



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:06 AM UTC

PDB ID : 6BSN / pdb_00006bsn
Title : Structure of proline utilization A (PutA) with proline bound in remote sites
Authors : Tanner, J.J.; Korasick, D.A.
Deposited on : 2017-12-04
Resolution : 2.15 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

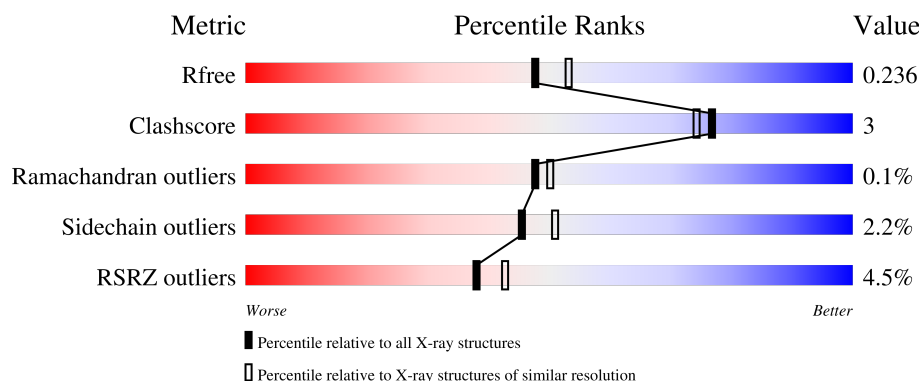
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

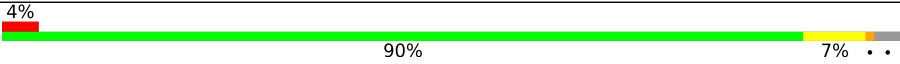
The reported resolution of this entry is 2.15 Å.

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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	1001	
1	B	1001	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	2009	-	-	X	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 15507 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.

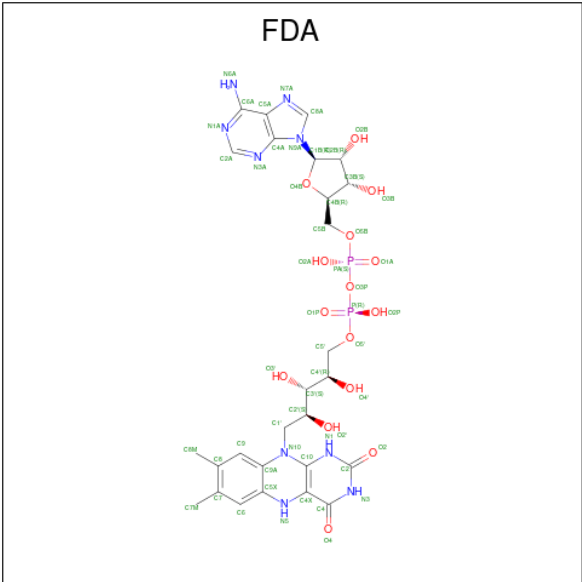
- Molecule 1 is a protein called Bifunctional protein PutA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	973	Total	C	N	O	S	0	2	0
			7269	4591	1316	1340	22			
1	B	973	Total	C	N	O	S	0	1	0
			7271	4593	1311	1345	22			

There are 6 discrepancies between the modelled and reference sequences:

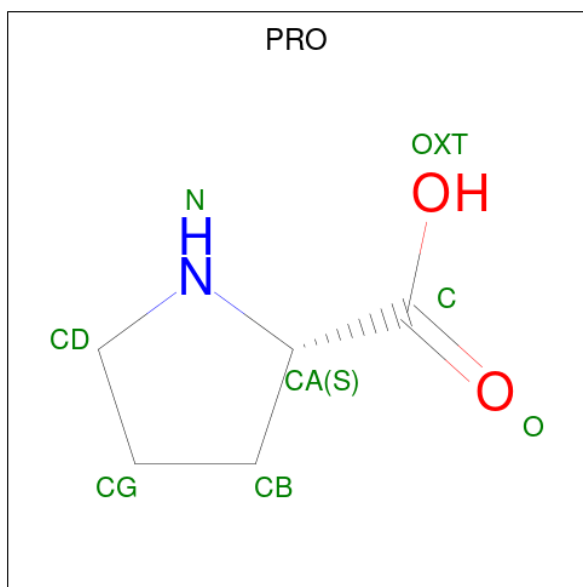
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q89E26
A	0	HIS	-	expression tag	UNP Q89E26
A	792	ALA	CYS	engineered mutation	UNP Q89E26
B	-1	GLY	-	expression tag	UNP Q89E26
B	0	HIS	-	expression tag	UNP Q89E26
B	792	ALA	CYS	engineered mutation	UNP Q89E26

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is PROLINE (CCD ID: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	5	1	2		
3	A	1	Total	C	N	O	0	0
			8	5	1	2		
3	A	1	Total	C	N	O	0	0
			8	5	1	2		
3	A	1	Total	C	N	O	0	0
			8	5	1	2		
3	A	1	Total	C	N	O	0	0
			8	5	1	2		
3	B	1	Total	C	N	O	0	0
			8	5	1	2		
3	B	1	Total	C	N	O	0	0
			8	5	1	2		
3	B	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	400	Total 400	O 400	0	0
5	B	319	Total 319	O 319	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.76Å 194.21Å 108.74Å 90.00° 121.39° 90.00°	Depositor
Resolution (Å)	47.02 – 2.15 47.02 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.02-2.15) 99.1 (47.02-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.16Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.209 , 0.239 0.205 , 0.236	Depositor DCC
R_{free} test set	7949 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15507	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FDA, SO4

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	0.36	0/7417	0.53	0/10086
1	B	0.32	0/7415	0.51	0/10082
All	All	0.34	0/14832	0.52	0/20168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7269	0	7244	43	0
1	B	7271	0	7237	40	0
2	A	53	0	33	1	0
2	B	53	0	33	0	0
3	A	40	0	35	2	0
3	B	32	0	28	2	0
4	A	35	0	0	2	0
4	B	35	0	0	1	0
5	A	400	0	0	3	0
5	B	319	0	0	1	0
All	All	15507	0	14610	84	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 3.

