



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:58 pm BST

PDB ID : 4D0L
Title : Phosphatidylinositol 4-kinase III beta-PIK93 in a complex with Rab11a- GTP gammaS
Authors : Burke, J.E.; Inglis, A.J.; Perisic, O.; Masson, G.R.; McLaughlin, S.H.; Rutaganira, F.; Shokat, K.M.; Williams, R.L.
Deposited on : 2014-04-29
Resolution : 2.94 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

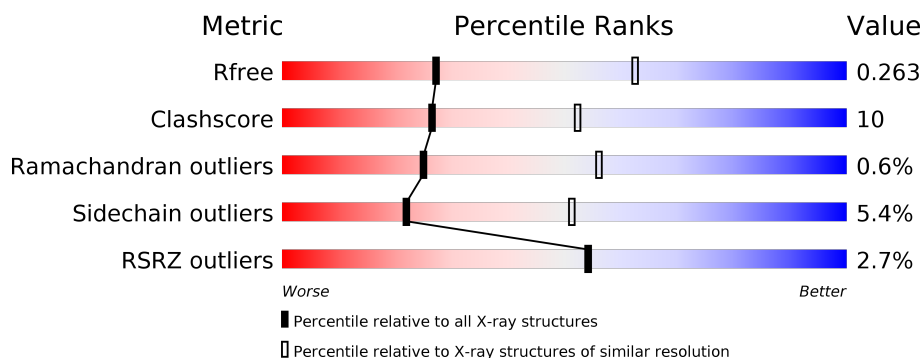
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	566	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>18%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	566	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>14%</div> <div>•</div> <div>16%</div> </div> </div>
1	E	566	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>17%</div> <div>•</div> <div>15%</div> </div> </div>
2	B	219	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>17%</div> <div>•</div> <div>21%</div> </div> </div>
2	D	219	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>16%</div> <div>•</div> <div>19%</div> </div> </div>
2	F	219	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>14%</div> <div>•</div> <div>19%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15864 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 PHOSPHATIDYLINOSITOL 4-KINASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	C	476	Total	C	N	O	S	0	0	0
			3833	2456	660	693	24			
1	E	479	Total	C	N	O	S	0	0	0
			3859	2473	666	696	24			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	expression tag	UNP Q9UBF8
A	120	SER	-	expression tag	UNP Q9UBF8
A	294	ALA	SER	engineered mutation	UNP Q9UBF8
C	119	GLY	-	expression tag	UNP Q9UBF8
C	120	SER	-	expression tag	UNP Q9UBF8
C	294	ALA	SER	engineered mutation	UNP Q9UBF8
E	119	GLY	-	expression tag	UNP Q9UBF8
E	120	SER	-	expression tag	UNP Q9UBF8
E	294	ALA	SER	engineered mutation	UNP Q9UBF8

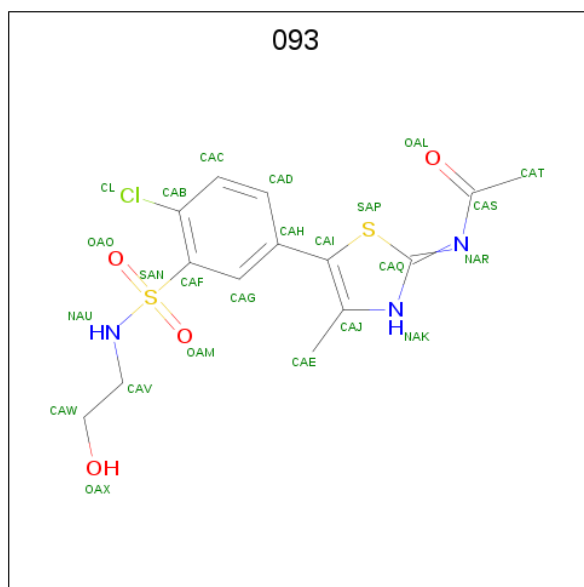
- Molecule 2 is a protein called RAS-RELATED PROTEIN RAB-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	D	177	Total	C	N	O	S	0	0	0
			1409	891	244	272	2			
2	F	177	Total	C	N	O	S	0	0	0
			1409	891	244	272	2			

There are 12 discrepancies between the modelled and reference sequences:

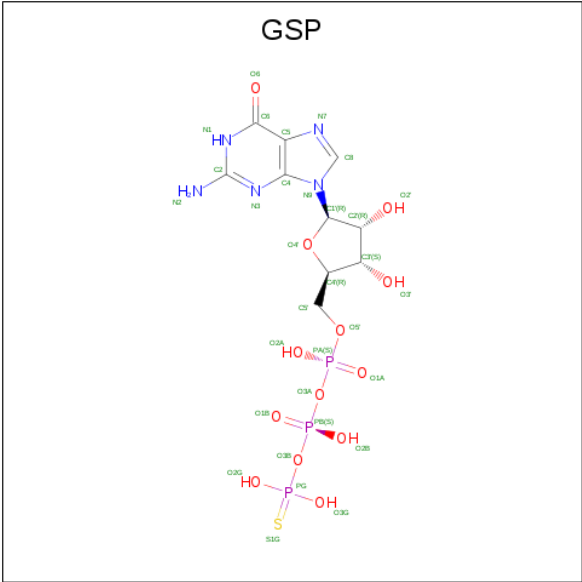
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62491
B	-1	SER	-	expression tag	UNP P62491
B	0	HIS	-	expression tag	UNP P62491
B	70	LEU	GLN	engineered mutation	UNP P62491
D	-2	GLY	-	expression tag	UNP P62491
D	-1	SER	-	expression tag	UNP P62491
D	0	HIS	-	expression tag	UNP P62491
D	70	LEU	GLN	engineered mutation	UNP P62491
F	-2	GLY	-	expression tag	UNP P62491
F	-1	SER	-	expression tag	UNP P62491
F	0	HIS	-	expression tag	UNP P62491
F	70	LEU	GLN	engineered mutation	UNP P62491

- Molecule 3 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIA ZOLE-2-YL)-ACETAMIDE (three-letter code: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	2	0
			24	14	1	3	4	2		
3	C	1	Total	C	Cl	N	O	S	0	0
			24	14	1	3	4	2		
3	E	1	Total	C	Cl	N	O	S	0	0
			24	14	1	3	4	2		

- Molecule 4 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	B	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	2	Total	O	0	0
			2	2		
6	C	1	Total	O	0	0
			1	1		

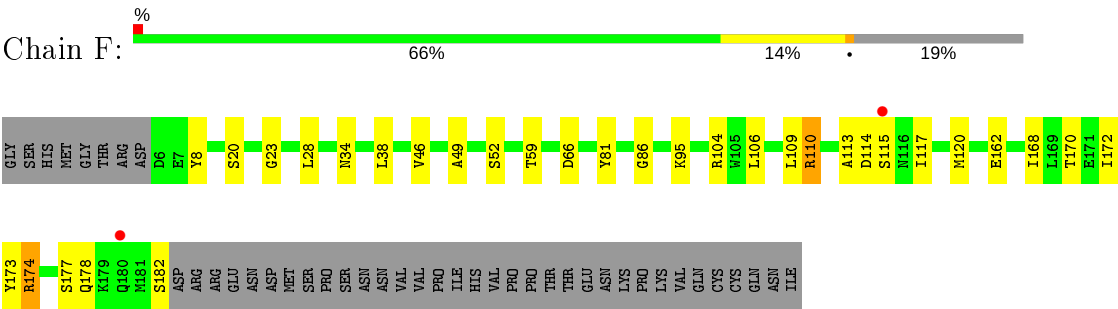
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	4	Total	O	0	0
			4	4		
6	F	3	Total	O	0	0
			3	3		



● Molecule 2: RAS-RELATED PROTEIN RAB-11A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	102.80Å 146.93Å 188.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	115.84 – 2.94 49.58 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (115.84-2.94) 99.7 (49.58-2.94)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.216 , 0.259 0.219 , 0.263	Depositor DCC
R_{free} test set	3095 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.710	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15864	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.26% 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: GSP, MG, 093

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	0.53	0/3866	0.75	1/5219 (0.0%)
1	C	0.53	0/3913	0.76	2/5285 (0.0%)
1	E	0.53	0/3940	0.75	2/5322 (0.0%)
2	B	0.50	0/1399	0.79	1/1892 (0.1%)
2	D	0.50	0/1431	0.70	0/1933
2	F	0.52	0/1431	0.74	0/1933
All	All	0.53	0/15980	0.75	6/21584 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	2
2	F	0	1
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	657	ARG	NE-CZ-NH1	6.79	123.70	120.30
2	B	88	LEU	CB-CG-CD1	6.40	121.89	111.00
1	E	348	LEU	C-N-CA	-5.49	98.94	122.00
1	C	143	MET	CG-SD-CE	5.17	108.48	100.20
1	A	739	MET	CG-SD-CE	-5.12	92.01	100.20
1	C	611	SER	N-CA-C	-5.09	97.25	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	C	403	ILE	Peptide
1	E	348	LEU	Peptide
1	E	750	GLY	Peptide
2	F	110	ARG	Peptide

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	3788	0	3839	77	1
1	C	3833	0	3870	57	0
1	E	3859	0	3895	106	0
2	B	1377	0	1370	32	0
2	D	1409	0	1405	25	0
2	F	1409	0	1407	23	0
3	A	24	0	16	7	0
3	C	24	0	16	5	0
3	E	24	0	16	7	0
4	B	32	0	12	3	0
4	D	32	0	12	2	0
4	F	32	0	12	3	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	8	0	0	0	0
6	B	2	0	0	1	0
6	C	1	0	0	0	0
6	E	4	0	0	1	0
6	F	3	0	0	0	0
All	All	15864	0	15870	328	1

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 10.

