



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:20 PM UTC

PDB ID : 4D0L / pdb_00004d0l
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 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

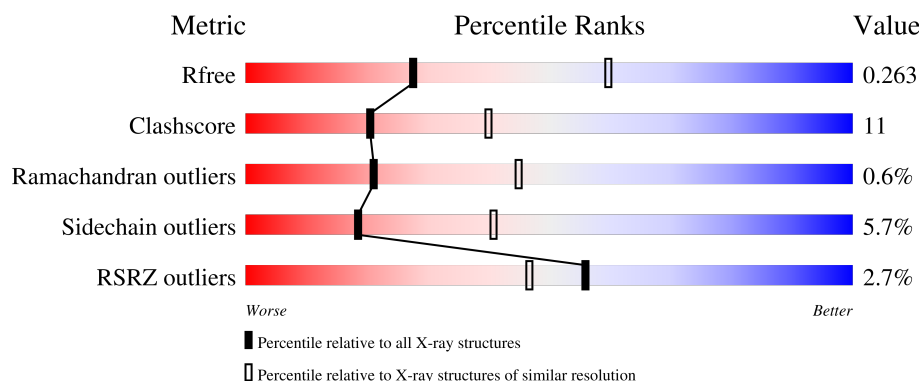
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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}	180053	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	566	2% 63% 19% 17%
1	C	566	2% 67% 14% 16%
1	E	566	4% 63% 18% 15%
2	B	219	3% 61% 16% 21%

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Mol	Chain	Length	Quality of chain
2	D	219	64% 16% 19%
2	F	219	% 65% 15% • 19%

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

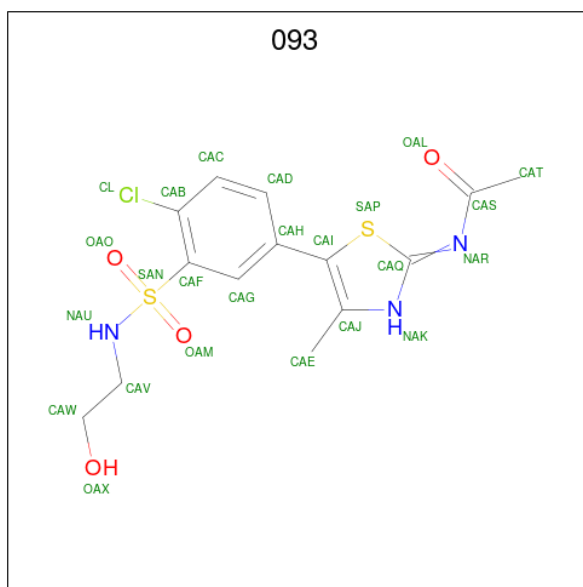
- Molecule 2 is a protein called RAS-RELATED PROTEIN RAB-11A.

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:

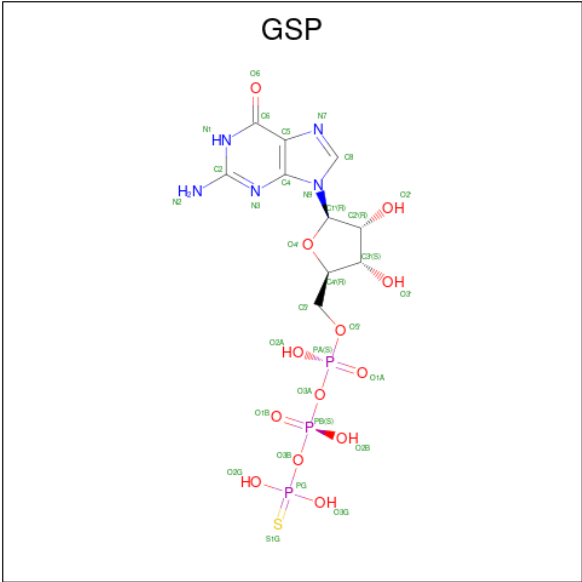
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62491
B	-1	SER	-	expression tag	UNP P62491
B	0	HIS	-	expression tag	UNP P62491
B	70	LEU	GLN	engineered mutation	UNP P62491
D	-2	GLY	-	expression tag	UNP P62491
D	-1	SER	-	expression tag	UNP P62491
D	0	HIS	-	expression tag	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 (CCD ID: 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 (CCD ID: 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 (CCD ID: 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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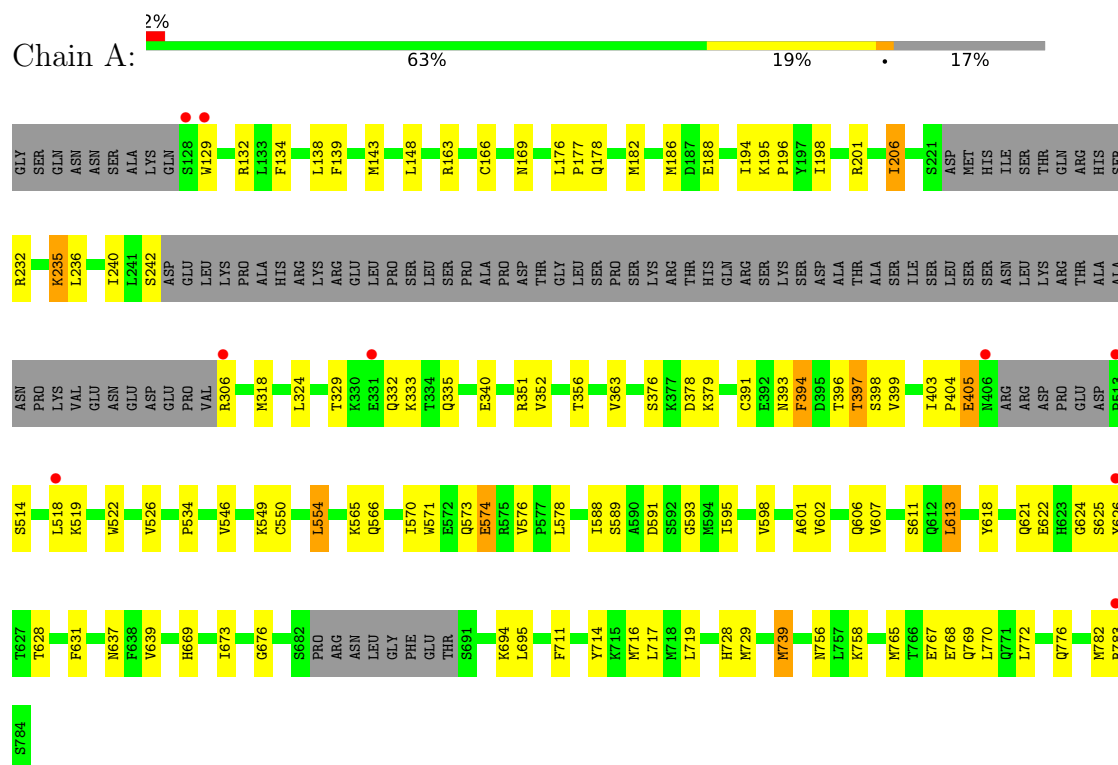
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	4	Total	O	0	0
			4	4		
6	F	3	Total	O	0	0
			3	3		

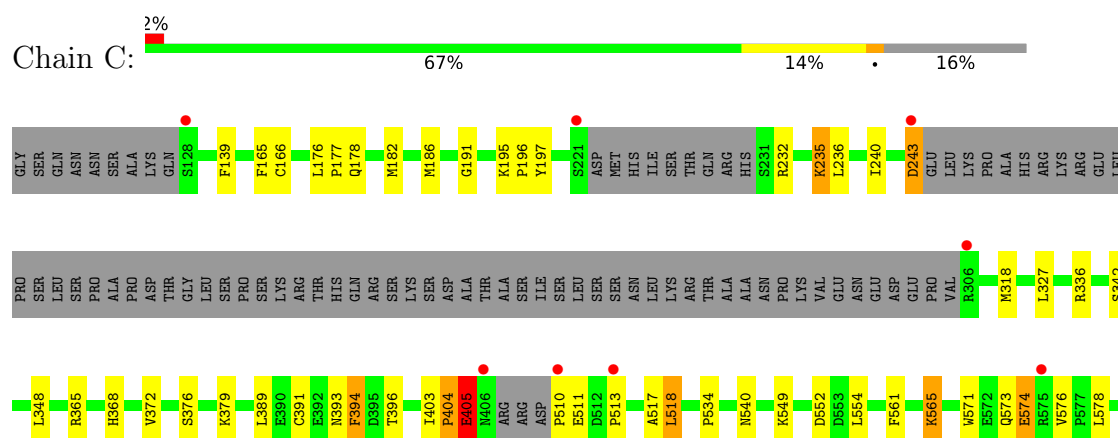
3 Residue-property plots

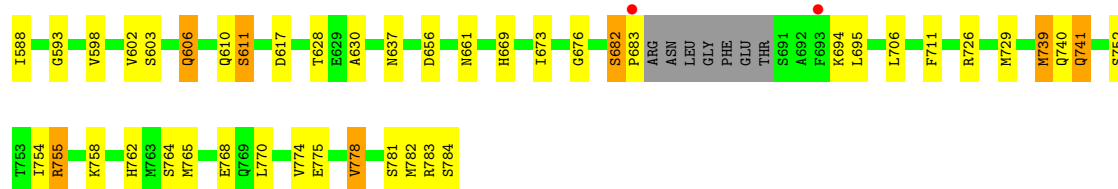
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PHOSPHATIDYLINOSITOL 4-KINASE BETA

