



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:58 PM UTC

PDB ID : 2LPR / pdb_00002lpr
Title : STRUCTURAL BASIS FOR BROAD SPECIFICITY IN ALPHA-LYTIC
PROTEASE MUTANTS
Authors : Bone, R.; Agard, D.A.
Deposited on : 1991-08-05
Resolution : 2.25 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

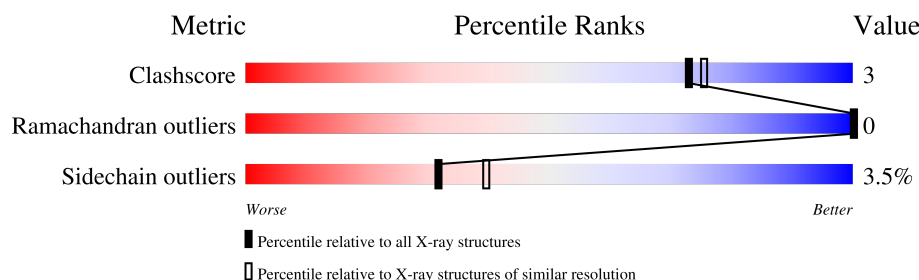
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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	198	 57% 37% 5%
2	P	5	 60% 20% 20%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1598 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 ALPHA-LYTIC PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1388	844	262	275	7			

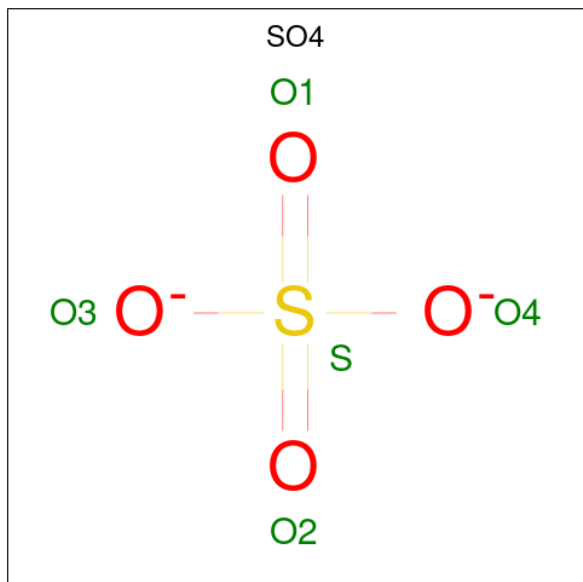
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	ALA	MET	conflict	UNP P00778

- Molecule 2 is a protein called METHOXYSUCCINYL-ALA-ALA-PRO-VALINE BORONIC ACID INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	4	Total	B	C	N	O	0	0	0
			25	1	15	4	5			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

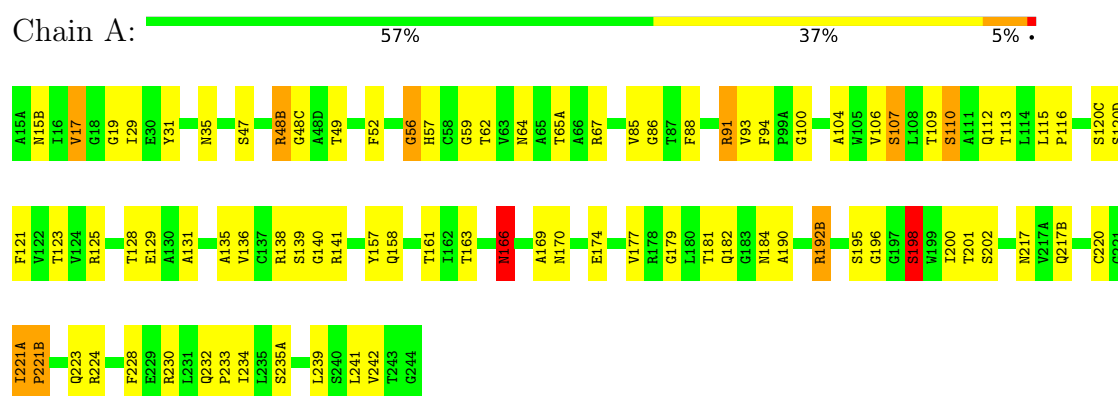
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		
4	P	2	Total	O	0	0
			2	2		

