



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:07 AM UTC

PDB ID : 1P13 / pdb_00001p13
Title : Crystal Structure of the Src SH2 Domain Complexed with Peptide (SD-pYANFK)
Authors : Sonnenburg, E.D.; Bilwes, A.; Hunter, T.; Noel, J.P.
Deposited on : 2003-04-11
Resolution : 1.63 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

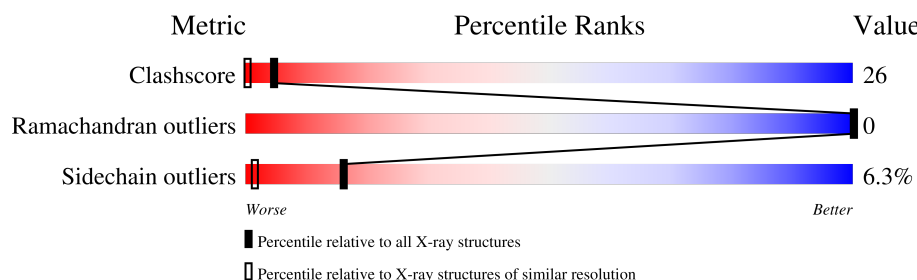
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	102	78% 15% 7%
1	B	102	69% 28% .
2	C	7	43% 43% 14%
2	D	7	43% 14% 43%

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
2	PTR	C	3	-	-	X	-
2	PTR	D	3	-	-	X	-
3	CAC	B	352	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2071 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.

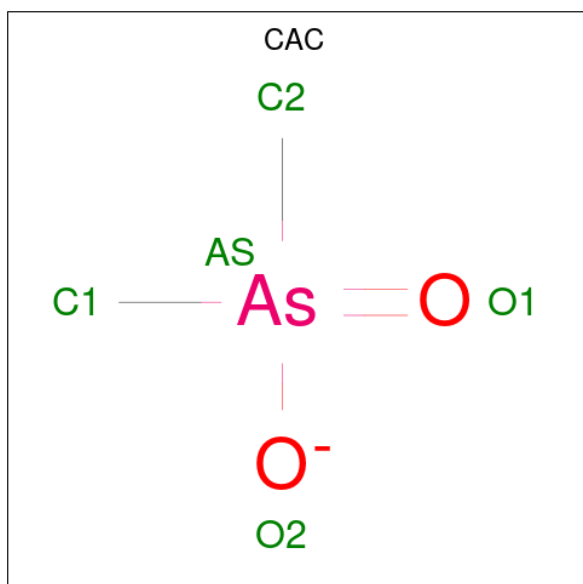
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	0
			827	521	148	155	3			
1	B	102	Total	C	N	O	S	0	0	0
			827	521	148	155	3			

- Molecule 2 is a protein called Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	P	S	0	0
			64	38	9	15	1	1		
2	D	7	Total	C	N	O	P	S	0	0
			64	38	9	15	1	1		

- Molecule 3 is CACODYLATE ION (CCD ID: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 4	As 1	C 2	O 1	0	0
3	A	1	Total 4	As 1	C 2	O 1	0	0
3	B	1	Total 4	As 1	C 2	O 1	0	0
3	B	1	Total 4	As 1	C 2	O 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total 119	O 119	0	0
4	B	117	Total 117	O 117	0	0
4	C	20	Total 20	O 20	0	0
4	D	17	Total 17	O 17	0	0

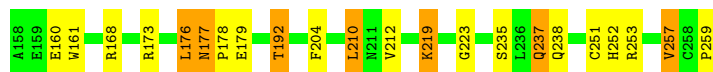
3 Residue-property plots [i](#)

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: Proto-oncogene tyrosine-protein kinase Src

Chain A: 



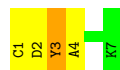
- Molecule 1: Proto-oncogene tyrosine-protein kinase Src

Chain B: 

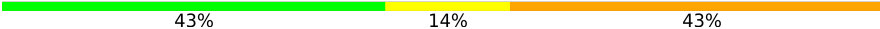


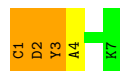
- Molecule 2: Peptide

Chain C: 