All (84) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ARG:NH1	4:A:2009:SO4:O1	2.22	0.73
1:A:964:PRO:HB3	3:B:1003:PRO:HB3	1.69	0.72
3:A:2003:PRO:HB3	1:B:964:PRO:HB3	1.73	0.70
1:B:581:HIS:ND1	4:B:1008:SO4:O1	2.28	0.65
1:B:660:PRO:HB2	1:B:689:ILE:HG21	1.79	0.65
1:A:546:THR:HG23	1:A:549:GLN:H	1.63	0.63
1:B:546:THR:HG23	1:B:549:GLN:H	1.62	0.63
1:A:581:HIS:ND1	4:A:2009:SO4:O4	2.30	0.62
1:B:623:GLY:HA3	1:B:673:MET:HE2	1.82	0.61
1:A:477:PRO:HB2	1:A:479:PRO:HD2	1.82	0.61
1:A:55:LEU:HD21	1:A:165:ASN:HD22	1.67	0.60
1:B:451:LEU:HB3	1:B:772:LEU:HD13	1.84	0.59
1:A:901:GLU:CD	1:A:932:ARG:HH22	2.12	0.57
1:A:901:GLU:OE1	1:A:932:ARG:NH2	2.32	0.57
1:A:308:GLY:HA3	1:A:337:MET:O	2.03	0.57
1:B:477:PRO:HB2	1:B:479:PRO:HD2	1.88	0.55
1:A:566:ARG:HH11	1:B:932:ARG:HA	1.72	0.55
1:B:507:PHE:O	1:B:510:GLU:HG2	2.06	0.55
1:A:116:VAL:HG11	1:A:773:PRO:HG2	1.90	0.54
1:A:542:ILE:HD12	1:A:687:PRO:HG2	1.89	0.54
1:B:109:THR:HG23	1:B:769:ALA:HB3	1.88	0.54
1:B:106:HIS:CD2	1:B:128:ARG:HD2	2.43	0.54
1:B:840:LYS:NZ	1:B:844:ASP:OD2	2.37	0.54
1:B:116:VAL:HG11	1:B:773:PRO:HG2	1.91	0.53
1:B:308:GLY:HA3	1:B:337:MET:O	2.08	0.52
1:B:761:GLY:HA2	1:B:912:TYR:CD1	2.45	0.52
1:A:451:LEU:HB3	1:A:772:LEU:HD13	1.91	0.52
1:B:317:ARG:O	1:B:321:VAL:HG23	2.10	0.51
1:A:904:LEU:HD13	1:A:932:ARG:HG2	1.91	0.51
1:A:542:ILE:HD13	1:A:691:ARG:HD3	1.94	0.50
1:A:109:THR:HG23	1:A:769:ALA:HB3	1.92	0.50
1:A:341:VAL:HG12	1:A:393:ALA:HB3	1.94	0.49
1:B:590:PHE:HD2	1:B:689:ILE:HD11	1.79	0.48
1:B:904:LEU:HD13	1:B:932:ARG:HG2	1.96	0.48
1:B:542:ILE:HD12	1:B:687:PRO:HG2	1.95	0.48
1:A:290:ASP:OD2	1:A:522:ARG:NH2	2.38	0.47
1:A:192:PHE:CE2	1:A:219:ILE:HG23	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ASN:HA	1:B:467:PHE:CD2	2.49	0.47
1:A:826:ASP:HB3	5:A:2424:HOH:O	2.14	0.47
1:B:404:LEU:HD22	1:B:429:LEU:HD11	1.97	0.47
1:A:593:LEU:HD11	1:A:692:GLU:HG3	1.97	0.46
1:A:684:GLU:OE1	1:A:713:ASP:HA	2.16	0.46
1:A:458:LEU:HD23	1:A:458:LEU:HA	1.72	0.46
1:B:608:GLU:HG3	1:B:662:ALA:HB2	1.98	0.45
3:B:1003:PRO:HA	5:B:1182:HOH:O	2.16	0.45
1:A:109:THR:HG22	5:A:2219:HOH:O	2.15	0.45
