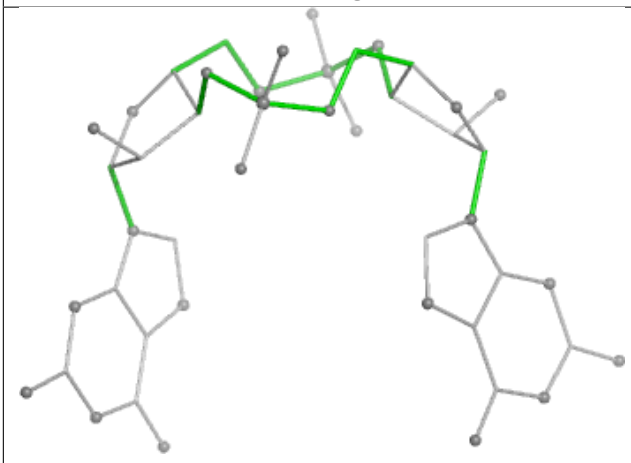
Ligand C2E B 503



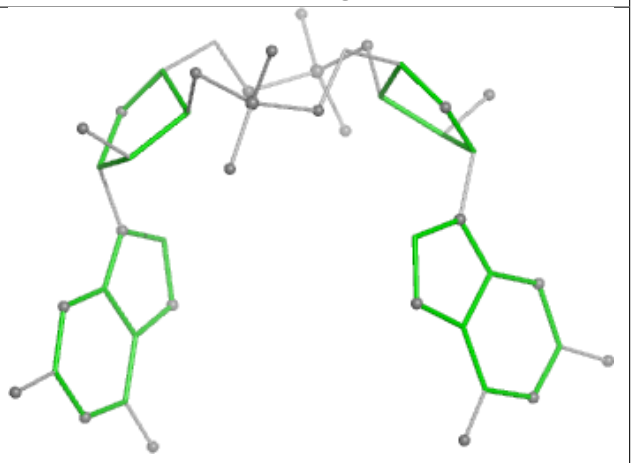
Bond lengths



Bond angles

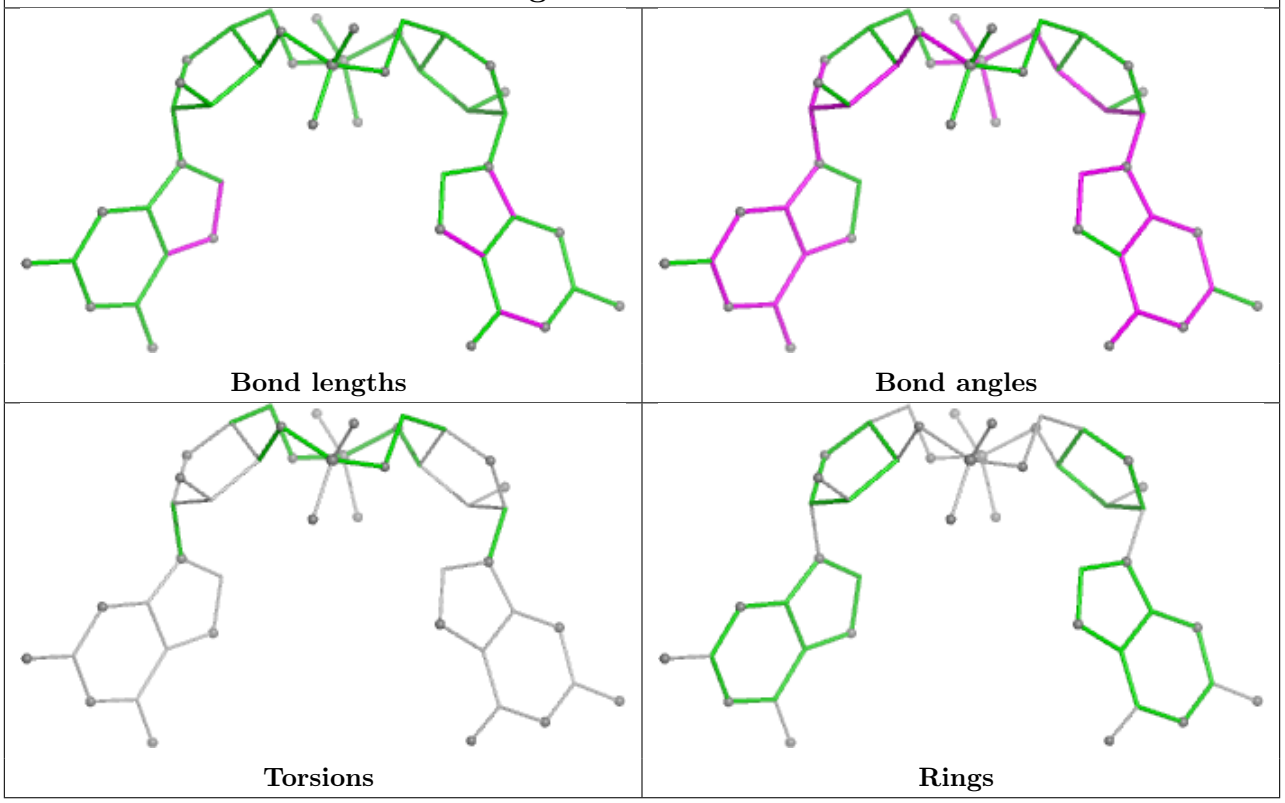


Torsions



Rings

Ligand C2E B 507



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, 95^{th} 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	458/459 (99%)	0.47	18 (3%)	43	34	2, 12, 21, 37	40 (8%)
1	B	441/459 (96%)	0.67	39 (8%)	15	11	2, 13, 27, 50	29 (6%)
All	All	899/918 (97%)	0.57	57 (6%)	26	19	2, 13, 25, 50	69 (7%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	ASN	4.0
1	B	186	GLU	3.9
1	B	150	ASP	3.6
1	B	149	LEU	3.5
1	B	452	LYS	3.3
1	B	422	GLY	3.1
1	B	454	ALA	3.1
1	B	217	LEU	3.1
1	A	341	ASP	3.0
1	B	222	ARG	2.9
1	B	407	GLU	2.8
1	A	288	LEU	2.8
1	A	70	ASP	2.8
1	A	164	ARG	2.7