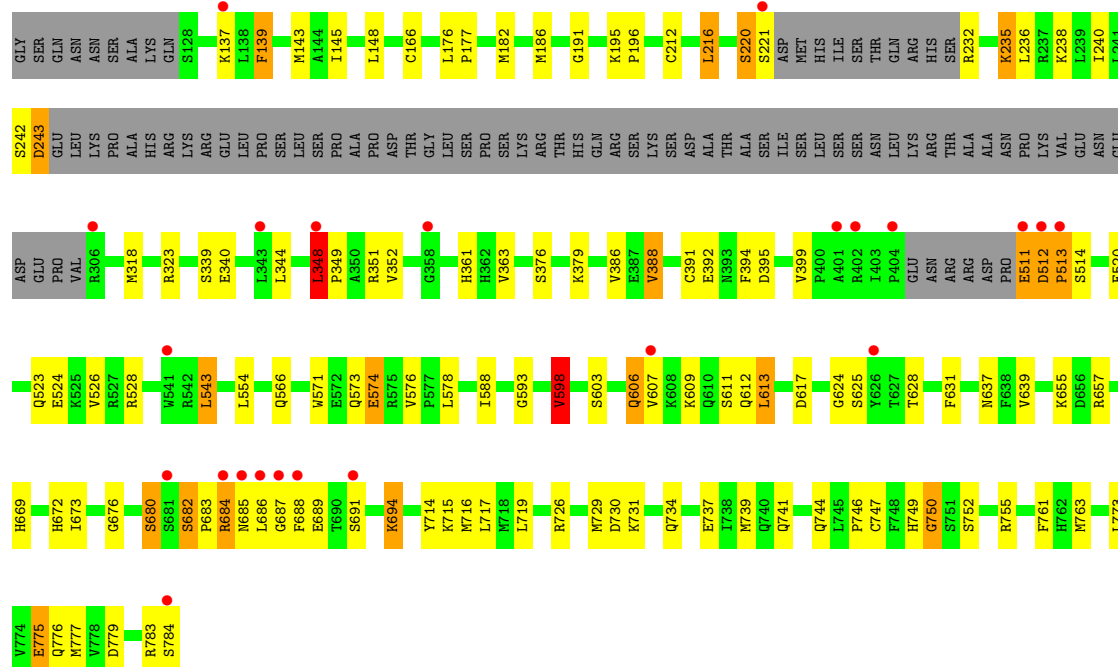


• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

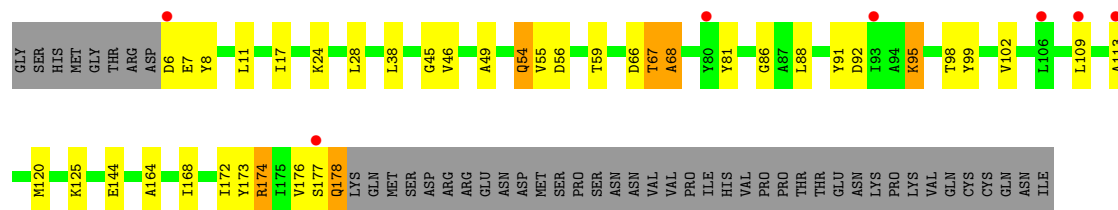




• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



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



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





• 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 – 2.94 115.84 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (115.84-2.94) 99.6 (115.84-2.94)	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	3175 reflections (5.07%)	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 , 39.1	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	0.72	0/3866	1.00	10/5219 (0.2%)
1	C	0.72	0/3913	0.99	11/5285 (0.2%)
1	E	0.71	0/3940	1.05	13/5322 (0.2%)
2	B	0.69	0/1399	0.98	1/1892 (0.1%)
2	D	0.71	0/1431	0.90	1/1933 (0.1%)
2	F	0.73	0/1431	0.96	2/1933 (0.1%)
All	All	0.71	0/15980	1.00	38/21584 (0.2%)

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 (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	348	LEU	CA-C-N	-16.72	98.94	119.84
1	E	348	LEU	C-N-CA	-16.72	98.94	119.84
2	B	67	THR	N-CA-C	9.89	123.86	111.69
1	A	676	GLY	N-CA-C	-9.33	100.60	112.54
1	E	676	GLY	N-CA-C	-8.60	101.54	112.54
1	C	611	SER	N-CA-C	-8.40	97.25	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	676	GLY	N-CA-C	-8.26	101.97	112.54
1	C	574	GLU	N-CA-C	-7.88	100.42	110.19
1	E	574	GLU	CA-C-N	-7.64	112.65	123.20
1	E	574	GLU	C-N-CA	-7.64	112.65	123.20
1	A	574	GLU	CA-C-N	-7.59	112.72	123.20
1	A	574	GLU	C-N-CA	-7.59	112.72	123.20
1	C	574	GLU	CA-C-N	-7.36	113.05	123.20
1	C	574	GLU	C-N-CA	-7.36	113.05	123.20
1	A	514	SER	N-CA-C	-7.09	104.09	112.89
1	A	574	GLU	N-CA-C	-7.03	101.48	110.19
1	C	404	PRO	N-CA-C	6.96	122.59	114.03
1	C	673	ILE	N-CA-C	6.90	123.69	109.34
1	E	673	ILE	N-CA-C	6.86	123.61	109.34
1	A	673	ILE	N-CA-C	6.83	123.55	109.34
1	E	673	ILE	CA-C-N	-6.78	113.43	122.85
1	E	673	ILE	C-N-CA	-6.78	113.43	122.85
2	D	175	ILE	N-CA-C	-6.77	103.72	110.62
2	F	76	ILE	CB-CA-C	-6.49	102.50	111.65
1	A	673	ILE	CA-C-N	-6.40	113.95	122.85
1	A	673	ILE	C-N-CA	-6.40	113.95	122.85
2	F	111	ASP	N-CA-C	-6.06	104.96	112.90
1	E	348	LEU	N-CA-C	6.00	123.08	109.81
1	E	741	GLN	N-CA-C	5.95	118.28	111.02
1	A	394	PHE	N-CA-C	5.81	117.61	111.28
1	E	598	VAL	N-CA-CB	5.71	116.95	110.72
1	C	673	ILE	CA-C-N	-5.67	114.38	122.77
1	C	673	ILE	C-N-CA	-5.67	114.38	122.77
1	C	139	PHE	N-CA-C	5.22	117.20	108.23
1	E	750	GLY	N-CA-C	5.17	121.63	112.64
1	A	206	ILE	N-CA-CB	5.02	120.44	110.95
1	C	741	GLN	N-CA-C	5.02	121.50	110.80
1	E	139	PHE	N-CA-C	5.00	116.84	108.23

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	82	1
1	C	3833	0	3870	65	0
1	E	3859	0	3895	115	0
2	B	1377	0	1370	34	0
2	D	1409	0	1405	25	0
2	F	1409	0	1407	24	0
3	A	24	0	16	8	0
3	C	24	0	16	6	0
3	E	24	0	16	8	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	355	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 11.

