Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 01:26 PM EDT

PDB ID	:	1SPS
Title	:	BINDING OF A HIGH AFFINITY PHOSPHOTYROSYL PEPTIDE TO THE SRC SH2 DOMAIN: CRYSTAL STRUCTURES OF THE COMPLEXED AND PEPTIDE-FREE FORMS
Authors	:	Waksman, G.; Kuriyan, J.
Deposited on	:	1993-03-05
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

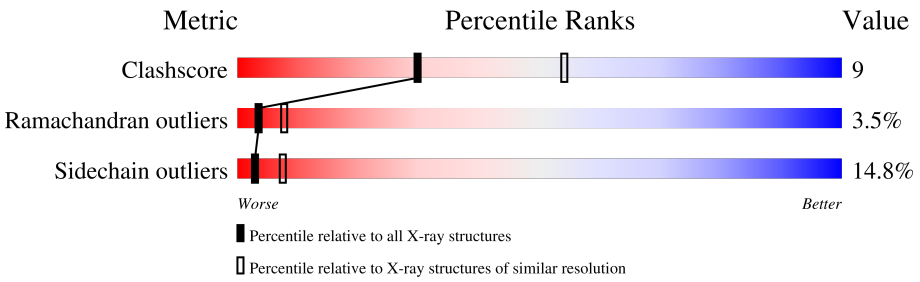
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	104	61% 28% 11% •
1	B	104	55% 36% 8% ••
1	C	104	62% 32% 5% ••
2	D	11	27% 27% 9% 36%
2	E	11	36% 9% 9% 45%
2	F	11	27% 55% 9% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3473 atoms, of which 721 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 SRC SH2 DOMAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	103	1040	525	206	149	157	3	0	0	0
1	B	103	1040	525	206	149	157	3	0	0	0
1	C	103	1040	525	206	149	157	3	0	0	0

- Molecule 2 is a protein called PEPTIDE YEEI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	D	7	66	38	5	7	15	1	0	0	0
2	E	6	65	35	7	7	15	1	0	0	0
2	F	10	102	58	11	11	21	1	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
3	A	10	30	20	10	0	0
3	B	16	48	32	16	0	0
3	E	3	9	6	3	0	0
3	C	8	24	16	8	0	0
3	F	3	9	6	3	0	0

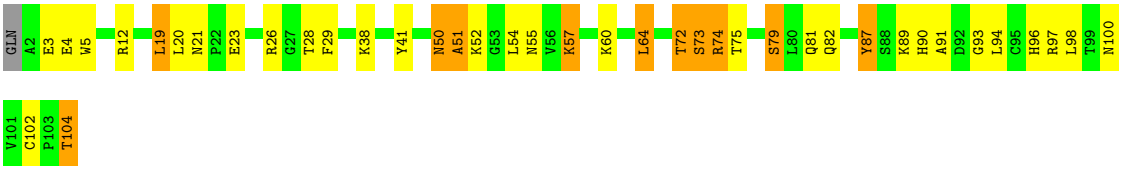
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

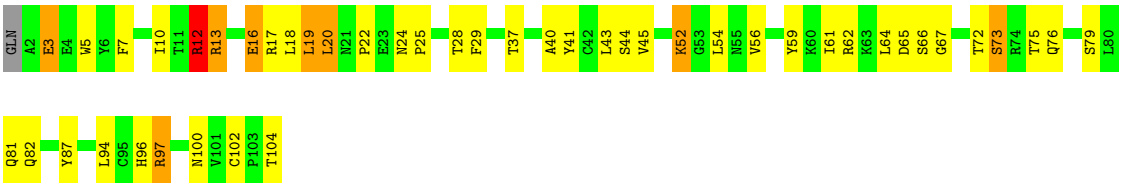
• Molecule 1: SRC SH2 DOMAIN

Chain A:



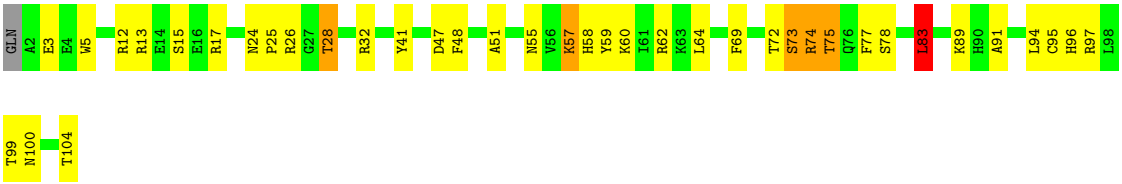
• Molecule 1: SRC SH2 DOMAIN

Chain B:



• Molecule 1: SRC SH2 DOMAIN

Chain C:

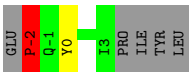


• Molecule 2: PEPTIDE YEEI

Chain D:

• Molecule 2: PEPTIDE YEEI

Chain E:



- Molecule 2: PEPTIDE YEEI

Chain F:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	93.30Å 93.30Å 55.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3473	wwPDB-VP
Average B, all atoms ($Å^2$)	32.0	wwPDB-VP

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: PTR

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	0.87	0/852	1.70	21/1147 (1.8%)
1	B	0.80	0/852	1.65	17/1147 (1.5%)
1	C	0.75	0/852	1.52	12/1147 (1.0%)
2	D	0.87	0/45	1.15	0/59
2	E	1.05	0/41	1.53	1/52 (1.9%)
2	F	0.98	0/73	1.89	4/94 (4.3%)
All	All	0.82	0/2715	1.62	55/3646 (1.5%)

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
2	D	0	1

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	5	TRP	CD1-CG-CD2	8.67	113.23	106.30
1	C	5	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	C	5	TRP	CB-CG-CD1	-8.30	116.21	127.00
1	C	5	TRP	CG-CD2-CE3	8.26	141.33	133.90
1	A	5	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	A	73	SER	N-CA-CB	8.13	122.69	110.50
1	C	5	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	A	73	SER	CB-CA-C	-7.79	95.29	110.10
1	B	5	TRP	CE2-CD2-CG	-7.70	101.14	107.30
1	A	5	TRP	CE2-CD2-CG	-7.61	101.22	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	83	LEU	CA-CB-CG	7.55	132.66	115.30
1	B	73	SER	N-CA-CB	7.40	121.60	110.50
1	B	5	TRP	CB-CG-CD1	-7.15	117.70	127.00
1	A	26	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	B	5	TRP	CG-CD2-CE3	7.10	140.29	133.90
1	A	104	THR	CA-CB-CG2	6.97	122.15	112.40
1	B	104	THR	CA-CB-CG2	6.88	122.04	112.40
1	A	51	ALA	CB-CA-C	-6.51	100.33	110.10
1	B	18	LEU	CA-CB-CG	6.51	130.28	115.30
1	B	12	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	B	13	ARG	CA-CB-CG	6.26	127.18	113.40
1	B	73	SER	CB-CA-C	-6.24	98.25	110.10
1	A	5	TRP	CB-CG-CD1	-6.21	118.92	127.00
1	A	74	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	C	28	THR	CA-CB-CG2	6.12	120.96	112.40
1	A	72	THR	CA-C-N	6.11	130.64	117.20
1	A	38	LYS	CA-CB-CG	-6.09	100.00	113.40
1	C	74	ARG	NE-CZ-NH1	6.05	123.32	120.30
2	F	6	TYR	O-C-N	6.03	132.35	122.70
1	A	41	TYR	CB-CG-CD1	-6.01	117.40	121.00
1	A	104	THR	CA-CB-OG1	-5.95	96.51	109.00
1	B	56	VAL	CG1-CB-CG2	-5.95	101.39	110.90
2	F	6	TYR	C-N-CA	5.82	136.25	121.70
1	A	5	TRP	CG-CD2-CE3	5.81	139.13	133.90
1	C	73	SER	N-CA-CB	5.74	119.11	110.50
1	B	97	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	C	17	ARG	NE-CZ-NH2	-5.66	117.47	120.30
2	F	-2	PRO	N-CA-CB	5.58	110.00	103.30
1	B	87	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	B	5	TRP	CG-CD1-NE1	-5.51	104.59	110.10
1	C	5	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	B	62	ARG	NE-CZ-NH1	5.45	123.03	120.30
2	E	-2	PRO	CA-N-CD	-5.41	103.93	111.50
1	C	59	TYR	CB-CG-CD2	-5.39	117.77	121.00
2	F	6	TYR	CA-C-N	-5.38	105.36	117.20
1	A	51	ALA	N-CA-CB	5.36	117.60	110.10
1	A	4	GLU	CA-CB-CG	5.34	125.15	113.40
1	A	87	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	B	41	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	A	5	TRP	CG-CD1-NE1	-5.22	104.88	110.10
1	A	79	SER	N-CA-CB	-5.18	102.72	110.50
1	B	59	TYR	CB-CG-CD2	-5.10	117.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	ASN	CA-C-N	5.05	128.30	117.20
1	C	41	TYR	CB-CG-CD2	-5.01	118.00	121.00
1	A	57	LYS	CG-CD-CE	-5.00	96.89	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	3	ILE	Peptide

