



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:20 AM UTC

PDB ID : 7LPR / pdb_00007lpr
Title : STRUCTURAL BASIS FOR BROAD SPECIFICITY IN ALPHA-LYTIC
PROTEASE MUTANTS
Authors : Fujishige, A.; Bone, R.; Agard, D.A.
Deposited on : 1991-08-05
Resolution : 2.05 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

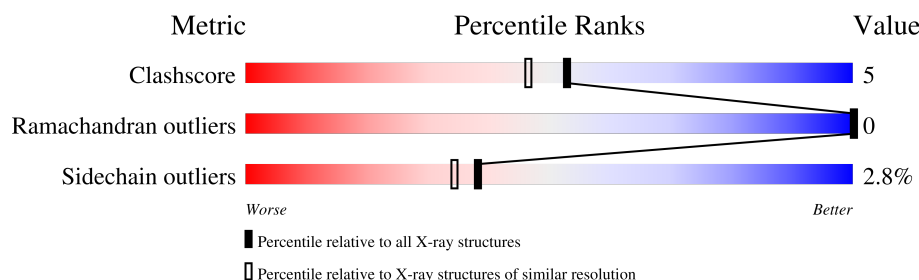
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)

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	51% 44% 5%
2	P	5	40% 40% 20%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1568 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			

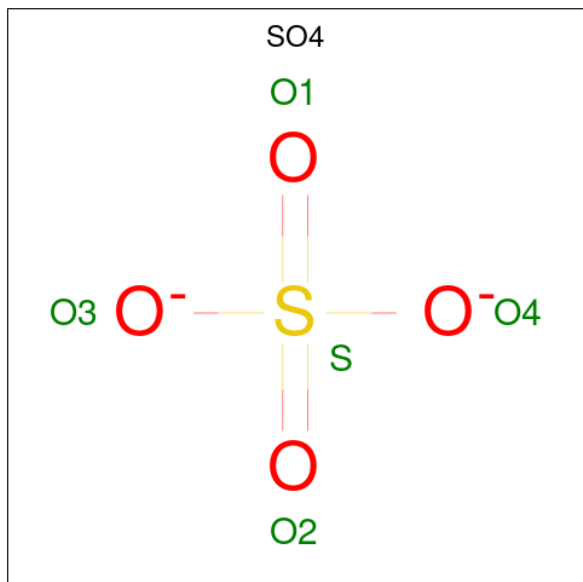
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ALA	MET	conflict	UNP P00778

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	4	Total	B	C	N	O	0	0	0
			26	1	16	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.

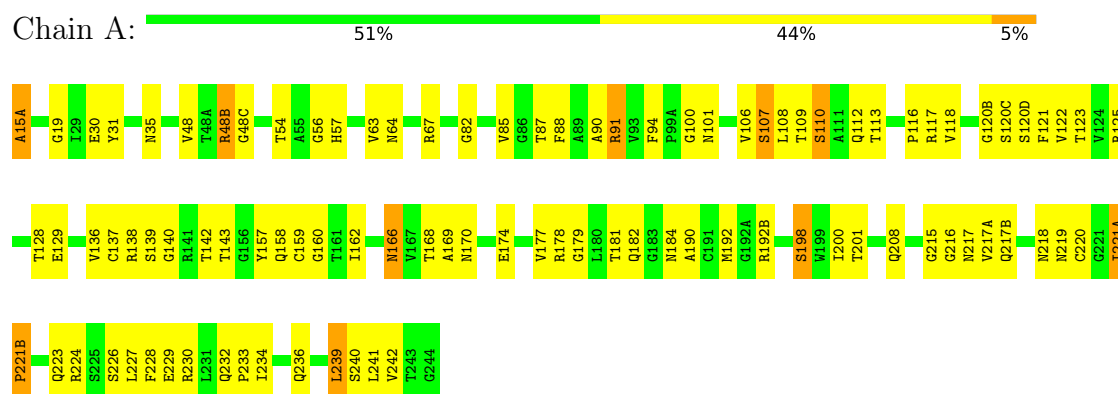
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total	O	0	0
			146	146		
4	P	3	Total	O	0	0
			3	3		

