



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:28 AM GMT

PDB ID : 3ESD
Title : cut-2b; NCN-Pt-Pincer-Cutinase Hybrid
Authors : Rutten, L.; Mannie, J.P.B.A.; Lutz, M.; Gros, P.
Deposited on : 2008-10-05
Resolution : 1.22 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

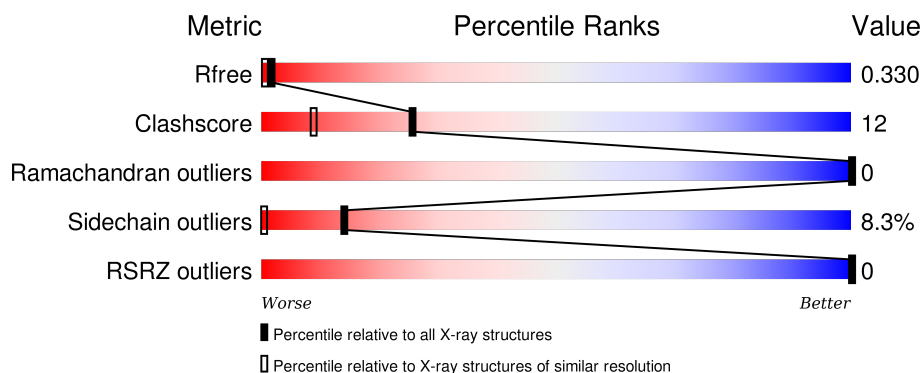
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.22 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}	91344	1197 (1.26-1.18)
Clashscore	102246	1295 (1.26-1.18)
Ramachandran outliers	100387	1239 (1.26-1.18)
Sidechain outliers	100360	1237 (1.26-1.18)
RSRZ outliers	91569	1201 (1.26-1.18)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	214	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1525 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.

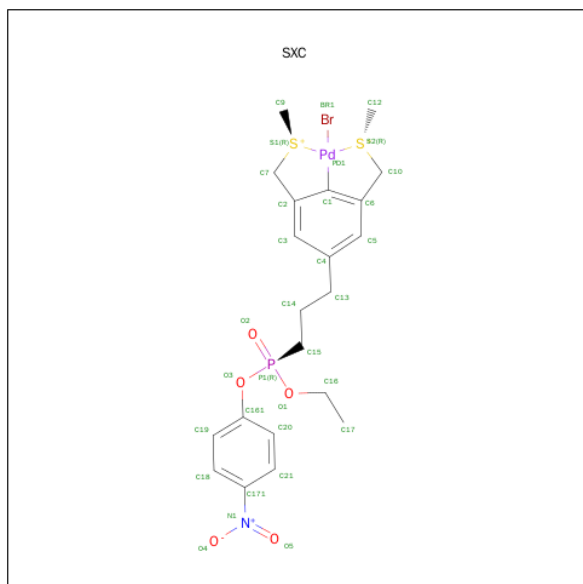
- Molecule 1 is a protein called Cutinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1430	890	258	277	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	ARG	SEE REMARK 999	UNP P00590
A	172	LYS	ASN	ENGINEERED	UNP P00590

- Molecule 2 is BROMO(4-{3-[(R)-ETHOXY(4-NITROPHENOXY)PHOSPHORYL]PROPYL}-2,6-BIS[(METHYLSULFANYL-KAPPAS)METHYL]PHENYL-KAPPAC 1)PALLADIUM(2+) (three-letter code: SXC) (formula: C₂₁H₂₇BrNO₅PPdS₂).

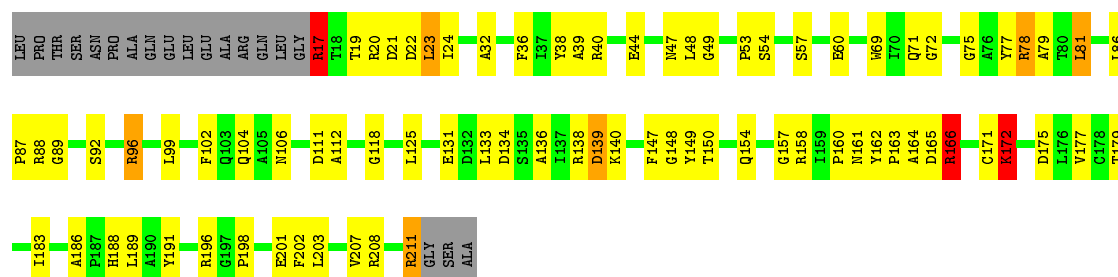


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	Br	C	O	P	Pd	S	0	0
			22	1	15	2	1	1	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total	O	0	0
			73	73		