All (328) 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)
2:B:56:ASP:OD2	2:B:174:ARG:NH1	1.72	1.20
1:C:240:ILE:O	1:C:243:ASP:OD1	1.75	1.04
1:E:323:ARG:NH1	1:E:340:GLU:OE2	1.90	1.03
1:E:686:LEU:HD22	1:E:688:PHE:CE2	1.98	0.98
1:C:694:LYS:HD3	1:C:784:SER:HA	1.46	0.95
1:A:232:ARG:O	1:A:235:LYS:NZ	1.99	0.94
1:A:549:LYS:NZ	3:A:2002:093:OAM	2.02	0.93
1:E:511:GLU:N	1:E:511:GLU:OE1	2.01	0.92
1:E:598:VAL:H	3:E:2002:093:HAK	1.18	0.92
1:E:686:LEU:HD13	1:E:688:PHE:CD2	2.04	0.91
1:E:686:LEU:HD13	1:E:688:PHE:CG	2.05	0.90
1:A:178:GLN:HA	1:A:739:MET:HE1	1.56	0.88
1:E:686:LEU:HB3	1:E:688:PHE:CE1	2.09	0.88
1:A:163:ARG:O	1:A:166:CYS:SG	2.33	0.86
2:B:95:LYS:O	2:B:98:THR:HG22	1.75	0.85
1:C:404:PRO:O	1:C:405:GLU:HB2	1.76	0.85
1:C:177:PRO:HB2	1:C:739:MET:HE1	1.58	0.84
1:E:344:LEU:O	1:E:348:LEU:HG	1.78	0.84
2:B:54:GLN:HG3	1:C:783:ARG:HD2	1.63	0.80
1:E:520:GLU:OE1	1:E:528:ARG:NH2	2.14	0.80
1:E:566:GLN:HE21	1:E:731:LYS:HB3	1.46	0.79
1:E:684:ARG:HA	1:E:684:ARG:CZ	2.12	0.79
1:E:686:LEU:HB3	1:E:688:PHE:CD1	2.19	0.78
2:D:181:MET:HA	2:D:181:MET:CE	2.14	0.78
1:E:607:VAL:O	1:E:611:SER:HB3	1.85	0.77
1:E:682:SER:CB	1:E:684:ARG:HB2	2.15	0.77
1:A:139:PHE:HA	1:A:143:MET:HE2	1.67	0.76
1:A:602:VAL:HG23	1:A:607:VAL:HG23	1.66	0.76
3:E:2002:093:HAE2	3:E:2002:093:HAD	1.69	0.75
2:F:110:ARG:HD3	2:F:114:ASP:O	1.88	0.74
3:C:2002:093:HAE2	3:C:2002:093:HAD	1.70	0.73
1:A:393:ASN:O	1:A:397:THR:OG1	2.06	0.72
1:A:611:SER:HB2	1:A:613:LEU:HD22	1.70	0.72
1:A:178:GLN:CD	1:A:739:MET:CE	2.58	0.72
1:E:520:GLU:OE2	1:E:524:GLU:HB3	1.89	0.72
1:C:365:ARG:NH2	1:C:405:GLU:OE2	2.22	0.72
1:E:684:ARG:NE	1:E:684:ARG:HA	2.03	0.71
2:D:110:ARG:NH1	2:D:114:ASP:O	2.24	0.71
1:C:232:ARG:O	1:C:235:LYS:HD2	1.92	0.70
1:E:682:SER:HB2	1:E:684:ARG:HB2	1.74	0.69
1:E:232:ARG:O	1:E:235:LYS:HD2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2002:093:CAE	3:C:2002:093:HAD	2.22	0.69
1:C:598:VAL:H	3:C:2002:093:HAK	1.39	0.69
1:E:726:ARG:CA	1:E:763:MET:HE1	2.22	0.69
3:A:2002:093:HAD	3:A:2002:093:HAE2	1.74	0.69
1:E:139:PHE:HA	1:E:143:MET:HE2	1.76	0.68
1:E:726:ARG:HA	1:E:763:MET:HE1	1.75	0.68
1:E:686:LEU:HB2	1:E:688:PHE:N	2.09	0.67
2:F:106:LEU:O	2:F:109:LEU:HB3	1.94	0.67
1:A:518:LEU:HG	1:A:519:LYS:H	1.60	0.67
1:E:682:SER:OG	1:E:684:ARG:NH1	2.28	0.66
1:A:618:TYR:CZ	1:A:622:GLU:HG3	2.30	0.66
1:E:607:VAL:O	1:E:611:SER:CB	2.43	0.66
2:F:81:TYR:HB3	2:F:113:ALA:HB2	1.77	0.66
2:B:81:TYR:HB3	2:B:113:ALA:HB2	1.78	0.65
2:B:120:MET:HE1	2:B:164:ALA:HB1	1.78	0.65
1:E:628:THR:HG23	1:E:631:PHE:H	1.61	0.65
1:A:611:SER:HB2	1:A:613:LEU:CD2	2.25	0.65
2:D:81:TYR:HB3	2:D:113:ALA:HB2	1.77	0.65
1:A:206:ILE:HD11	1:A:394:PHE:HE2	1.62	0.65
1:A:765:MET:HA	1:A:769:GLN:OE1	1.97	0.65
1:E:682:SER:HB3	1:E:684:ARG:N	2.12	0.65
3:A:2002:093:CAE	3:A:2002:093:HAD	2.28	0.63
1:E:232:ARG:O	1:E:235:LYS:CD	2.46	0.63
1:A:178:GLN:CA	1:A:739:MET:HE1	2.25	0.63
1:E:238:LYS:O	1:E:242:SER:HB3	1.97	0.63
1:C:232:ARG:O	1:C:235:LYS:CD	2.46	0.63
3:E:2002:093:CAE	3:E:2002:093:HAD	2.29	0.62
1:E:752:SER:HB2	1:E:755:ARG:CZ	2.29	0.62
1:A:628:THR:HG23	1:A:631:PHE:H	1.64	0.62
2:B:45:GLY:O	2:B:67:THR:O	2.18	0.62
1:C:694:LYS:HD3	1:C:784:SER:CA	2.24	0.62
1:A:637:ASN:HB3	1:A:669:HIS:CD2	2.35	0.61
2:F:110:ARG:HD2	2:F:115:SER:HA	1.80	0.61
2:B:67:THR:O	2:B:68:ALA:HB3	2.00	0.60
1:C:404:PRO:O	1:C:405:GLU:CB	2.45	0.60
1:E:686:LEU:HD22	1:E:688:PHE:CZ	2.36	0.60
1:E:682:SER:N	1:E:683:PRO:HA	2.16	0.60
1:E:783:ARG:O	1:E:784:SER:OG	2.16	0.60
1:C:740:GLN:OE1	1:C:754:ILE:HD13	2.01	0.60
1:E:212:CYS:O	1:E:216:LEU:HD12	2.03	0.59
1:A:767:GLU:HA	1:A:770:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PHE:O	1:A:163:ARG:NH1	2.36	0.59
1:C:637:ASN:HB3	1:C:669:HIS:CD2	2.38	0.59
1:E:352:VAL:HG12	1:E:363:VAL:HG11	1.84	0.59
2:B:8:TYR:CE2	2:B:11:LEU:HB2	2.38	0.59
2:D:38:LEU:HA	4:D:2000:GSP:O2'	2.03	0.59
4:F:2000:GSP:O2B	4:F:2000:GSP:O3G	2.20	0.59
1:A:602:VAL:HG23	1:A:607:VAL:CG2	2.34	0.58
2:B:92:ASP:H	2:B:98:THR:HG21	1.68	0.58
1:C:510:PRO:O	1:C:511:GLU:HB2	2.03	0.58
1:A:598:VAL:H	3:A:2002:093:HAK	1.51	0.58
1:E:607:VAL:O	1:E:611:SER:N	2.37	0.58
1:E:682:SER:HB3	1:E:684:ARG:HB2	1.85	0.58
1:C:774:VAL:O	1:C:778:VAL:HG12	2.04	0.58
1:A:242:SER:O	1:A:306:ARG:HD3	2.04	0.57
2:D:85:VAL:HG13	2:D:172:ILE:HD13	1.87	0.57
1:A:518:LEU:HG	1:A:519:LYS:N	2.19	0.57
1:E:637:ASN:HB3	1:E:669:HIS:CD2	2.40	0.57
1:E:686:LEU:HD13	1:E:688:PHE:CB	2.34	0.56
2:B:28:LEU:HD22	2:B:66:ASP:HB2	1.87	0.56
1:A:570:ILE:HG23	1:A:728:HIS:HD2	1.71	0.56
1:E:686:LEU:CB	1:E:688:PHE:CD1	2.87	0.56
1:C:628:THR:HG22	1:C:630:ALA:N	2.21	0.56
2:F:28:LEU:HD22	2:F:66:ASP:HB2	1.88	0.56
1:A:188:GLU:HG3	1:A:232:ARG:HH12	1.71	0.55
1:A:306:ARG:O	1:A:351:ARG:NH1	2.40	0.55
1:E:682:SER:N	1:E:683:PRO:CA	2.68	0.55
2:F:170:THR:O	2:F:174:ARG:HG3	2.07	0.55
2:B:8:TYR:HA	2:B:59:THR:OG1	2.06	0.55
1:E:139:PHE:HD1	1:E:143:MET:HE2	1.71	0.55
2:D:28:LEU:HD22	2:D:66:ASP:HB2	1.88	0.55
2:F:110:ARG:HE	2:F:117:ILE:HG22	1.72	0.55
1:C:182:MET:HA	1:C:186:MET:HG3	1.89	0.55
2:D:8:TYR:CE2	2:D:11:LEU:HB2	2.43	0.54
1:E:686:LEU:HB2	1:E:687:GLY:CA	2.37	0.54
1:E:598:VAL:O	3:E:2002:093:NAR	2.40	0.54
1:E:686:LEU:HD13	1:E:688:PHE:HB2	1.90	0.54
1:A:403:ILE:HG22	1:A:534:PRO:HB3	1.90	0.54
4:B:2000:GSP:O2B	4:B:2000:GSP:O3G	2.26	0.54
1:E:139:PHE:HD1	1:E:143:MET:CE	2.21	0.54
1:A:178:GLN:CD	1:A:739:MET:HE3	2.27	0.54
1:E:512:ASP:N	1:E:513:PRO:HD3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:GLU:HA	2:B:144:GLU:OE1	2.07	0.54
1:A:182:MET:HA	1:A:186:MET:HG3	1.90	0.53
1:E:598:VAL:N	3:E:2002:093:HAK	1.98	0.53
1:A:379:LYS:HD2	1:A:550:CYS:SG	2.49	0.53
2:B:67:THR:O	2:B:68:ALA:CB	2.55	0.53
1:E:361:HIS:HB2	1:E:388:VAL:HG13	1.90	0.53
1:A:139:PHE:HD1	1:A:143:MET:CE	2.20	0.53
1:E:730:ASP:O	1:E:734:GLN:HB2	2.09	0.53
1:A:139:PHE:HD1	1:A:143:MET:HE2	1.73	0.52
1:C:554:LEU:HD13	1:C:593:GLY:HA3	1.90	0.52
1:E:571:TRP:CE2	1:E:578:LEU:HD12	2.45	0.52
1:E:683:PRO:O	1:E:684:ARG:HB3	2.08	0.52
2:D:181:MET:HA	2:D:181:MET:HE3	1.92	0.52
2:F:8:TYR:HA	2:F:59:THR:OG1	2.10	0.52
1:A:329:THR:HG23	1:A:332:GLN:H	1.73	0.52
1:E:603:SER:OG	1:E:606:GLN:HB2	2.10	0.52
1:E:588:ILE:HD12	1:E:593:GLY:HA2	1.91	0.51
1:E:243:ASP:OD1	1:E:243:ASP:N	2.43	0.51
1:A:625:SER:O	1:A:628:THR:HG22	2.11	0.51
1:A:598:VAL:N	3:A:2002:093:HAK	2.08	0.51
1:A:570:ILE:HG23	1:A:728:HIS:CD2	2.46	0.51
2:F:173:TYR:O	2:F:173:TYR:CG	2.63	0.51
2:F:110:ARG:CD	2:F:115:SER:HA	2.41	0.51
1:E:182:MET:HA	1:E:186:MET:HG3	1.92	0.51
2:B:24:LYS:HE2	6:B:3001:HOH:O	2.09	0.51
1:C:178:GLN:CD	1:C:739:MET:HE2	2.31	0.51
2:B:56:ASP:OD2	2:B:174:ARG:CZ	2.55	0.50
1:A:178:GLN:CG	1:A:739:MET:CE	2.90	0.50
1:A:768:GLU:H	1:A:768:GLU:CD	2.13	0.50
1:C:588:ILE:HD12	1:C:593:GLY:HA2	1.93	0.50
1:A:404:PRO:O	1:A:405:GLU:CB	2.59	0.50
1:E:395:ASP:N	6:E:3002:HOH:O	2.44	0.50
1:C:774:VAL:O	1:C:778:VAL:CG1	2.60	0.50
2:B:6:ASP:O	1:E:628:THR:HA	2.11	0.50
1:E:657:ARG:HD2	1:E:672:HIS:CE1	2.47	0.50
1:A:169:ASN:OD1	1:A:201:ARG:CZ	2.59	0.49
1:A:195:LYS:HB3	1:A:196:PRO:HD3	1.94	0.49
1:A:626:TYR:HA	1:A:631:PHE:CD2	2.47	0.49
1:E:216:LEU:O	1:E:220:SER:HB2	2.12	0.49
2:F:106:LEU:HA	2:F:109:LEU:HB2	1.95	0.49
