



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:13 AM UTC

PDB ID : 6R2B / pdb_00006r2b
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis KGD after soaking with succinylphosphonate
Authors : Wagner, T.; Alzari, P.M.; Bellinzoni, M.
Deposited on : 2019-03-15
Resolution : 1.96 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

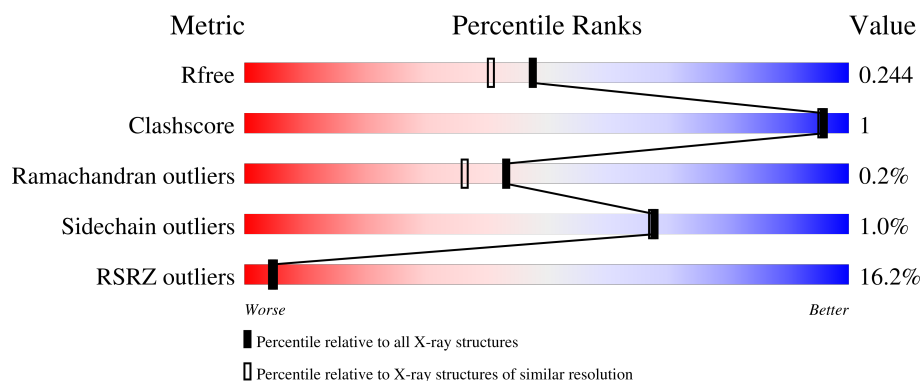
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	868	17% 94%
1	B	868	14% 93%
1	C	868	15% 93%
1	D	868	18% 93%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27742 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.

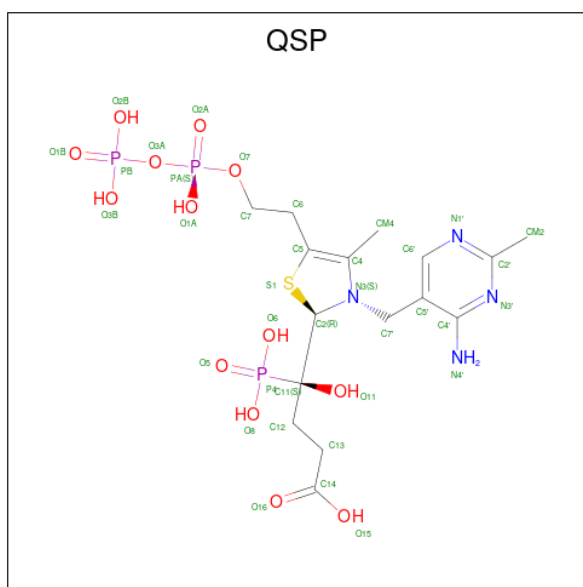
- Molecule 1 is a protein called Multifunctional 2-oxoglutarate metabolism enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	844	Total	C	N	O	S	0	1	0
			6550	4119	1159	1248	24			
1	B	840	Total	C	N	O	S	0	2	0
			6561	4127	1159	1251	24			
1	C	844	Total	C	N	O	S	0	1	0
			6575	4138	1164	1249	24			
1	D	839	Total	C	N	O	S	0	2	0
			6540	4116	1159	1241	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	expression tag	UNP A0R2B1
B	360	GLY	-	expression tag	UNP A0R2B1
C	360	GLY	-	expression tag	UNP A0R2B1
D	360	GLY	-	expression tag	UNP A0R2B1

- Molecule 2 is (4 {S})-4-[(2 {R})-3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-4-methyl-5-[2-[oxidanyl(phosphonooxy)phosphoryl]oxyethyl]-2 {H}-1,3-thiazol-2-yl]-4-oxidanyl-4-phosphono-butanoic acid (CCD ID: QSP) (formula: C₁₆H₂₇N₄O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 37	C 16	N 4	O 13	P 3	S 1	0	0
2	B	1	Total 37	C 16	N 4	O 13	P 3	S 1	0	0
2	C	1	Total 37	C 16	N 4	O 13	P 3	S 1	0	0
2	D	1	Total 37	C 16	N 4	O 13	P 3	S 1	0	0

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

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0

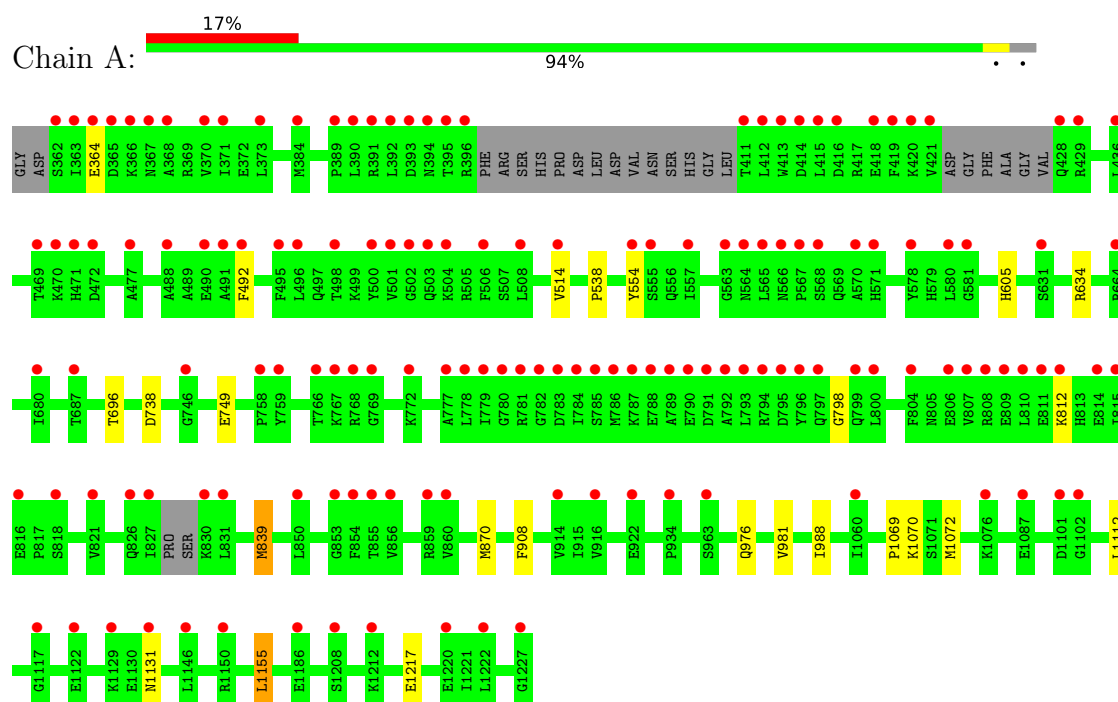
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	326	Total 326	O 326	0	0
5	B	351	Total 351	O 351	0	0
5	C	355	Total 355	O 355	0	0
5	D	328	Total 328	O 328	0	0

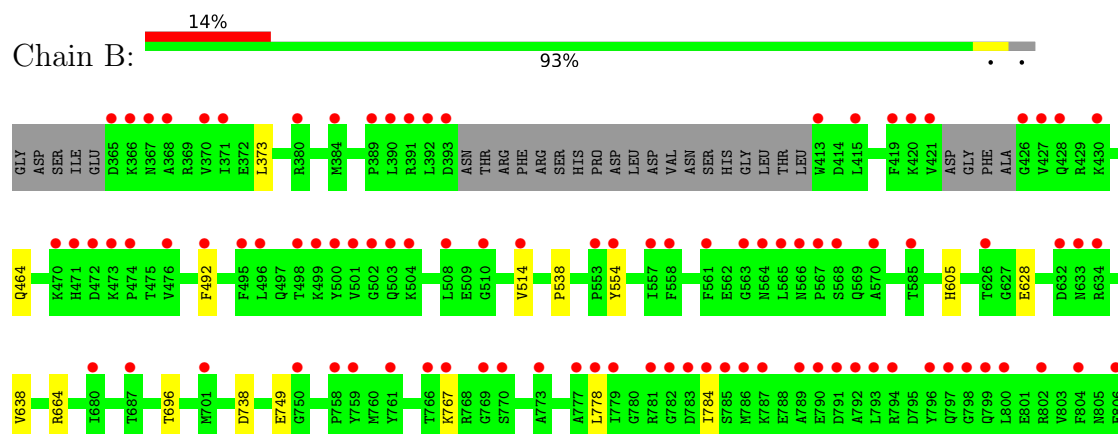
3 Residue-property plots [i](#)

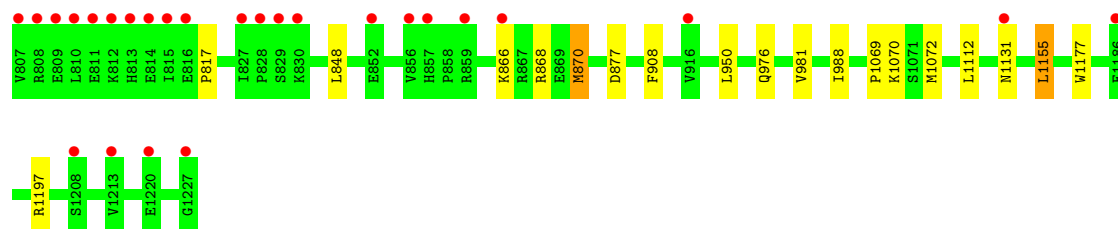
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