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	834	206	818	16	0
1	B	834	206	818	17	0
1	C	834	206	818	16	0
2	D	61	5	48	3	0
2	E	58	7	47	1	0
2	F	91	11	67	4	0
3	A	10	20	0	0	0
3	B	16	32	0	1	0
3	C	8	16	0	0	0
3	E	3	6	0	0	0
3	F	3	6	0	0	0
All	All	2752	721	2616	50	0

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

All (50) 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:B:28:THR:HG22	1:B:100:ASN:HB3	1.47	0.95
1:B:7:PHE:HB3	1:B:10:ILE:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LYS:HB3	2:F:1:GLU:HG3	1.77	0.65
1:B:12:ARG:NH2	2:E:-2:PRO:HB3	2.11	0.64
1:C:97:ARG:NH1	1:C:99:THR:HG22	2.18	0.57
1:B:16:GLU:O	1:B:20:LEU:HB2	2.05	0.56
1:A:57:LYS:HB3	2:D:1:GLU:HG3	1.86	0.56
1:C:97:ARG:HH11	1:C:99:THR:HG22	1.69	0.56
1:C:57:LYS:HG3	1:C:95:CYS:SG	2.46	0.56
1:B:37:THR:HB	1:B:40:ALA:HB3	1.90	0.54
1:A:93:GLY:HA3	2:D:3:ILE:HG23	1.90	0.53
1:A:21:ASN:OD1	1:A:23:GLU:HG2	2.08	0.52
1:C:24:ASN:HB3	1:C:28:THR:HG21	1.92	0.51
1:C:28:THR:HA	1:C:100:ASN:O	2.10	0.51
1:C:26:ARG:HG3	1:C:47:ASP:HA	1.93	0.50
1:A:96:HIS:HD2	1:A:97:ARG:O	1.94	0.50
1:C:77:PHE:CD2	1:C:83:LEU:HD22	2.48	0.49
1:C:62:ARG:O	1:C:69:PHE:HA	2.14	0.48
1:A:19:LEU:CD1	1:A:102:CYS:SG	3.02	0.48
1:A:29:PHE:CD1	1:A:98:LEU:HB3	2.50	0.47
1:B:96:HIS:HD2	1:B:97:ARG:O	1.98	0.47
1:A:79:SER:HB3	1:A:82:GLN:HB2	1.96	0.47
1:C:60:LYS:HB2	1:C:60:LYS:HE3	1.73	0.46
1:B:94:LEU:HD23	1:B:96:HIS:O	2.16	0.46
1:C:47:ASP:CB	1:C:57:LYS:HD3	2.46	0.46
1:C:12:ARG:HG3	1:C:58:HIS:CE1	2.51	0.45
1:B:25:PRO:O	1:B:28:THR:HG23	2.17	0.45
1:B:52:LYS:HG2	3:B:1038:HOH:O	2.16	0.45
1:B:20:LEU:HD12	1:B:54:LEU:HD12	1.98	0.44
2:F:7:LEU:HA	2:F:7:LEU:HD23	1.68	0.44
1:A:50:ASN:O	1:A:51:ALA:HB3	2.18	0.43
1:B:29:PHE:HA	1:B:44:SER:O	2.19	0.43
1:A:19:LEU:HD13	1:A:102:CYS:SG	2.59	0.43
1:A:60:LYS:HB2	1:A:60:LYS:HE3	1.76	0.43
1:B:64:LEU:HD22	1:B:76:GLN:OE1	2.19	0.43
1:A:28:THR:HA	1:A:100:ASN:HB3	2.01	0.43
1:C:15:SER:OG	1:C:32:ARG:HD3	2.19	0.42
1:C:94:LEU:HD12	2:F:3:ILE:HD11	2.01	0.42
1:A:74:ARG:HE	1:A:74:ARG:HB2	1.69	0.42
1:A:87:TYR:CD1	1:A:94:LEU:HD22	2.55	0.41
1:B:52:LYS:HD2	1:B:52:LYS:N	2.36	0.41
1:B:19:LEU:HD13	1:B:102:CYS:SG	2.61	0.41
1:A:91:ALA:O	1:A:94:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ASN:HA	1:B:25:PRO:HD2	1.94	0.41
1:C:74:ARG:HE	1:C:74:ARG:HB2	1.77	0.41
1:A:64:LEU:HG	2:F:7:LEU:HG	2.04	0.40
1:B:28:THR:HA	1:B:100:ASN:O	2.21	0.40
1:B:43:LEU:HB2	1:B:61:ILE:HD11	2.03	0.40
1:A:12:ARG:CZ	2:D:-2:PRO:HB2	2.51	0.40
1:C:75:THR:HG22	1:C:77:PHE:CZ	2.56	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	101/104 (97%)	93 (92%)	6 (6%)	2 (2%)	7 19
1	B	101/104 (97%)	94 (93%)	2 (2%)	5 (5%)	2 4
1	C	101/104 (97%)	89 (88%)	8 (8%)	4 (4%)	3 6
2	D	4/11 (36%)	4 (100%)	0	0	100 100
2	E	3/11 (27%)	3 (100%)	0	0	100 100
2	F	7/11 (64%)	7 (100%)	0	0	100 100
All	All	317/345 (92%)	290 (92%)	16 (5%)	11 (4%)	3 8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	65	ASP
1	B	73	SER
1	A	73	SER
1	B	3	GLU
1	B	66	SER