- Molecule 1: Cutinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	72.36 Å 72.36 Å 110.77 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.00 – 1.22 41.50 – 1.22	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.00-1.22) 97.0 (41.50-1.22)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.22 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.199 , 0.222 0.319 , 0.330	Depositor DCC
R_{free} test set	3141 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.5	EDS
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 61944 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1525	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.70% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.03	5/1453 (0.3%)	2.84	88/1971 (4.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ARG	CZ-NH1	8.57	1.44	1.33
1	A	40	ARG	NE-CZ	-7.37	1.23	1.33
1	A	148	GLY	C-N	5.88	1.47	1.34
1	A	77	TYR	CE1-CZ	-5.77	1.31	1.38
1	A	148	GLY	CA-C	-5.38	1.43	1.51

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	NE-CZ-NH2	48.28	144.44	120.30
1	A	211	ARG	NE-CZ-NH1	25.80	133.20	120.30
1	A	22	ASP	CB-CG-OD2	23.43	139.38	118.30
1	A	20	ARG	NE-CZ-NH1	21.95	131.28	120.30
1	A	177	VAL	O-C-N	21.05	156.38	122.70
1	A	40	ARG	NE-CZ-NH1	-17.86	111.37	120.30
1	A	112	ALA	O-C-N	17.01	149.91	122.70
1	A	157	GLY	O-C-N	15.59	147.65	122.70
1	A	162	TYR	CG-CD2-CE2	15.46	133.66	121.30
1	A	138	ARG	NE-CZ-NH1	15.09	127.85	120.30
1	A	148	GLY	CA-C-O	14.55	146.78	120.60
1	A	40	ARG	CD-NE-CZ	14.05	143.28	123.60
1	A	20	ARG	NE-CZ-NH2	-14.01	113.30	120.30
1	A	40	ARG	NH1-CZ-NH2	-13.86	104.15	119.40
1	A	149	TYR	CZ-CE2-CD2	13.38	131.84	119.80
1	A	44	GLU	O-C-N	13.31	144.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ARG	NE-CZ-NH2	-12.23	114.18	120.30
1	A	211	ARG	NE-CZ-NH2	-11.63	114.49	120.30
1	A	32	ALA	O-C-N	11.56	141.19	122.70
1	A	125	LEU	O-C-N	10.73	139.87	122.70
1	A	148	GLY	O-C-N	-10.61	105.72	122.70
1	A	158	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	A	147	PHE	CB-CG-CD1	-10.03	113.78	120.80
1	A	149	TYR	CG-CD2-CE2	-9.79	113.47	121.30
1	A	149	TYR	CG-CD1-CE1	9.50	128.90	121.30
1	A	162	TYR	CZ-CE2-CD2	-9.33	111.40	119.80
1	A	138	ARG	CD-NE-CZ	9.14	136.40	123.60
1	A	79	ALA	O-C-N	9.13	137.31	122.70
1	A	162	TYR	CB-CG-CD1	9.01	126.41	121.00
1	A	172	LYS	O-C-N	8.96	137.03	122.70
1	A	157	GLY	CA-C-O	-8.94	104.50	120.60
1	A	162	TYR	CD1-CE1-CZ	8.74	127.66	119.80
1	A	175	ASP	CB-CG-OD1	8.72	126.15	118.30
1	A	177	VAL	CA-C-O	-8.65	101.93	120.10