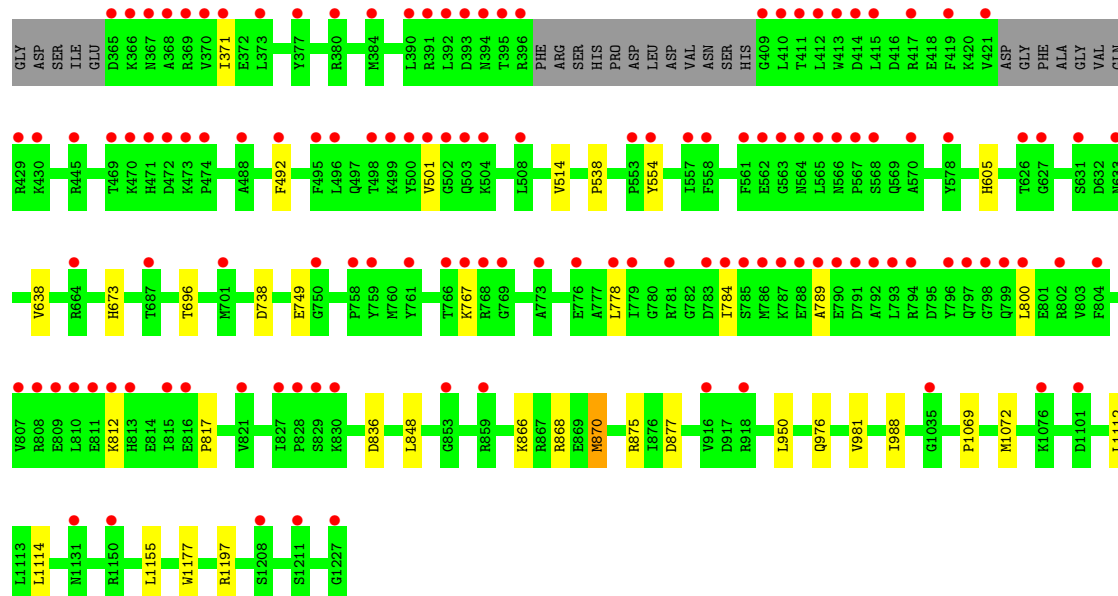
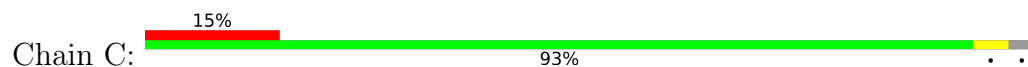


- Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme

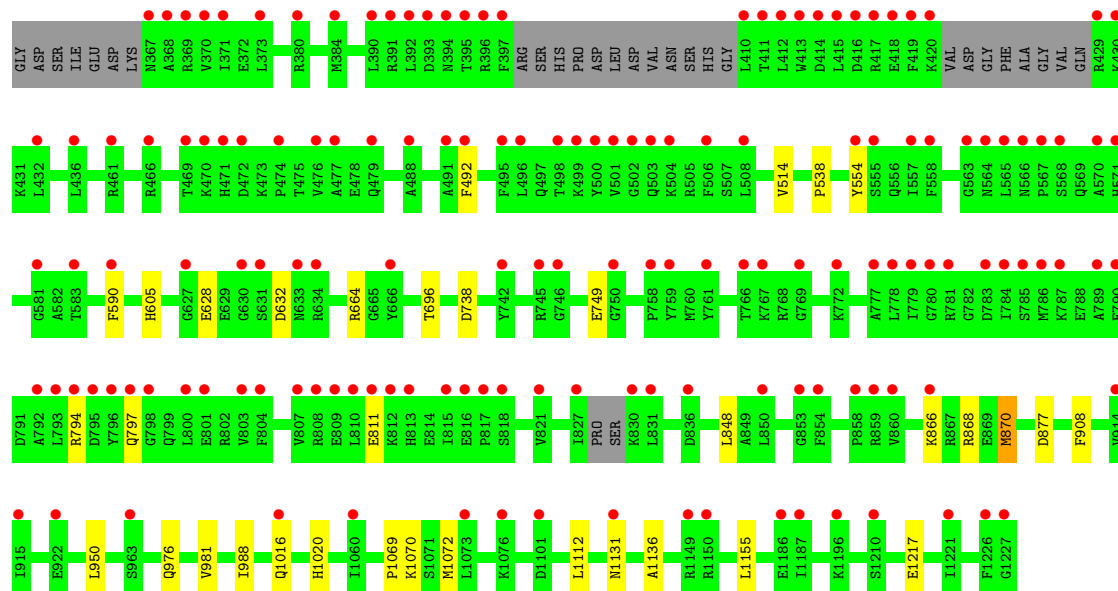
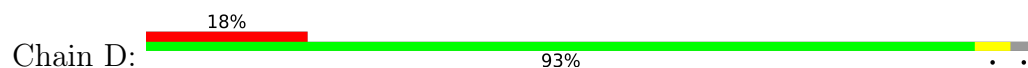




• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme



• Molecule 1: Multifunctional 2-oxoglutarate metabolism enzyme



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.12Å 82.76Å 162.97Å 98.55° 97.52° 102.18°	Depositor
Resolution (Å)	158.87 – 1.96 158.87 – 1.96	Depositor EDS
% Data completeness (in resolution range)	97.1 (158.87-1.96) 97.1 (158.87-1.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.97Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.228 , 0.245 0.226 , 0.244	Depositor DCC
R_{free} test set	14370 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27742	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0215e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: QSP, MG, CA

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	0.84	2/6684 (0.0%)	1.16	4/9058 (0.0%)
1	B	0.84	1/6700 (0.0%)	1.15	2/9074 (0.0%)
1	C	0.84	1/6713 (0.0%)	1.15	3/9099 (0.0%)
1	D	0.84	1/6678 (0.0%)	1.15	2/9045 (0.0%)
All	All	0.84	5/26775 (0.0%)	1.15	11/36276 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	870	MET	SD-CE	-7.90	1.59	1.79
1	B	870	MET	SD-CE	-7.88	1.59	1.79
1	C	870	MET	SD-CE	-7.12	1.61	1.79
1	A	870	MET	SD-CE	-5.76	1.65	1.79
1	A	839	MET	SD-CE	-5.08	1.66	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	GLU	CA-C-N	6.57	129.38	120.44
1	A	364	GLU	C-N-CA	6.57	129.38	120.44
1	A	798	GLY	CA-C-N	5.20	127.20	120.44
1	A	798	GLY	C-N-CA	5.20	127.20	120.44
1	B	638	VAL	N-CA-C	5.19	113.58	107.77
1	D	877	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	877	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	836	ASP	CA-CB-CG	5.08	117.69	112.60
1	C	638	VAL	N-CA-C	5.07	113.45	107.77
1	D	632	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	877	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6550	0	6354	13	0
1	B	6561	0	6412	15	0
1	C	6575	0	6399	16	0
1	D	6540	0	6373	17	0
2	A	37	0	0	0	0
2	B	37	0	0	0	0
2	C	37	0	0	0	0
2	D	37	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	326	0	0	0	0
5	B	351	0	0	0	0
5	C	355	0	0	1	0
5	D	328	0	0	0	0
All	All	27742	0	25538	57	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (57) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:866:LYS:HE2	1:C:870:MET:HE3	1.78	0.66
1:D:866:LYS:HE2	1:D:870:MET:HE3	1.79	0.65
1:D:1112:LEU:HD21	1:D:1155:LEU:HD22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:794:ARG:HA	1:D:797:GLN:HG2	1.83	0.60
1:B:866:LYS:HE2	1:B:870:MET:HE3	1.83	0.58
1:C:492:PHE:HD2	1:C:554:TYR:HE1	1.52	0.56
1:C:749:GLU:CD	1:C:749:GLU:H	2.14	0.55
1:B:492:PHE:HD1	1:B:554:TYR:HE1	1.57	0.52
1:C:673:HIS:HB3	5:C:2444:HOH:O	2.09	0.51
1:A:492:PHE:HD1	1:A:554:TYR:HE1	1.59	0.50
1:A:1112:LEU:HD21	1:A:1155:LEU:HD22	1.94	0.50
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.94	0.48
1:A:749:GLU:H	1:A:749:GLU:CD	2.21	0.48
1:B:696:THR:HG21	1:B:738:ASP:HB2	1.96	0.48
1:C:749:GLU:CD	1:C:749:GLU:N	2.72	0.48
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.97	0.47
1:A:839:MET:HE3	1:A:839:MET:HA	1.97	0.46
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.96	0.46
1:C:817:PRO:HB3	1:D:1217:GLU:HG2	1.98	0.46
1:B:778:LEU:HB3	1:B:784:ILE:HG12	1.97	0.46
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.98	0.46
1:D:492:PHE:HD1	1:D:554:TYR:HE2	1.63	0.46
1:B:848:LEU:HD12	1:B:868:ARG:HD3	1.99	0.45
1:A:749:GLU:CD	1:A:749:GLU:N	2.75	0.45
1:B:1069:PRO:HB2	1:B:1072:MET:HB3	1.99	0.45
1:D:749:GLU:CD	1:D:749:GLU:N	2.75	0.44
1:D:848:LEU:HD12	1:D:868:ARG:HD2	1.99	0.44
1:C:778:LEU:HB3	1:C:784:ILE:HG12	1.99	0.44
1:A:634:ARG:HD2	1:D:590:PHE:CD1	2.51	0.44
1:C:696:THR:HG21	1:C:738:ASP:HB2	1.99	0.44
1:A:696:THR:HG21	1:A:738:ASP:HB2	1.98	0.44
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	2.00	0.44
1:B:492:PHE:CD1	1:B:554:TYR:HE1	2.34	0.44
1:C:1069:PRO:HB2	1:C:1072:MET:HB3	1.99	0.43
1:C:784:ILE:HD12	1:C:789:ALA:HB2	2.00	0.43
1:C:848:LEU:HD12	1:C:868:ARG:HD2	2.00	0.43
1:B:628:GLU:HG2	1:B:664:ARG:O	2.19	0.43
1:A:1069:PRO:HB2	1:A:1072:MET:HB3	2.00	0.42
1:A:1069:PRO:CB	1:A:1072:MET:HB3	2.50	0.42
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.54	0.42
1:C:870:MET:HE2	1:C:875:ARG:O	2.18	0.42
1:D:1016:GLN:HB3	1:D:1020:HIS:HB2	2.01	0.42
1:D:1069:PRO:CB	1:D:1072:MET:HB3	2.50	0.41
1:A:908:PHE:CZ	1:A:1070:LYS:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1112:LEU:HD23	1:C:1114:LEU:HD11	2.02	0.41
1:D:696:THR:HG21	1:D:738:ASP:HB2	2.03	0.41
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.56	0.41
1:D:1069:PRO:HB2	1:D:1072:MET:HB3	2.02	0.41
1:D:628:GLU:HG2	1:D:664:ARG:O	2.21	0.41
1:B:1069:PRO:CB	1:B:1072:MET:HB3	2.51	0.41
1:A:634:ARG:HD2	1:D:590:PHE:HD1	1.85	0.41
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.56	0.41
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.56	0.40
1:A:1217:GLU:HG2	1:B:817:PRO:HB3	2.02	0.40
1:B:749:GLU:N	1:B:749:GLU:CD	2.80	0.40
1:D:1112:LEU:HD12	1:D:1136:ALA:HB3	2.03	0.40
1:C:1069:PRO:CB	1:C:1072:MET:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	837/868 (96%)	817 (98%)	18 (2%)	2 (0%)	43	36
1	B	836/868 (96%)	814 (97%)	20 (2%)	2 (0%)	43	36
1	C	839/868 (97%)	816 (97%)	21 (2%)	2 (0%)	43	36
1	D	833/868 (96%)	810 (97%)	21 (2%)	2 (0%)	43	36
All	All	3345/3472 (96%)	3257 (97%)	80 (2%)	8 (0%)	43	36