All (355) 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
2:D:181:MET:HA	2:D:181:MET:HE3	1.37	1.04
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LYS:NZ	3:A:2002:093:OAM	2.02	0.93
1:E:511:GLU:OE1	1:E:511:GLU:N	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: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: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:CZ	1:E:684:ARG:HA	2.12	0.79
1:E:686:LEU:HB3	1:E:688:PHE:CD1	2.19	0.78
1:A:178:GLN:CD	1:A:739:MET:CE	2.58	0.77
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
2:D:181:MET:HA	2:D:181:MET:CE	2.14	0.77
1:A:602:VAL:HG23	1:A:607:VAL:HG23	1.66	0.76
1:A:139:PHE:HA	1:A:143:MET:HE2	1.68	0.75
1:A:178:GLN:HA	1:A:739:MET:HE1	1.69	0.74
2:F:110:ARG:HD3	2:F:114:ASP:O	1.88	0.74
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: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:C:778:VAL:HG23	1:C:782:MET:HE3	1.70	0.71
1:E:684:ARG:HA	1:E:684:ARG:NE	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:139:PHE:HA	1:E:143:MET:HE2	1.74	0.69
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
3:C:2002:093:HAD	3:C:2002:093:CAE	2.22	0.69
1:C:598:VAL:H	3:C:2002:093:HAK	1.39	0.69
1:E:726:ARG:HA	1:E:763:MET:HE1	1.74	0.69
3:C:2002:093:HAD	3:C:2002:093:HAE3	1.73	0.68
1:E:726:ARG:CA	1:E:763:MET:HE1	2.23	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:178:GLN:CD	1:C:739:MET:HE2	2.20	0.65
2:B:81:TYR:HB3	2:B:113:ALA:HB2	1.78	0.65
1:C:695:LEU:HD23	1:C:782:MET:HE2	1.77	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:E:238:LYS:O	1:E:242:SER:HB3	1.97	0.63
2:B:88:LEU:HD21	2:B:120:MET:HE2	1.79	0.63
1:A:178:GLN:CA	1:A:739:MET:HE1	2.27	0.63
1:C:232:ARG:O	1:C:235:LYS:CD	2.46	0.63
3:E:2002:093:HAD	3:E:2002:093:CAE	2.29	0.63
1:E:752:SER:HB2	1:E:755:ARG:CZ	2.29	0.62
1:A:178:GLN:CD	1:A:739:MET:HE3	2.24	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:178:GLN:HG3	1:A:739:MET:HE2	1.82	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
3:A:2002:093:HAD	3:A:2002:093:HAE3	1.83	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:120:MET:HE1	2:B:164:ALA:O	2.03	0.57
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:768:GLU:CD	1:A:768:GLU:H	2.13	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
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
1:A:129:TRP:CD1	1:A:129:TRP:H	2.24	0.54
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:A:139:PHE:HD1	1:A:143:MET:HE2	1.71	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:O3G	4:B:2000:GSP:O2B	2.26	0.54
1:E:139:PHE:HD1	1:E:143:MET:CE	2.21	0.54
3:C:2002:093:HAE3	3:C:2002:093:CAD	2.37	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: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
1:A:178:GLN:NE2	1:A:739:MET:HE3	2.25	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
3:E:2002:093:HAD	3:E:2002:093:HAE3	1.91	0.52
1:E:588:ILE:HD12	1:E:593:GLY:HA2	1.91	0.51
1:E:243:ASP:N	1:E:243:ASP:OD1	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
1:E:686:LEU:HB2	1:E:687:GLY:C	2.35	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:139:PHE:HD1	1:E:143:MET:HE2	1.75	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
3:A:2002:093:HAE3	3:A:2002:093:CAD	2.41	0.51
3:E:2002:093:HAE3	3:E:2002:093:CAD	2.41	0.51
2:B:56:ASP:OD2	2:B:174:ARG:CZ	2.55	0.50
1:A:711:PHE:CZ	1:A:782:MET:HE1	2.47	0.50
1:A:178:GLN:CG	1:A:739:MET:CE	2.90	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
2:B:6:ASP:O	1:E:628:THR:HA	2.11	0.50
1:C:774:VAL:O	1:C:778:VAL:CG1	2.60	0.50
2:B:88:LEU:CD2	2:B:120:MET:HE2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:120:MET:HE1	2:B:164:ALA:C	2.37	0.49
1:C:177:PRO:C	1:C:739:MET:HE1	2.37	0.49
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:C:177:PRO:HB2	1:C:739:MET:CE	2.43	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:E:773:LEU:HG	1:E:777:MET:HE3	1.96	0.47
1:A:621:GLN:NE2	1:A:622:GLU:OE2	2.46	0.47
2:B:28:LEU:HD11	2:B:49:ALA:HB3	1.96	0.47
1:C:571:TRP:CD2	1:C:578:LEU:HD12	2.49	0.47
2:D:10:TYR:HE2	2:D:58:LYS:HZ2	1.61	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:C:394:PHE:C	1:C:396:THR:H	2.23	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:E:694:LYS:HD3	1:E:784:SER:HB2	1.96	0.47
1:E:716:MET:HE1	1:E:719:LEU:HD23	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:E:657:ARG:HD3	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: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: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:86:GLY:HA3	2:D:172:ILE:HD11	1.98	0.45
1:A:236:LEU:O	1:A:240:ILE:HG13	2.16	0.45
1:C:393:ASN:C	1:C:394:PHE:O	2.57	0.45
1:E:386:VAL:O	1:E:543:LEU:CD2	2.64	0.45
1:C:573:GLN:C	1:C:574:GLU:O	2.57	0.45
1:C:177:PRO:HB2	1:C:739:MET:HE1	1.98	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:C:517:ALA:C	1:C:518:LEU:HG	2.41	0.45
2:D:120:MET:HE1	2:D:167:THR:HB	1.98	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
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:682:SER:N	1:E:683:PRO:C	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:778:VAL:O	1:C:781:SER:OG	2.30	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
2:D:173:TYR:O	2:D:173:TYR:CG	2.69	0.44
1:E:176:LEU:N	1:E:177:PRO:CD	2.81	0.44
1:E:682:SER:HB3	1:E:683:PRO:C	2.42	0.44
2:F:178:GLN:O	2:F:182:SER:N	2.51	0.44
2:B:173:TYR:O	2:B:173:TYR:CG	2.67	0.44
1:C:342:SER:OG	1:C:368:HIS:CD2	2.71	0.44
1:E:682:SER:CA	1:E:683:PRO:C	2.91	0.44
1:A:756:ASN:CG	2:F:34:ASN:ND2	2.76	0.43
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
1:A:573:GLN:C	1:A:574:GLU:O	2.58	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:C:178:GLN:NE2	1:C:739:MET:HE2	2.34	0.43
1:C:778:VAL:HG23	1:C:782:MET:CE	2.46	0.43
1:E:512:ASP:N	1:E:512:ASP:OD1	2.52	0.43
1:E:682:SER:CB	1:E:683:PRO:C	2.91	0.43
1:C:740:GLN:CD	1:C:754:ILE:CD1	2.92	0.43
2:D:110:ARG:NH1	2:D:117:ILE:HG22	2.34	0.43
1:A:178:GLN:NE2	1:A:739:MET:CE	2.79	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:C:711:PHE:HZ	1:C:782:MET:HE1	1.84	0.42
1:A:624:GLY:HA3	1:A:628:THR:HG21	2.00	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:E:511:GLU:C	1:E:513:PRO:HD3	2.44	0.42
1:A:306:ARG:C	1:A:351:ARG:HH22	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:HG3	1:A:739:MET:CE	2.47	0.42
1:E:573:GLN:C	1:E:574:GLU:O	2.59	0.42
1:C:598:VAL:N	3:C:2002:093:HAK	2.11	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:HA	1:C:755:ARG:HD2	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
3:E:2002:093:CAE	3:E:2002:093:CAD	2.93	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:716:MET:HE1	1:A:719:LEU:HD23	2.02	0.42
1:E:729:MET:HG3	1:E:761:PHE:CG	2.54	0.42
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
2:B:28:LEU:CD2	2:B:66:ASP:HB2	2.50	0.41
1:E:511:GLU:N	1:E:511:GLU:CD	2.77	0.41
1:C:695:LEU:HD12	1:C:695:LEU:HA	1.94	0.41
1:E:386:VAL:O	1:E:543:LEU:HD23	2.20	0.41
3:E:2002:093:OAL	3:E:2002:093:SAP	2.78	0.41
1:A:405:GLU:HG3	1:A:534:PRO:HG3	2.02	0.41
1:A:695:LEU:HD12	1:A:695:LEU:HA	1.95	0.41
1:C:178:GLN:CD	1:C:739:MET:CE	2.92	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:688:PHE:O	1:E:689:GLU:C	2.63	0.41
1:A:578:LEU:CD2	1:A:717:LEU:HB3	2.51	0.41
2:B:173:TYR:CD2	2:B:173:TYR:C	2.98	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
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:A:178:GLN:N	1:A:739:MET:HE1	2.35	0.40
1:E:191:GLY:HA3	1:E:232:ARG:HH21	1.86	0.40
1:A:549:LYS:HD2	1:A:595:ILE:HD12	2.03	0.40
1:A:601:ALA:O	3:A:2002:093:HAT2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:MET:HE1	1:A:758:LYS:HB3	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
1:E:686:LEU:N	1:E:687:GLY:HA2	2.34	0.40
2:D:28:LEU:CD2	2:D:66:ASP:HB2	2.51	0.40
2:D:175:ILE:O	2:D:179:LYS:HG2	2.21	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: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
2:D:137:ASP:OD1	2:D:140:ARG:NH2	2.47	0.40
1:E:139:PHE:CA	1:E:143:MET:HE2	2.48	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%)	30 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	466/566 (82%)	445 (96%)	16 (3%)	5 (1%)	11	29
1	E	471/566 (83%)	446 (95%)	22 (5%)	3 (1%)	21	45
2	B	171/219 (78%)	164 (96%)	6 (4%)	1 (1%)	21	45
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%)	21	45

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%)	405 (96%)	17 (4%)	28	53
1	C	428/508 (84%)	403 (94%)	25 (6%)	18	40
1	E	429/508 (84%)	394 (92%)	35 (8%)	10	26
2	B	147/191 (77%)	140 (95%)	7 (5%)	23	47
2	D	151/191 (79%)	143 (95%)	8 (5%)	20	43
2	F	151/191 (79%)	144 (95%)	7 (5%)	24	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1728/2097 (82%)	1629 (94%)	99 (6%)	18	41