1:E:625:SER:O	1:E:628:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:613:LEU:HG	1:E:617:ASP:HB3	1.94	0.49
1:A:324:LEU:O	1:A:333:LYS:HE3	2.12	0.49
1:A:588:ILE:HD12	1:A:593:GLY:HA2	1.94	0.49
1:A:571:TRP:CE2	1:A:578:LEU:HD12	2.48	0.49
1:A:206:ILE:HD11	1:A:394:PHE:CE2	2.45	0.48
1:C:571:TRP:CE2	1:C:578:LEU:HD12	2.48	0.48
1:C:195:LYS:HB3	1:C:196:PRO:HD3	1.95	0.48
1:C:740:GLN:OE1	1:C:754:ILE:CD1	2.61	0.48
1:A:549:LYS:HD3	1:A:554:LEU:HD21	1.95	0.48
2:D:58:LYS:HE3	2:D:173:TYR:OH	2.13	0.48
1:C:561:PHE:CZ	1:C:565:LYS:HD3	2.48	0.48
1:E:655:LYS:HA	1:E:691:SER:O	2.14	0.48
2:F:120:MET:CB	2:F:168:ILE:HD12	2.44	0.48
1:C:602:VAL:CG1	1:C:606:GLN:HG2	2.43	0.48
1:C:694:LYS:HD3	1:C:784:SER:CB	2.44	0.48
1:E:351:ARG:HG3	1:E:399:VAL:CG1	2.43	0.48
1:E:195:LYS:HB3	1:E:196:PRO:HD3	1.95	0.48
1:E:686:LEU:H	1:E:687:GLY:HA2	1.78	0.48
1:A:571:TRP:CD2	1:A:578:LEU:HD12	2.49	0.47
1:C:628:THR:HG22	1:C:630:ALA:H	1.79	0.47
1:A:621:GLN:NE2	1:A:622:GLU:OE2	2.46	0.47
2:B:173:TYR:CG	2:B:173:TYR:O	2.67	0.47
2:B:28:LEU:HD11	2:B:49:ALA:HB3	1.96	0.47
1:A:695:LEU:HD23	1:A:782:MET:HE2	1.96	0.47
1:C:571:TRP:CD2	1:C:578:LEU:HD12	2.49	0.47
1:A:356:THR:HG21	1:A:546:VAL:HG12	1.95	0.47
2:B:99:TYR:O	2:B:102:VAL:HG22	2.15	0.47
1:E:694:LYS:HD3	1:E:784:SER:HB2	1.96	0.47
1:E:571:TRP:CD2	1:E:578:LEU:HD12	2.49	0.47
1:E:684:ARG:NE	1:E:684:ARG:CA	2.74	0.47
1:C:405:GLU:HG3	1:C:534:PRO:HG3	1.97	0.47
1:E:746:PRO:O	1:E:749:HIS:HB2	2.15	0.47
2:D:28:LEU:HD11	2:D:49:ALA:HB3	1.96	0.47
3:C:2002:093:CAE	3:C:2002:093:CAD	2.91	0.47
2:B:38:LEU:HA	4:B:2000:GSP:O2'	2.15	0.46
1:E:657:ARG:HD3	1:E:657:ARG:HA	1.59	0.46
1:E:680:SER:HB2	1:E:747:CYS:O	2.15	0.46
2:B:17:ILE:HD13	2:B:109:LEU:HD11	1.97	0.46
2:B:91:TYR:HB2	2:B:98:THR:HG23	1.96	0.46
1:E:236:LEU:O	1:E:240:ILE:HG13	2.16	0.46
1:E:686:LEU:HB2	1:E:687:GLY:C	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:MET:CE	1:A:758:LYS:HA	2.45	0.46
2:F:28:LEU:HD11	2:F:49:ALA:HB3	1.96	0.46
1:C:191:GLY:HA3	1:C:232:ARG:HH21	1.80	0.46
2:B:120:MET:HB2	2:B:168:ILE:HD12	1.97	0.46
1:C:394:PHE:O	1:C:396:THR:N	2.48	0.46
1:C:177:PRO:CB	1:C:739:MET:HE1	2.40	0.46
1:E:684:ARG:HG3	1:E:684:ARG:O	2.16	0.46
1:E:752:SER:HB3	1:E:755:ARG:NH2	2.30	0.46
1:C:729:MET:CE	1:C:758:LYS:HA	2.46	0.46
1:E:523:GLN:HA	1:E:526:VAL:HG12	1.98	0.46
1:E:715:LYS:NZ	1:E:775:GLU:OE2	2.42	0.46
1:C:236:LEU:O	1:C:240:ILE:HG13	2.16	0.46
2:D:173:TYR:CG	2:D:173:TYR:O	2.69	0.46
2:D:86:GLY:HA3	2:D:172:ILE:HD11	1.98	0.45
1:A:178:GLN:NE2	1:A:739:MET:CE	2.79	0.45
1:A:178:GLN:HG3	1:A:739:MET:CE	2.47	0.45
1:A:178:GLN:NE2	1:A:739:MET:HE2	2.31	0.45
1:A:236:LEU:O	1:A:240:ILE:HG13	2.16	0.45
3:E:2002:093:CAE	3:E:2002:093:CAD	2.93	0.45
1:E:386:VAL:O	1:E:543:LEU:CD2	2.64	0.45
1:C:778:VAL:HG23	1:C:782:MET:CE	2.46	0.45
1:E:352:VAL:CG1	1:E:363:VAL:HG11	2.46	0.45
1:E:624:GLY:HA3	1:E:628:THR:HG21	1.99	0.45
2:F:109:LEU:HG	2:F:110:ARG:HG2	1.99	0.45
3:A:2002:093:CAE	3:A:2002:093:CAD	2.95	0.45
1:E:779:ASP:HB3	1:E:783:ARG:NH2	2.32	0.45
2:B:92:ASP:HB3	2:B:98:THR:HG21	2.00	0.44
1:C:682:SER:HB3	1:C:683:PRO:HD3	1.98	0.44
1:A:133:LEU:O	1:A:136:SER:OG	2.28	0.44
2:D:31:PHE:O	2:D:51:ARG:NH1	2.44	0.44
1:A:756:ASN:OD1	2:F:34:ASN:ND2	2.50	0.44
1:E:686:LEU:HB2	1:E:687:GLY:HA2	1.99	0.44
1:C:549:LYS:HE3	1:C:552:ASP:OD2	2.17	0.44
1:E:752:SER:CB	1:E:755:ARG:CZ	2.95	0.44
1:C:726:ARG:NH2	1:C:762:HIS:O	2.50	0.44
2:D:21:GLY:O	4:D:2000:GSP:H5'1	2.17	0.44
1:E:726:ARG:HA	1:E:763:MET:CE	2.45	0.44
1:E:176:LEU:N	1:E:177:PRO:CD	2.81	0.44
2:F:178:GLN:O	2:F:182:SER:N	2.51	0.44
1:C:342:SER:OG	1:C:368:HIS:CD2	2.71	0.44
2:D:181:MET:HA	2:D:181:MET:HE2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:174:ARG:O	2:F:178:GLN:NE2	2.51	0.43
1:A:235:LYS:HG2	1:A:236:LEU:N	2.33	0.43
2:F:86:GLY:HA3	2:F:172:ILE:HD11	2.01	0.43
1:A:783:ARG:HD3	2:F:170:THR:HG21	1.99	0.43
1:A:176:LEU:N	1:A:177:PRO:CD	2.81	0.43
2:B:92:ASP:H	2:B:98:THR:CG2	2.30	0.43
1:C:176:LEU:N	1:C:177:PRO:CD	2.82	0.43
2:B:125:LYS:HG2	4:B:2000:GSP:C6	2.53	0.43
1:E:682:SER:CB	1:E:684:ARG:NH1	2.82	0.43
1:A:352:VAL:HG23	1:A:363:VAL:HB	2.00	0.43
1:A:576:VAL:HG12	1:A:578:LEU:HG	2.01	0.43
1:E:512:ASP:OD1	1:E:512:ASP:N	2.52	0.43
2:D:110:ARG:NH1	2:D:117:ILE:HG22	2.34	0.43
2:D:170:THR:O	2:D:174:ARG:HG3	2.19	0.43
1:E:639:VAL:HG13	1:E:714:TYR:HB2	2.01	0.43
2:F:38:LEU:HA	4:F:2000:GSP:O2'	2.19	0.43
1:E:139:PHE:CD1	1:E:143:MET:HE2	2.52	0.42
1:A:624:GLY:HA3	1:A:628:THR:HG21	2.00	0.42
2:B:88:LEU:HD21	2:B:120:MET:HE2	2.01	0.42
2:F:23:GLY:HA2	4:F:2000:GSP:O1A	2.18	0.42
1:A:589:SER:OG	1:A:591:ASP:HB2	2.19	0.42
1:A:772:LEU:HG	1:A:776:GLN:NE2	2.35	0.42
1:E:686:LEU:HB2	1:E:688:PHE:H	1.81	0.42
1:C:598:VAL:N	3:C:2002:093:HAK	2.11	0.42
1:C:394:PHE:C	1:C:396:THR:H	2.23	0.42
1:E:686:LEU:CD1	1:E:688:PHE:CD2	2.91	0.42
1:C:576:VAL:HG12	1:C:578:LEU:HG	2.01	0.42
1:C:755:ARG:HD2	1:C:755:ARG:HA	1.82	0.42
2:D:120:MET:HB2	2:D:168:ILE:HD12	2.01	0.42
1:E:683:PRO:O	1:E:684:ARG:CB	2.68	0.42
1:C:552:ASP:O	1:C:554:LEU:HD12	2.20	0.42
2:D:110:ARG:NH2	2:D:117:ILE:HG22	2.35	0.42
1:E:232:ARG:O	1:E:235:LYS:HG3	2.19	0.42
2:B:86:GLY:HA3	2:B:172:ILE:HD11	2.01	0.42
1:C:765:MET:HB3	1:C:770:LEU:HD12	2.02	0.42
1:A:711:PHE:CZ	1:A:782:MET:HE1	2.54	0.42
1:E:729:MET:HG3	1:E:761:PHE:CG	2.54	0.42
1:A:573:GLN:C	1:A:574:GLU:O	2.58	0.41
2:D:58:LYS:CE	2:D:173:TYR:OH	2.68	0.41
1:E:232:ARG:O	1:E:235:LYS:CG	2.68	0.41
2:F:120:MET:HB3	2:F:168:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:LEU:CD2	2:B:66:ASP:HB2	2.50	0.41
1:C:695:LEU:HA	1:C:695:LEU:HD12	1.94	0.41
3:E:2002:093:OAL	3:E:2002:093:SAP	2.78	0.41
1:E:386:VAL:O	1:E:543:LEU:HD23	2.20	0.41
1:A:405:GLU:HG3	1:A:534:PRO:HG3	2.02	0.41
1:A:695:LEU:HA	1:A:695:LEU:HD12	1.95	0.41
2:B:120:MET:HE1	2:B:164:ALA:CB	2.50	0.41
1:A:639:VAL:HG13	1:A:714:TYR:HB2	2.03	0.41
1:E:513:PRO:CG	1:E:514:SER:H	2.33	0.41
1:E:394:PHE:O	1:E:395:ASP:CB	2.69	0.41
1:E:576:VAL:HG12	1:E:578:LEU:HG	2.02	0.41
1:A:578:LEU:CD2	1:A:717:LEU:HB3	2.51	0.41
2:F:8:TYR:HE1	2:F:52:SER:HB2	1.86	0.41
2:B:178:GLN:NE2	2:B:178:GLN:HA	2.36	0.41
1:C:365:ARG:NE	1:C:405:GLU:OE2	2.52	0.41
1:C:393:ASN:C	1:C:394:PHE:O	2.57	0.40
1:C:573:GLN:C	1:C:574:GLU:O	2.57	0.40
1:E:191:GLY:HA3	1:E:232:ARG:HH21	1.86	0.40
1:A:601:ALA:O	3:A:2002:093:HAT2	2.21	0.40
1:A:549:LYS:HD2	1:A:595:ILE:HD12	2.03	0.40
2:B:176:VAL:HG23	2:B:177:SER:N	2.35	0.40
1:C:165:PHE:CZ	1:C:197:TYR:HA	2.56	0.40
1:C:389:LEU:HD22	1:C:540:ASN:HB3	2.03	0.40
1:C:656:ASP:O	1:C:661:ASN:ND2	2.53	0.40
2:D:114:ASP:OD1	2:D:115:SER:N	2.54	0.40
2:D:10:TYR:HE2	2:D:58:LYS:HZ2	1.68	0.40
1:E:686:LEU:N	1:E:687:GLY:HA2	2.34	0.40
2:D:175:ILE:O	2:D:179:LYS:HG2	2.21	0.40
2:D:28:LEU:CD2	2:D:66:ASP:HB2	2.51	0.40
1:E:511:GLU:N	1:E:513:PRO:HD3	2.36	0.40
1:E:578:LEU:CD2	1:E:717:LEU:HB3	2.52	0.40
1:E:773:LEU:HG	1:E:777:MET:HE3	2.03	0.40
1:A:393:ASN:ND2	1:A:396:THR:HG22	2.36	0.40
1:A:522:TRP:O	1:A:526:VAL:HG23	2.22	0.40
1:C:694:LYS:HD3	1:C:784:SER:HB2	2.02	0.40
1:C:778:VAL:HG23	1:C:782:MET:HE3	2.02	0.40
2:D:137:ASP:OD1	2:D:140:ARG:NH2	2.47	0.40
1:E:686:LEU:HD22	1:E:688:PHE:CD2	2.54	0.40
1:A:194:ILE:HG22	1:A:198:ILE:HD12	2.03	0.40
1:C:327:LEU:HD21	1:C:336:ARG:NH2	2.37	0.40
1:E:394:PHE:O	1:E:395:ASP:HB2	2.21	0.40