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	PRO
1	B	538	PRO

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Mol	Chain	Res	Type
1	B	605	HIS
1	C	538	PRO
1	C	605	HIS
1	D	538	PRO
1	A	605	HIS
1	D	605	HIS

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	680/726 (94%)	675 (99%)	5 (1%)	76	76
1	B	689/726 (95%)	681 (99%)	8 (1%)	63	61
1	C	685/726 (94%)	676 (99%)	9 (1%)	61	58
1	D	682/726 (94%)	677 (99%)	5 (1%)	76	76
All	All	2736/2904 (94%)	2709 (99%)	27 (1%)	68	67

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	514	VAL
1	A	812	LYS
1	A	976	GLN
1	A	1131	ASN
1	A	1155	LEU
1	B	373	LEU
1	B	464	GLN
1	B	514	VAL
1	B	767	LYS
1	B	950	LEU
1	B	976	GLN
1	B	1131	ASN
1	B	1155	LEU
1	C	371	ILE
1	C	501	VAL

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Mol	Chain	Res	Type
1	C	514	VAL
1	C	767	LYS
1	C	800	LEU
1	C	812	LYS
1	C	950	LEU
1	C	976	GLN
1	C	1155	LEU
1	D	514	VAL
1	D	811	GLU
1	D	950	LEU
1	D	976	GLN
1	D	1131	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	487	ASN
1	A	679	GLN
1	A	797	GLN
1	A	976	GLN
1	A	1001	GLN
1	A	1061	GLN
1	B	556	GLN
1	B	679	GLN
1	B	976	GLN
1	B	1061	GLN
1	B	1107	ASN
1	C	556	GLN
1	C	679	GLN
1	C	797	GLN
1	C	976	GLN
1	C	1016	GLN
1	C	1061	GLN
1	D	556	GLN
1	D	679	GLN
1	D	947	ASN
1	D	976	GLN
1	D	1030	GLN
1	D	1107	ASN

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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$
2	QSP	B	2001	3	33,38,38	2.41	10 (30%)	48,59,59	1.40	7 (14%)
2	QSP	A	2001	3	33,38,38	1.98	11 (33%)	48,59,59	1.32	6 (12%)
2	QSP	C	2001	3	33,38,38	2.28	11 (33%)	48,59,59	1.35	7 (14%)
2	QSP	D	2001	3	33,38,38	2.15	9 (27%)	48,59,59	1.47	6 (12%)

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
2	QSP	B	2001	3	-	2/29/54/54	0/2/2/2
2	QSP	A	2001	3	-	2/29/54/54	0/2/2/2
2	QSP	C	2001	3	-	2/29/54/54	0/2/2/2
2	QSP	D	2001	3	-	1/29/54/54	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	QSP	PA-O3A	-8.12	1.50	1.59
2	C	2001	QSP	PA-O3A	-8.01	1.50	1.59
2	D	2001	QSP	PA-O3A	-7.63	1.51	1.59
2	A	2001	QSP	PA-O3A	-5.20	1.53	1.59
2	C	2001	QSP	C4'-N3'	4.03	1.40	1.35
2	B	2001	QSP	C4'-N3'	3.97	1.40	1.35
2	D	2001	QSP	C4'-N3'	3.72	1.40	1.35
2	B	2001	QSP	O11-C11	-3.59	1.40	1.43
2	B	2001	QSP	C2-N3	3.58	1.50	1.46
2	B	2001	QSP	C4-N3	3.56	1.45	1.36
2	D	2001	QSP	C2-S1	3.33	1.90	1.83
2	C	2001	QSP	C4-N3	3.28	1.45	1.36
2	A	2001	QSP	PA-O7	3.15	1.71	1.59
2	B	2001	QSP	C2-S1	3.10	1.89	1.83
2	D	2001	QSP	PA-O7	2.92	1.70	1.59
2	A	2001	QSP	C4'-N3'	2.89	1.38	1.35
2	C	2001	QSP	C5'-C4'	2.87	1.47	1.42
2	A	2001	QSP	C2-S1	2.81	1.89	1.83
2	B	2001	QSP	C7'-N3	2.80	1.51	1.46
2	D	2001	QSP	C4-N3	2.78	1.43	1.36
2	C	2001	QSP	C2-S1	2.75	1.89	1.83
2	D	2001	QSP	C2'-N1'	2.71	1.38	1.34
2	A	2001	QSP	O7-C7	-2.65	1.34	1.44
2	C	2001	QSP	C7'-N3	2.56	1.50	1.46
2	A	2001	QSP	CM4-C4	2.56	1.53	1.49
2	C	2001	QSP	PA-O7	2.55	1.69	1.59
2	B	2001	QSP	O7-C7	-2.54	1.34	1.44
2	B	2001	QSP	C13-C14	2.52	1.56	1.50
2	B	2001	QSP	C5'-C4'	2.52	1.47	1.42
2	C	2001	QSP	O7-C7	-2.49	1.34	1.44
2	D	2001	QSP	O7-C7	-2.47	1.34	1.44
2	A	2001	QSP	C4-N3	2.46	1.42	1.36
2	A	2001	QSP	C5-C4	2.43	1.40	1.35
2	C	2001	QSP	C13-C14	2.41	1.56	1.50
2	A	2001	QSP	C6'-N1'	2.31	1.39	1.34
2	C	2001	QSP	C6-C7	2.30	1.58	1.51
2	C	2001	QSP	C2'-N1'	2.26	1.37	1.34
2	D	2001	QSP	C6-C5	-2.22	1.45	1.50
2	A	2001	QSP	O11-C11	-2.22	1.41	1.43
2	D	2001	QSP	C6-C7	2.18	1.57	1.51
2	A	2001	QSP	C2-N3	2.14	1.48	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	QSP	S1-C2-N3	-4.47	103.22	106.91
2	D	2001	QSP	O1A-PA-O3A	3.86	117.71	107.27
2	A	2001	QSP	O1A-PA-O3A	3.80	117.55	107.27
2	B	2001	QSP	S1-C2-N3	-3.72	103.84	106.91
2	B	2001	QSP	O1A-PA-O3A	3.32	116.25	107.27
2	B	2001	QSP	C13-C12-C11	3.12	121.53	114.43
2	C	2001	QSP	O11-C11-C2	-2.93	105.40	110.91
2	C	2001	QSP	O1A-PA-O3A	2.93	115.19	107.27
2	C	2001	QSP	C2'-N3'-C4'	-2.87	113.68	118.10
2	D	2001	QSP	C2'-N3'-C4'	-2.78	113.82	118.10
2	D	2001	QSP	CM4-C4-N3	2.66	122.37	119.89
2	A	2001	QSP	C13-C12-C11	2.58	120.29	114.43
2	B	2001	QSP	C2'-N3'-C4'	-2.54	114.19	118.10
2	A	2001	QSP	O11-C11-C2	-2.48	106.26	110.91
2	C	2001	QSP	C13-C12-C11	2.39	119.86	114.43
2	B	2001	QSP	O3B-PB-O2B	2.39	116.75	107.80
2	D	2001	QSP	O3B-PB-O2B	2.38	116.72	107.80
2	B	2001	QSP	O11-C11-C2	-2.36	106.47	110.91
2	A	2001	QSP	O3B-PB-O2B	2.35	116.61	107.80
2	D	2001	QSP	O6-P4-O5	2.31	118.63	112.96
2	C	2001	QSP	C5'-C7'-N3	2.30	116.60	113.14
2	C	2001	QSP	S1-C2-N3	-2.25	105.05	106.91
2	A	2001	QSP	C2'-N3'-C4'	-2.11	114.85	118.10
2	C	2001	QSP	O8-P4-O6	2.09	114.14	108.24
2	A	2001	QSP	C4-C5-S1	2.07	113.03	110.74
2	B	2001	QSP	O6-P4-O5	2.02	117.91	112.96

There are no chirality outliers.