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ARG
1	A	138	LEU
1	A	148	LEU
1	A	235	LYS
1	A	318	MET
1	A	335	GLN
1	A	376	SER
1	A	378	ASP
1	A	391	CYS
1	A	397	THR
1	A	554	LEU
1	A	565	LYS
1	A	566	GLN
1	A	606	GLN
1	A	613	LEU
1	A	694	LYS
1	A	739	MET
2	B	7	GLU
2	B	46	VAL
2	B	54	GLN
2	B	55	VAL
2	B	95	LYS
2	B	174	ARG
2	B	178	GLN
1	C	166	CYS
1	C	235	LYS
1	C	243	ASP
1	C	318	MET
1	C	348	LEU
1	C	372	VAL
1	C	376	SER
1	C	379	LYS
1	C	391	CYS
1	C	405	GLU
1	C	518	LEU
1	C	565	LYS
1	C	603	SER

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Mol	Chain	Res	Type
1	C	606	GLN
1	C	610	GLN
1	C	611	SER
1	C	617	ASP
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	46	VAL
2	D	95	LYS
2	D	162	GLU
2	D	175	ILE
2	D	177	SER
2	D	181	MET
2	D	182	SER
1	E	137	LYS
1	E	145	ILE
1	E	148	LEU
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
1	E	339	SER
1	E	376	SER
1	E	379	LYS
1	E	388	VAL
1	E	391	CYS
1	E	392	GLU
1	E	511	GLU
1	E	512	ASP
1	E	543	LEU
1	E	554	LEU
1	E	598	VAL
1	E	606	GLN

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Mol	Chain	Res	Type
1	E	609	LYS
1	E	612	GLN
1	E	613	LEU
1	E	680	SER
1	E	682	SER
1	E	684	ARG
1	E	685	ASN
1	E	694	LYS
1	E	737	GLU
1	E	739	MET
1	E	744	GLN
1	E	775	GLU
1	E	776	GLN
2	F	46	VAL
2	F	95	LYS
2	F	104	ARG
2	F	108	GLU
2	F	162	GLU
2	F	174	ARG
2	F	177	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	393	ASN
1	A	606	GLN
1	A	659	ASN
1	A	728	HIS
1	A	776	GLN
1	C	185	HIS
1	C	207	ASN
1	C	566	GLN
1	C	610	GLN
1	C	612	GLN
1	C	659	ASN
1	C	728	HIS
1	E	204	GLN
1	E	207	ASN
1	E	335	GLN
1	E	368	HIS
1	E	540	ASN

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Mol	Chain	Res	Type
1	E	568	GLN
1	E	621	GLN
1	E	659	ASN
1	E	728	HIS
1	E	776	GLN
2	F	34	ASN
2	F	178	GLN

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 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	B	2000	5	33,34,34	1.38	6 (18%)	47,54,54	1.95	11 (23%)
3	093	A	2002	-	25,25,25	3.32	9 (36%)	33,36,36	5.50	13 (39%)
4	GSP	F	2000	5	33,34,34	1.35	7 (21%)	47,54,54	1.94	14 (29%)
3	093	C	2002	-	25,25,25	2.93	6 (24%)	33,36,36	4.85	15 (45%)
3	093	E	2002	-	25,25,25	2.94	9 (36%)	33,36,36	4.50	10 (30%)
4	GSP	D	2000	5	33,34,34	1.39	7 (21%)	47,54,54	1.86	10 (21%)

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	B	2000	5	-	3/21/38/38	0/3/3/3
3	093	A	2002	-	-	8/19/19/19	0/2/2/2
4	GSP	F	2000	5	-	2/21/38/38	0/3/3/3
3	093	C	2002	-	-	7/19/19/19	0/2/2/2
3	093	E	2002	-	-	9/19/19/19	0/2/2/2
4	GSP	D	2000	5	-	2/21/38/38	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2002	093	CAQ-NAR	8.48	1.45	1.32
3	A	2002	093	CAQ-SAP	-8.20	1.60	1.73
3	C	2002	093	CAQ-SAP	-8.11	1.60	1.73
3	E	2002	093	CAQ-NAR	8.05	1.45	1.32
3	A	2002	093	CAI-SAP	-7.73	1.55	1.74
3	C	2002	093	CAQ-NAR	7.57	1.44	1.32
3	E	2002	093	CAQ-SAP	-6.80	1.62	1.73
3	C	2002	093	CAI-SAP	-6.32	1.58	1.74
3	E	2002	093	CAI-SAP	-6.06	1.59	1.74
3	C	2002	093	CAJ-NAK	3.79	1.47	1.37
3	E	2002	093	CAJ-NAK	3.75	1.47	1.37
3	A	2002	093	SAN-NAU	3.74	1.67	1.61
3	A	2002	093	CAJ-NAK	3.71	1.47	1.37
3	A	2002	093	CAV-CAW	-3.61	1.38	1.50
4	B	2000	GSP	C6-N1	-3.23	1.32	1.38
4	D	2000	GSP	C5-C4	3.14	1.47	1.38
4	F	2000	GSP	C5-N7	-3.06	1.32	1.39
3	E	2002	093	CAS-NAR	3.04	1.44	1.38
3	C	2002	093	CAS-NAR	2.99	1.44	1.38
4	B	2000	GSP	C5-C4	2.87	1.46	1.38
3	A	2002	093	CAS-NAR	2.79	1.44	1.38
3	A	2002	093	CAT-CAS	2.63	1.53	1.49
4	D	2000	GSP	PG-O3G	2.63	1.63	1.54
4	D	2000	GSP	PA-O3A	2.58	1.62	1.59
4	F	2000	GSP	PG-O3G	2.57	1.63	1.54
4	D	2000	GSP	C5-N7	-2.49	1.34	1.39
4	F	2000	GSP	C6-N1	-2.45	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2000	GSP	C6-N1	-2.43	1.34	1.38
4	B	2000	GSP	C5-N7	-2.40	1.34	1.39
4	B	2000	GSP	PG-O3G	2.38	1.62	1.54
3	E	2002	093	CAT-CAS	2.36	1.53	1.49
3	E	2002	093	OAM-SAN	-2.36	1.40	1.43
3	C	2002	093	CAT-CAS	2.31	1.52	1.49
4	B	2000	GSP	C4-N9	-2.26	1.32	1.38
4	F	2000	GSP	C5-C4	2.26	1.44	1.38
3	E	2002	093	CAB-CAF	2.25	1.43	1.40
3	A	2002	093	OAM-SAN	-2.19	1.41	1.43
4	F	2000	GSP	C4-N9	-2.14	1.32	1.38
4	F	2000	GSP	PG-O2G	2.11	1.61	1.54
4	D	2000	GSP	PG-S1G	2.05	1.95	1.90
3	E	2002	093	CAB-CL	2.04	1.78	1.73
4	D	2000	GSP	C4-N9	-2.03	1.32	1.38
4	B	2000	GSP	PG-O2G	2.02	1.61	1.54
4	F	2000	GSP	PA-O3A	2.00	1.61	1.59