1:B:138:GLY:HA2	1:B:922:ILE:HG23	1.98	0.45
1:A:507:PHE:O	1:A:510:GLU:HG2	2.16	0.45
1:A:705:SER:HA	1:A:708:TYR:OH	2.18	0.44
1:A:761:GLY:HA2	1:A:912:TYR:CD1	2.53	0.44
1:A:953:PRO:HB2	1:A:965:LYS:HD3	2.00	0.43
1:A:623:GLY:HA3	1:A:673:MET:HE2	2.00	0.43
1:B:489:ILE:O	1:B:491:ARG:N	2.45	0.43
1:B:215:ALA:O	1:B:219:ILE:HG12	2.18	0.43
1:B:304:TRP:CZ3	1:B:307:PHE:HB2	2.54	0.43
1:A:854:ALA:HB1	1:A:874:GLU:O	2.18	0.43
2:A:2001:FDA:H8A	5:A:2358:HOH:O	2.18	0.42
1:B:143:LEU:HD12	1:B:143:LEU:HA	1.88	0.42
1:B:713:ASP:OD2	1:B:713:ASP:N	2.47	0.42
1:A:774:GLU:HA	1:A:811:MET:SD	2.59	0.42
1:B:201:THR:O	1:B:204:ASP:HB2	2.19	0.42
1:B:451:LEU:O	1:B:455:VAL:HG23	2.20	0.42
1:A:436:ILE:HD13	1:A:436:ILE:HA	1.87	0.42
1:B:123:LEU:N	1:B:123:LEU:HD12	2.34	0.42
1:A:138:GLY:HA2	1:A:922:ILE:HG23	2.02	0.41
1:B:96:GLU:HG2	1:B:157:ARG:HH22	1.85	0.41
1:B:542:ILE:HD13	1:B:691:ARG:HD3	2.03	0.41
1:B:953:PRO:HB2	1:B:965:LYS:HD3	2.02	0.41
1:B:341:VAL:HG12	1:B:393:ALA:HB3	2.02	0.41
1:A:102:GLY:HA3	1:A:130:ILE:HG21	2.02	0.41
1:B:170:GLY:O	1:B:446:SER:HA	2.21	0.41
1:A:660:PRO:HB2	1:A:689:ILE:HG21	2.03	0.41
1:B:110:LYS:NZ	1:B:803:ASP:OD2	2.46	0.41
1:A:404:LEU:HD13	1:A:436:ILE:HD11	2.03	0.41
1:A:954:PHE:CE1	3:A:2002:PRO:HG2	2.55	0.41
1:A:31:PRO:HB2	1:A:32:PRO:HD3	2.03	0.41
1:A:497:HIS:ND1	1:A:498:PRO:HD2	2.35	0.41
1:A:168:VAL:HB	1:A:444:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:THR:CG2	1:B:769:ALA:HB3	2.51	0.40
1:B:385:ARG:NH1	1:B:411:SER:O	2.54	0.40
1:A:317:ARG:O	1:A:321:VAL:HG23	2.21	0.40
1:A:489:ILE:O	1:A:491:ARG:N	2.49	0.40
1:B:489:ILE:O	1:B:490:VAL:HG22	2.22	0.40
1:A:566:ARG:HH21	1:A:566:ARG:HG3	1.87	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	967/1001 (97%)	951 (98%)	15 (2%)	1 (0%)	48	50
1	B	966/1001 (96%)	951 (98%)	15 (2%)	0	100	100
All	All	1933/2002 (97%)	1902 (98%)	30 (2%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	490	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	712/757 (94%)	695 (98%)	17 (2%)	43	47
1	B	712/757 (94%)	697 (98%)	15 (2%)	47	52
All	All	1424/1514 (94%)	1392 (98%)	32 (2%)	45	51