- Molecule 2: Peptide

Chain D: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.38Å 58.79Å 62.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.88 – 1.63	Depositor
% Data completeness (in resolution range)	99.3 (42.88-1.63)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2071	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, 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	0.77	0/845	1.08	2/1137 (0.2%)
1	B	0.85	0/845	1.16	6/1137 (0.5%)
2	C	0.79	0/47	0.91	0/58
2	D	0.68	0/47	0.81	0/58
All	All	0.81	0/1784	1.11	8/2390 (0.3%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ASN	N-CA-C	7.98	119.70	109.65
1	A	257	VAL	N-CA-C	-7.34	100.12	109.58
1	B	229	SER	N-CA-C	7.18	119.97	111.71
1	B	255	THR	CA-C-N	-6.89	111.99	122.81
1	B	255	THR	C-N-CA	-6.89	111.99	122.81
1	B	227	ILE	N-CA-C	-6.33	106.02	113.42
1	B	256	ASN	N-CA-C	6.03	119.36	109.72
1	A	223	GLY	N-CA-C	-5.23	106.09	112.68

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	827	0	809	31	0
1	B	827	0	810	35	0
2	C	64	0	52	13	0
2	D	64	0	52	16	0
3	A	8	0	0	2	0
3	B	8	0	0	6	0
4	A	119	0	0	7	0
4	B	117	0	0	7	0
4	C	20	0	0	0	0
4	D	17	0	0	0	0
All	All	2071	0	1723	88	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 26.