3 Residue-property plots [i](#)

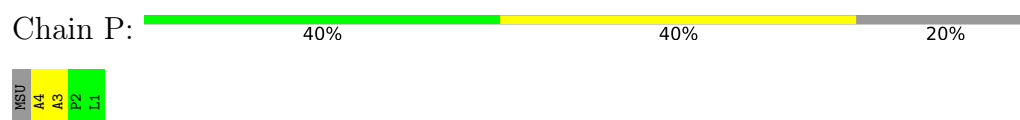
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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-LEUCINE 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	66.31Å 66.31Å 80.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.05	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.136 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1568	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: SO4, BLE

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	1.54	3/1406 (0.2%)	2.77	132/1906 (6.9%)
2	P	1.68	0/17	4.06	4/23 (17.4%)
All	All	1.55	3/1423 (0.2%)	2.79	136/1929 (7.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	GLY	N-CA	6.49	1.52	1.45
1	A	234	ILE	CA-CB	6.44	1.62	1.54
1	A	215	GLY	N-CA	5.01	1.51	1.45

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48(B)	ARG	CD-NE-CZ	17.84	149.37	124.40
1	A	184	ASN	OD1-CG-ND2	-12.88	109.72	122.60
2	P	3	ALA	O-C-N	12.50	131.30	121.55
1	A	91	ARG	CD-NE-CZ	11.76	140.86	124.40
1	A	88	PHE	CA-C-O	-11.69	107.26	120.70
1	A	200	ILE	CA-C-O	-11.46	109.99	121.45
1	A	221(A)	ILE	N-CA-CB	11.41	119.70	111.83
1	A	110	SER	CA-CB-OG	-10.60	89.91	111.10
1	A	110	SER	CB-CA-C	-10.58	91.06	110.63
1	A	224	ARG	CA-C-O	-10.48	108.79	121.36
1	A	110	SER	O-C-N	9.99	133.91	122.22
1	A	67	ARG	NE-CZ-NH1	9.46	130.96	121.50
1	A	106	VAL	CA-C-O	-9.45	110.47	120.48
1	A	170	ASN	CA-CB-CG	-9.28	103.32	112.60
1	A	157	TYR	CA-C-O	-9.17	111.00	120.54
1	A	35	ASN	OD1-CG-ND2	9.04	131.64	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	SER	CA-C-O	-8.96	109.98	120.10
1	A	158	GLN	CA-C-O	-8.62	111.37	121.11
1	A	48(B)	ARG	NE-CZ-NH1	-8.57	112.93	121.50
1	A	57	HIS	CA-C-O	-8.54	107.95	119.05
2	P	4	ALA	CB-CA-C	-8.53	97.71	110.50
2	P	3	ALA	CA-C-O	-8.45	112.27	120.64
1	A	190	ALA	N-CA-C	-8.36	98.71	110.50
1	A	226	SER	CA-C-O	-8.35	111.13	120.32
1	A	107	SER	CA-CB-OG	-8.31	94.48	111.10
1	A	120(D)	SER	N-CA-CB	-8.03	96.33	110.14
1	A	208	GLN	OE1-CD-NE2	7.91	130.51	122.60
1	A	217(B)	GLN	CG-CD-NE2	7.84	128.16	116.40
1	A	113	THR	CA-CB-OG1	-7.81	97.88	109.60
1	A	64	ASN	CA-C-O	-7.79	108.80	119.16
1	A	230	ARG	NE-CZ-NH2	-7.67	112.30	119.20
1	A	35	ASN	CA-CB-CG	-7.62	104.98	112.60
1	A	230	ARG	NE-CZ-NH1	7.56	129.06	121.50
1	A	192(B)	ARG	NE-CZ-NH2	-7.53	112.42	119.20
1	A	200	ILE	O-C-N	7.50	130.99	122.82
1	A	109	THR	CA-C-N	7.48	131.06	120.28
1	A	109	THR	C-N-CA	7.48	131.06	120.28
1	A	123	THR	CA-C-O	-7.46	112.54	121.05
1	A	170	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	A	48(B)	ARG	NH1-CZ-NH2	7.32	128.82	119.30
1	A	228	PHE	CA-CB-CG	7.22	121.02	113.80
1	A	91	ARG	NE-CZ-NH1	7.02	128.52	121.50
1	A	218	ASN	CB-CG-ND2	6.93	126.80	116.40
1	A	120(C)	SER	CA-CB-OG	-6.90	97.31	111.10
1	A	85	VAL	CA-C-O	-6.87	111.90	118.98
1	A	217(A)	VAL	CA-C-O	-6.84	114.54	121.59
1	A	230	ARG	CA-C-O	-6.84	113.66	121.19
1	A	169	ALA	N-CA-C	-6.82	98.61	109.59
1	A	121	PHE	CA-C-O	-6.76	113.22	121.06
1	A	216	GLY	CA-C-O	-6.75	115.22	121.63
1	A	166	ASN	CA-CB-CG	-6.71	105.89	112.60
1	A	177	VAL	N-CA-CB	6.63	120.26	111.64
1	A	142	THR	CA-C-O	-6.62	110.62	120.42
1	A	128	THR	CA-CB-OG1	-6.61	99.69	109.60
1	A	54	THR	CA-CB-CG2	6.60	121.72	110.50
1	A	110	SER	N-CA-CB	-6.52	100.19	110.22
1	A	143	THR	CA-C-O	-6.42	112.05	119.56