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	55	LEU
1	A	123	LEU
1	A	183	ARG
1	A	197	GLU
1	A	235	SER
1	A	255	VAL
1	A	314	TYR
1	A	542	ILE
1	A	546	THR
1	A	658	ASN
1	A	681	LYS
1	A	713	ASP
1	A	758	GLU
1	A	849	ARG
1	A	883	GLU
1	A	909	ARG
1	B	29	LEU
1	B	55	LEU
1	B	123	LEU
1	B	197	GLU
1	B	235	SER
1	B	314	TYR
1	B	490	VAL
1	B	510	GLU
1	B	542	ILE
1	B	546	THR
1	B	658	ASN
1	B	681	LYS
1	B	713	ASP
1	B	758	GLU
1	B	902	ARG

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

Mol	Chain	Res	Type
1	A	165	ASN
1	A	461	ASN
1	A	470	GLN
1	A	919	HIS
1	B	106	HIS
1	B	433	HIS
1	B	461	ASN
1	B	698	HIS
1	B	919	HIS
1	B	970	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 ligands are modelled in this entry.

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	FDA	B	1001	-	57,58,58	2.82	22 (38%)	78,89,89	2.02	17 (21%)
3	PRO	B	1003	-	8,8,8	1.19	0	10,10,10	0.95	0
4	SO4	B	1011	-	4,4,4	0.27	0	6,6,6	0.13	0
4	SO4	A	2013	-	4,4,4	0.24	0	6,6,6	0.28	0
3	PRO	A	2003	-	8,8,8	1.18	0	10,10,10	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	2011	-	4,4,4	0.26	0	6,6,6	0.11	0
4	SO4	A	2007	-	4,4,4	0.21	0	6,6,6	0.18	0
4	SO4	B	1008	-	4,4,4	0.25	0	6,6,6	0.16	0
4	SO4	B	1012	-	4,4,4	0.24	0	6,6,6	0.09	0
3	PRO	B	1004	-	8,8,8	1.18	0	10,10,10	1.26	2 (20%)
3	PRO	B	1005	-	8,8,8	1.13	0	10,10,10	0.96	0
4	SO4	B	1006	-	4,4,4	0.25	0	6,6,6	0.13	0
4	SO4	B	1009	-	4,4,4	0.21	0	6,6,6	0.11	0
4	SO4	B	1007	-	4,4,4	0.25	0	6,6,6	0.14	0
3	PRO	A	2006	-	8,8,8	1.08	0	10,10,10	1.24	1 (10%)
4	SO4	A	2009	-	4,4,4	0.21	0	6,6,6	0.19	0
4	SO4	A	2012	-	4,4,4	0.21	0	6,6,6	0.13	0
3	PRO	A	2005	-	8,8,8	1.14	0	10,10,10	1.17	1 (10%)
4	SO4	A	2008	-	4,4,4	0.29	0	6,6,6	0.22	0
4	SO4	A	2010	-	4,4,4	0.24	0	6,6,6	0.14	0
3	PRO	B	1002	-	8,8,8	1.13	0	10,10,10	0.91	0
3	PRO	A	2004	-	8,8,8	1.09	0	10,10,10	1.20	1 (10%)
4	SO4	B	1010	-	4,4,4	0.29	0	6,6,6	0.09	0
3	PRO	A	2002	-	8,8,8	1.11	0	10,10,10	1.14	0
2	FDA	A	2001	-	57,58,58	2.89	22 (38%)	78,89,89	2.00	20 (25%)