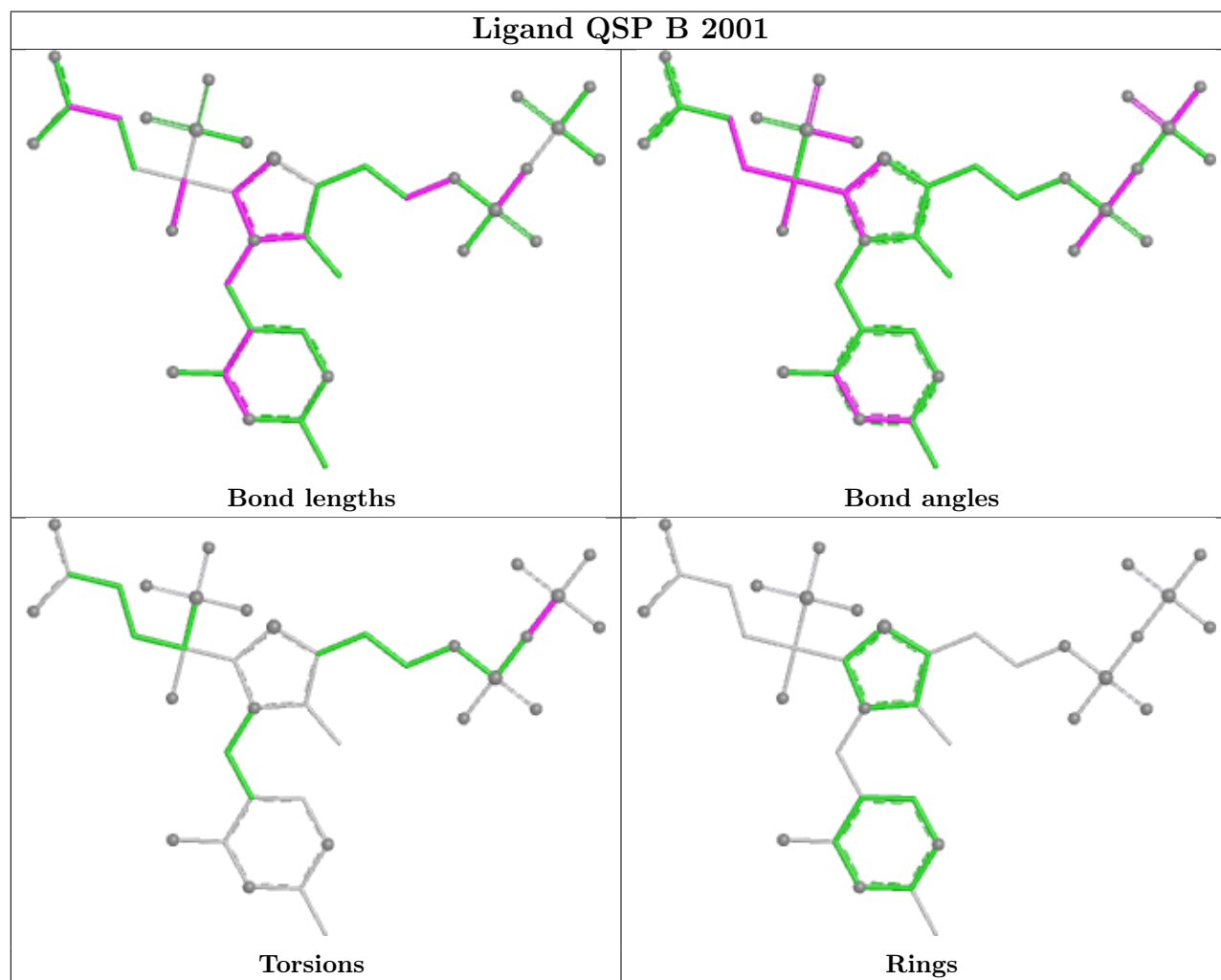
All (7) torsion outliers are listed below:

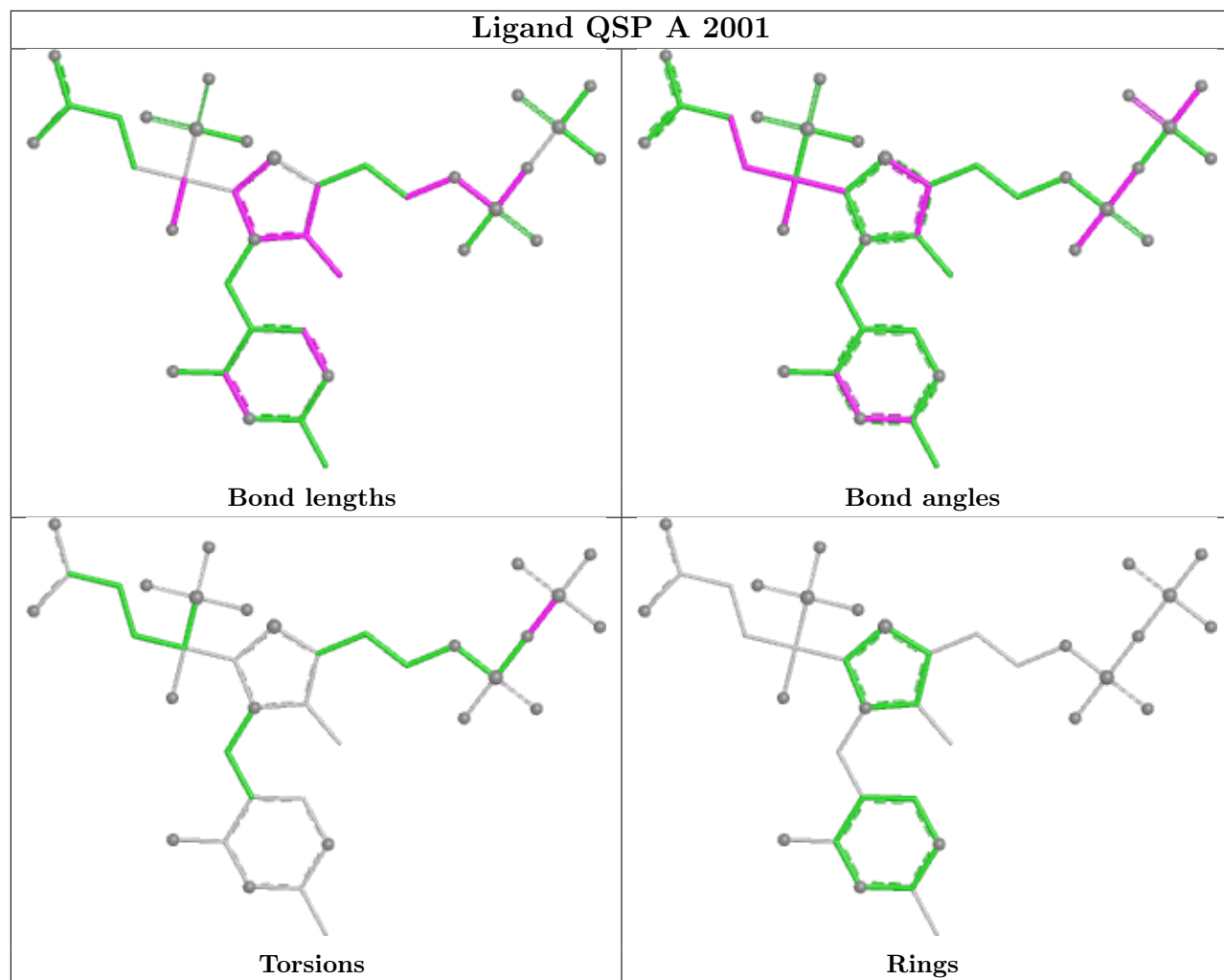
Mol	Chain	Res	Type	Atoms
2	A	2001	QSP	PA-O3A-PB-O2B
2	B	2001	QSP	PA-O3A-PB-O2B
2	B	2001	QSP	PA-O3A-PB-O3B
2	D	2001	QSP	PA-O3A-PB-O2B
2	A	2001	QSP	PA-O3A-PB-O3B
2	C	2001	QSP	PA-O3A-PB-O3B
2	C	2001	QSP	C2-C11-C12-C13