1	A	63	VAL	CA-C-O	-6.36	113.84	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	A	230	ARG	CD-NE-CZ	-6.29	115.59	124.40
1	A	220	CYS	CA-C-O	-6.24	111.58	119.31
1	A	234	ILE	N-CA-C	-6.22	104.68	110.53
1	A	19	GLY	O-C-N	6.22	129.68	122.65
1	A	15(A)	ALA	O-C-N	6.21	132.64	122.70
1	A	31	TYR	CA-C-O	-6.21	114.62	121.33
1	A	160	GLY	N-CA-C	-6.21	98.46	113.18
1	A	241	LEU	N-CA-CB	-6.15	101.31	110.17
1	A	94	PHE	CA-C-O	-6.15	111.74	120.16
1	A	192(B)	ARG	CG-CD-NE	-6.15	98.48	112.00
1	A	112	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	A	162	ILE	CA-C-O	-6.12	113.87	120.85
1	A	181	THR	CA-CB-OG1	-6.10	100.45	109.60
1	A	184	ASN	CB-CG-OD1	6.07	132.94	120.80
1	A	123	THR	O-C-N	6.07	130.17	123.01
1	A	109	THR	O-C-N	-6.05	115.90	122.79
1	A	219	ASN	N-CA-C	-6.00	104.61	112.41
1	A	178	ARG	CD-NE-CZ	-5.96	116.05	124.40
1	A	182	GLN	CB-CG-CD	-5.94	102.51	112.60
1	A	217(A)	VAL	CA-CB-CG1	5.93	120.48	110.40
1	A	201	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	139	SER	CA-C-O	-5.89	113.89	120.66
1	A	90	ALA	O-C-N	5.86	129.27	123.46
1	A	216	GLY	O-C-N	5.84	130.38	123.61
1	A	239	LEU	CA-C-O	-5.83	114.55	121.66
1	A	122	VAL	N-CA-C	-5.80	100.06	108.17
1	A	118	VAL	O-C-N	5.79	129.29	123.10
1	A	234	ILE	CA-C-O	-5.78	114.64	121.05
1	A	239	LEU	O-C-N	5.78	129.56	123.03
1	A	178	ARG	N-CA-CB	-5.77	102.11	110.70
1	A	240	SER	CA-C-O	-5.76	114.14	120.36
1	A	116	PRO	CA-C-O	-5.73	117.07	121.31
1	A	136	VAL	N-CA-CB	-5.70	100.31	112.00
1	A	217(A)	VAL	N-CA-CB	-5.68	99.36	110.45
1	A	224	ARG	O-C-N	5.66	129.40	123.06
1	A	108	LEU	N-CA-CB	-5.64	101.76	110.56
1	A	19	GLY	CA-C-O	-5.62	113.25	119.27
1	A	107	SER	O-C-N	5.59	129.59	123.22
1	A	113	THR	O-C-N	5.53	130.10	123.13
1	A	30	GLU	CB-CG-CD	-5.53	103.20	112.60
1	A	117	ARG	NH1-CZ-NH2	-5.50	112.14	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	SER	N-CA-CB	-5.45	101.14	111.00
1	A	157	TYR	N-CA-CB	-5.44	101.40	110.37
1	A	31	TYR	N-CA-C	-5.43	100.81	109.07
1	A	91	ARG	NH1-CZ-NH2	-5.42	112.25	119.30
1	A	170	ASN	CA-C-O	-5.39	115.35	121.39
1	A	129	GLU	CG-CD-OE2	-5.36	106.08	118.40
1	A	201	THR	N-CA-C	-5.35	102.60	110.52
1	A	236	GLN	OE1-CD-NE2	-5.33	117.27	122.60
1	A	120(B)	GLY	N-CA-C	-5.31	101.08	110.86
1	A	174	GLU	CG-CD-OE2	-5.30	106.21	118.40
1	A	158	GLN	O-C-N	5.30	130.08	123.19
2	P	4	ALA	N-CA-C	5.29	125.83	111.00
1	A	64	ASN	O-C-N	5.25	127.39	121.87
1	A	221(B)	PRO	O-C-N	5.24	131.09	122.70
1	A	142	THR	O-C-N	5.24	128.37	122.19
1	A	48(C)	GLY	N-CA-C	-5.21	102.50	111.47
1	A	57	HIS	N-CA-C	-5.21	106.75	113.01
1	A	142	THR	CA-C-N	-5.20	114.33	122.65
1	A	142	THR	C-N-CA	-5.20	114.33	122.65
1	A	48	VAL	CA-C-O	-5.19	116.25	121.49
1	A	217(B)	GLN	OE1-CD-NE2	-5.18	117.42	122.60
1	A	217	ASN	N-CA-CB	-5.17	103.59	110.57
1	A	87	THR	CA-CB-OG1	-5.13	101.90	109.60
1	A	82	GLY	CA-C-O	-5.11	113.28	119.00
1	A	178	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	A	67	ARG	NH1-CZ-NH2	-5.08	112.70	119.30
1	A	118	VAL	CA-C-O	-5.08	114.99	120.67
1	A	236	GLN	CG-CD-OE1	5.07	130.94	120.80
1	A	88	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	242	VAL	CA-C-O	-5.05	115.09	120.85
1	A	136	VAL	CA-C-O	-5.05	116.40	121.45
1	A	168	THR	CA-CB-OG1	-5.05	102.03	109.60
1	A	100	GLY	CA-C-O	5.04	129.35	120.57
1	A	227	LEU	N-CA-CB	-5.04	102.78	110.85
1	A	121	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	56	GLY	O-C-N	5.01	127.00	122.19