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: ALPHA-LYTIC PROTEASE



• Molecule 2: METHOXYSUCCINYL-ALA-ALA-PRO-VALINE BORONIC ACID INHIBITOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.25Å 66.25Å 80.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.127 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1598	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: B2V, 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	1.38	1/1406 (0.1%)	2.58	115/1906 (6.0%)
2	P	1.12	0/17	2.05	1/23 (4.3%)
All	All	1.38	1/1423 (0.1%)	2.58	116/1929 (6.0%)

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
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	GLY	N-CA	5.57	1.51	1.45

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48(B)	ARG	NE-CZ-NH2	-13.04	107.47	119.20
1	A	166	ASN	CA-CB-CG	-11.36	101.24	112.60
1	A	228	PHE	CA-CB-CG	10.69	124.49	113.80
1	A	67	ARG	NE-CZ-NH1	10.24	131.74	121.50
1	A	221(A)	ILE	N-CA-CB	9.79	118.59	111.83
1	A	88	PHE	CA-C-O	-9.73	109.29	120.58
1	A	192(B)	ARG	CD-NE-CZ	-9.66	110.88	124.40
1	A	110	SER	CA-CB-OG	-9.37	92.35	111.10
1	A	57	HIS	CA-C-O	-9.11	107.20	119.05
1	A	121	PHE	CA-C-O	-8.89	110.75	121.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	VAL	CA-C-O	-8.48	110.24	118.98
1	A	170	ASN	CA-CB-CG	-8.25	104.35	112.60
1	A	128	THR	CA-CB-OG1	-8.12	97.41	109.60
1	A	91	ARG	CD-NE-CZ	7.97	135.56	124.40
1	A	109	THR	CA-C-N	7.96	131.28	120.38
1	A	109	THR	C-N-CA	7.96	131.28	120.38
1	A	112	GLN	OE1-CD-NE2	-7.91	114.69	122.60
1	A	106	VAL	CA-C-O	-7.90	112.11	120.48
1	A	48(B)	ARG	NE-CZ-NH1	7.79	129.29	121.50
1	A	91	ARG	NE-CZ-NH1	7.75	129.25	121.50
1	A	116	PRO	CA-C-O	-7.74	115.58	121.31
1	A	242	VAL	CA-C-O	-7.67	112.10	120.85
1	A	184	ASN	OD1-CG-ND2	-7.65	114.95	122.60
1	A	136	VAL	CA-C-O	-7.53	113.92	121.45
1	A	125	ARG	NE-CZ-NH1	-7.44	114.06	121.50
1	A	192(B)	ARG	NE-CZ-NH1	7.43	128.93	121.50
1	A	192(B)	ARG	NE-CZ-NH2	-7.36	112.58	119.20
1	A	35	ASN	OD1-CG-ND2	7.33	129.94	122.60
1	A	112	GLN	CG-CD-OE1	7.32	135.44	120.80
1	A	120(D)	SER	N-CA-CB	-7.28	97.61	110.14
1	A	107	SER	CA-CB-OG	-7.27	96.57	111.10
1	A	109	THR	CA-C-O	7.13	130.22	121.81
1	A	67	ARG	NE-CZ-NH2	-6.94	112.95	119.20
1	A	190	ALA	N-CA-C	-6.92	100.24	110.48
1	A	217(B)	GLN	CG-CD-NE2	6.91	126.76	116.40
1	A	93	VAL	CA-C-O	-6.85	113.35	120.27
2	P	3	ALA	O-C-N	6.83	126.73	121.88
1	A	182	GLN	CB-CG-CD	-6.80	101.03	112.60
1	A	113	THR	CA-CB-OG1	-6.75	99.47	109.60
1	A	64	ASN	CA-C-O	-6.66	110.30	119.16
1	A	195	SER	CA-C-O	-6.65	113.88	121.19
1	A	15(B)	ASN	CB-CG-ND2	6.63	126.34	116.40
1	A	181	THR	CA-CB-OG1	-6.61	99.68	109.60
1	A	110	SER	O-C-N	6.57	129.08	122.12
1	A	157	TYR	CA-C-O	-6.57	113.33	120.36
1	A	121	PHE	O-C-N	6.56	130.88	123.27
1	A	31	TYR	N-CA-C	-6.50	99.19	109.07
1	A	161	THR	CA-CB-CG2	6.49	121.53	110.50
1	A	200	ILE	CA-C-O	-6.44	114.56	121.19
1	A	235(A)	SER	CA-C-O	-6.38	113.16	120.24