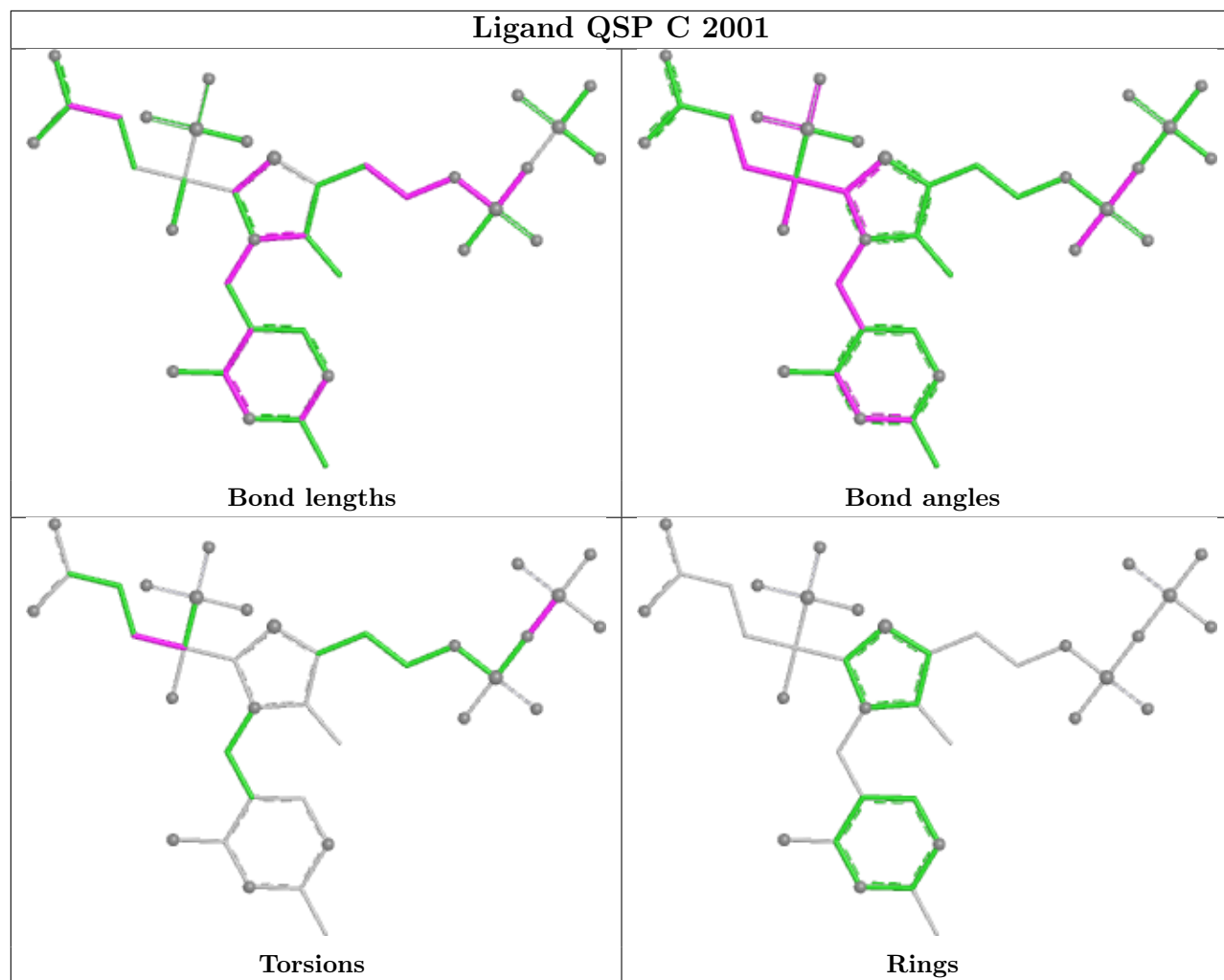
There are no ring outliers.

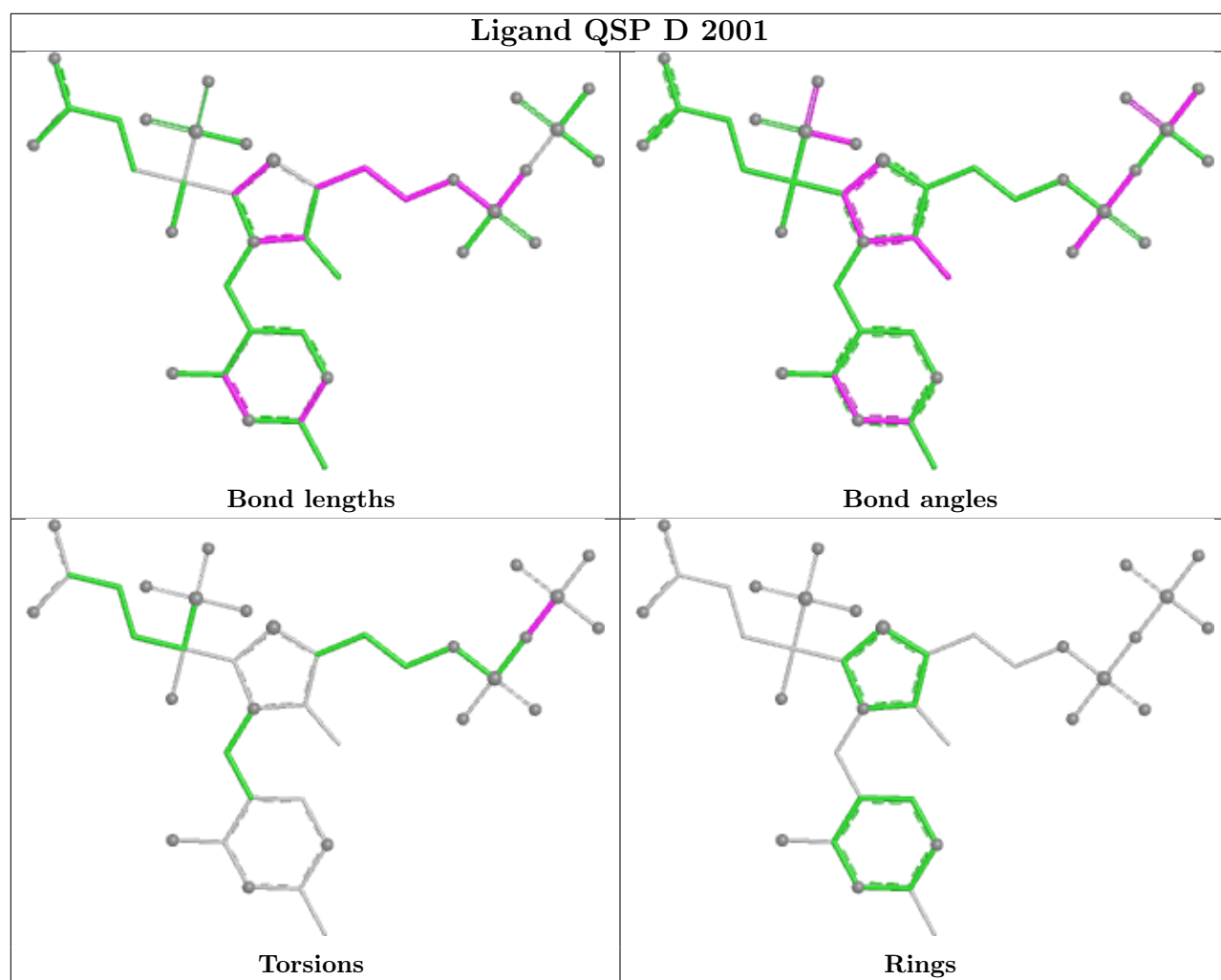
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	844/868 (97%)	1.01	147 (17%) 4 4	18, 31, 60, 98	1 (0%)
1	B	840/868 (96%)	0.91	120 (14%) 6 7	18, 30, 58, 89	2 (0%)
1	C	844/868 (97%)	0.89	128 (15%) 5 6	14, 29, 57, 92	1 (0%)
1	D	839/868 (96%)	1.04	152 (18%) 3 3	18, 30, 58, 85	2 (0%)
All	All	3367/3472 (96%)	0.96	547 (16%) 4 5	14, 30, 58, 98	6 (0%)