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
3	PRO	A	2003	-	-	4/4/11/11	0/1/1/1
2	FDA	B	1001	-	-	6/34/50/50	0/6/6/6
3	PRO	B	1003	-	-	4/4/11/11	0/1/1/1
3	PRO	B	1005	-	-	2/4/11/11	0/1/1/1
3	PRO	B	1002	-	-	0/4/11/11	0/1/1/1
3	PRO	A	2004	-	-	2/4/11/11	0/1/1/1
3	PRO	A	2002	-	-	1/4/11/11	0/1/1/1
3	PRO	A	2006	-	-	0/4/11/11	0/1/1/1
3	PRO	B	1004	-	-	0/4/11/11	0/1/1/1
2	FDA	A	2001	-	-	5/34/50/50	0/6/6/6
3	PRO	A	2005	-	-	3/4/11/11	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FDA	PA-O3P	-9.17	1.49	1.59
2	A	2001	FDA	O4-C4	7.33	1.37	1.23
2	B	1001	FDA	PA-O3P	-7.14	1.51	1.59
2	B	1001	FDA	O4-C4	7.07	1.37	1.23
2	A	2001	FDA	C6-C5X	6.85	1.50	1.39
2	A	2001	FDA	O2-C2	6.76	1.37	1.23
2	B	1001	FDA	C6-C5X	6.58	1.49	1.39
2	B	1001	FDA	O2-C2	6.46	1.37	1.23
2	B	1001	FDA	C9-C9A	5.57	1.48	1.39
2	A	2001	FDA	C9-C9A	5.49	1.48	1.39
2	B	1001	FDA	P-O3P	5.48	1.65	1.59
2	B	1001	FDA	C4X-N5	4.62	1.45	1.35
2	A	2001	FDA	P-O3P	4.44	1.64	1.59
2	A	2001	FDA	C10-N1	4.35	1.44	1.37
2	B	1001	FDA	C2-N1	4.31	1.44	1.37
2	B	1001	FDA	C10-N1	4.13	1.44	1.37
2	A	2001	FDA	C4X-N5	4.09	1.44	1.35
2	A	2001	FDA	C6A-N6A	3.88	1.44	1.34
2	B	1001	FDA	C6A-N6A	3.81	1.43	1.34
2	A	2001	FDA	C5X-N5	3.57	1.46	1.39
2	A	2001	FDA	C2-N1	3.55	1.43	1.37
2	B	1001	FDA	C5X-N5	3.39	1.45	1.39
2	A	2001	FDA	C5X-C9A	-3.37	1.36	1.40
2	B	1001	FDA	C10-N10	3.33	1.44	1.38
2	B	1001	FDA	C5X-C9A	-3.27	1.37	1.40
2	A	2001	FDA	C10-N10	3.07	1.43	1.38
2	A	2001	FDA	C2-N3	3.02	1.42	1.37
2	B	1001	FDA	C9A-N10	2.98	1.46	1.41
2	B	1001	FDA	O2'-C2'	-2.77	1.37	1.43
2	B	1001	FDA	C2-N3	2.76	1.42	1.37
2	A	2001	FDA	PA-O5B	-2.74	1.48	1.59
2	B	1001	FDA	C4X-C4	2.69	1.49	1.41
2	A	2001	FDA	PA-O2A	-2.68	1.42	1.55
2	A	2001	FDA	C4X-C4	2.54	1.49	1.41
2	B	1001	FDA	PA-O5B	-2.49	1.49	1.59
2	A	2001	FDA	C9A-N10	2.45	1.45	1.41
2	B	1001	FDA	PA-O2A	-2.44	1.44	1.55
2	B	1001	FDA	O3B-C3B	-2.40	1.37	1.43
2	A	2001	FDA	O3B-C3B	-2.38	1.37	1.43
2	A	2001	FDA	O3'-C3'	-2.36	1.37	1.43
2	B	1001	FDA	C2B-C3B	-2.22	1.47	1.53
2	B	1001	FDA	O4'-C4'	-2.17	1.38	1.43
2	A	2001	FDA	C6-C7	2.16	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FDA	O2'-C2'	-2.16	1.38	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	FDA	N3A-C2A-N1A	-6.11	119.33	128.58
2	A	2001	FDA	N3A-C2A-N1A	-6.06	119.41	128.58
2	B	1001	FDA	C4-N3-C2	-5.60	118.66	126.37
2	A	2001	FDA	O2P-P-O3P	-5.40	92.68	107.27
2	A	2001	FDA	C4-N3-C2	-4.91	119.61	126.37
2	A	2001	FDA	C5A-C4A-N3A	-4.91	119.96	126.72
2	B	1001	FDA	C5A-C4A-N3A	-4.75	120.18	126.72
2	B	1001	FDA	O2P-P-O3P	-4.50	95.10	107.27
2	B	1001	FDA	N3A-C4A-N9A	4.42	134.69	127.17
2	A	2001	FDA	N3A-C4A-N9A	4.29	134.47	127.17
2	A	2001	FDA	O3P-P-O1P	4.20	123.33	110.70
2	B	1001	FDA	O3P-P-O1P	4.17	123.26	110.70
2	B	1001	FDA	C5A-N7A-C8A	3.89	109.56	103.45
2	A	2001	FDA	C2A-N3A-C4A	3.88	121.31	111.83
2	A	2001	FDA	C5A-N7A-C8A	3.88	109.54	103.45
2	B	1001	FDA	C2A-N3A-C4A	3.78	121.06	111.83
2	B	1001	FDA	N9A-C8A-N7A	-3.64	108.77	113.94
2	A	2001	FDA	N9A-C8A-N7A	-3.36	109.17	113.94
2	A	2001	FDA	O4-C4-C4X	-3.34	119.21	127.26
2	B	1001	FDA	N3-C2-N1	3.24	120.83	115.74
2	B	1001	FDA	O2A-PA-O5B	-3.16	93.25	107.57
2	B	1001	FDA	C4X-C4-N3	3.05	120.51	112.13
2	B	1001	FDA	O4-C4-C4X	-3.03	119.95	127.26
2	A	2001	FDA	N3-C2-N1	3.03	120.50	115.74
2	B	1001	FDA	O2A-PA-O3P	-2.86	99.55	107.27
2	A	2001	FDA	O2A-PA-O5B	-2.85	94.67	107.57
2	B	1001	FDA	C4A-N9A-C8A	2.84	108.72	105.74
2	A	2001	FDA	C4X-C4-N3	2.76	119.71	112.13
2	A	2001	FDA	C4A-C5A-N7A	-2.72	107.47	110.58
2	A	2001	FDA	O2-C2-N1	-2.57	117.29	121.86
2	A	2001	FDA	O5'-P-O1P	2.54	119.02	108.94
2	B	1001	FDA	C5X-C9A-N10	2.45	120.78	118.01
2	B	1001	FDA	C4A-C5A-N7A	-2.41	107.83	110.58
2	A	2001	FDA	C4A-N9A-C8A	2.39	108.25	105.74
3	A	2006	PRO	OXT-C-CA	2.37	121.53	113.51
3	B	1004	PRO	OXT-C-O	-2.34	118.77	124.08
3	A	2004	PRO	OXT-C-CA	2.19	120.93	113.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1004	PRO	OXT-C-CA	2.16	120.81	113.51
3	A	2005	PRO	OXT-C-O	-2.12	119.27	124.08
2	A	2001	FDA	O2A-PA-O3P	-2.08	101.65	107.27
2	A	2001	FDA	C4'-C3'-C2'	2.06	117.01	113.57
2	A	2001	FDA	O5B-PA-O1A	2.05	117.06	108.94