All (1) 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:A:340:GLU:OE1	1:A:626:TYR:OH[4_595]	2.16	0.04

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	460/566 (81%)	445 (97%)	13 (3%)	2 (0%)	34	64
1	C	466/566 (82%)	445 (96%)	16 (3%)	5 (1%)	14	40
1	E	471/566 (83%)	446 (95%)	22 (5%)	3 (1%)	25	56
2	B	171/219 (78%)	164 (96%)	6 (4%)	1 (1%)	25	56
2	D	175/219 (80%)	170 (97%)	5 (3%)	0	100	100
2	F	175/219 (80%)	168 (96%)	7 (4%)	0	100	100
All	All	1918/2355 (81%)	1838 (96%)	69 (4%)	11 (1%)	25	56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	513	PRO
1	E	513	PRO
1	C	405	GLU
2	B	68	ALA
1	C	682	SER
1	A	405	GLU
1	C	394	PHE
1	C	741	GLN
1	A	399	VAL
1	E	348	LEU
1	E	349	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/508 (83%)	409 (97%)	13 (3%)	40	71
1	C	428/508 (84%)	403 (94%)	25 (6%)	20	48
1	E	429/508 (84%)	398 (93%)	31 (7%)	14	37
2	B	147/191 (77%)	139 (95%)	8 (5%)	22	51
2	D	151/191 (79%)	142 (94%)	9 (6%)	19	46
2	F	151/191 (79%)	144 (95%)	7 (5%)	27	57
All	All	1728/2097 (82%)	1635 (95%)	93 (5%)	22	51

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	148	LEU
1	A	235	LYS
1	A	318	MET
1	A	335	GLN
1	A	378	ASP
1	A	391	CYS
1	A	397	THR
1	A	565	LYS
1	A	606	GLN
1	A	613	LEU
1	A	694	LYS
1	A	739	MET
2	B	7	GLU
2	B	11	LEU
2	B	20	SER
2	B	33	ARG
2	B	46	VAL
2	B	54	GLN
2	B	55	VAL
2	B	174	ARG
1	C	166	CYS

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Mol	Chain	Res	Type
1	C	235	LYS
1	C	243	ASP
1	C	318	MET
1	C	348	LEU
1	C	379	LYS
1	C	391	CYS
1	C	405	GLU
1	C	518	LEU
1	C	565	LYS
1	C	603	SER
1	C	606	GLN
1	C	609	LYS
1	C	610	GLN
1	C	611	SER
1	C	617	ASP
1	C	633	SER
1	C	706	LEU
1	C	739	MET
1	C	752	SER
1	C	755	ARG
1	C	764	SER
1	C	768	GLU
1	C	775	GLU
1	C	778	VAL
2	D	7	GLU
2	D	11	LEU
2	D	20	SER
2	D	46	VAL
2	D	95	LYS
2	D	162	GLU
2	D	177	SER
2	D	181	MET
2	D	182	SER
1	E	137	LYS
1	E	145	ILE
1	E	166	CYS
1	E	216	LEU
1	E	220	SER
1	E	221	SER
1	E	235	LYS
1	E	243	ASP
1	E	318	MET

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Mol	Chain	Res	Type
1	E	339	SER
1	E	379	LYS
1	E	391	CYS
1	E	392	GLU
1	E	512	ASP
1	E	543	LEU
1	E	565	LYS
1	E	598	VAL
1	E	606	GLN
1	E	609	LYS
1	E	612	GLN
1	E	613	LEU
1	E	633	SER
1	E	680	SER
1	E	682	SER
1	E	684	ARG
1	E	685	ASN
1	E	737	GLU
1	E	739	MET
1	E	744	GLN
1	E	775	GLU
1	E	776	GLN
2	F	20	SER
2	F	46	VAL
2	F	95	LYS
2	F	104	ARG
2	F	162	GLU
2	F	174	ARG
2	F	177	SER

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

Mol	Chain	Res	Type
1	A	393	ASN
1	A	540	ASN
1	A	606	GLN
1	A	776	GLN
2	B	178	GLN
1	C	185	HIS
1	C	540	ASN
1	C	612	GLN
1	E	150	ASN

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Mol	Chain	Res	Type
1	E	185	HIS
1	E	204	GLN
1	E	335	GLN
1	E	368	HIS
1	E	540	ASN
1	E	566	GLN
1	E	728	HIS
2	F	34	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	GSP	F	2000	5	26,34,34	1.22	4 (15%)	28,54,54	2.07	9 (32%)
4	GSP	D	2000	5	26,34,34	1.37	4 (15%)	28,54,54	2.21	10 (35%)
3	093	A	2002	-	20,25,25	2.01	6 (30%)	23,36,36	4.99	9 (39%)
3	093	E	2002	-	20,25,25	2.03	7 (35%)	23,36,36	4.10	7 (30%)
3	093	C	2002	1	20,25,25	1.68	4 (20%)	23,36,36	4.55	11 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GSP	B	2000	5	26,34,34	1.29	3 (11%)	28,54,54	1.98	8 (28%)