All (547) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	827	ILE	9.5
1	B	421	VAL	7.9
1	A	421	VAL	7.8
1	D	412	LEU	7.8
1	C	421	VAL	7.7
1	D	410	LEU	7.6
1	D	420	LYS	6.9
1	A	794	ARG	6.9
1	D	371	ILE	6.8
1	C	409	GLY	6.7
1	A	827	ILE	6.6
1	C	827	ILE	6.5
1	B	796	TYR	6.5
1	C	790	GLU	6.4
1	A	796	TYR	6.4
1	D	411	THR	6.3
1	A	396	ARG	6.2
1	B	570	ALA	6.2
1	C	828	PRO	6.2
1	C	796	TYR	6.1
1	C	392	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	827	ILE	6.0
1	A	411	THR	6.0
1	D	796	TYR	5.9
1	C	793	LEU	5.8
1	B	828	PRO	5.8
1	A	570	ALA	5.7
1	C	413	TRP	5.7
1	C	794	ARG	5.6
1	D	808	ARG	5.6
1	A	394	ASN	5.6
1	D	392	LEU	5.5
1	C	410	LEU	5.5
1	A	363	ILE	5.5
1	D	793	LEU	5.5
1	D	419	PHE	5.5
1	A	797	GLN	5.4
1	C	554	TYR	5.4
1	A	392	LEU	5.4
1	B	392	LEU	5.4
1	D	415	LEU	5.4
1	A	412	LEU	5.3
1	A	793	LEU	5.3
1	D	570	ALA	5.3
1	B	794	ARG	5.3
1	D	395	THR	5.3
1	B	793	LEU	5.2
1	A	790	GLU	5.2
1	D	413	TRP	5.2
1	A	395	THR	5.1
1	B	554	TYR	5.0
1	D	1227	GLY	5.0
1	A	568	SER	5.0
1	C	394	ASN	5.0
1	B	413	TRP	4.9
1	D	397	PHE	4.9
1	C	501	VAL	4.9
1	D	568	SER	4.9
1	B	790	GLU	4.9
1	C	778	LEU	4.8
1	B	390	LEU	4.8
1	D	367	ASN	4.7
1	A	368	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	784	ILE	4.7
1	C	829	SER	4.7
1	C	368	ALA	4.7
1	B	498	THR	4.6
1	D	555	SER	4.6
1	C	415	LEU	4.6
1	B	393	ASP	4.6
1	B	501	VAL	4.6
1	B	808	ARG	4.5
1	A	415	LEU	4.5
1	D	794	ARG	4.5
1	B	786	MET	4.5
1	A	781	ARG	4.5
1	C	789	ALA	4.5
1	A	370	VAL	4.5
1	B	502	GLY	4.5
1	B	568	SER	4.5
1	A	792	ALA	4.5
1	A	787	LYS	4.4
1	D	391	ARG	4.4
1	D	368	ALA	4.4
1	A	786	MET	4.4
1	C	417	ARG	4.4
1	A	362	SER	4.3
1	A	364	GLU	4.3
1	C	412	LEU	4.3
1	D	554	TYR	4.3
1	D	414	ASP	4.3
1	B	391	ARG	4.2
1	B	427	VAL	4.2
1	B	426	GLY	4.2
1	B	781	ARG	4.2
1	B	787	LYS	4.2
1	D	790	GLU	4.2
1	D	502	GLY	4.1
1	D	394	ASN	4.1
1	C	804	PHE	4.1
1	B	503	GLN	4.1
1	C	1227	GLY	4.1
1	C	366	LYS	4.0
1	A	778	LEU	4.0
1	B	368	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	370	VAL	4.0
1	D	492	PHE	4.0
1	B	809	GLU	4.0
1	D	815	ILE	4.0
1	A	554	TYR	4.0
1	D	390	LEU	4.0
1	D	786	MET	4.0
1	C	570	ALA	4.0
1	B	829	SER	3.9
1	A	807	VAL	3.9
1	B	366	LYS	3.9
1	B	804	PHE	3.9
1	D	472	ASP	3.9
1	B	759	TYR	3.9
1	A	563	GLY	3.9
1	A	1102	GLY	3.9
1	B	779	ILE	3.9
1	C	797	GLN	3.8
1	B	761	TYR	3.8
1	A	413	TRP	3.8
1	A	471	HIS	3.8
1	D	781	ARG	3.8
1	A	367	ASN	3.8
1	A	810	LEU	3.7
1	C	391	ARG	3.7
1	C	784	ILE	3.7
1	C	808	ARG	3.7
1	A	1101	ASP	3.7
1	C	498	THR	3.7
1	B	778	LEU	3.7
1	A	504	LYS	3.7
1	D	767	LYS	3.7
1	C	786	MET	3.7
1	C	504	LYS	3.7
1	C	766	THR	3.7
1	D	807	VAL	3.7
1	D	566	ASN	3.7
1	C	816	GLU	3.6
1	D	816	GLU	3.6
1	C	503	GLN	3.6
1	C	562	GLU	3.6
1	A	795	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	365	ASP	3.6
1	D	830	LYS	3.6
1	D	797	GLN	3.6
1	C	365	ASP	3.6
1	B	807	VAL	3.6
1	D	501	VAL	3.6
1	D	804	PHE	3.6
1	D	787	LYS	3.6
1	A	390	LEU	3.6
1	A	502	GLY	3.5
1	C	411	THR	3.5
1	D	498	THR	3.5
1	A	766	THR	3.5
1	A	371	ILE	3.5
1	B	815	ILE	3.5
1	B	565	LEU	3.5
1	C	502	GLY	3.5
1	D	504	LYS	3.5
1	C	779	ILE	3.5
1	A	501	VAL	3.5
1	C	812	LYS	3.5
1	D	393	ASP	3.5
1	B	626	THR	3.4
1	A	769	GLY	3.4
1	A	812	LYS	3.4
1	C	627	GLY	3.4
1	A	414	ASP	3.4
1	C	626	THR	3.4
1	A	1227	GLY	3.4
1	D	800	LEU	3.4
1	B	566	ASN	3.4
1	C	384	MET	3.4
1	B	811	GLU	3.4
1	C	809	GLU	3.4
1	A	779	ILE	3.4
1	D	491	ALA	3.4
1	A	419	PHE	3.4
1	A	859	ARG	3.4
1	D	859	ARG	3.4
1	A	853	GLY	3.3
1	D	784	ILE	3.3
1	A	366	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	767	LYS	3.3
1	D	429	ARG	3.3
1	D	564	ASN	3.3
1	B	415	LEU	3.3
1	D	583	THR	3.3
1	C	631	SER	3.3
1	B	773	ALA	3.3
1	B	810	LEU	3.3
1	D	810	LEU	3.3
1	C	492	PHE	3.3
1	D	1186	GLU	3.2
1	C	395	THR	3.2
1	A	782	GLY	3.2
1	C	471	HIS	3.2
1	A	391	ARG	3.2
1	A	759	TYR	3.2
1	B	859	ARG	3.2
1	C	557	ILE	3.2
1	D	766	THR	3.2
1	C	566	ASN	3.2
1	D	633	ASN	3.2
1	B	504	LYS	3.2
1	B	783	ASP	3.2
1	C	791	ASP	3.2
1	A	830	LYS	3.2
1	D	627	GLY	3.2
1	D	1150	ARG	3.2
1	A	783	ASP	3.2
1	A	470	LYS	3.1
1	C	564	ASN	3.1
1	C	815	ILE	3.1
1	B	799	GLN	3.1
1	D	759	TYR	3.1
1	B	1227	GLY	3.1
1	C	859	ARG	3.1
1	D	471	HIS	3.1
1	B	472	ASP	3.1
1	C	830	LYS	3.1
1	D	567	PRO	3.1
1	A	780	GLY	3.1
1	D	780	GLY	3.1
1	A	800	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	810	LEU	3.1
1	D	811	GLU	3.1
1	A	564	ASN	3.1
1	B	766	THR	3.1
1	A	488	ALA	3.1
1	A	567	PRO	3.1
1	A	746	GLY	3.1
1	B	557	ILE	3.1
1	D	557	ILE	3.1
1	A	831	LEU	3.1
1	C	390	LEU	3.1
1	B	567	PRO	3.1
1	A	784	ILE	3.0
1	C	393	ASP	3.0
1	D	831	LEU	3.0
1	B	384	MET	3.0
1	C	1150	ARG	3.0
1	A	393	ASP	3.0
1	C	787	LYS	3.0
1	A	373	LEU	3.0
1	A	1222	LEU	3.0
1	C	807	VAL	3.0
1	C	785	SER	3.0
1	D	836	ASP	3.0
1	A	826	GLN	3.0
1	D	396	ARG	3.0
1	D	418	GLU	3.0
1	A	498	THR	3.0
1	B	492	PHE	3.0
1	A	789	ALA	3.0
1	A	566	ASN	3.0
1	D	778	LEU	2.9
1	D	1101	ASP	2.9
1	A	768	ARG	2.9
1	D	417	ARG	2.9
1	D	581	GLY	2.9
1	A	1087	GLU	2.9
1	B	792	ALA	2.9
1	D	1076	LYS	2.9
1	D	914	VAL	2.9
1	C	367	ASN	2.9
1	A	804	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	812	LYS	2.9
1	A	365	ASP	2.9
1	A	806	GLU	2.9
1	A	492	PHE	2.9
1	B	777	ALA	2.9
1	A	816	GLU	2.9
1	B	496	LEU	2.9
1	C	371	ILE	2.9
1	A	469	THR	2.8
1	A	428	GLN	2.8
1	B	561	PHE	2.8
1	A	811	GLU	2.8
1	C	414	ASP	2.8
1	B	785	SER	2.8
1	B	370	VAL	2.8
1	D	558	PHE	2.8
1	C	769	GLY	2.8
1	D	436	LEU	2.8
1	C	567	PRO	2.8
1	A	860	VAL	2.8
1	C	500	TYR	2.8
1	C	759	TYR	2.8
1	C	761	TYR	2.8
1	D	500	TYR	2.8
1	D	590	PHE	2.8
1	C	429	ARG	2.8
1	A	788	GLU	2.8
1	C	800	LEU	2.8
1	C	821	VAL	2.8
1	A	1208	SER	2.7
1	C	568	SER	2.7
1	B	500	TYR	2.7
1	B	634	ARG	2.7
1	C	419	PHE	2.7
1	B	814	GLU	2.7
1	D	809	GLU	2.7
1	A	687	THR	2.7
1	C	469	THR	2.7
1	C	373	LEU	2.7
1	C	495	PHE	2.7
1	D	373	LEU	2.7
1	D	461	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	785	SER	2.7
1	B	564	ASN	2.7
1	C	811	GLU	2.7
1	B	471	HIS	2.7
1	B	789	ALA	2.7
1	A	500	TYR	2.7
1	B	797	GLN	2.7
1	C	802	ARG	2.7
1	D	812	LYS	2.7
1	D	476	VAL	2.7
1	A	491	ALA	2.6
1	B	563	GLY	2.6
1	C	563	GLY	2.6
1	A	472	ASP	2.6
1	C	783	ASP	2.6
1	A	855	THR	2.6
1	B	806	GLU	2.6
1	D	470	LYS	2.6
1	B	633	ASN	2.6
1	D	813	HIS	2.6
1	A	808	ARG	2.6
1	C	380	ARG	2.6
1	D	430	LYS	2.6
1	A	508	LEU	2.6
1	B	371	ILE	2.6
1	C	396	ARG	2.6
1	D	769	GLY	2.6
1	C	370	VAL	2.6
1	D	792	ALA	2.6
1	D	860	VAL	2.6
1	B	430	LYS	2.6
1	C	1076	LYS	2.6
1	A	631	SER	2.6
1	B	389	PRO	2.6
1	B	419	PHE	2.6
1	B	800	LEU	2.6
1	D	1149	ARG	2.6
1	A	809	GLU	2.6
1	A	814	GLU	2.6
1	A	1186	GLU	2.6
1	B	1220	GLU	2.6
1	C	798	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	420	LYS	2.6
1	C	792	ALA	2.6
1	B	802	ARG	2.5
1	B	769	GLY	2.5
1	B	367	ASN	2.5
1	A	856	VAL	2.5
1	C	781	ARG	2.5
1	A	384	MET	2.5
1	A	934	PRO	2.5
1	B	474	PRO	2.5
1	A	1212	LYS	2.5
1	D	854	PHE	2.5
1	C	565	LEU	2.5
1	D	745	ARG	2.5
1	C	687	THR	2.5
1	D	817	PRO	2.5
1	C	473	LYS	2.5
1	A	565	LEU	2.5
1	B	510	GLY	2.5
1	A	818	SER	2.5
1	D	477	ALA	2.5
1	A	821	VAL	2.5
1	A	1129	LYS	2.5
1	B	791	ASP	2.5
1	D	858	PRO	2.5
1	C	1035	GLY	2.4
1	D	563	GLY	2.4
1	A	496	LEU	2.4
1	B	813	HIS	2.4
1	D	496	LEU	2.4
1	A	503	GLN	2.4
1	D	503	GLN	2.4
1	A	815	ILE	2.4
1	B	798	GLY	2.4
1	D	750	GLY	2.4
1	D	801	GLU	2.4
1	C	508	LEU	2.4
1	A	767	LYS	2.4
1	B	473	LYS	2.4
1	A	557	ILE	2.4
1	C	1101	ASP	2.4
1	A	477	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	369	ARG	2.4
1	B	553	PRO	2.4
1	B	758	PRO	2.4
1	B	852	GLU	2.4
1	B	1208	SER	2.4
1	D	565	LEU	2.4
1	A	495	PHE	2.4
1	B	495	PHE	2.4
1	B	558	PHE	2.4
1	A	1150	ARG	2.4
1	B	680	ILE	2.4
1	C	768	ARG	2.4
1	D	1221	ILE	2.4
1	D	488	ALA	2.4
1	B	514	VAL	2.4
1	C	430	LYS	2.4
1	D	416	ASP	2.3
1	D	783	ASP	2.3
1	D	466[A]	ARG	2.3
1	C	561	PHE	2.3
1	B	585	THR	2.3
1	D	1131	ASN	2.3
1	C	750	GLY	2.3
1	A	1076	LYS	2.3
1	C	1208	SER	2.3
1	D	821	VAL	2.3
1	A	429	ARG	2.3
1	C	664	ARG	2.3
1	D	1073	LEU	2.3
1	C	813	HIS	2.3
1	C	1131	ASN	2.3
1	D	779	ILE	2.3
1	B	499	LYS	2.3
1	C	916	VAL	2.3
1	B	816	GLU	2.3
1	C	788	GLU	2.3
1	C	496	LEU	2.3
1	D	432	LEU	2.3
1	D	571	HIS	2.3
1	A	854	PHE	2.3
1	D	495	PHE	2.3
1	D	742	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	758	PRO	2.3
1	C	773	ALA	2.3
1	A	1060	ILE	2.3
1	C	369	ARG	2.3
1	A	785	SER	2.3
1	A	772	LYS	2.3
1	B	1186	GLU	2.2
1	C	474	PRO	2.2
1	D	758	PRO	2.2
1	D	761	TYR	2.2
1	A	916	VAL	2.2
1	A	1131	ASN	2.2
1	D	380	ARG	2.2
1	A	418	GLU	2.2
1	A	580	LEU	2.2
1	A	850	LEU	2.2
1	A	555	SER	2.2
1	A	799	GLN	2.2
1	A	1117	GLY	2.2
1	C	553	PRO	2.2
1	D	798	GLY	2.2
1	B	420	LYS	2.2
1	B	470	LYS	2.2
1	C	767	LYS	2.2
1	D	499	LYS	2.2
1	D	866	LYS	2.2
1	B	428	GLN	2.2
1	D	508	LEU	2.2
1	D	850	LEU	2.2
1	A	416	ASP	2.2
1	A	791	ASP	2.2
1	A	963	SER	2.2
1	C	472	ASP	2.2
1	D	474	PRO	2.2
1	A	506	PHE	2.2
1	D	506	PHE	2.2
1	A	680	ILE	2.2
1	A	436	LEU	2.2
1	A	1146	LEU	2.2
1	B	508	LEU	2.2
1	A	571	HIS	2.1
1	A	664	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	380	ARG	2.2
1	D	772	LYS	2.2
1	C	633	ASN	2.1
1	A	922	GLU	2.1
1	C	776	GLU	2.1
1	D	1226	PHE	2.1
1	D	1187	ILE	2.1
1	D	795	ASP	2.1
1	A	914	VAL	2.1
1	B	770	SER	2.1
1	D	631	SER	2.1
1	C	853	GLY	2.1
1	D	630	GLY	2.1
1	D	746	GLY	2.1
1	C	470	LYS	2.1
1	D	1196	LYS	2.1
1	B	857	HIS	2.1
1	D	384	MET	2.1
1	D	777	ALA	2.1
1	D	1016	GLN	2.1
1	C	377	TYR	2.1
1	D	1060	ILE	2.1
1	B	687	THR	2.1
1	D	469	THR	2.1
1	B	750	GLY	2.1
1	D	803	VAL	2.1
1	C	499	LYS	2.1
1	B	1131	ASN	2.1
1	D	479	GLN	2.1
1	D	666	TYR	2.1
1	C	918	ARG	2.1
1	A	1122	GLU	2.1
1	B	830	LYS	2.1
1	D	922	GLU	2.1
1	D	853	GLY	2.1
1	A	514	VAL	2.1
1	B	476	VAL	2.1
1	B	916	VAL	2.1
1	A	777	ALA	2.1
1	D	634	ARG	2.1
1	A	490	GLU	2.0
1	C	558	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	1211	SER	2.0
1	D	818	SER	2.0
1	D	915	ILE	2.0
1	D	1210[A]	SER	2.0
1	A	578	TYR	2.0
1	C	701	MET	2.0
1	B	782	GLY	2.0
1	A	389	PRO	2.0
1	B	856	VAL	2.0
1	C	488	ALA	2.0
1	D	789	ALA	2.0
1	B	632	ASP	2.0
1	A	1220	GLU	2.0
1	B	866	LYS	2.0
1	D	963	SER	2.0
1	B	701	MET	2.0
1	A	581	GLY	2.0
1	C	799	GLN	2.0
1	C	578	TYR	2.0
1	C	758	PRO	2.0
1	B	1213	VAL	2.0
1	C	445	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	QSP	C	2001	37/37	0.95	0.10	14,20,29,31	0