1	B	135	SER	2.7
1	B	207	ASN	2.7
1	A	336	ASP	2.6
1	B	453	ALA	2.6
1	A	404	HIS	2.6
1	A	55	MET	2.6
1	B	319	ASP	2.5
1	B	424	GLY	2.5
1	A	86	ASP	2.5
1	A	234	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	210	GLY	2.4
1	B	418	SER	2.4
1	A	109	ASP	2.4
1	B	213	PHE	2.4
1	A	287	GLU	2.4
1	B	195	PRO	2.3
1	B	160	ASP	2.3
1	B	419	ALA	2.3
1	B	404	HIS	2.3
1	A	104	THR	2.3
1	B	197	ASP	2.2
1	B	43	ALA	2.2
1	A	223	THR	2.2
1	B	2	SER	2.2
1	A	445	GLY	2.1
1	A	71	ASP	2.1
1	B	225	GLN	2.1
1	A	459	HIS	2.1
1	B	184	ASP	2.1
1	B	336	ASP	2.1
1	B	420	THR	2.1
1	B	16	ARG	2.1
1	A	340	HIS	2.1
1	B	248	VAL	2.1
1	B	427	PRO	2.1
1	B	283	ASP	2.1
1	B	408	MET	2.0
1	A	349	GLU	2.0
1	B	411	VAL	2.0
1	B	204	ALA	2.0
1	B	101	ASP	2.0
1	B	233	ASP	2.0
1	B	33	MET	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)