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	GSP	F	2000	5	-	1/17/38/38	0/3/3/3
4	GSP	D	2000	5	-	2/17/38/38	0/3/3/3
3	093	A	2002	-	-	8/17/19/19	0/2/2/2
3	093	E	2002	-	-	9/17/19/19	0/2/2/2
3	093	C	2002	1	-	11/17/19/19	0/2/2/2
4	GSP	B	2000	5	-	3/17/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2002	093	CAH-CAI	4.62	1.52	1.48
3	A	2002	093	CAQ-NAR	4.26	1.45	1.33
3	E	2002	093	CAQ-NAR	4.04	1.45	1.33
4	D	2000	GSP	C6-C5	3.96	1.48	1.41
3	C	2002	093	CAQ-NAR	3.78	1.44	1.33
3	A	2002	093	SAN-NAU	3.64	1.67	1.61
4	B	2000	GSP	C6-C5	3.49	1.47	1.41
3	A	2002	093	CAV-CAW	-3.44	1.38	1.50
3	E	2002	093	CAS-NAR	3.02	1.44	1.37
3	C	2002	093	CAS-NAR	2.98	1.44	1.37
3	C	2002	093	CAH-CAI	2.96	1.51	1.48
4	F	2000	GSP	O4'-C1'	2.91	1.45	1.41
3	A	2002	093	CAS-NAR	2.78	1.44	1.37
3	A	2002	093	CAT-CAS	2.63	1.53	1.49
4	F	2000	GSP	C6-C5	2.59	1.45	1.41
4	D	2000	GSP	PG-O3G	2.57	1.63	1.54
4	F	2000	GSP	PG-O3G	2.51	1.63	1.54
4	D	2000	GSP	C5-C4	2.43	1.47	1.40
3	E	2002	093	OAM-SAN	-2.37	1.40	1.43
3	E	2002	093	CAT-CAS	2.36	1.53	1.49
4	B	2000	GSP	PG-O3G	2.32	1.62	1.54
3	C	2002	093	CAT-CAS	2.32	1.52	1.49
3	A	2002	093	OAM-SAN	-2.20	1.41	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2002	093	CAB-CAF	2.15	1.43	1.40
4	B	2000	GSP	C5-C4	2.15	1.46	1.40
4	D	2000	GSP	PG-S1G	2.04	1.95	1.90
4	F	2000	GSP	PG-O2G	2.04	1.61	1.54
3	E	2002	093	CAB-CL	2.02	1.78	1.73

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	093	OAO-SAN-OAM	-20.87	93.89	119.55
3	C	2002	093	OAO-SAN-OAM	-17.94	97.50	119.55
3	E	2002	093	OAO-SAN-OAM	-16.87	98.81	119.55
3	E	2002	093	OAO-SAN-NAU	5.87	116.21	107.04
3	C	2002	093	OAO-SAN-NAU	5.51	115.65	107.04
3	C	2002	093	OAM-SAN-CAF	5.35	116.47	107.66
3	A	2002	093	OAO-SAN-NAU	5.10	115.01	107.04
3	A	2002	093	OAM-SAN-NAU	4.90	114.70	107.04
4	D	2000	GSP	C2-N3-C4	4.50	120.50	115.36
4	F	2000	GSP	C5-C6-N1	-4.47	117.31	123.43
4	B	2000	GSP	C6-C5-C4	-4.29	116.70	120.80
4	D	2000	GSP	C5-C6-N1	-4.27	117.60	123.43
4	B	2000	GSP	C2-N3-C4	4.23	120.19	115.36
3	A	2002	093	OAO-SAN-CAF	4.20	114.58	107.66
4	F	2000	GSP	C2-N3-C4	4.08	120.01	115.36
4	F	2000	GSP	C6-N1-C2	4.07	122.40	115.93
3	C	2002	093	OAO-SAN-CAF	4.05	114.32	107.66
3	A	2002	093	CAT-CAS-NAR	4.02	121.08	114.85
4	D	2000	GSP	C6-N1-C2	3.97	122.24	115.93
3	C	2002	093	CAB-CAF-SAN	-3.89	120.71	123.25
4	D	2000	GSP	PA-O3A-PB	-3.86	119.58	132.83
4	F	2000	GSP	PA-O3A-PB	-3.80	119.79	132.83
3	E	2002	093	CAF-CAB-CL	3.80	124.27	121.49
4	F	2000	GSP	N3-C2-N1	-3.61	122.41	127.22
3	A	2002	093	OAX-CAW-CAV	-3.52	98.72	111.59
4	B	2000	GSP	C6-N1-C2	3.45	121.42	115.93
3	A	2002	093	OAM-SAN-CAF	3.34	113.16	107.66
4	D	2000	GSP	C6-C5-C4	-3.29	117.66	120.80
3	E	2002	093	OAM-SAN-CAF	3.28	113.06	107.66
4	B	2000	GSP	C5-C6-N1	-3.27	118.96	123.43
4	D	2000	GSP	N3-C2-N1	-3.24	122.90	127.22
4	D	2000	GSP	C3'-C2'-C1'	3.14	105.70	100.98
3	C	2002	093	CAF-SAN-NAU	-3.03	103.89	107.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2002	093	CAF-CAB-CL	-3.03	119.27	121.49
4	B	2000	GSP	PA-O3A-PB	-3.01	122.49	132.83
4	D	2000	GSP	C4-C5-N7	-2.91	106.36	109.40
3	C	2002	093	CAC-CAB-CAF	2.88	122.01	120.05
3	E	2002	093	CAT-CAS-NAR	2.86	119.28	114.85
3	C	2002	093	CAD-CAH-CAG	2.73	122.03	118.16
4	F	2000	GSP	C6-C5-C4	-2.72	118.20	120.80
3	E	2002	093	OAO-SAN-CAF	2.72	112.13	107.66
4	B	2000	GSP	C4-C5-N7	-2.72	106.57	109.40
3	A	2002	093	CAD-CAH-CAG	2.71	121.99	118.16
4	B	2000	GSP	N3-C2-N1	-2.71	123.61	127.22
3	A	2002	093	OAL-CAS-NAR	-2.69	118.52	123.67
3	C	2002	093	CAT-CAS-NAR	2.58	118.85	114.85
3	C	2002	093	CAQ-NAR-CAS	2.57	122.79	116.11
4	B	2000	GSP	O2G-PG-O3B	2.48	112.93	104.64
4	D	2000	GSP	C2'-C3'-C4'	2.44	107.39	102.64
4	D	2000	GSP	O2G-PG-O3B	2.24	112.11	104.64
4	F	2000	GSP	O3'-C3'-C2'	-2.21	104.69	111.82
3	E	2002	093	CAQ-NAR-CAS	2.20	121.82	116.11
4	F	2000	GSP	O2B-PB-O1B	2.11	122.68	112.24
4	F	2000	GSP	C4-C5-N7	-2.08	107.24	109.40

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2002	093	NAU-CAV-CAW-OAX
3	E	2002	093	CAB-CAF-SAN-OAM
3	E	2002	093	CAB-CAF-SAN-OAO
3	E	2002	093	CAB-CAF-SAN-NAU
3	E	2002	093	CAG-CAF-SAN-NAU
3	E	2002	093	CAW-CAV-NAU-SAN
3	C	2002	093	CAB-CAF-SAN-OAO
3	C	2002	093	CAB-CAF-SAN-NAU
3	C	2002	093	NAU-CAV-CAW-OAX
4	B	2000	GSP	C5'-O5'-PA-O2A
3	A	2002	093	CAV-NAU-SAN-OAO
3	E	2002	093	CAG-CAF-SAN-OAO
3	C	2002	093	CAD-CAH-CAI-CAJ
3	C	2002	093	CAG-CAF-SAN-OAO
3	A	2002	093	CAB-CAF-SAN-OAO
3	C	2002	093	CAB-CAF-SAN-OAM

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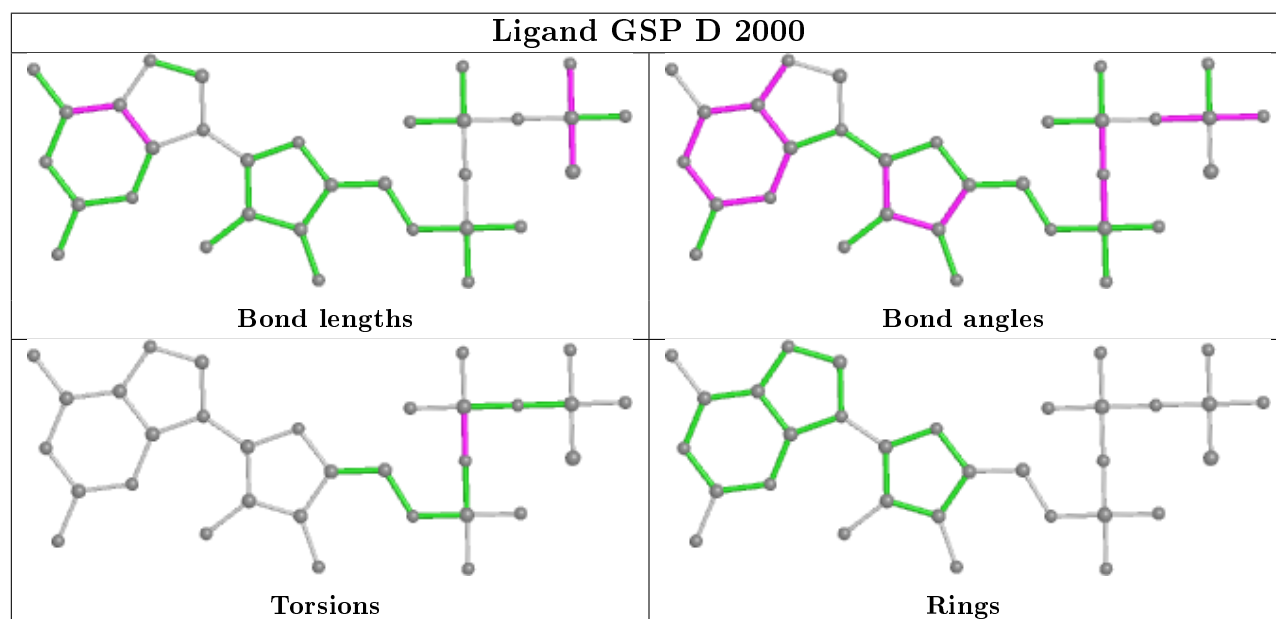
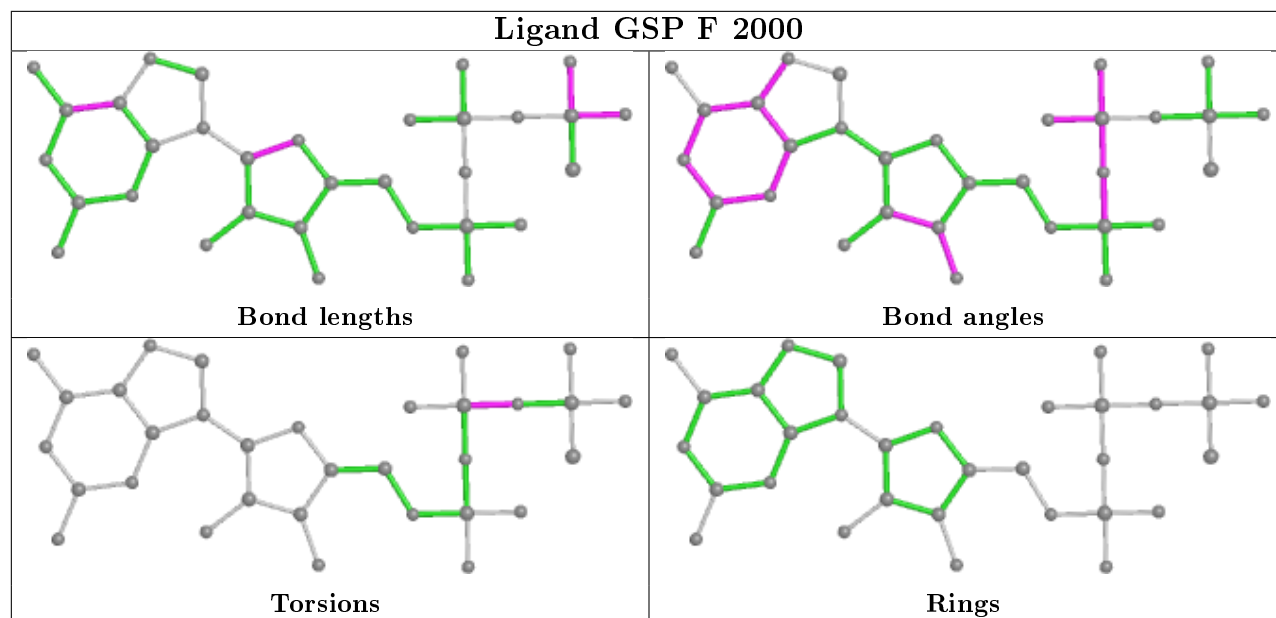
Mol	Chain	Res	Type	Atoms
3	E	2002	093	CAG-CAF-SAN-OAM
3	E	2002	093	CAV-NAU-SAN-OAO
3	C	2002	093	CAV-NAU-SAN-OAO
3	A	2002	093	CAV-NAU-SAN-CAF
3	A	2002	093	CAV-NAU-SAN-OAM
4	D	2000	GSP	PA-O3A-PB-O1B
3	C	2002	093	CAG-CAH-CAI-CAJ
4	B	2000	GSP	C5'-O5'-PA-O3A
4	B	2000	GSP	C5'-O5'-PA-O1A
3	C	2002	093	CAV-NAU-SAN-CAF
4	D	2000	GSP	PA-O3A-PB-O2B
3	A	2002	093	CAD-CAH-CAI-CAJ
3	E	2002	093	CAV-NAU-SAN-CAF
3	A	2002	093	CAG-CAF-SAN-OAO
4	F	2000	GSP	PG-O3B-PB-O1B
3	C	2002	093	CAG-CAF-SAN-NAU
3	C	2002	093	CAG-CAF-SAN-OAM
3	A	2002	093	CAG-CAH-CAI-CAJ