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	1388	0	1356	14	0
2	P	26	0	28	0	0
3	A	5	0	0	0	0
4	A	146	0	0	1	0
4	P	3	0	0	0	0
All	All	1568	0	1384	14	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 5.

All (14) 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:HG2	1:A:239:LEU:HD23	1.84	0.60
1:A:137:CYS:HA	1:A:159:CYS:HA	1.88	0.54
1:A:166:ASN:HD22	1:A:179:GLY:HA2	1.72	0.54
1:A:221(A):ILE:HB	1:A:221(B):PRO:HD2	1.92	0.52
1:A:48(B):ARG:CG	1:A:239:LEU:HD23	2.40	0.50
1:A:221(B):PRO:HG2	1:A:223:GLN:NE2	2.30	0.46
1:A:138:ARG:HA	1:A:198:SER:O	2.15	0.46
1:A:166:ASN:ND2	1:A:179:GLY:HA2	2.31	0.44
1:A:15(A):ALA:N	4:A:345:HOH:O	2.49	0.44
1:A:232:GLN:N	1:A:233:PRO:HD2	2.33	0.44
1:A:166:ASN:HA	1:A:179:GLY:HA2	2.00	0.43
1:A:138:ARG:HD2	1:A:192:MET:HE3	2.00	0.42
1:A:101:ASN:HB3	1:A:229:GLU:OE2	2.22	0.40
1:A:138:ARG:HD2	1:A:192:MET:CE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	137 (97%)	4 (3%)	38	34
2	P	1/1 (100%)	1 (100%)	0	100	100
All	All	142/142 (100%)	138 (97%)	4 (3%)	38	34

All (4) 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	198	SER

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

Mol	Chain	Res	Type
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	BLE	P	1	1,2	3,8,8	0.33	0	4,10,10	0.89	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	BLE	P	1	1,2	-	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	0.74	0	6,6,6	1.22	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	1	SO4	O3-S-O1	-2.31	97.48	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.