1	A	47	ASN	OD1-CG-ND2	8.64	141.76	121.90
1	A	138	ARG	O-C-N	-8.28	109.45	122.70
1	A	49	GLY	O-C-N	-8.22	109.54	122.70
1	A	88	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	77	TYR	CB-CG-CD1	-7.83	116.31	121.00
1	A	22	ASP	CB-CG-OD1	-7.76	111.31	118.30
1	A	77	TYR	CD1-CE1-CZ	7.71	126.73	119.80
1	A	125	LEU	CA-C-O	-7.66	104.02	120.10
1	A	77	TYR	CB-CG-CD2	7.63	125.58	121.00
1	A	22	ASP	OD1-CG-OD2	-7.54	108.98	123.30
1	A	77	TYR	CG-CD1-CE1	-7.46	115.33	121.30
1	A	158	ARG	CD-NE-CZ	7.31	133.84	123.60
1	A	149	TYR	CB-CG-CD1	7.23	125.34	121.00
1	A	202	PHE	CD1-CE1-CZ	7.19	128.73	120.10
1	A	44	GLU	CA-C-N	-7.19	101.38	117.20
1	A	38	TYR	CB-CG-CD1	-7.15	116.71	121.00
1	A	22	ASP	CA-CB-CG	7.11	129.05	113.40
1	A	177	VAL	CA-C-N	-7.06	101.66	117.20
1	A	186	ALA	N-CA-CB	7.04	119.95	110.10
1	A	47	ASN	CB-CG-ND2	-6.96	100.00	116.70
1	A	139	ASP	CA-C-O	6.72	134.20	120.10
1	A	23	LEU	O-C-N	-6.68	112.01	122.70
1	A	162	TYR	CG-CD1-CE1	-6.64	115.99	121.30
1	A	154	GLN	CG-CD-OE1	6.46	134.52	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ARG	O-C-N	6.45	134.16	123.20
1	A	211	ARG	NH1-CZ-NH2	-6.44	112.31	119.40
1	A	112	ALA	CA-C-O	-6.43	106.59	120.10
1	A	179	THR	C-N-CA	6.28	135.49	122.30
1	A	49	GLY	CA-C-O	6.28	131.91	120.60
1	A	112	ALA	CA-C-N	-6.23	103.49	117.20
1	A	158	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	78	ARG	CA-CB-CG	6.13	126.88	113.40
1	A	138	ARG	CA-C-O	6.12	132.95	120.10
1	A	38	TYR	CB-CG-CD2	6.08	124.65	121.00
1	A	102	PHE	CB-CG-CD1	5.99	124.99	120.80
1	A	202	PHE	CG-CD2-CE2	5.88	127.27	120.80
1	A	139	ASP	O-C-N	-5.79	113.44	122.70
1	A	20	ARG	O-C-N	-5.77	113.47	122.70
1	A	60	GLU	OE1-CD-OE2	5.71	130.16	123.30
1	A	149	TYR	CD1-CE1-CZ	-5.67	114.70	119.80
1	A	166	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	89	GLY	O-C-N	5.47	131.46	122.70
1	A	36	PHE	CB-CG-CD1	-5.45	116.99	120.80
1	A	77	TYR	CZ-CE2-CD2	-5.41	114.93	119.80
1	A	191	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	A	77	TYR	CG-CD2-CE2	5.24	125.49	121.30
1	A	69	TRP	CD1-CG-CD2	5.20	110.46	106.30
1	A	36	PHE	CB-CG-CD2	5.20	124.44	120.80
1	A	69	TRP	CG-CD2-CE3	5.16	138.54	133.90
1	A	164	ALA	O-C-N	-5.13	114.49	122.70
1	A	79	ALA	CA-C-O	-5.11	109.38	120.10
1	A	17	ARG	CD-NE-CZ	5.04	130.66	123.60
1	A	102	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	A	72	GLY	CA-C-O	5.01	129.62	120.60

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	1430	0	1422	36	0
2	A	22	0	17	2	0
3	A	73	0	0	1	0
All	All	1525	0	1439	36	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 12.