All (88) 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:C:2:ASP:C	2:C:3:PTR:N	2.16	1.04
1:B:219:LYS:HE2	4:B:499:HOH:O	1.56	1.02
1:A:160:GLU:HG2	1:A:257:VAL:HG11	1.45	0.97
1:B:251:CYS:SG	3:B:352:CAC:AS	2.83	0.96
1:B:205:ASP:HB2	1:B:208:LYS:HB2	1.48	0.95
2:D:3:PTR:C	2:D:4:ALA:N	2.35	0.89
2:D:2:ASP:C	2:D:3:PTR:HN2	1.77	0.89
1:A:177:ASN:ND2	1:A:179:GLU:HG2	1.90	0.87
2:D:2:ASP:CA	2:D:3:PTR:N	2.39	0.84
1:A:178:PRO:HD3	1:B:206:ASN:O	1.81	0.80
1:A:237:GLN:H	1:A:237:GLN:CD	1.90	0.78
1:B:169:ARG:HG3	4:B:505:HOH:O	1.84	0.77
1:B:252:HIS:HE1	4:B:501:HOH:O	1.65	0.77
2:C:3:PTR:C	2:C:4:ALA:N	2.48	0.77
1:B:235:SER:HB2	1:B:237:GLN:HE21	1.50	0.76
1:B:190:SER:HA	3:B:399:CAC:C1	2.16	0.75
1:B:238:GLN:HB3	4:B:492:HOH:O	1.86	0.74
1:A:173:ARG:NH1	4:A:470:HOH:O	2.20	0.74
1:A:192:THR:HG23	4:A:442:HOH:O	1.88	0.74
1:A:252:HIS:HD2	1:A:253:ARG:O	1.71	0.72
1:A:251:CYS:SG	3:A:351:CAC:O1	2.46	0.71
1:B:251:CYS:SG	3:B:352:CAC:O1	2.49	0.70
2:C:1:CYS:SG	2:C:2:ASP:N	2.66	0.69
2:D:3:PTR:HA	2:D:4:ALA:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:ASP:HA	2:D:3:PTR:N	2.08	0.67
1:A:177:ASN:HD21	1:A:179:GLU:HG2	1.59	0.67
1:B:180:ASN:OD1	1:B:259:PRO:OXT	2.14	0.66
1:A:259:PRO:HA	4:A:474:HOH:O	1.94	0.66
2:D:2:ASP:HA	2:D:3:PTR:HN2	1.60	0.65
2:D:2:ASP:CA	2:D:3:PTR:HN2	2.07	0.65
1:A:176:LEU:HD13	1:A:212:VAL:HG23	1.79	0.64
1:A:219:LYS:HE2	4:A:464:HOH:O	1.98	0.63
2:D:2:ASP:HB2	2:D:3:PTR:H	1.63	0.63
1:B:235:SER:HB2	1:B:237:GLN:NE2	2.13	0.63
1:B:205:ASP:O	1:B:209:GLY:N	2.29	0.62
1:A:177:ASN:HD22	1:A:179:GLU:H	1.47	0.62
1:B:237:GLN:H	1:B:237:GLN:CD	2.08	0.62
2:C:3:PTR:O	2:C:4:ALA:CA	2.47	0.62
1:A:219:LYS:NZ	4:A:447:HOH:O	2.24	0.62
2:D:3:PTR:O	2:D:4:ALA:N	2.32	0.62
2:D:3:PTR:CA	2:D:4:ALA:N	2.63	0.61
2:D:2:ASP:CA	2:D:3:PTR:H	2.14	0.59
1:A:177:ASN:HD22	1:A:177:ASN:C	2.13	0.57
2:D:2:ASP:C	2:D:3:PTR:H	2.06	0.57
2:D:2:ASP:CB	2:D:3:PTR:H	2.18	0.56
2:C:3:PTR:CD1	2:C:3:PTR:HN2	2.18	0.56
2:C:2:ASP:C	2:C:3:PTR:H	2.10	0.55
1:A:176:LEU:O	1:B:206:ASN:HB3	2.08	0.54
1:B:161:TRP:HA	1:B:257:VAL:HG13	1.90	0.54
2:C:3:PTR:HA	2:C:4:ALA:N	2.23	0.54
1:B:190:SER:CA	3:B:399:CAC:C1	2.87	0.53
1:B:203:ASP:OD2	1:B:213:LYS:NZ	2.33	0.53
1:A:177:ASN:ND2	1:A:179:GLU:H	2.07	0.52
1:B:251:CYS:SG	3:B:352:CAC:C2	2.97	0.52
1:A:168:ARG:HD2	2:D:3:PTR:O3P	2.09	0.52
1:B:252:HIS:HD2	1:B:253:ARG:O	1.93	0.52
1:A:204:PHE:HD1	1:A:210:LEU:HD13	1.75	0.51
1:B:235:SER:OG	1:B:237:GLN:HG2	2.10	0.51
1:A:178:PRO:HG2	1:B:207:ALA:HB2	1.93	0.50
1:A:176:LEU:HG	1:B:206:ASN:OD1	2.11	0.50
2:C:3:PTR:N	2:C:3:PTR:CD1	2.75	0.49
1:B:205:ASP:CB	1:B:208:LYS:HB2	2.31	0.49
1:A:177:ASN:HD22	1:A:178:PRO:N	2.11	0.49
1:A:237:GLN:CD	1:A:237:GLN:N	2.64	0.47
2:D:1:CYS:HB3	2:D:2:ASP:H	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ASN:CB	4:B:461:HOH:O	2.62	0.47
1:B:204:PHE:CE1	1:B:209:GLY:HA2	2.50	0.47
2:C:2:ASP:O	2:C:3:PTR:N	2.44	0.46
1:B:258:CYS:HA	1:B:259:PRO:C	2.40	0.46
2:C:3:PTR:CA	2:C:4:ALA:N	2.77	0.46
1:A:237:GLN:CD	4:A:483:HOH:O	2.58	0.46
1:B:204:PHE:CE2	1:B:206:ASN:HA	2.51	0.46
1:B:161:TRP:CA	1:B:257:VAL:HG13	2.46	0.45
1:A:160:GLU:HG2	1:A:257:VAL:CG1	2.32	0.45
1:B:160:GLU:HB2	1:B:257:VAL:HG11	1.98	0.45
1:A:204:PHE:C	1:A:204:PHE:CD2	2.95	0.45
1:A:251:CYS:CB	3:A:351:CAC:AS	3.24	0.44
1:A:237:GLN:HG3	4:A:483:HOH:O	2.18	0.44
2:D:3:PTR:O	2:D:4:ALA:C	2.61	0.44
3:B:352:CAC:AS	4:B:508:HOH:O	2.97	0.43
1:B:179:GLU:O	1:B:179:GLU:HG3	2.18	0.42
2:C:2:ASP:C	2:C:3:PTR:CA	2.91	0.41
1:A:178:PRO:HG2	1:B:207:ALA:CB	2.50	0.41
1:A:235:SER:OG	1:A:237:GLN:HG2	2.20	0.41
1:B:168:ARG:HD2	2:C:3:PTR:O3P	2.20	0.41
1:A:161:TRP:HB3	1:A:257:VAL:HG22	2.02	0.41
1:B:168:ARG:HB2	2:C:3:PTR:O3P	2.20	0.41
1:B:221:ASP:HA	4:B:486:HOH:O	2.21	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	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
1	B	100/102 (98%)	97 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	2/7 (29%)	2 (100%)	0	0	100	100
2	D	2/7 (29%)	2 (100%)	0	0	100	100
All	All	204/218 (94%)	197 (97%)	7 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	90/90 (100%)	83 (92%)	7 (8%)	11	1
1	B	90/90 (100%)	87 (97%)	3 (3%)	33	8
2	C	5/5 (100%)	5 (100%)	0	100	100
2	D	5/5 (100%)	3 (60%)	2 (40%)	0	0
All	All	190/190 (100%)	178 (94%)	12 (6%)	16	1