There are no chirality outliers.

All (27) torsion outliers are listed below:

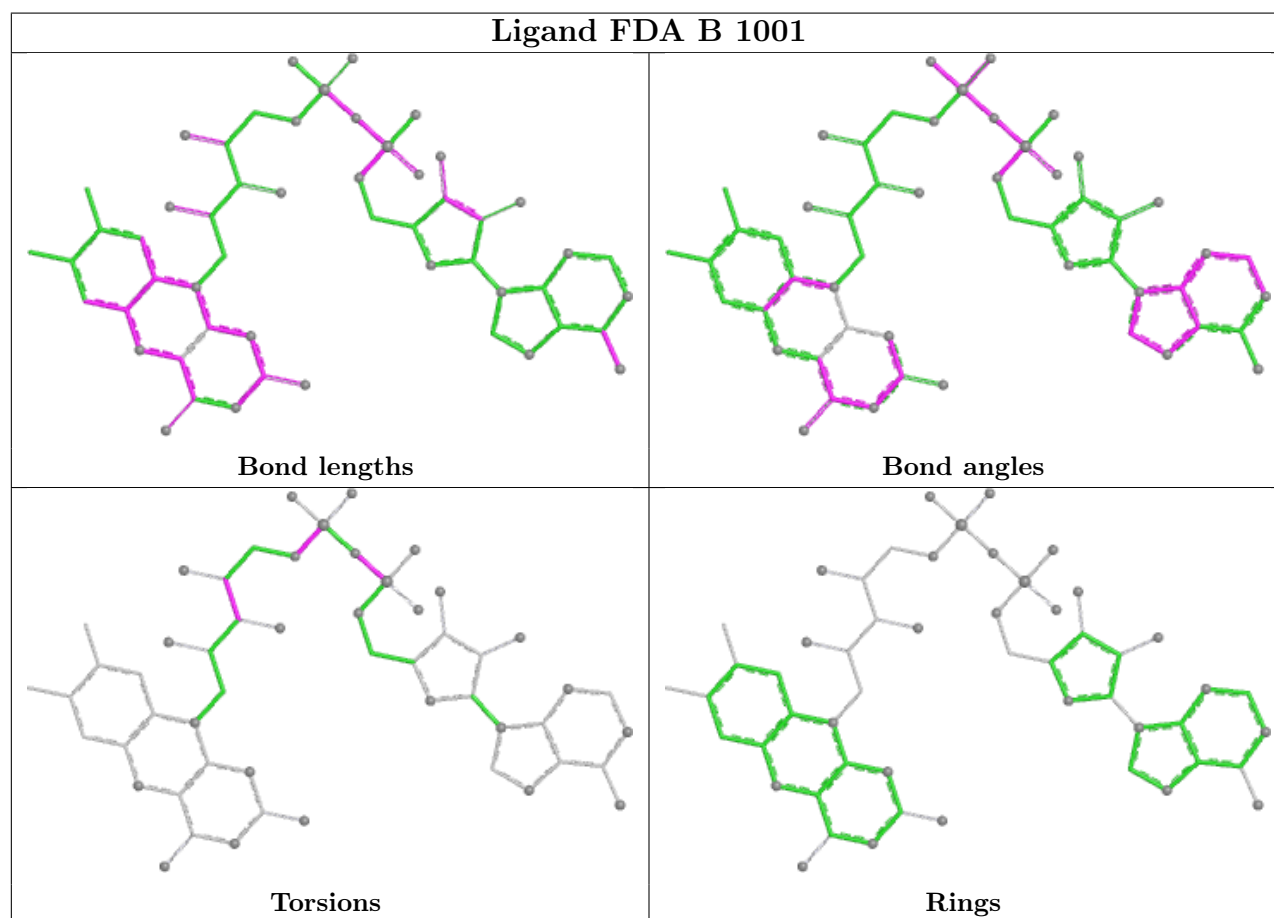
Mol	Chain	Res	Type	Atoms
2	A	2001	FDA	P-O3P-PA-O5B
3	A	2003	PRO	O-C-CA-N
3	A	2003	PRO	OXT-C-CA-N
3	A	2003	PRO	O-C-CA-CB
3	A	2003	PRO	OXT-C-CA-CB
3	B	1003	PRO	O-C-CA-N
3	B	1003	PRO	OXT-C-CA-N
3	B	1003	PRO	O-C-CA-CB
3	B	1003	PRO	OXT-C-CA-CB
2	A	2001	FDA	O3'-C3'-C4'-C5'
2	A	2001	FDA	O3'-C3'-C4'-O4'
2	A	2001	FDA	C2'-C3'-C4'-O4'
2	A	2001	FDA	C2'-C3'-C4'-C5'
2	B	1001	FDA	C2'-C3'-C4'-C5'
2	B	1001	FDA	C2'-C3'-C4'-O4'
2	B	1001	FDA	O3'-C3'-C4'-C5'
2	B	1001	FDA	O3'-C3'-C4'-O4'
2	B	1001	FDA	C5'-O5'-P-O1P
3	A	2002	PRO	O-C-CA-CB
3	A	2004	PRO	OXT-C-CA-CB
3	A	2005	PRO	O-C-CA-N
3	A	2004	PRO	O-C-CA-CB
3	A	2005	PRO	O-C-CA-CB
3	B	1005	PRO	O-C-CA-CB
3	B	1005	PRO	OXT-C-CA-CB
2	B	1001	FDA	P-O3P-PA-O5B
3	A	2005	PRO	OXT-C-CA-N