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	093	OAO-SAN-OAM	-21.10	93.89	119.52
3	A	2002	093	CAQ-SAP-CAI	19.53	100.51	88.35
3	C	2002	093	OAO-SAN-OAM	-18.13	97.50	119.52
3	E	2002	093	OAO-SAN-OAM	-17.05	98.81	119.52
3	C	2002	093	CAQ-SAP-CAI	16.38	98.55	88.35
3	E	2002	093	CAQ-SAP-CAI	15.41	97.94	88.35
3	E	2002	093	OAO-SAN-NAU	5.90	116.21	107.03
4	D	2000	GSP	C5-C4-N3	-5.85	119.09	128.39
4	B	2000	GSP	C5-C4-N3	-5.83	119.11	128.39
3	C	2002	093	OAO-SAN-NAU	5.54	115.65	107.03
4	F	2000	GSP	C5-C4-N3	-5.48	119.66	128.39
3	C	2002	093	OAM-SAN-CAF	5.32	116.47	107.68
4	B	2000	GSP	PB-O3B-PG	-5.24	114.00	133.17
3	A	2002	093	OAO-SAN-NAU	5.13	115.01	107.03
3	A	2002	093	OAM-SAN-NAU	4.93	114.70	107.03
4	D	2000	GSP	C2-N3-C4	4.76	120.50	112.30
4	F	2000	GSP	N9-C4-N3	4.70	135.34	125.95
4	B	2000	GSP	C2-N3-C4	4.58	120.19	112.30
3	A	2002	093	CAE-CAJ-CAI	-4.57	125.60	130.98
4	F	2000	GSP	C2-N3-C4	4.48	120.01	112.30
4	D	2000	GSP	N9-C4-N3	4.33	134.61	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2002	093	CAT-CAS-NAR	4.21	121.08	114.84
4	B	2000	GSP	N9-C4-N3	4.19	134.34	125.95
3	A	2002	093	OAO-SAN-CAF	4.18	114.58	107.68
3	C	2002	093	OAO-SAN-CAF	4.02	114.32	107.68
3	E	2002	093	CAF-CAB-CL	3.81	124.27	121.52
3	E	2002	093	CAE-CAJ-CAI	-3.80	126.51	130.98
4	F	2000	GSP	PB-O3B-PG	-3.67	119.73	133.17
3	C	2002	093	CAE-CAJ-CAI	-3.62	126.72	130.98
3	C	2002	093	CAB-CAF-SAN	-3.60	120.71	123.19
4	B	2000	GSP	C6-C5-N7	3.54	136.73	130.29
3	A	2002	093	OAX-CAW-CAV	-3.48	98.72	111.50
3	A	2002	093	OAM-SAN-CAF	3.31	113.16	107.68
3	E	2002	093	CAH-CAI-SAP	3.29	125.70	117.32
3	E	2002	093	OAM-SAN-CAF	3.26	113.06	107.68
4	D	2000	GSP	PB-O3B-PG	-3.17	121.58	133.17
4	D	2000	GSP	C6-C5-N7	3.12	135.98	130.29
3	C	2002	093	CAF-CAB-CL	-3.10	119.27	121.52
3	E	2002	093	CAI-CAJ-NAK	3.03	110.28	105.70
3	C	2002	093	CAC-CAB-CAF	3.02	122.01	120.04
3	E	2002	093	CAT-CAS-NAR	3.00	119.28	114.84
3	C	2002	093	CAF-SAN-NAU	-2.92	103.89	107.86
4	F	2000	GSP	C2'-C1'-N9	-2.86	105.30	113.25
4	D	2000	GSP	C4-C5-N7	-2.72	106.36	110.67
4	F	2000	GSP	O4'-C1'-N9	2.71	114.50	108.36
3	C	2002	093	CAT-CAS-NAR	2.71	118.85	114.84
3	E	2002	093	OAO-SAN-CAF	2.69	112.13	107.68
3	A	2002	093	OAL-CAS-NAR	-2.67	118.52	123.63
4	B	2000	GSP	C4-C5-N7	-2.59	106.57	110.67
4	B	2000	GSP	O2G-PG-O3B	2.48	112.93	104.64
4	D	2000	GSP	C2'-C3'-C4'	2.47	107.39	102.61
4	F	2000	GSP	N9-C8-N7	-2.46	108.83	113.40
3	C	2002	093	CAH-CAI-SAP	2.46	123.59	117.32
3	C	2002	093	CAD-CAH-CAG	2.40	122.03	119.25
3	C	2002	093	CAS-NAR-CAQ	2.39	122.79	117.26
4	F	2000	GSP	C8-N9-C4	2.38	110.48	106.03
3	A	2002	093	CAD-CAH-CAG	2.37	121.99	119.25
4	F	2000	GSP	C8-N7-C5	2.35	108.45	104.26
4	F	2000	GSP	C6-C5-N7	2.35	134.56	130.29
4	B	2000	GSP	C5-C6-N1	2.24	118.96	113.25
4	D	2000	GSP	C3'-C2'-C1'	2.24	105.70	101.46
4	D	2000	GSP	O2G-PG-O3B	2.24	112.11	104.64
4	F	2000	GSP	O3'-C3'-C2'	-2.22	104.69	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	2000	GSP	O6-C6-C5	-2.21	120.69	126.53
4	F	2000	GSP	O2B-PB-O1B	2.20	122.68	112.44
3	C	2002	093	CAI-CAJ-NAK	2.19	109.02	105.70
4	B	2000	GSP	O3A-PB-O1B	-2.18	104.16	110.70
4	F	2000	GSP	C4-C5-N7	-2.17	107.24	110.67
3	A	2002	093	CAI-CAJ-NAK	2.11	108.89	105.70
4	D	2000	GSP	C8-N7-C5	2.05	107.91	104.26
4	B	2000	GSP	C2-N1-C6	-2.04	121.42	125.11
3	A	2002	093	CAE-CAJ-NAK	2.04	125.50	121.36
4	B	2000	GSP	O2B-PB-O1B	2.03	121.90	112.44

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2002	093	NAU-CAV-CAW-OAX
3	A	2002	093	NAK-CAQ-NAR-CAS
3	A	2002	093	SAP-CAQ-NAR-CAS
3	C	2002	093	CAB-CAF-SAN-OAO
3	C	2002	093	CAB-CAF-SAN-NAU
3	C	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
4	B	2000	GSP	C5'-O5'-PA-O2A
4	B	2000	GSP	C5'-O5'-PA-O3A
3	A	2002	093	CAV-NAU-SAN-OAO
3	E	2002	093	CAG-CAF-SAN-OAO
3	A	2002	093	CAB-CAF-SAN-OAO
3	C	2002	093	CAB-CAF-SAN-OAM
3	C	2002	093	CAV-NAU-SAN-OAO
3	E	2002	093	CAV-NAU-SAN-OAO
3	A	2002	093	CAV-NAU-SAN-CAF
3	C	2002	093	CAG-CAF-SAN-OAO
3	A	2002	093	CAV-NAU-SAN-OAM
3	E	2002	093	CAG-CAF-SAN-OAM
4	D	2000	GSP	PA-O3A-PB-O1B
4	B	2000	GSP	C5'-O5'-PA-O1A
4	D	2000	GSP	PA-O3A-PB-O2B
3	C	2002	093	CAV-NAU-SAN-CAF

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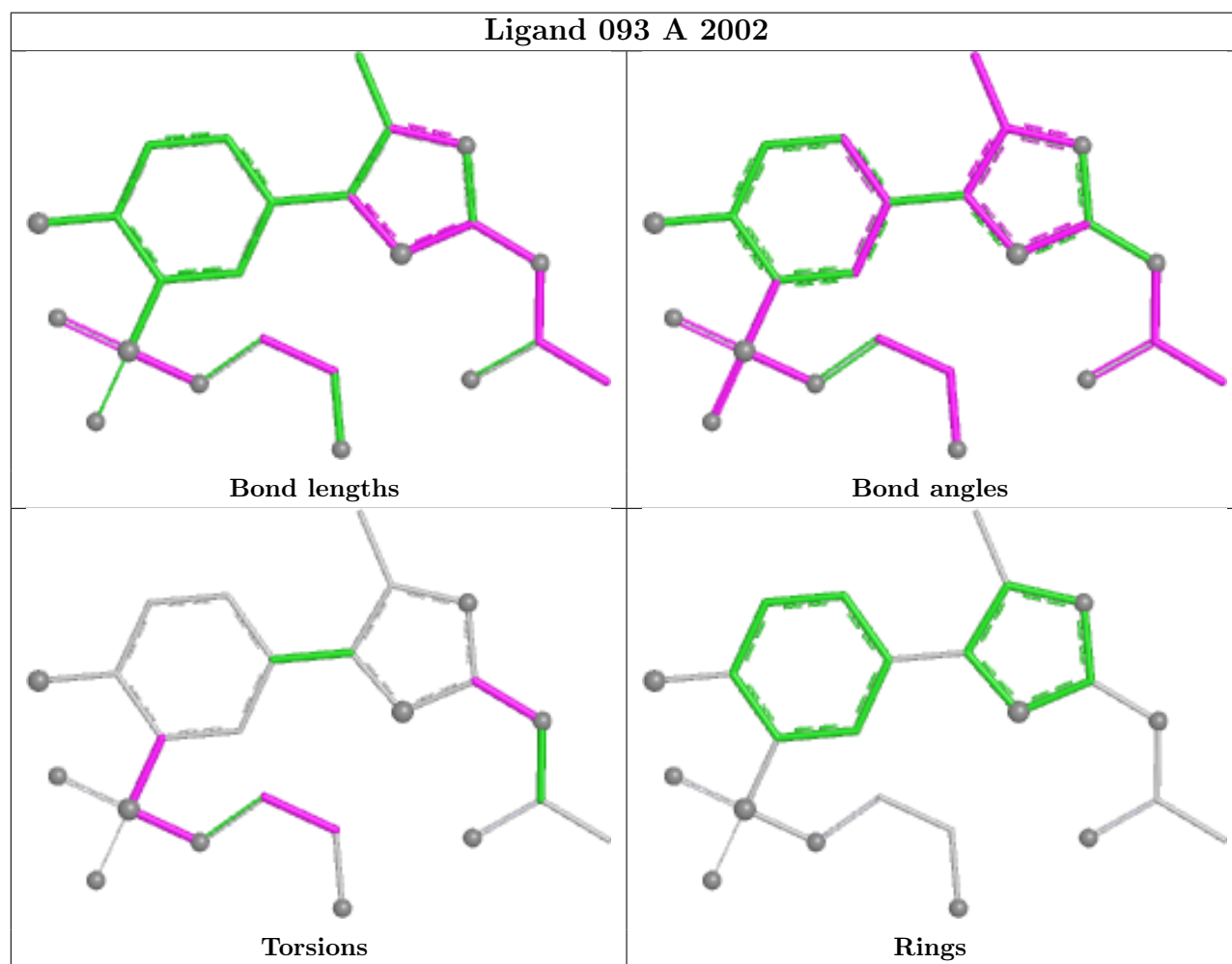
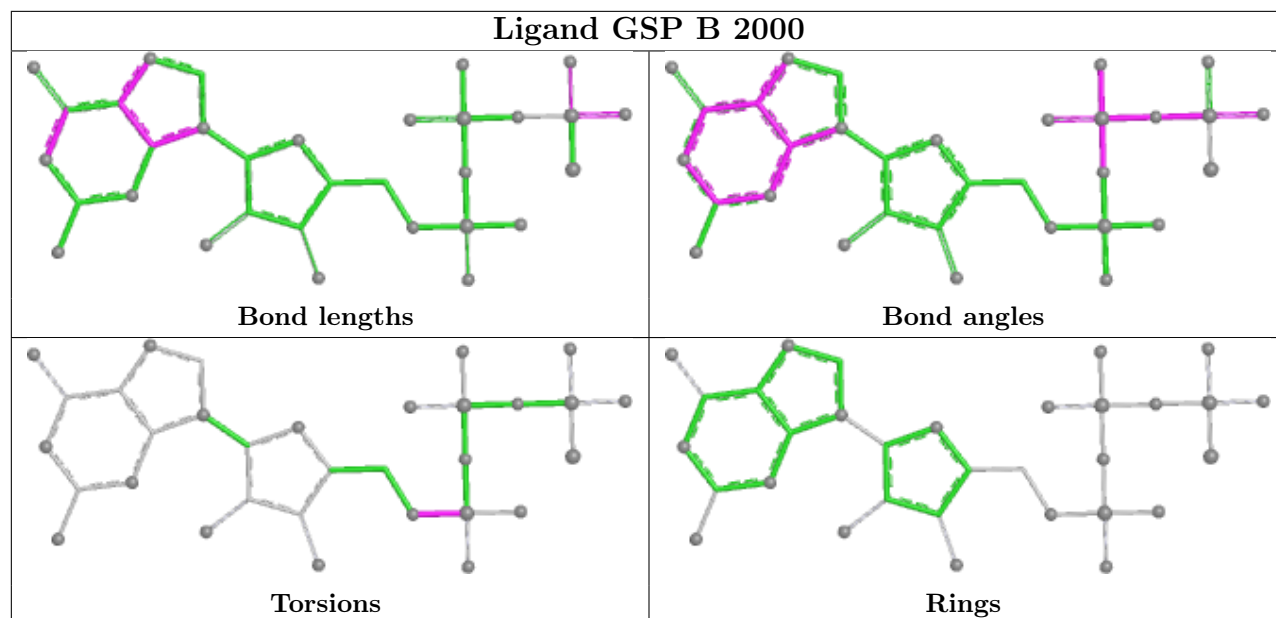
Mol	Chain	Res	Type	Atoms
3	A	2002	093	CAG-CAF-SAN-OAO
3	E	2002	093	CAV-NAU-SAN-CAF
4	F	2000	GSP	PG-O3B-PB-O1B
4	F	2000	GSP	PA-O3A-PB-O1B