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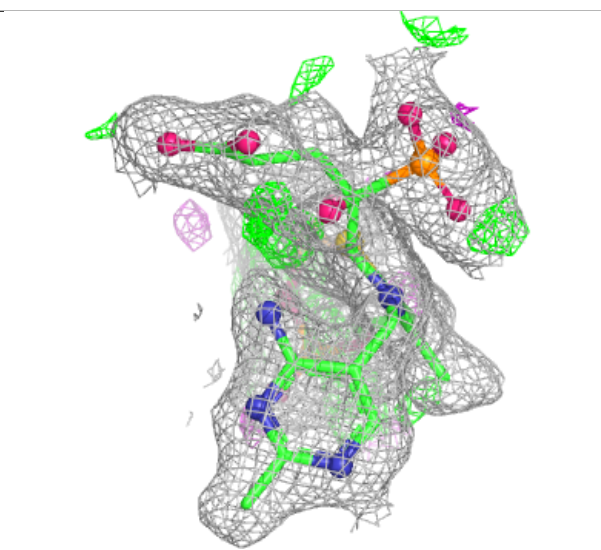
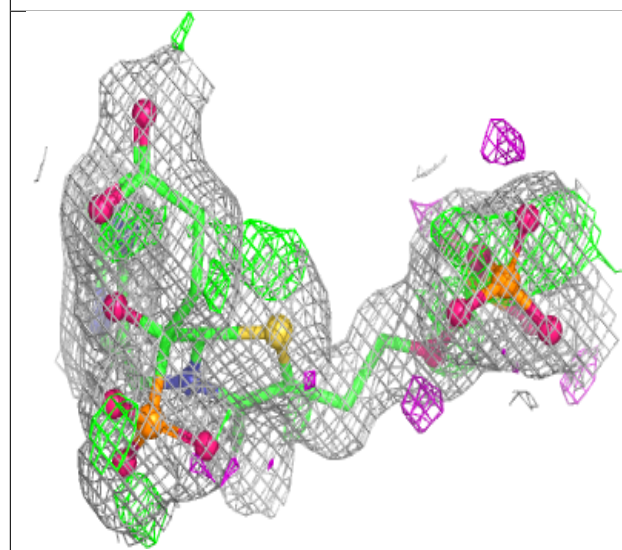
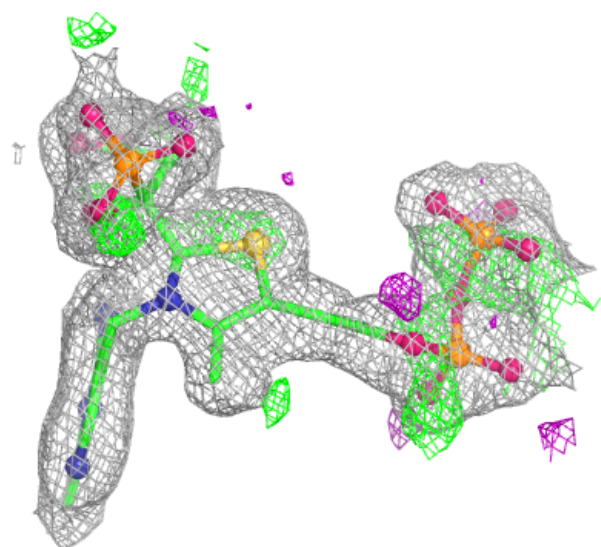
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	2002	1/1	0.95	0.04	20,20,20,20	0
3	MG	D	2002	1/1	0.95	0.05	19,19,19,19	0
2	QSP	D	2001	37/37	0.96	0.08	15,21,30,31	0
3	MG	B	2002	1/1	0.96	0.03	19,19,19,19	0
2	QSP	B	2001	37/37	0.96	0.09	17,21,30,31	0
2	QSP	A	2001	37/37	0.96	0.09	14,22,30,31	0
3	MG	A	2002	1/1	0.97	0.05	20,20,20,20	0
4	CA	A	2003	1/1	0.98	0.07	28,28,28,28	0
4	CA	C	2003	1/1	0.98	0.08	26,26,26,26	0
4	CA	D	2003	1/1	0.98	0.13	27,27,27,27	0
4	CA	B	2003	1/1	0.99	0.07	26,26,26,26	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.