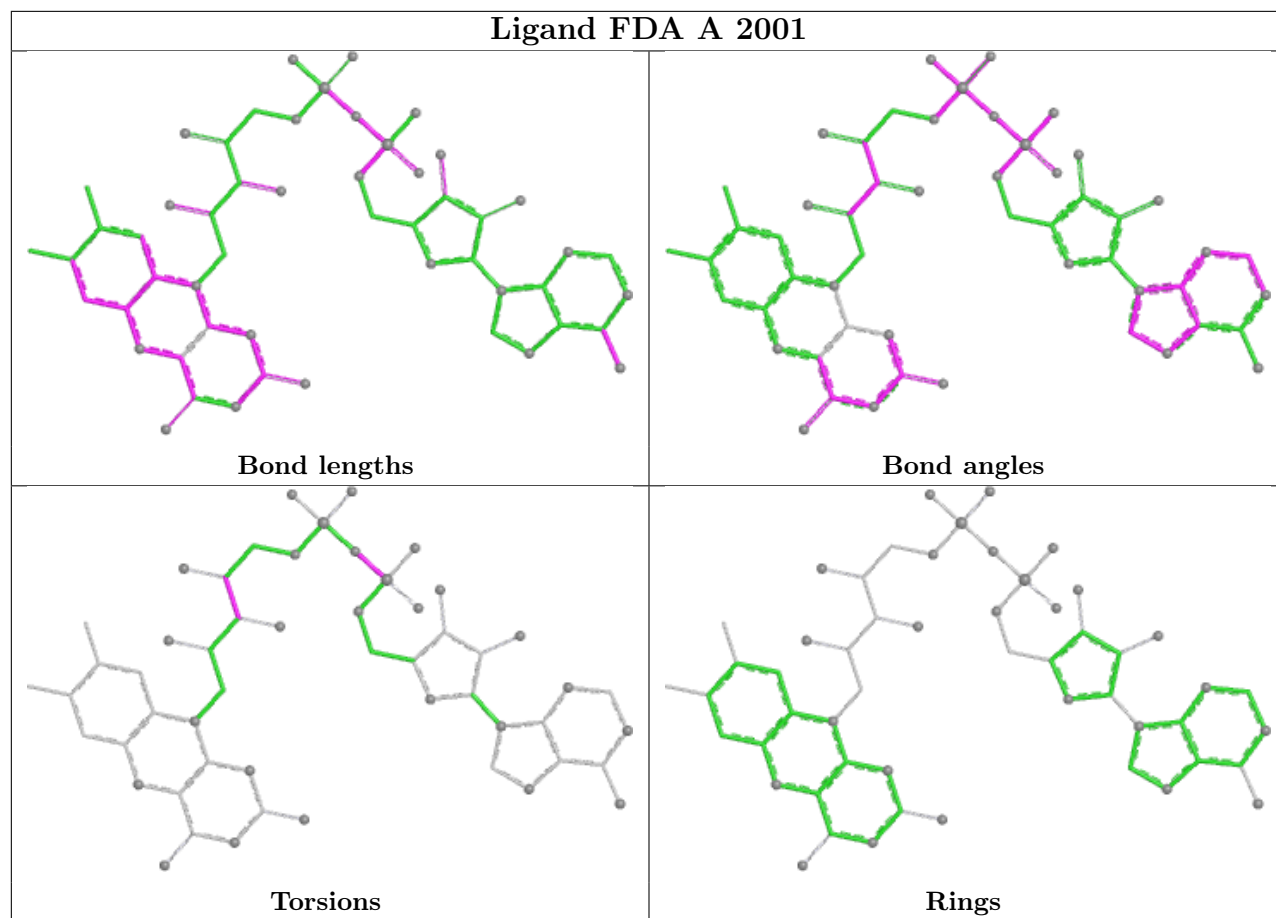
There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1003	PRO	2	0
3	A	2003	PRO	1	0
4	B	1008	SO4	1	0
4	A	2009	SO4	2	0
3	A	2002	PRO	1	0
2	A	2001	FDA	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	973/1001 (97%)	0.08	42 (4%)	40 45	21, 34, 61, 98	2 (0%)
1	B	973/1001 (97%)	0.20	45 (4%)	37 42	24, 39, 66, 100	1 (0%)
All	All	1946/2002 (97%)	0.14	87 (4%)	38 43	21, 36, 64, 100	3 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	987	ALA	8.9
1	B	987	ALA	7.4
1	A	988	ALA	7.1
1	B	51	ARG	6.1
1	B	184	SER	6.1
1	B	988	ALA	5.9
1	B	129	VAL	5.9
1	A	55	LEU	5.8
1	A	51	ARG	5.2
1	B	409	GLY	5.2
1	A	409	GLY	5.1
1	A	29	LEU	5.1
1	B	123	LEU	5.1
1	A	434	ALA	5.1
1	A	542	ILE	5.0
1	B	55	LEU	5.0
1	A	184	SER	4.9
1	B	542	ILE	4.7
1	B	183	ARG	4.6
1	B	460	GLU	4.5
1	A	123	LEU	4.2
1	B	225	ASN	3.9
1	A	131	GLN	3.9
1	A	28	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	29	LEU	3.9
1	B	4	ILE	3.8
1	A	459	LEU	3.8
1	B	56	GLY	3.6
1	B	223	ALA	3.5
1	B	131	GLN	3.5
1	A	1	MET	3.5
1	B	54	ARG	3.4
1	B	464	ASN	3.4
1	A	132	PRO	3.4
1	A	463	ALA	3.4
1	B	130	ILE	3.3
1	A	460	GLU	3.3
1	B	132	PRO	3.2
1	B	459	LEU	3.2
1	B	189	ARG	3.2
1	B	28	HIS	3.2
1	B	490	VAL	3.1
1	A	133	GLY	3.1
1	B	122	ALA	3.1
1	A	226	HIS	3.1
1	A	472	ALA	3.1
1	A	464	ASN	3.0
1	B	185	GLY	3.0
1	A	56	GLY	3.0
1	A	130	ILE	3.0
1	A	185	GLY	3.0
1	A	543	ALA	2.9
1	A	221	LYS	2.9
1	A	183	ARG	2.8
1	B	121	TRP	2.7
1	B	408	GLU	2.6
1	A	121	TRP	2.6
1	B	543	ALA	2.6
1	A	223	ALA	2.6
1	B	434	ALA	2.6
1	A	410	SER	2.5
1	B	934	GLN	2.4
1	A	50	LYS	2.4
1	A	510	GLU	2.4
1	B	837	VAL	2.4
1	B	472	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	410	SER	2.3
1	A	861	PRO	2.3
1	B	222	ALA	2.3
1	A	182	PRO	2.3
1	B	456	ARG	2.3
1	B	713	ASP	2.3
1	B	182	PRO	2.2
1	A	122	ALA	2.2
1	A	30	SER	2.2
1	A	490	VAL	2.1
1	A	181	LYS	2.1
1	B	864	GLU	2.1
1	A	456	ARG	2.1
1	A	475	ARG	2.1
1	B	22	ARG	2.1
1	A	484	ARG	2.0
1	A	474	TYR	2.0
1	B	461	ASN	2.0
1	B	31	PRO	2.0
1	B	188	THR	2.0
1	B	474	TYR	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
4	SO4	A	2010	5/5	0.71	0.17	82,82,83,86	5
4	SO4	B	1007	5/5	0.72	0.17	76,82,83,84	5