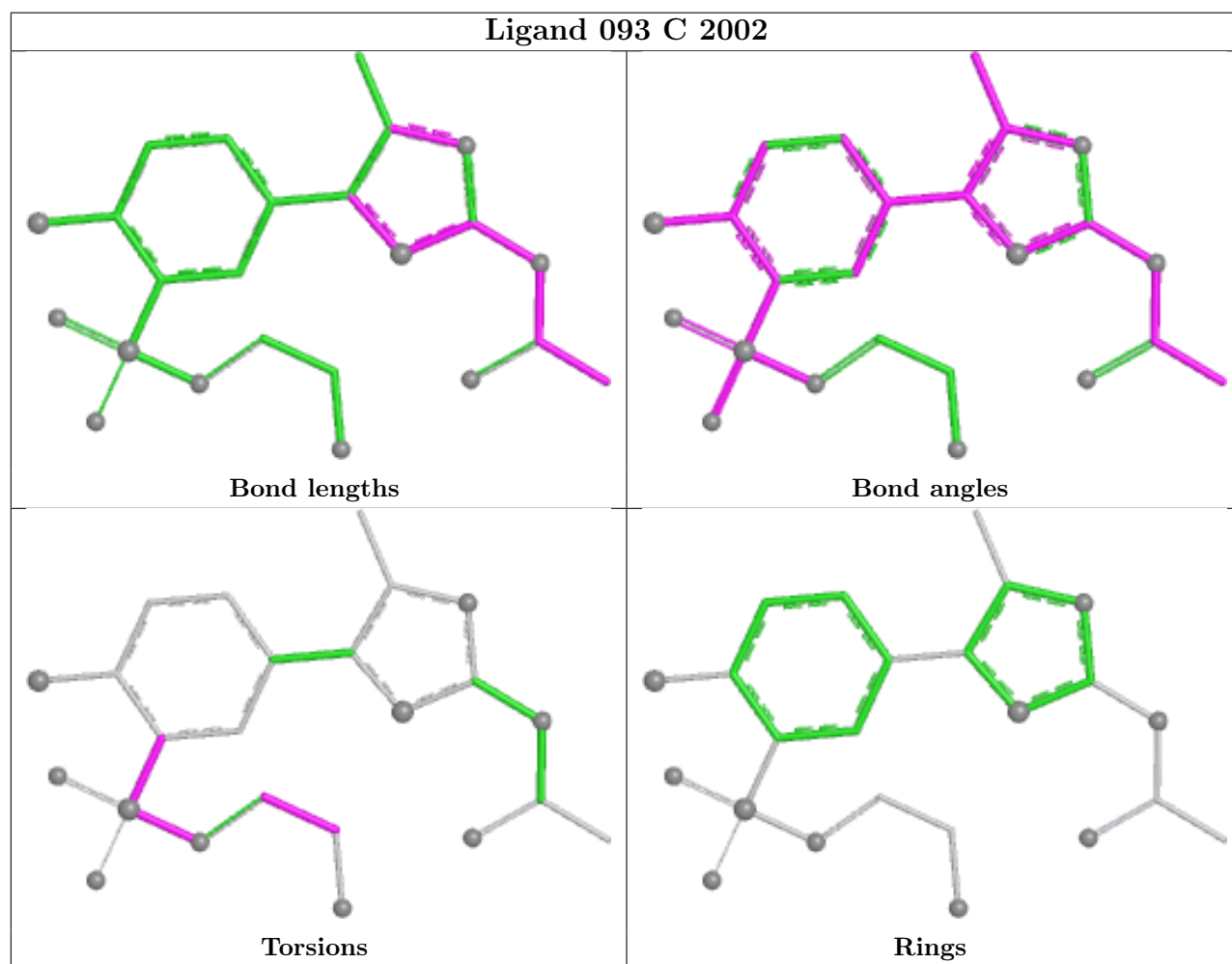
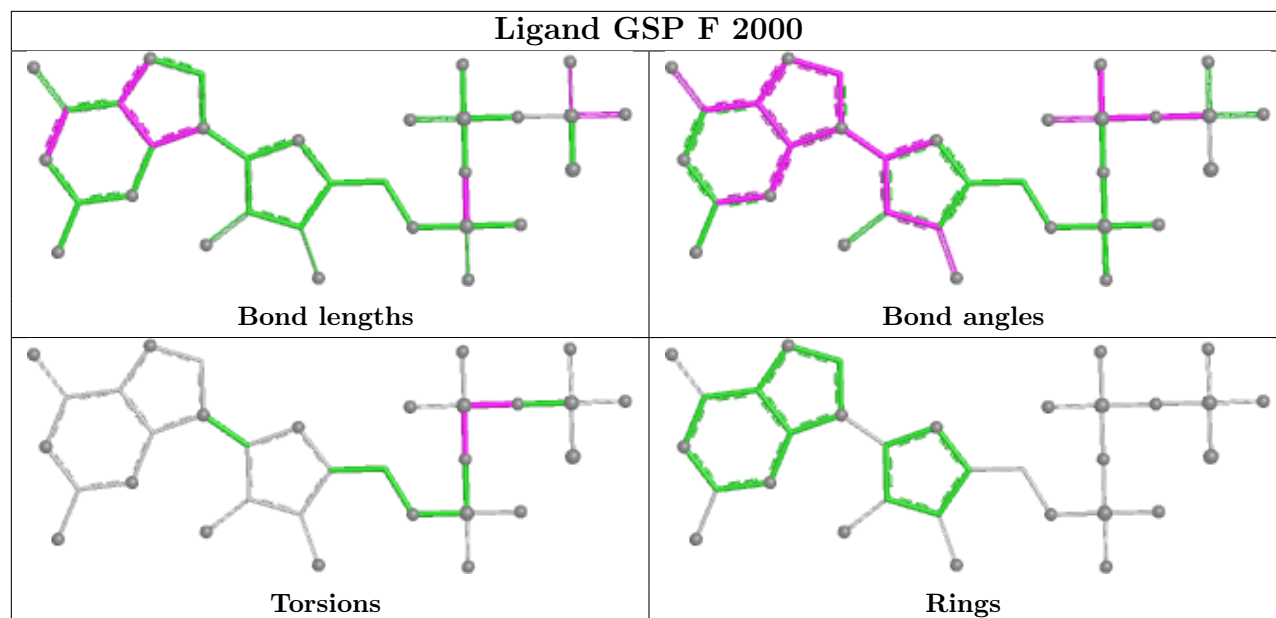
There are no ring outliers.