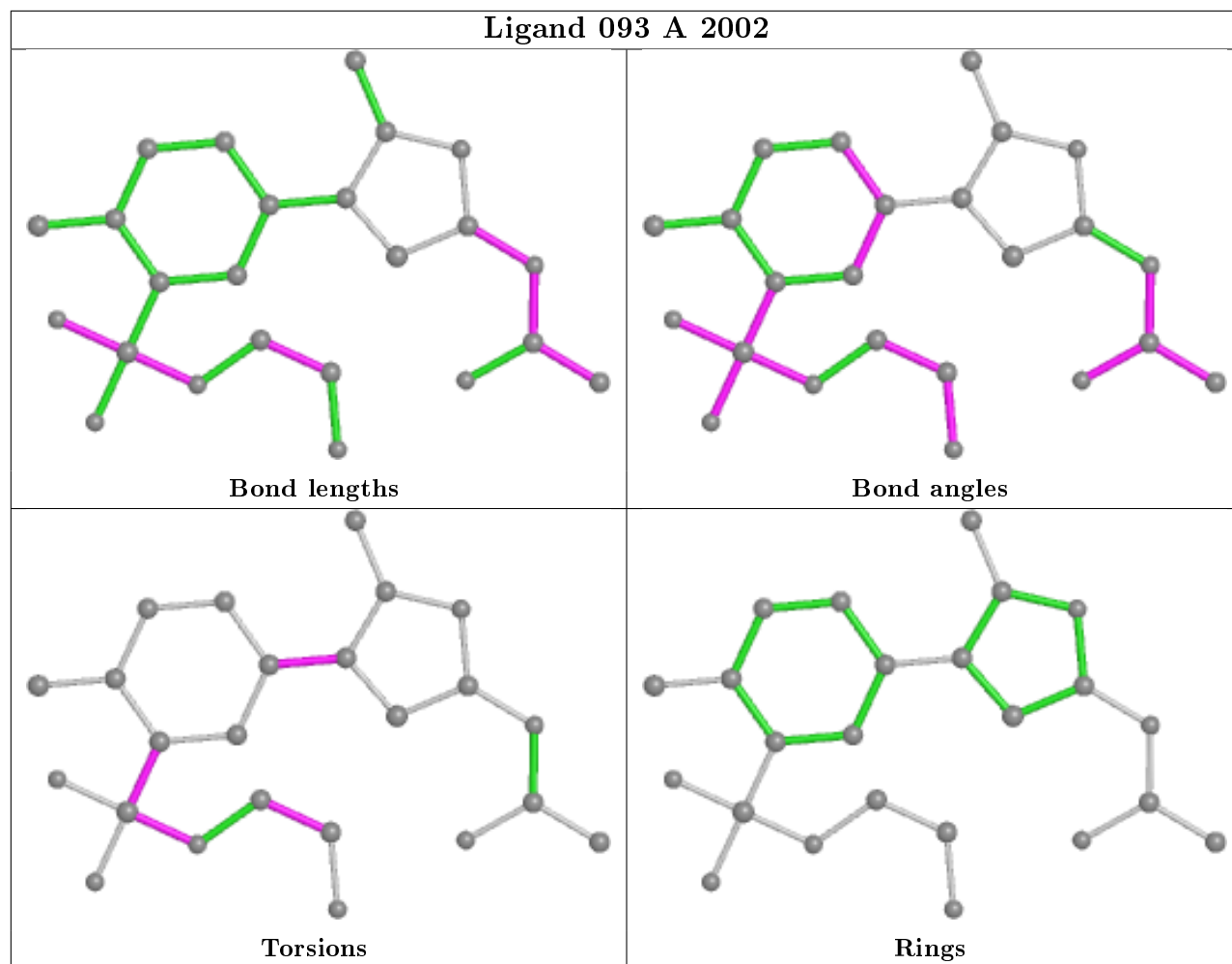
There are no ring outliers.

6 monomers are involved in 27 short contacts:

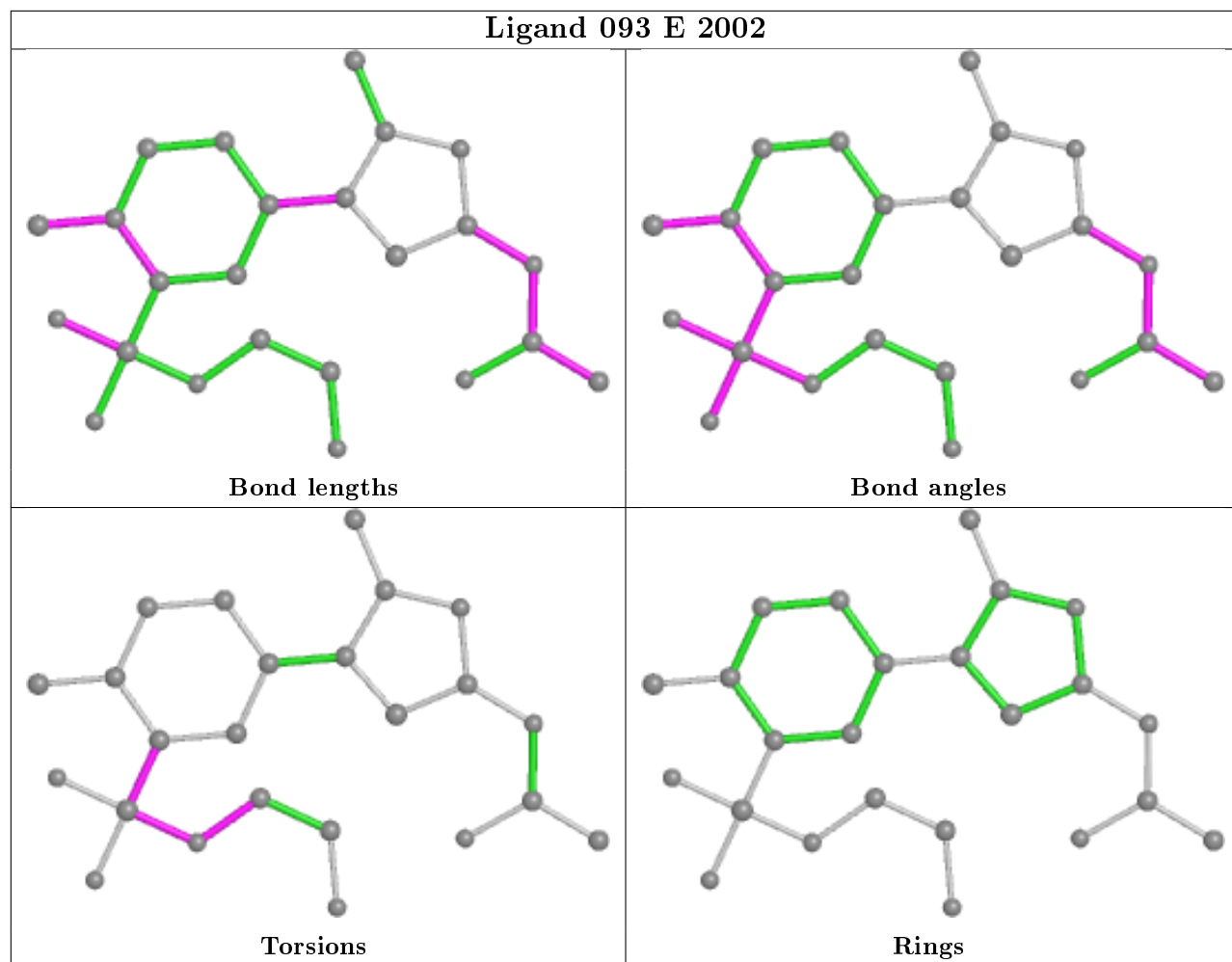
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	2000	GSP	3	0
4	D	2000	GSP	2	0
3	A	2002	093	7	0
3	E	2002	093	7	0
3	C	2002	093	5	0
4	B	2000	GSP	3	0