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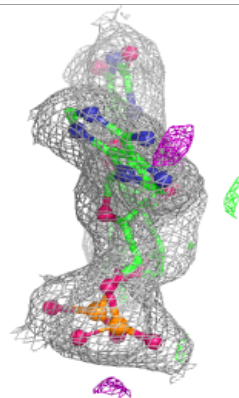
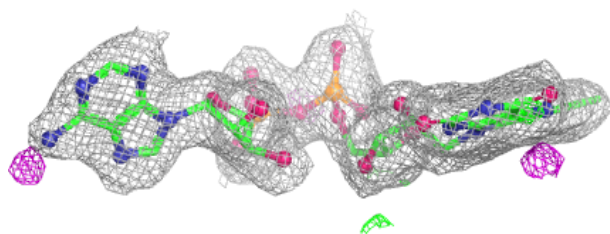
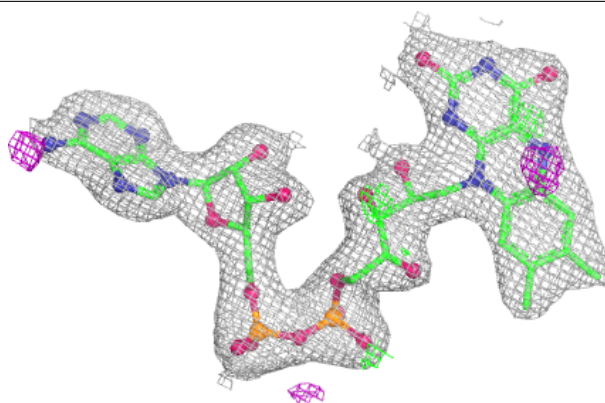
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	1010	5/5	0.78	0.28	92,93,95,95	5
4	SO4	B	1012	5/5	0.78	0.16	91,95,95,96	5
4	SO4	A	2013	5/5	0.80	0.17	73,79,81,81	5
4	SO4	B	1009	5/5	0.82	0.15	99,101,103,104	0
4	SO4	B	1011	5/5	0.83	0.14	75,76,81,84	5
3	PRO	B	1003	8/8	0.84	0.15	40,46,60,62	0
4	SO4	A	2011	5/5	0.84	0.14	83,84,86,88	5
4	SO4	A	2012	5/5	0.85	0.22	96,97,98,99	0
3	PRO	B	1004	8/8	0.86	0.18	57,62,64,65	0
3	PRO	A	2006	8/8	0.86	0.15	38,43,47,47	8
4	SO4	A	2008	5/5	0.87	0.12	56,59,64,66	5
4	SO4	B	1008	5/5	0.87	0.13	80,80,83,86	5
3	PRO	A	2003	8/8	0.89	0.14	32,37,65,67	8
3	PRO	A	2004	8/8	0.90	0.13	40,48,52,53	0
3	PRO	A	2005	8/8	0.90	0.15	53,54,55,57	8
3	PRO	B	1005	8/8	0.91	0.13	51,56,57,57	0
4	SO4	A	2009	5/5	0.92	0.11	56,58,63,66	5
4	SO4	A	2007	5/5	0.95	0.10	49,52,52,52	5
4	SO4	B	1006	5/5	0.95	0.09	50,53,56,57	5
3	PRO	A	2002	8/8	0.96	0.07	28,35,38,40	0
2	FDA	B	1001	53/53	0.96	0.07	26,34,44,53	0
3	PRO	B	1002	8/8	0.97	0.07	31,35,38,39	0
2	FDA	A	2001	53/53	0.97	0.06	19,29,38,42	0

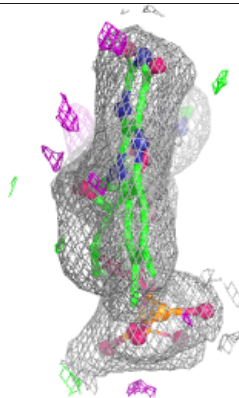
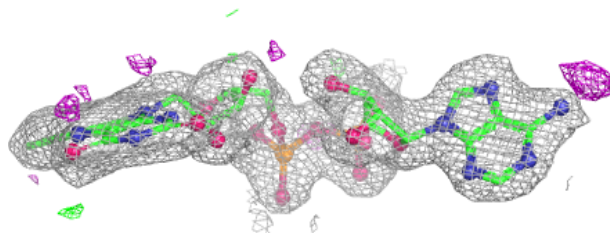
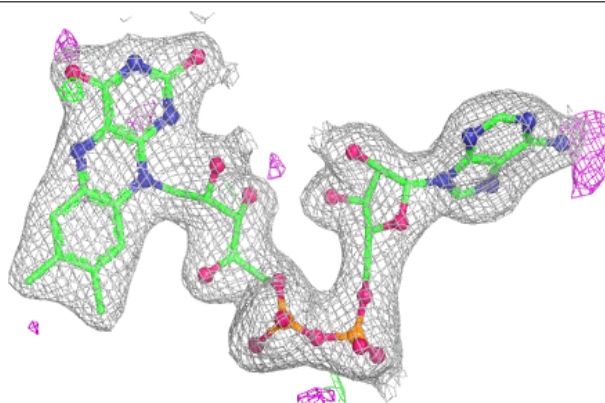
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FDA B 1001:

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

**Electron density around FDA 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 [i](#)

There are no such residues in this entry.