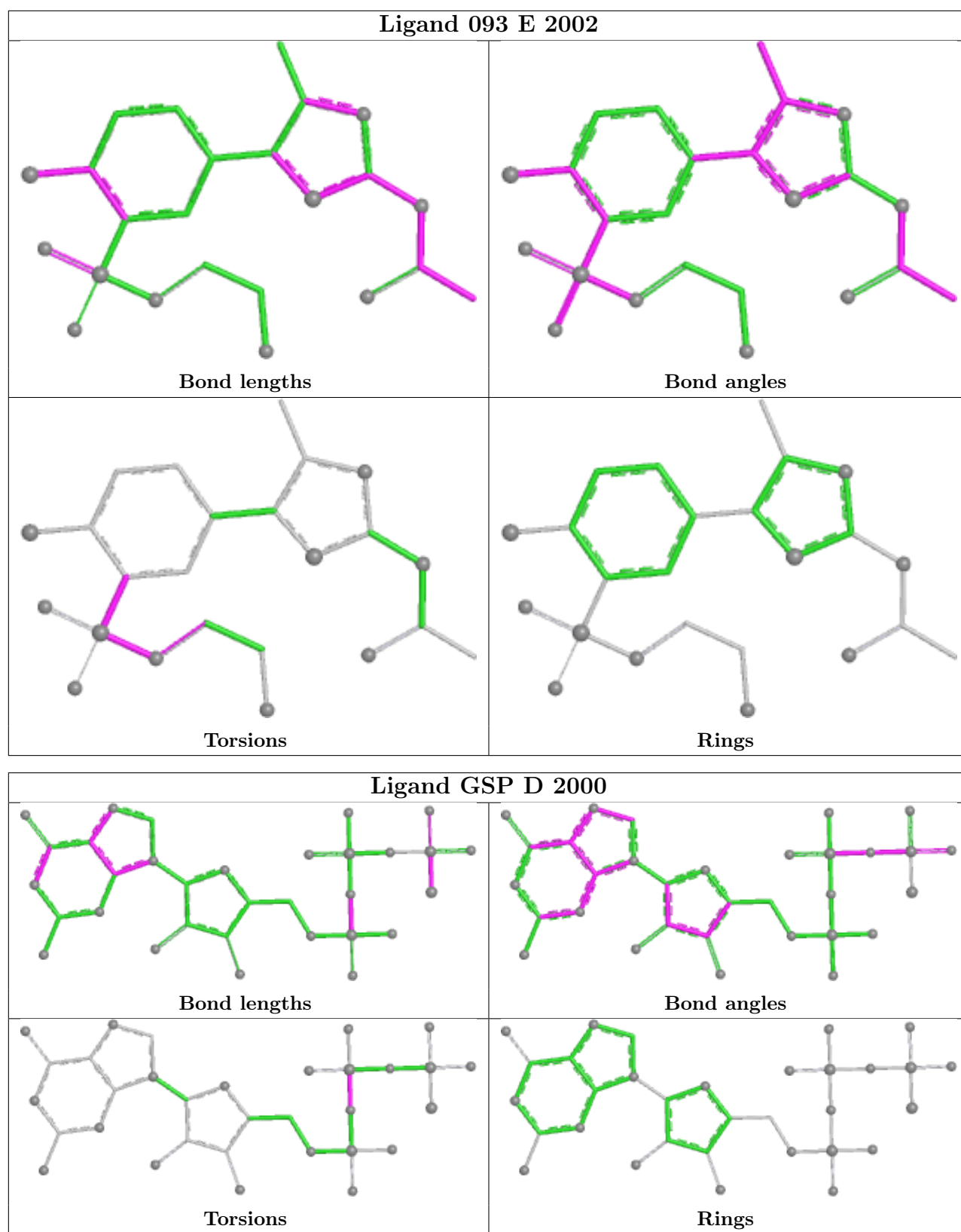
6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2000	GSP	3	0
3	A	2002	093	8	0
4	F	2000	GSP	3	0
3	C	2002	093	6	0
3	E	2002	093	8	0
4	D	2000	GSP	2	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 ⓘ

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%)	0.01	9 (1%) 66 58	39, 61, 99, 117	0
1	C	476/566 (84%)	-0.05	10 (2%) 63 54	38, 61, 98, 146	0
1	E	479/566 (84%)	0.18	23 (4%) 35 29	42, 67, 110, 171	0
2	B	173/219 (78%)	0.52	7 (4%) 42 34	53, 82, 113, 139	0
2	D	177/219 (80%)	0.07	1 (0%) 85 81	45, 65, 106, 149	0
2	F	177/219 (80%)	0.14	3 (1%) 69 61	41, 65, 109, 136	0
All	All	1952/2355 (82%)	0.10	53 (2%) 56 47	38, 65, 106, 171	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	510	PRO	4.2
1	C	221	SER	4.1
2	F	109	LEU	4.0
1	A	513	PRO	3.9
1	E	687	GLY	3.8
1	E	686	LEU	3.8
1	E	607	VAL	3.5
1	C	243	ASP	3.5
1	A	129	TRP	3.4
1	E	688	PHE	3.2
1	C	513	PRO	3.1
1	E	404	PRO	3.0
1	E	511	GLU	3.0
1	C	683	PRO	3.0
2	B	106	LEU	2.9
1	E	513	PRO	2.8
1	A	518	LEU	2.7
2	B	109	LEU	2.7
1	E	137	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	358	GLY	2.6
2	B	177	SER	2.6
1	A	626	TYR	2.5
1	E	306	ARG	2.5
1	E	402	ARG	2.5
2	F	179	LYS	2.5
1	E	348	LEU	2.5
1	A	128	SER	2.4
1	E	626	TYR	2.4
1	E	685	ASN	2.4
1	A	306	ARG	2.3
2	B	113	ALA	2.3
1	E	512	ASP	2.3
2	B	80	TYR	2.3
1	E	691	SER	2.3
1	C	693	PHE	2.2
2	B	6	ASP	2.2
2	F	56	ASP	2.2
1	C	128	SER	2.2
1	E	784	SER	2.2
1	E	221	SER	2.2
1	E	401	ALA	2.2
2	D	68	ALA	2.2
1	C	306	ARG	2.2
1	C	406	ASN	2.2
1	C	575	ARG	2.1
1	E	541	TRP	2.1
1	E	684	ARG	2.1
1	A	331	GLU	2.1
1	E	681	SER	2.1
2	B	93	ILE	2.1
1	A	783	ARG	2.1
1	A	406	ASN	2.1
1	E	343	LEU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

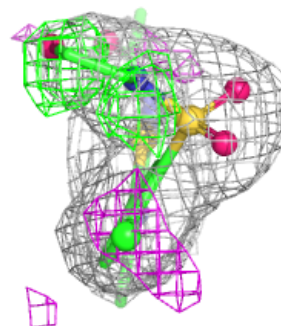
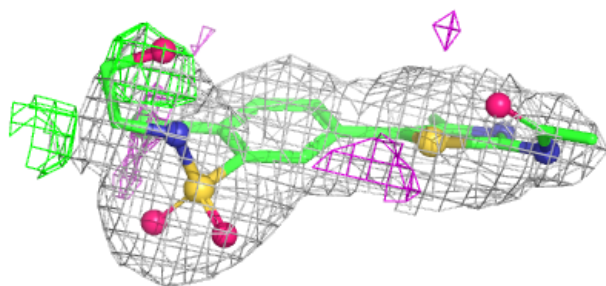
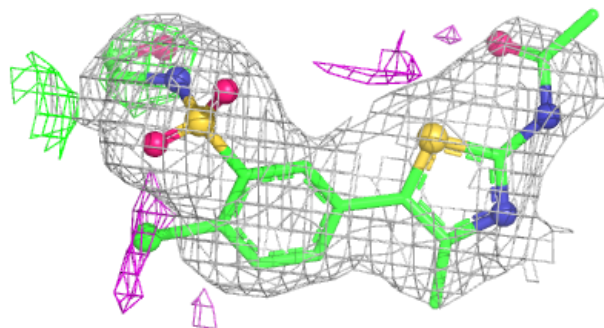
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	MG	D	2001	1/1	0.90	0.09	72,72,72,72	0
5	MG	B	2001	1/1	0.91	0.14	87,87,87,87	0
3	093	A	2002	24/24	0.92	0.13	57,75,105,130	2
3	093	C	2002	24/24	0.94	0.10	57,66,75,123	0
3	093	E	2002	24/24	0.94	0.10	65,72,83,124	0
5	MG	F	2001	1/1	0.94	0.13	59,59,59,59	0
4	GSP	D	2000	32/32	0.96	0.07	46,55,65,72	0
4	GSP	F	2000	32/32	0.97	0.06	43,47,58,61	0
4	GSP	B	2000	32/32	0.97	0.06	47,58,76,86	0