1	A	195	SER	O-C-N	6.36	130.69	122.87
1	A	15(B)	ASN	OD1-CG-ND2	-6.35	116.25	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	LEU	CA-C-O	-6.34	114.06	121.16
1	A	170	ASN	CA-C-O	-6.32	114.98	122.13
1	A	221(B)	PRO	CB-CA-C	6.32	119.26	110.98
1	A	141	ARG	CA-C-O	-6.25	110.92	119.05
1	A	224	ARG	CA-C-O	-6.23	113.75	120.92
1	A	200	ILE	O-C-N	6.21	129.83	123.00
1	A	86	GLY	CA-C-O	-6.16	114.75	120.97
1	A	120(D)	SER	CA-C-O	-6.14	113.30	121.46
1	A	107	SER	N-CA-CB	6.08	120.19	110.16
1	A	49	THR	CA-CB-OG1	-6.08	100.48	109.60
1	A	139	SER	N-CA-CB	-6.07	100.02	111.00
1	A	123	THR	CA-C-O	-6.04	113.80	120.69
1	A	196	GLY	CA-C-O	-6.00	112.56	119.10
1	A	220	CYS	CA-C-O	-6.00	112.00	119.38
1	A	113	THR	O-C-N	5.97	130.66	123.13
1	A	201	THR	CA-CB-OG1	-5.96	100.66	109.60
1	A	230	ARG	NE-CZ-NH1	5.92	127.42	121.50
1	A	91	ARG	NH1-CZ-NH2	-5.90	111.62	119.30
1	A	17	VAL	N-CA-CB	-5.89	101.77	111.44
1	A	64	ASN	CB-CG-ND2	5.77	125.05	116.40
1	A	202	SER	O-C-N	5.76	130.15	122.43
1	A	174	GLU	CG-CD-OE2	-5.72	105.24	118.40
1	A	131	ALA	CA-C-O	-5.71	115.21	121.89
1	A	161	THR	CA-CB-OG1	-5.69	101.07	109.60
1	A	228	PHE	O-C-N	5.69	130.24	123.24
1	A	158	GLN	CA-C-O	-5.67	114.70	121.11
1	A	106	VAL	N-CA-CB	-5.66	103.55	111.25
1	A	163	THR	O-C-N	5.62	129.28	122.48
1	A	59	GLY	CA-C-O	-5.60	115.13	121.68
1	A	232	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	A	135	ALA	CA-C-O	-5.55	115.09	121.47
1	A	65(A)	THR	CA-CB-OG1	-5.53	101.31	109.60
1	A	241	LEU	N-CA-CB	-5.52	101.86	109.97
1	A	129	GLU	CG-CD-OE2	-5.45	105.87	118.40
1	A	239	LEU	O-C-N	5.43	129.35	123.10
1	A	239	LEU	CA-C-O	-5.42	114.89	121.28
1	A	48(C)	GLY	N-CA-C	-5.40	102.18	111.47
1	A	35	ASN	N-CA-CB	-5.38	103.95	112.08
1	A	184	ASN	O-C-N	5.37	129.19	122.22
1	A	94	PHE	CA-C-O	-5.36	112.81	120.16
1	A	177	VAL	N-CA-CB	5.36	119.11	111.82
1	A	56	GLY	O-C-N	5.36	127.39	122.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	THR	CA-C-O	-5.35	115.08	121.56
1	A	52	PHE	CA-C-O	-5.35	114.85	121.06
1	A	107	SER	O-C-N	5.32	129.28	123.22
1	A	136	VAL	O-C-N	5.27	128.57	122.82
1	A	121	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	169	ALA	N-CA-C	-5.22	100.67	109.07
1	A	120(C)	SER	CB-CA-C	-5.21	100.62	110.01
1	A	125	ARG	NH1-CZ-NH2	5.21	126.07	119.30
1	A	62	THR	CA-CB-CG2	-5.20	101.66	110.50
1	A	217	ASN	CB-CG-ND2	-5.19	108.61	116.40
1	A	31	TYR	CA-C-O	-5.19	115.73	121.33
1	A	123	THR	CA-CB-OG1	-5.18	101.83	109.60
1	A	94	PHE	O-C-N	5.17	127.27	121.32
1	A	198	SER	N-CA-C	5.10	117.83	110.28
1	A	230	ARG	CA-C-O	-5.10	115.58	121.19
1	A	100	GLY	CA-C-O	5.07	129.38	120.57
1	A	129	GLU	CA-C-O	-5.03	114.95	120.69
1	A	234	ILE	N-CA-C	-5.03	105.80	110.53
1	A	47	SER	CB-CA-C	-5.02	101.06	109.65
1	A	115	LEU	CB-CA-C	5.02	116.65	108.87
1	A	19	GLY	N-CA-C	5.02	120.66	114.69
1	A	224	ARG	O-C-N	5.01	128.97	123.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	192(B)	ARG	Sidechain