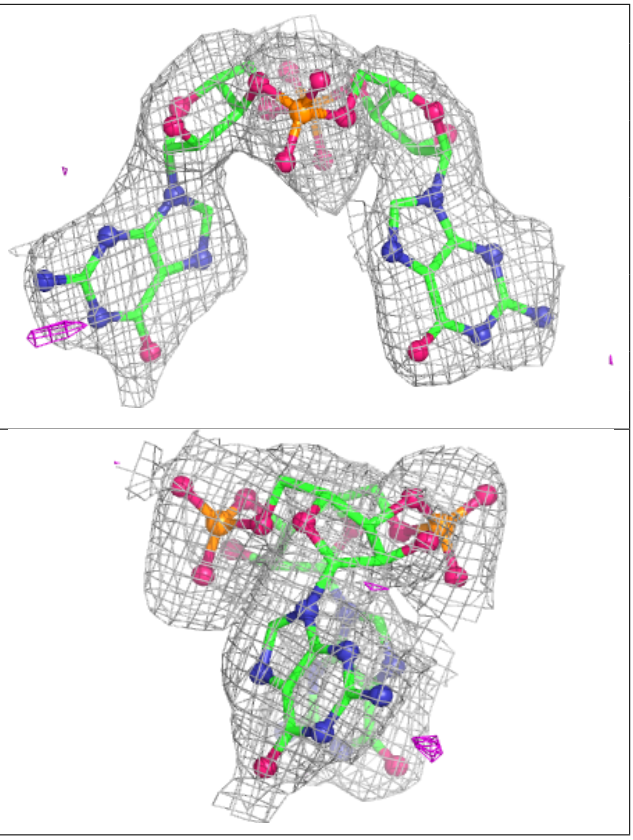
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

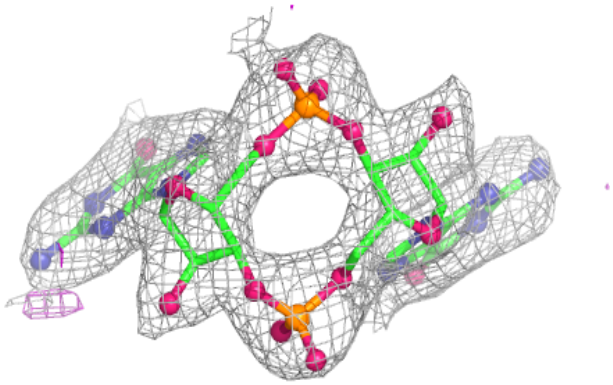
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	502	1/1	0.90	0.07	15,15,15,15	0
5	SO4	A	1460	5/5	0.90	0.21	31,34,41,44	0
3	MG	B	509	1/1	0.93	0.09	29,29,29,29	0
2	BEF	A	501	4/4	0.93	0.16	13,14,19,23	0
4	C2E	B	507	46/46	0.95	0.08	2,17,24,28	0
2	BEF	B	501	4/4	0.95	0.07	3,5,6,7	0
5	SO4	B	1455	5/5	0.95	0.16	32,33,36,41	0
4	C2E	B	505	46/46	0.96	0.08	2,10,16,23	0
5	SO4	A	1461	5/5	0.96	0.07	21,28,33,34	0
4	C2E	B	503	46/46	0.96	0.07	6,16,22,25	0
4	C2E	A	503	46/46	0.97	0.06	2,2,9,13	0
4	C2E	A	505	46/46	0.97	0.07	2,5,14,18	0
3	MG	B	502	1/1	0.98	0.04	12,12,12,12	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 C2E B 507:

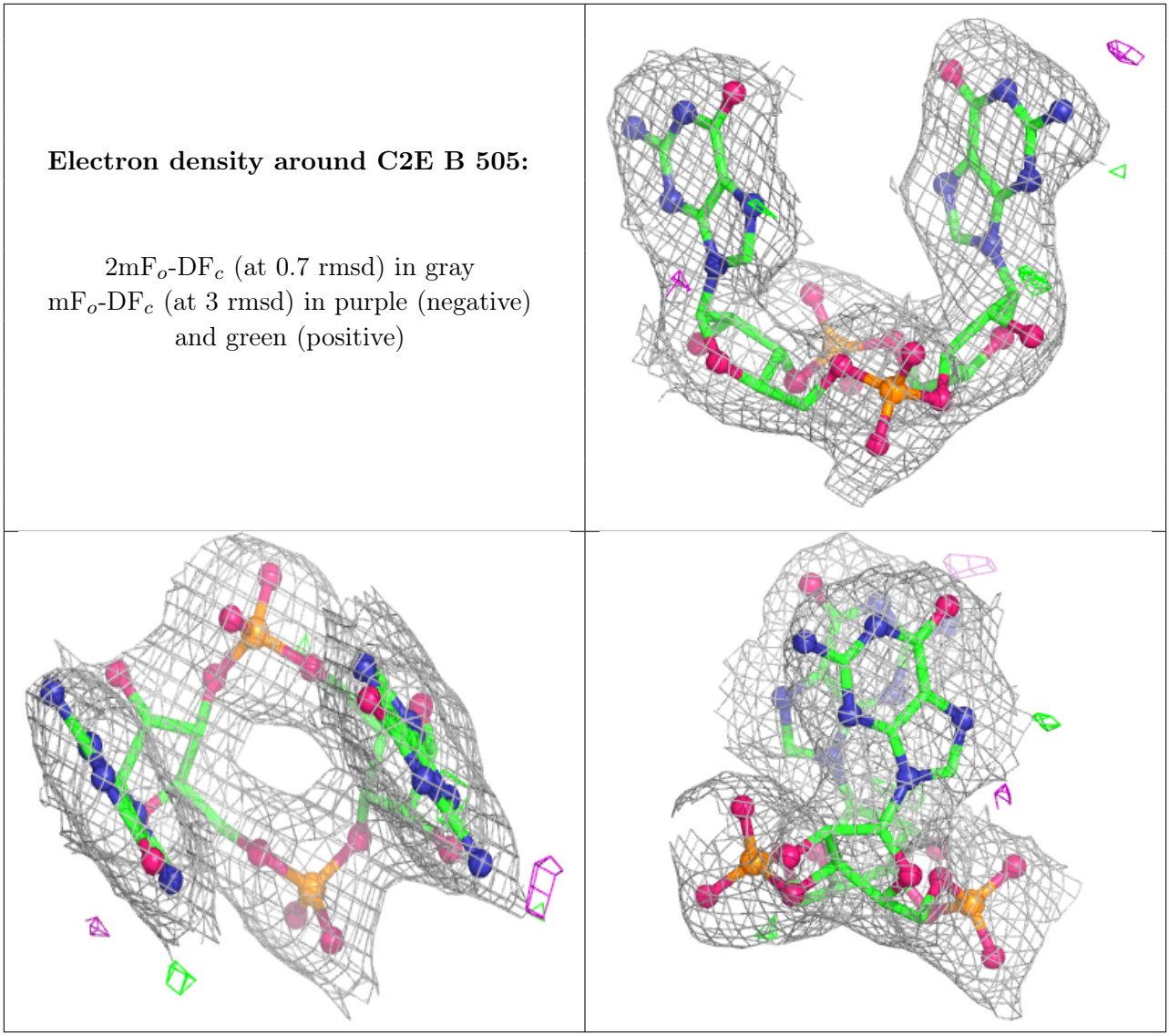
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





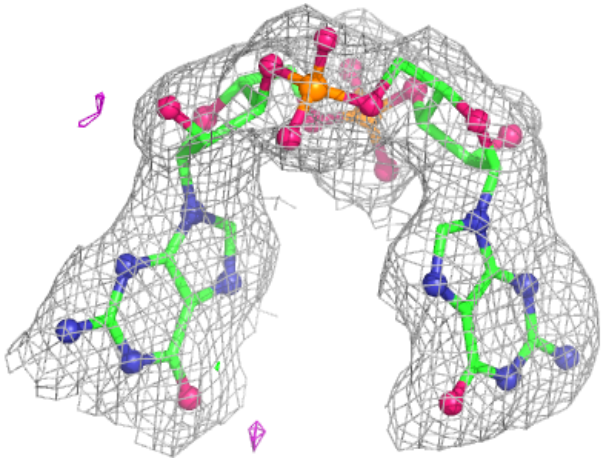
Electron density around C2E B 505:

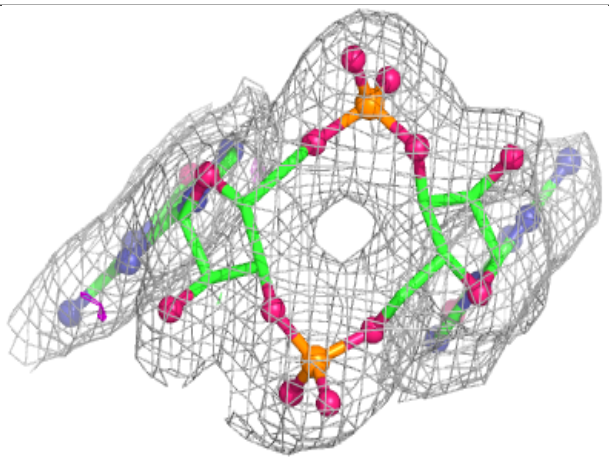
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

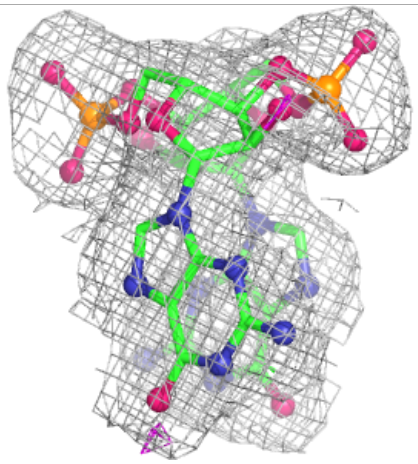


Electron density around C2E B 503:

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

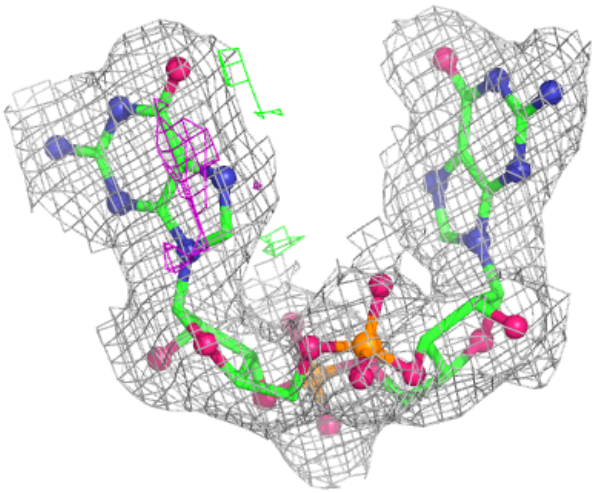


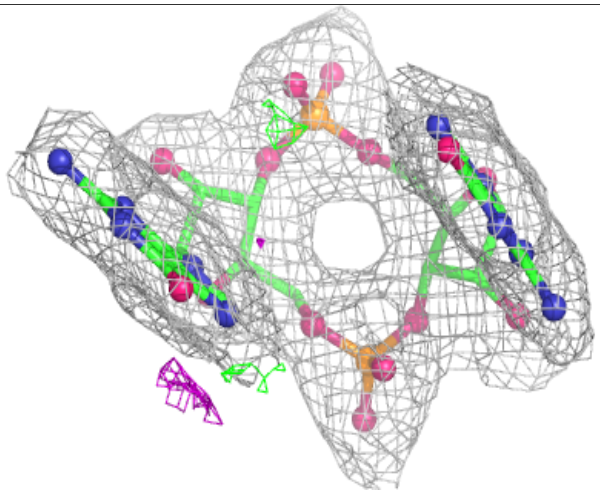


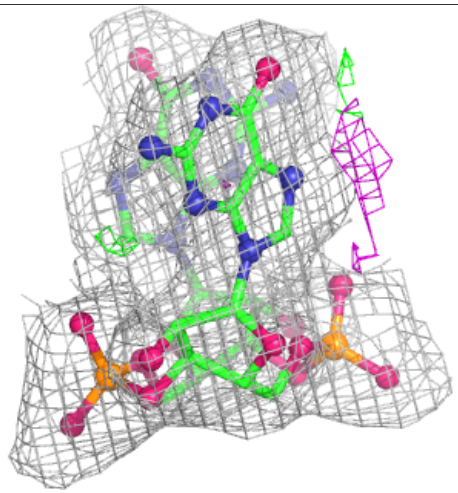


Electron density around C2E A 503:

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

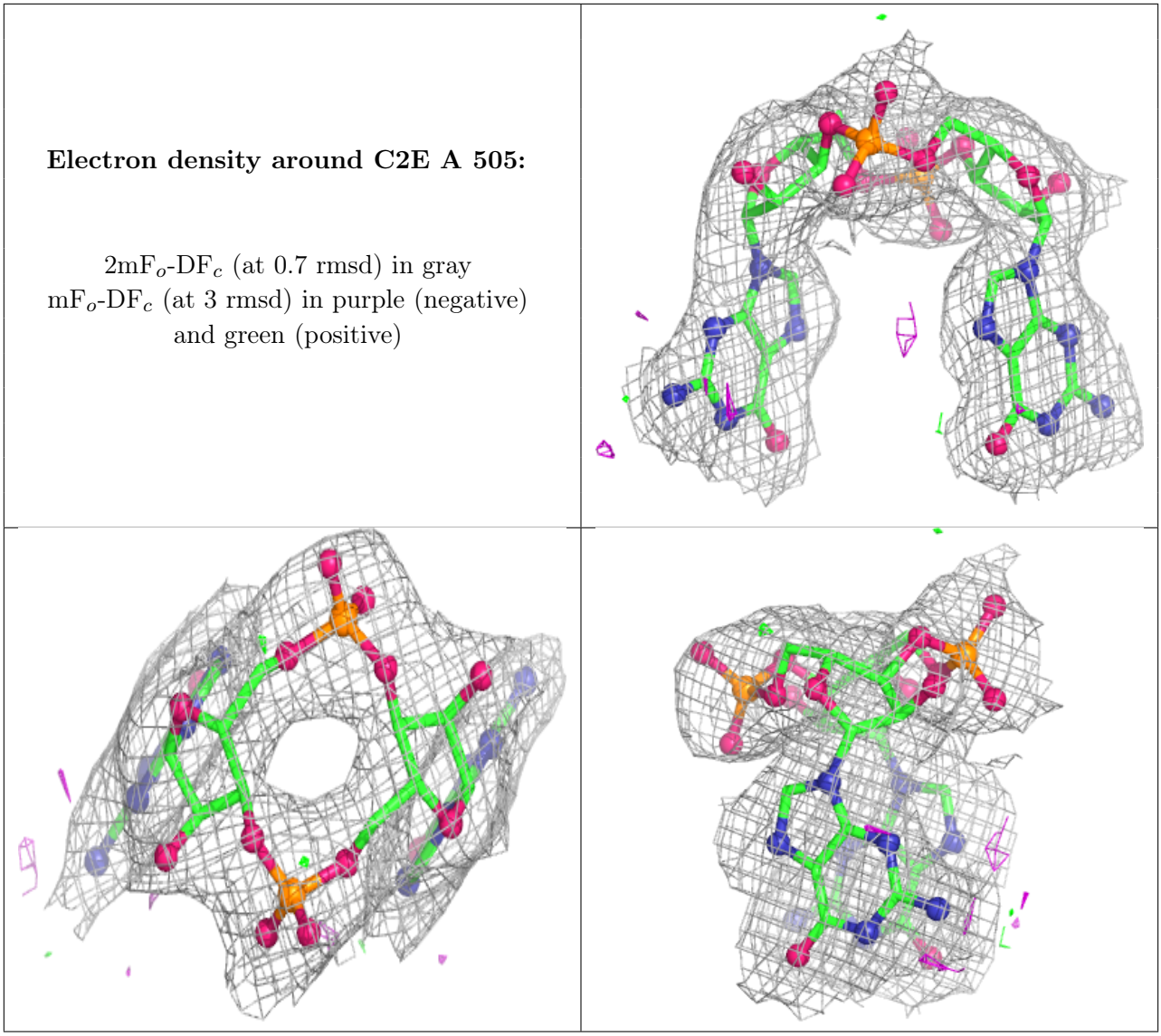






Electron density around C2E A 505:

$2mF_o$-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

There are no such residues in this entry.