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LEU
1	A	177	ASN
1	A	192	THR
1	A	210	LEU
1	A	219	LYS
1	A	237	GLN
1	A	238	GLN
1	B	194	LYS
1	B	237	GLN
1	B	246	HIS
2	D	1	CYS
2	D	2	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	238	GLN
1	A	252	HIS
1	B	237	GLN
1	B	252	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	D	3	2	15,16,17	2.12	5 (33%)	17,22,24	1.69	3 (17%)
2	PTR	C	3	2	15,16,17	1.59	3 (20%)	17,22,24	1.64	3 (17%)

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	D	3	2	-	0/10/11/13	0/1/1/1
2	PTR	C	3	2	-	0/10/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	PTR	P-OH	-6.26	1.48	1.59
2	C	3	PTR	P-OH	-4.01	1.52	1.59
2	D	3	PTR	CE1-CZ	2.72	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	PTR	CD1-CG	2.42	1.43	1.38
2	D	3	PTR	CE1-CD1	2.29	1.42	1.38
2	C	3	PTR	CE1-CZ	2.25	1.43	1.38
2	D	3	PTR	CD1-CG	2.11	1.43	1.38
2	D	3	PTR	CA-N	-2.05	1.42	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	PTR	O3P-P-OH	-3.72	94.31	105.32
2	D	3	PTR	OH-CZ-CE1	3.24	128.94	119.22
2	C	3	PTR	OH-CZ-CE1	3.21	128.85	119.22
2	D	3	PTR	OH-CZ-CE2	-2.86	110.64	119.22
2	C	3	PTR	OH-CZ-CE2	-2.57	111.53	119.22
2	C	3	PTR	P-OH-CZ	2.33	132.17	123.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	PTR	15	0
2	C	3	PTR	12	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	CAC	B	352	-	0,3,4	-	-	0,3,6	-	-
3	CAC	B	399	1	0,3,4	-	-	0,3,6	-	-
3	CAC	A	351	1	0,3,4	-	-	0,3,6	-	-
3	CAC	A	398	1	0,3,4	-	-	0,3,6	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	352	CAC	4	0
3	B	399	CAC	2	0
3	A	351	CAC	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	2
2	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3:PTR	C	4:ALA	N	2.48
1	D	3:PTR	C	4:ALA	N	2.35
1	C	2:ASP	C	3:PTR	N	2.16
1	D	2:ASP	C	3:PTR	N	2.03

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.