All (36) 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:163:PRO:HG2	1:A:166:ARG:HD2	1.51	0.91
1:A:198:PRO:HA	1:A:201:GLU:HG2	1.68	0.76
1:A:17:ARG:HG3	1:A:19:THR:H	1.54	0.71
1:A:150:THR:HB	3:A:246:HOH:O	1.94	0.68
1:A:24:ILE:HA	1:A:104:GLN:HE22	1.59	0.67
1:A:17:ARG:HE	1:A:19:THR:N	1.94	0.66
1:A:23:LEU:HD11	1:A:104:GLN:HG2	1.78	0.64
1:A:48:LEU:HB3	1:A:53:PRO:HD3	1.80	0.64
1:A:203:LEU:O	1:A:207:VAL:HG23	2.01	0.59
1:A:24:ILE:HG22	1:A:71:GLN:HE22	1.69	0.58
1:A:81:LEU:O	2:A:215:SXC:H17	2.05	0.56
1:A:24:ILE:HA	1:A:104:GLN:NE2	2.23	0.54
1:A:17:ARG:HE	1:A:19:THR:H	1.55	0.54
1:A:134:ASP:OD1	1:A:136:ALA:HB3	2.09	0.53
1:A:188:HIS:NE2	2:A:215:SXC:H216	2.23	0.53
1:A:160:PRO:O	1:A:161:ASN:HB2	2.11	0.51
1:A:198:PRO:HA	1:A:201:GLU:CG	2.41	0.47
1:A:54:SER:HB3	1:A:196:ARG:HG2	1.97	0.45
1:A:39:ALA:O	1:A:118:GLY:HA2	2.17	0.45
1:A:208:ARG:O	1:A:211:ARG:O	2.34	0.45
1:A:17:ARG:NH2	1:A:19:THR:OG1	2.49	0.45
1:A:99:LEU:HA	1:A:99:LEU:HD23	1.84	0.45
1:A:163:PRO:CG	1:A:166:ARG:HD2	2.34	0.45
1:A:139:ASP:O	1:A:166:ARG:NH2	2.50	0.45
1:A:75:GLY:O	1:A:78:ARG:NH1	2.49	0.45
1:A:163:PRO:HB2	1:A:165:ASP:OD1	2.17	0.45
1:A:96:ARG:HG3	1:A:96:ARG:HH11	1.82	0.44
1:A:17:ARG:CG	1:A:19:THR:H	2.29	0.44
1:A:131:GLU:HG2	1:A:131:GLU:O	2.17	0.43
1:A:96:ARG:NH1	1:A:96:ARG:HG3	2.35	0.42
1:A:48:LEU:CB	1:A:53:PRO:HD3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HB3	1:A:87:PRO:HD2	2.02	0.42
1:A:198:PRO:CA	1:A:201:GLU:HG2	2.45	0.42
1:A:21:ASP:HB3	1:A:24:ILE:CG2	2.50	0.41
1:A:172:LYS:HZ3	1:A:172:LYS:HG3	1.69	0.41
1:A:106:ASN:OD1	1:A:140:LYS:HE3	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	193/214 (90%)	190 (98%)	3 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	145/159 (91%)	133 (92%)	12 (8%)	14	0

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

Mol	Chain	Res	Type
1	A	17	ARG

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Mol	Chain	Res	Type
1	A	57	SER
1	A	81	LEU
1	A	92	SER
1	A	96	ARG
1	A	111	ASP
1	A	133	LEU
1	A	166	ARG
1	A	171	CYS
1	A	172	LYS
1	A	183	ILE
1	A	189	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	84	ASN
1	A	104	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	SXC	A	215	1	19,24,35	1.88	5 (26%)	20,36,53	1.89	6 (30%)

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	SXC	A	215	1	-	0/5/35/46	0/3/3/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	215	SXC	PD1-S2	-2.38	2.27	2.30
2	A	215	SXC	C1-C6	-2.17	1.36	1.40
2	A	215	SXC	C10-S2	2.13	1.85	1.82
2	A	215	SXC	C5-C6	2.33	1.43	1.39
2	A	215	SXC	C1-PD1	6.07	2.05	1.98

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	215	SXC	C6-C5-C4	-5.04	113.61	121.80
2	A	215	SXC	C3-C2-C1	-3.02	115.61	119.76
2	A	215	SXC	C10-C6-C5	-2.71	116.33	120.87
2	A	215	SXC	C15-C14-C13	-2.09	107.72	112.12
2	A	215	SXC	C13-C4-C5	-2.01	117.19	120.56
2	A	215	SXC	C5-C4-C3	3.09	123.51	118.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	215	SXC	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	195/214 (91%)	-0.51	0 100 100	9, 21, 33, 51	0

There are no RSRZ outliers to report.

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	SXC	A	215	22/32	1.00	0.06	0.48	8,15,22,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.