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Mol	Chain	Res	Type
1	A	3	GLU
1	C	25	PRO
1	C	51	ALA
1	C	73	SER
1	C	91	ALA
1	B	67	GLY

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	91/92 (99%)	79 (87%)	12 (13%)	4 9
1	B	91/92 (99%)	76 (84%)	15 (16%)	2 5
1	C	91/92 (99%)	78 (86%)	13 (14%)	3 8
2	D	5/10 (50%)	5 (100%)	0	100 100
2	E	5/10 (50%)	4 (80%)	1 (20%)	1 3
2	F	7/10 (70%)	5 (71%)	2 (29%)	0 1
All	All	290/306 (95%)	247 (85%)	43 (15%)	3 7

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	20	LEU
1	A	52	LYS
1	A	54	LEU
1	A	55	ASN
1	A	64	LEU
1	A	72	THR
1	A	75	THR
1	A	81	GLN
1	A	89	LYS
1	A	90	HIS
1	A	104	THR

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Mol	Chain	Res	Type
1	B	3	GLU
1	B	12	ARG
1	B	13	ARG
1	B	16	GLU
1	B	17	ARG
1	B	19	LEU
1	B	20	LEU
1	B	22	PRO
1	B	45	VAL
1	B	52	LYS
1	B	72	THR
1	B	75	THR
1	B	79	SER
1	B	81	GLN
1	B	82	GLN
2	E	-2	PRO
1	C	3	GLU
1	C	13	ARG
1	C	48	PHE
1	C	55	ASN
1	C	57	LYS
1	C	64	LEU
1	C	72	THR
1	C	75	THR
1	C	78	SER
1	C	83	LEU
1	C	89	LYS
1	C	96	HIS
1	C	104	THR
2	F	-1	GLN
2	F	6	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	B	82	GLN
1	B	96	HIS
2	E	-1	GLN
1	C	81	GLN
1	C	82	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	PTR	E	0	2	15,16,17	1.44	2 (13%)	19,22,24	1.18	2 (10%)
2	PTR	D	0	2	15,16,17	0.92	0	19,22,24	1.08	1 (5%)
2	PTR	F	0	2	15,16,17	1.27	2 (13%)	19,22,24	1.42	3 (15%)

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	PTR	E	0	2	-	1/10/11/13	0/1/1/1
2	PTR	D	0	2	-	1/10/11/13	0/1/1/1
2	PTR	F	0	2	-	1/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	0	PTR	P-OH	3.70	1.65	1.59
2	F	0	PTR	CB-CA	-2.55	1.48	1.53
2	E	0	PTR	OH-CZ	2.48	1.46	1.40
2	F	0	PTR	P-OH	-2.19	1.55	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	0	PTR	CE2-CZ-CE1	3.20	125.11	120.18
2	E	0	PTR	CG-CB-CA	2.84	119.85	114.10
2	F	0	PTR	CD1-CE1-CZ	-2.69	116.45	119.73
2	F	0	PTR	CD2-CG-CD1	2.25	121.70	118.17
2	D	0	PTR	O2P-P-OH	2.17	112.03	105.24
2	E	0	PTR	O2P-P-OH	2.00	111.51	105.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	0	PTR	CZ-OH-P-O1P
2	F	0	PTR	C-CA-CB-CG
2	D	0	PTR	CZ-OH-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.