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	1388	0	1356	9	0
2	P	25	0	26	0	0
3	A	5	0	0	1	0
4	A	178	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	2	0	0	0	0
All	All	1598	0	1382	9	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 (9) 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:48(B):ARG:HD2	4:A:354:HOH:O	1.85	0.76
1:A:166:ASN:HD22	1:A:179:GLY:HA2	1.65	0.60
1:A:221(B):PRO:HG2	1:A:223:GLN:NE2	2.22	0.54
1:A:166:ASN:ND2	1:A:179:GLY:HA2	2.23	0.53
1:A:221(A):ILE:HB	1:A:221(B):PRO:HD2	1.91	0.53
1:A:138:ARG:HA	1:A:198:SER:O	2.13	0.48
1:A:17:VAL:O	1:A:29:ILE:HG12	2.14	0.47
1:A:233:PRO:HB3	3:A:1:SO4:O4	2.16	0.45
1:A:56:GLY:HA2	1:A:104:ALA:HB2	1.99	0.44

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	196/198 (99%)	187 (95%)	9 (5%)	0	100	100
2	P	2/5 (40%)	2 (100%)	0	0	100	100
All	All	198/203 (98%)	189 (96%)	9 (4%)	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	141/141 (100%)	136 (96%)	5 (4%)	32	39
2	P	1/1 (100%)	1 (100%)	0	100	100
All	All	142/142 (100%)	137 (96%)	5 (4%)	32	39

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	107	SER
1	A	110	SER
1	A	166	ASN
1	A	198	SER

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	101	ASN
1	A	112	GLN
1	A	166	ASN
1	A	182	GLN
1	A	223	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	B2V	P	1	2,1	2,7,7	0.39	0	4,9,9	1.03	0

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	B2V	P	1	2,1	-	0/4/8/8	-

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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	SO4	A	1	-	4,4,4	0.69	0	6,6,6	1.15	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	SO4	1	0

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

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.