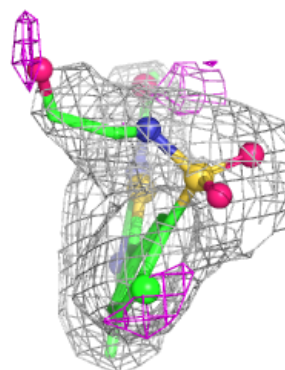
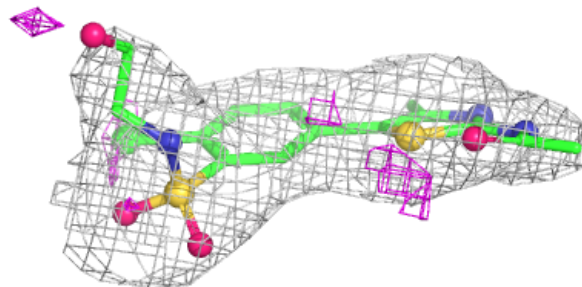
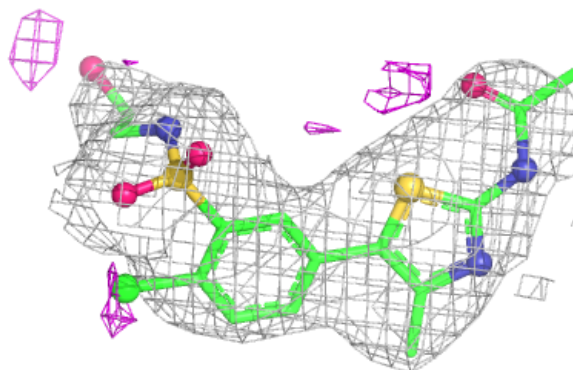
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 093 A 2002:

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

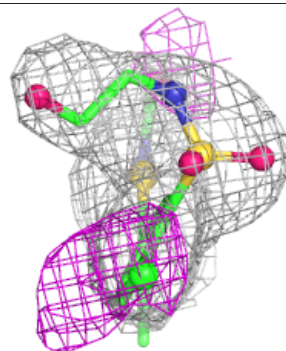
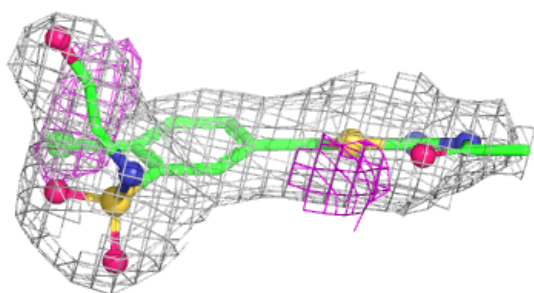
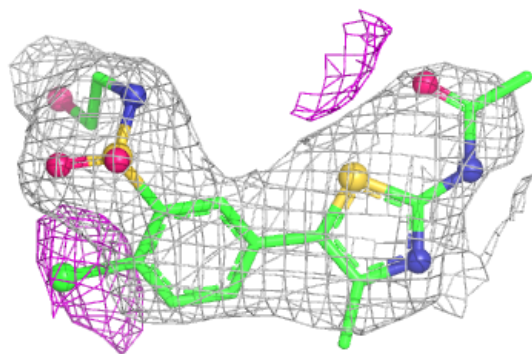
**Electron density around 093 C 2002:**

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

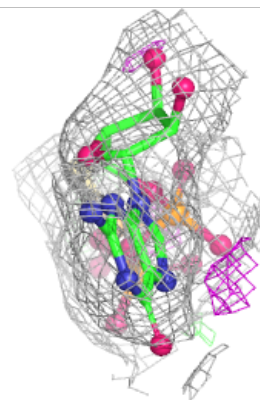
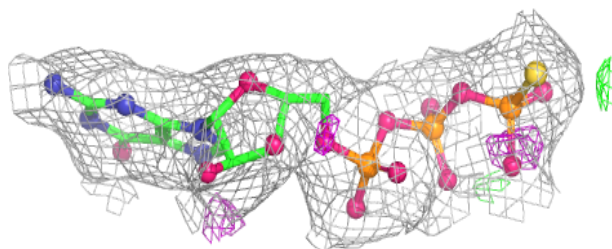
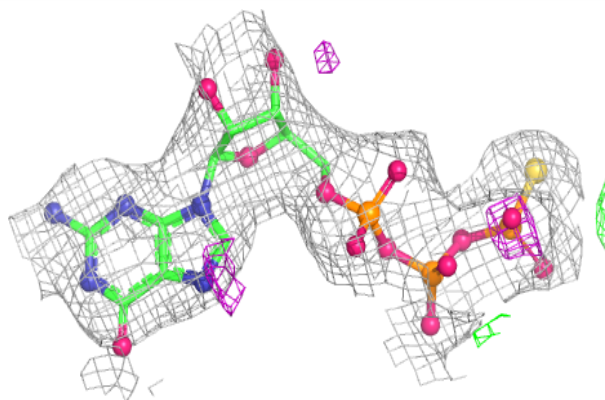


Electron density around 093 E 2002:

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

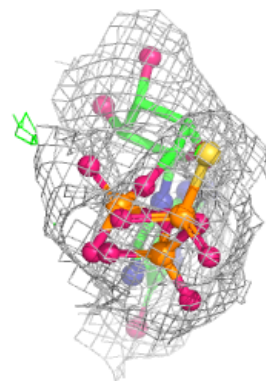
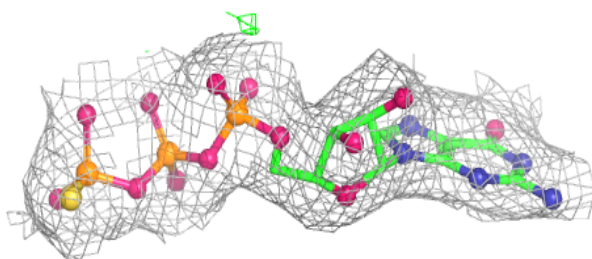
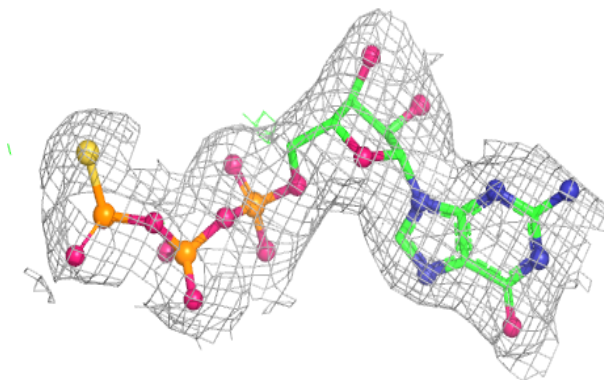
**Electron density around GSP D 2000:**

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

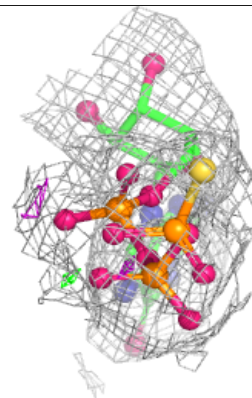
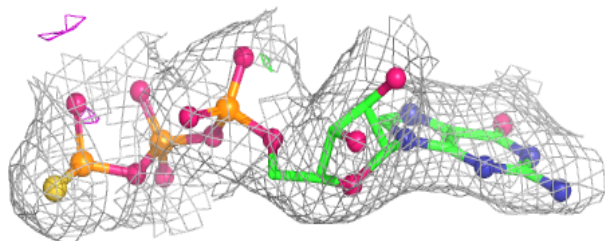
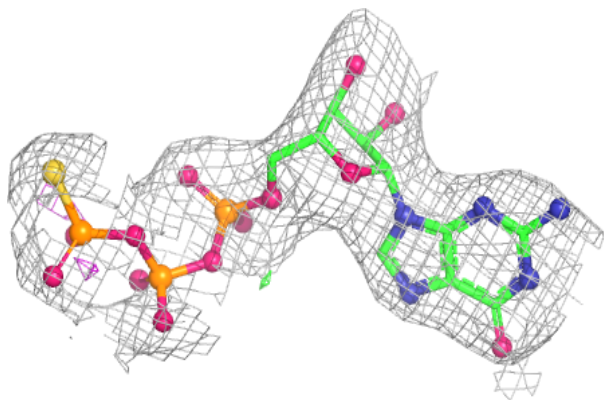


Electron density around GSP F 2000:

$2mF_o-DF_c$ (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.