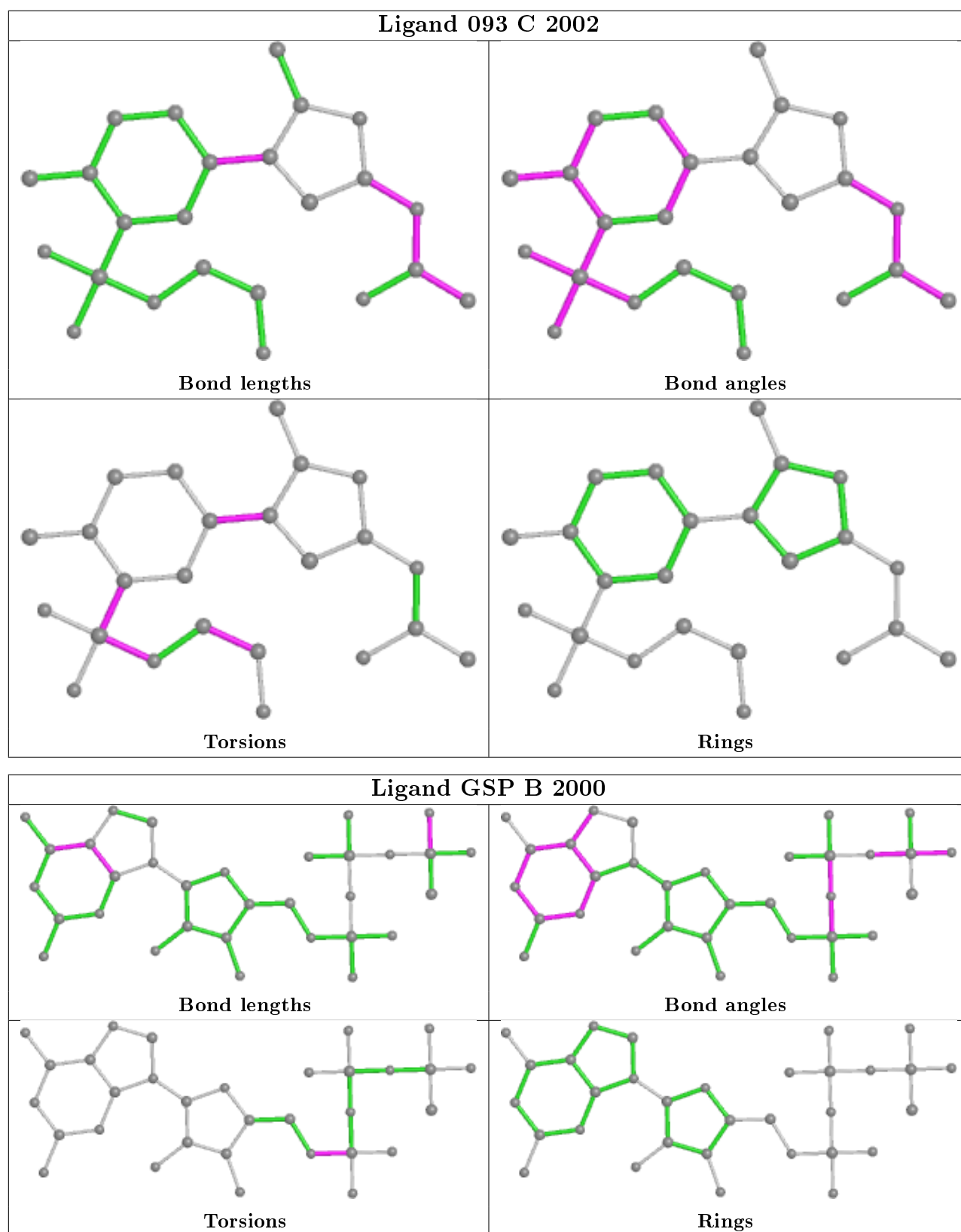
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand 093 E 2002





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	470/566 (83%)	0.03	7 (1%) 73 75	39, 61, 99, 117	0
1	C	476/566 (84%)	0.01	4 (0%) 86 87	38, 61, 98, 146	0
1	E	479/566 (84%)	0.15	25 (5%) 27 26	42, 67, 110, 171	0
2	B	173/219 (78%)	0.21	6 (3%) 44 42	53, 82, 113, 139	0
2	D	177/219 (80%)	0.28	8 (4%) 33 32	45, 65, 106, 149	0
2	F	177/219 (80%)	0.10	2 (1%) 80 82	41, 65, 109, 136	0
All	All	1952/2355 (82%)	0.10	52 (2%) 54 54	38, 65, 106, 171	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	686	LEU	6.1
1	C	683	PRO	3.8
1	E	687	GLY	3.8
1	E	401	ALA	3.7
1	E	688	PHE	3.7
1	E	682	SER	3.5
1	E	615	LEU	3.1
2	B	6	ASP	3.0
1	E	398	SER	2.9
1	E	684	ARG	2.9
2	F	115	SER	2.9
2	D	181	MET	2.8
2	D	182	SER	2.8
1	E	685	ASN	2.7
1	C	612	GLN	2.7
2	D	104	ARG	2.7
1	C	243	ASP	2.6
1	E	784	SER	2.6
1	E	351	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	180	GLN	2.5
1	E	348	LEU	2.4
2	D	175	ILE	2.4
1	A	128	SER	2.4
1	E	344	LEU	2.4
1	A	607	VAL	2.3
1	E	626	TYR	2.3
1	A	241	LEU	2.3
2	B	53	ILE	2.3
1	E	399	VAL	2.3
2	D	116	ASN	2.3
1	A	396	THR	2.3
2	D	179	LYS	2.3
1	E	537	HIS	2.2
2	B	104	ARG	2.2
1	E	346	HIS	2.2
1	E	137	LYS	2.2
2	B	99	TYR	2.2
2	B	105	TRP	2.2
2	D	142	PHE	2.2
1	E	396	THR	2.1
1	E	690	THR	2.1
1	E	350	ALA	2.1
2	B	80	TYR	2.1
1	A	129	TRP	2.1
1	E	402	ARG	2.1
1	E	609	LYS	2.1
1	E	129	TRP	2.1
1	C	129	TRP	2.0
1	A	406	ASN	2.0
1	A	604	ILE	2.0
1	E	389	LEU	2.0
2	D	178	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

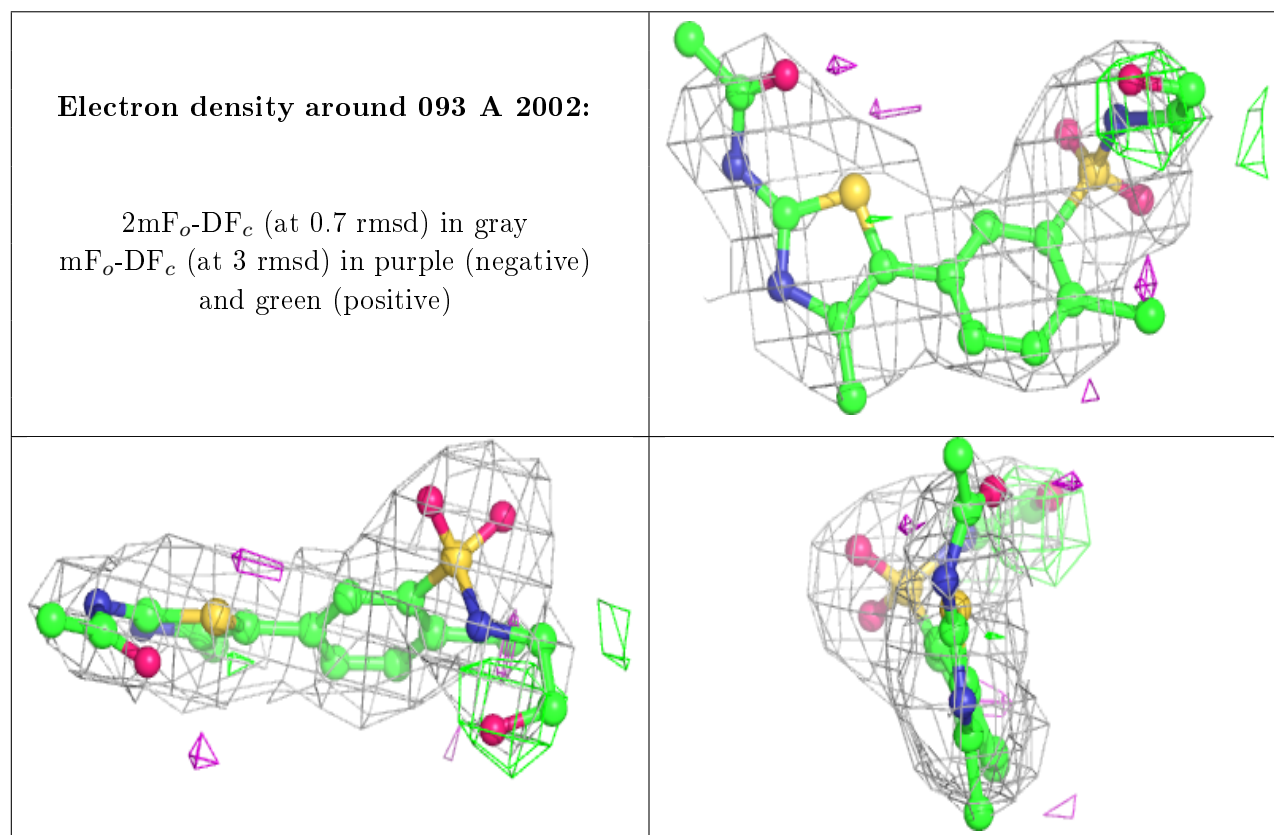
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