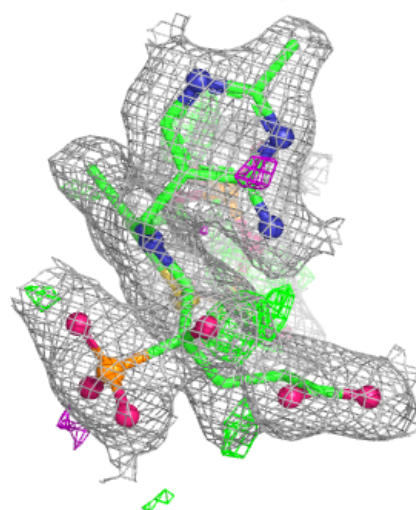
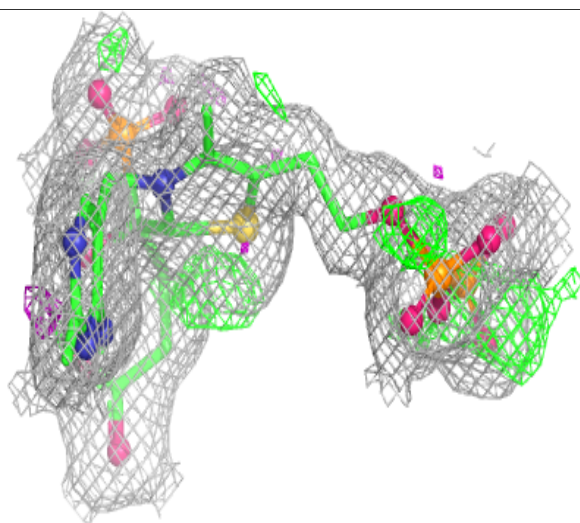
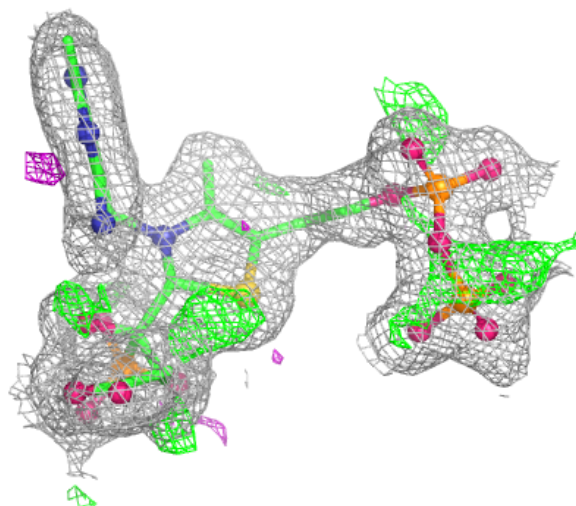
Electron density around QSP C 2001:

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



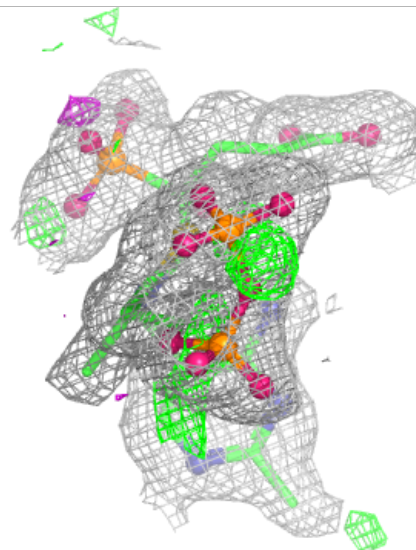
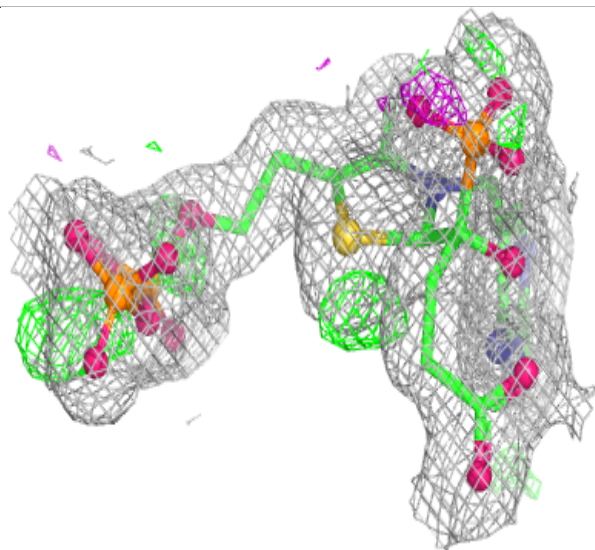
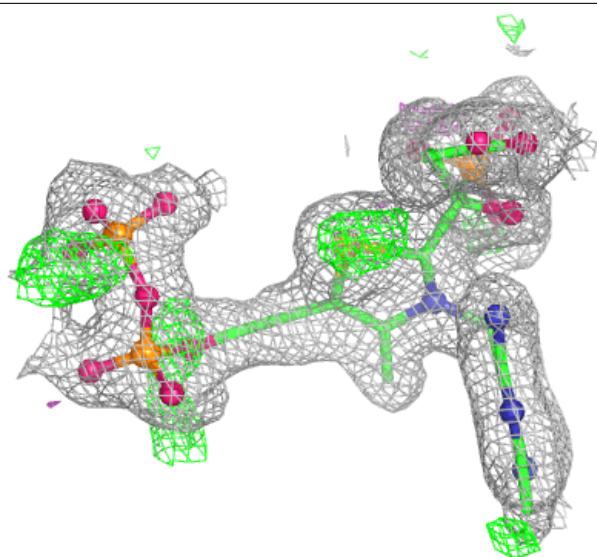
Electron density around QSP D 2001:

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



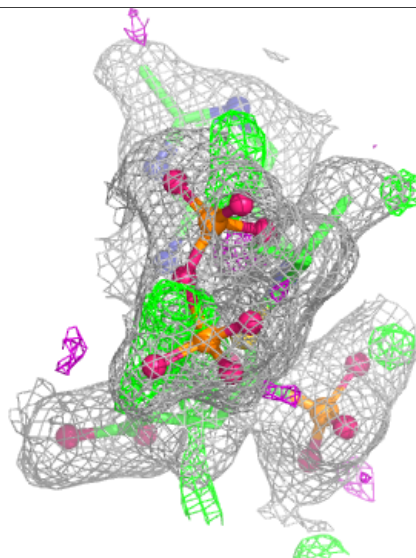
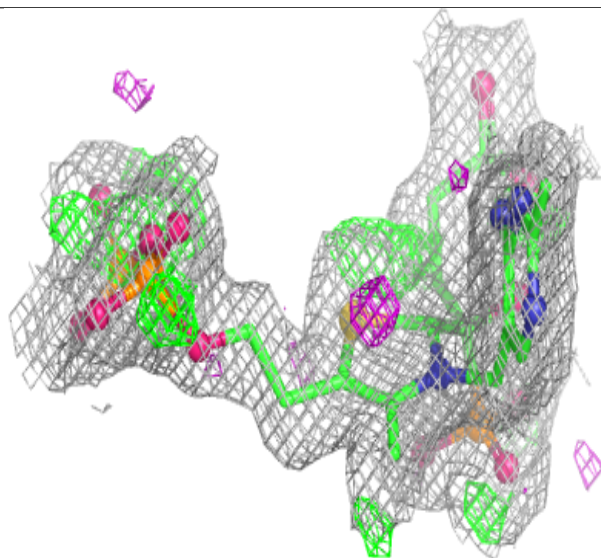
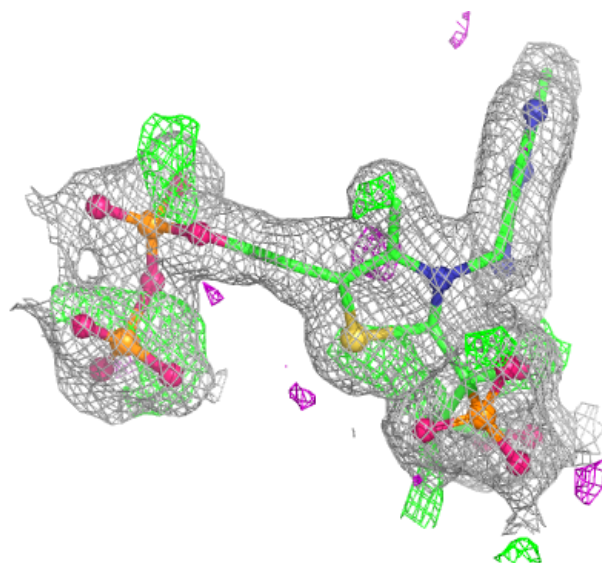
Electron density around QSP B 2001:

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



Electron density around QSP A 2001:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.