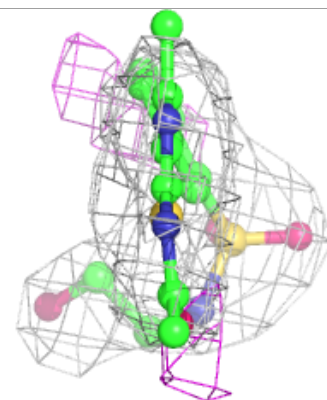
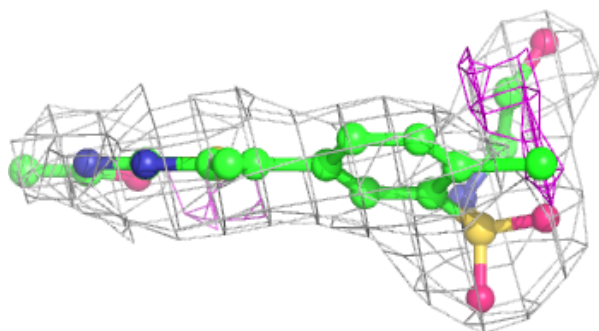
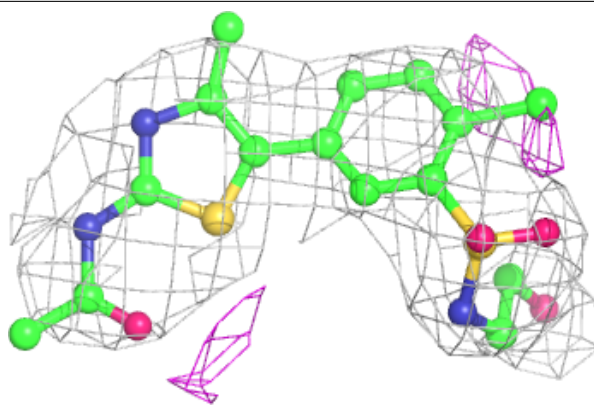
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	D	2001	1/1	0.87	0.10	72,72,72,72	0
5	MG	B	2001	1/1	0.91	0.06	87,87,87,87	0
3	093	A	2002	24/24	0.95	0.22	57,75,105,130	2
5	MG	F	2001	1/1	0.95	0.14	59,59,59,59	0
3	093	E	2002	24/24	0.96	0.20	65,72,83,124	0
3	093	C	2002	24/24	0.96	0.19	57,66,75,123	0
4	GSP	D	2000	32/32	0.97	0.16	46,55,65,72	0
4	GSP	B	2000	32/32	0.97	0.13	47,58,76,86	0
4	GSP	F	2000	32/32	0.98	0.13	43,47,58,61	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.

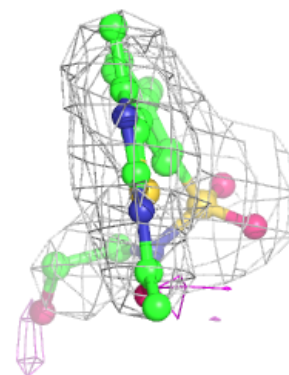
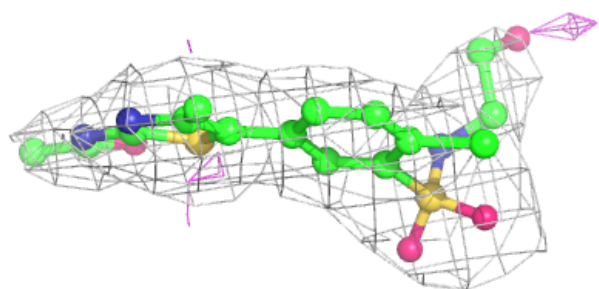
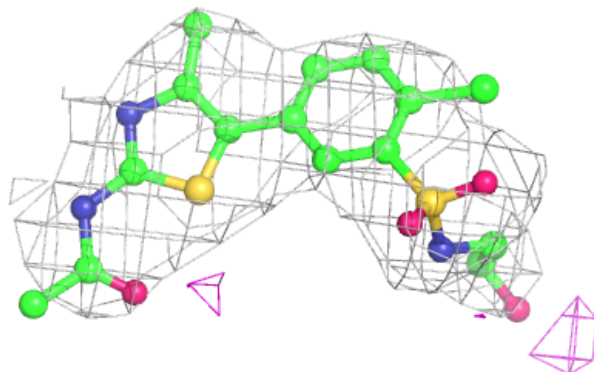


Electron density around 093 E 2002:

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

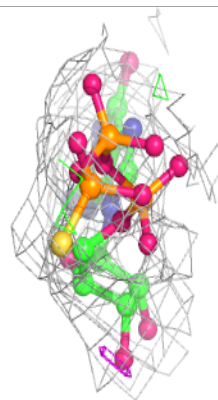
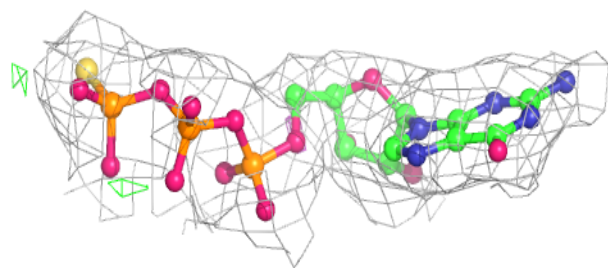
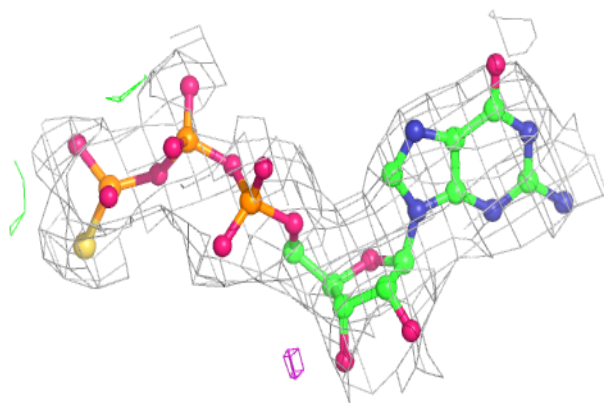
**Electron density around 093 C 2002:**

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

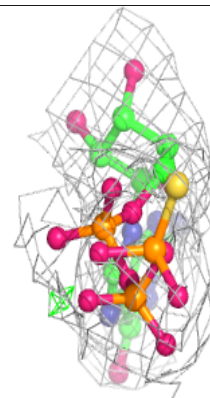
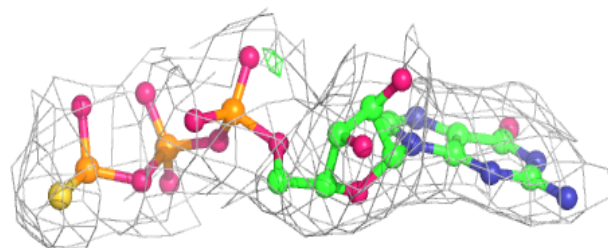
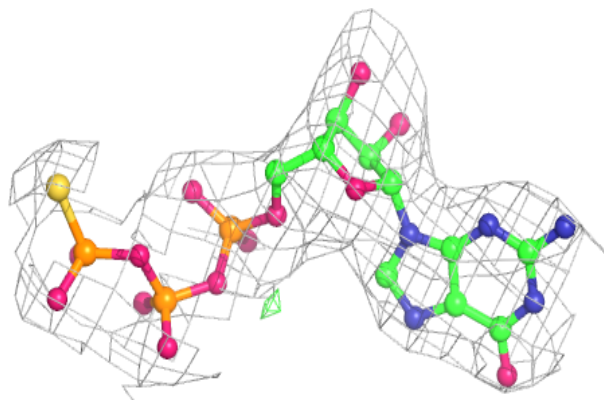


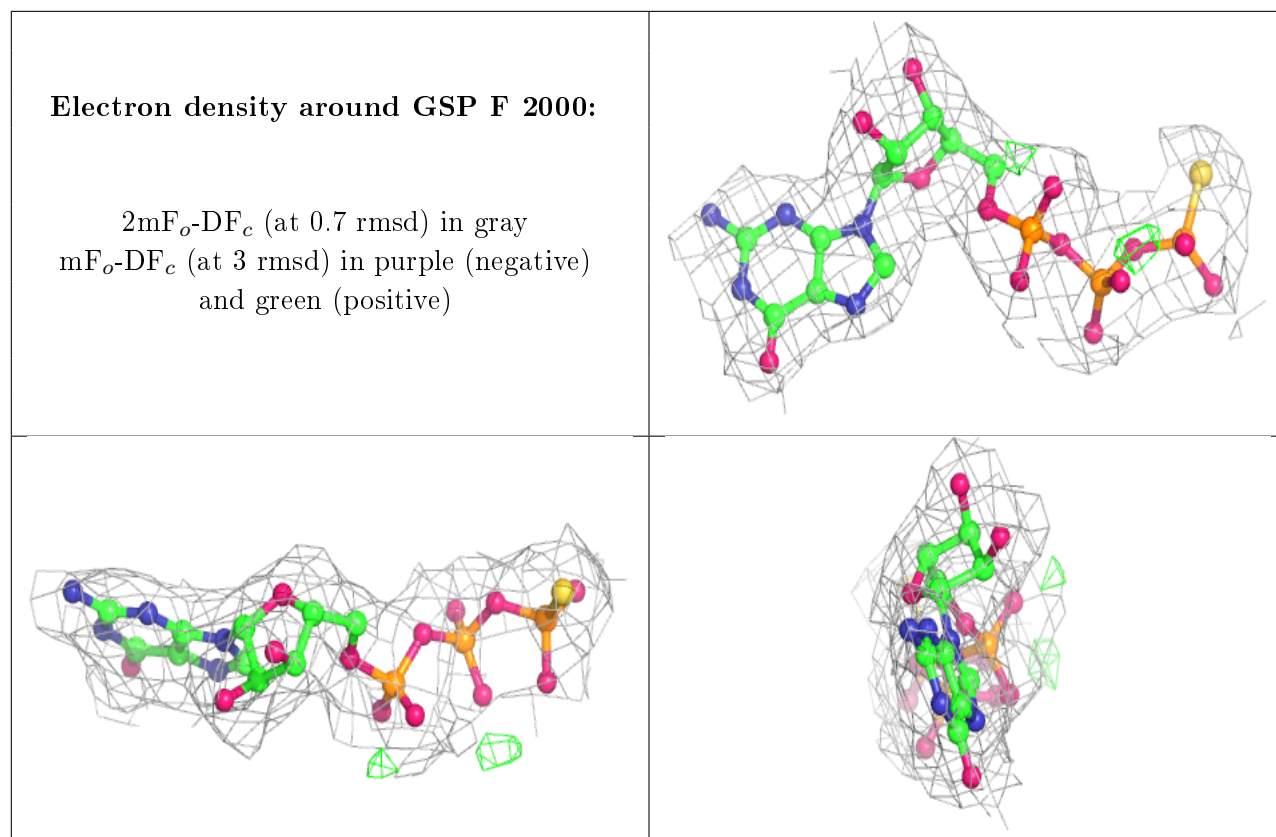
Electron density around GSP D 2000:

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

**Electron density around GSP B 2000:**

$2mF_o-DF_c$ (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.