



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:06 AM UTC

PDB ID : 6LPR / pdb_00006lpr
Title : STRUCTURAL BASIS FOR BROAD SPECIFICITY IN ALPHA-LYTIC
PROTEASE MUTANTS
Authors : Bone, R.; Agard, D.A.
Deposited on : 1991-08-05
Resolution : 2.10 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

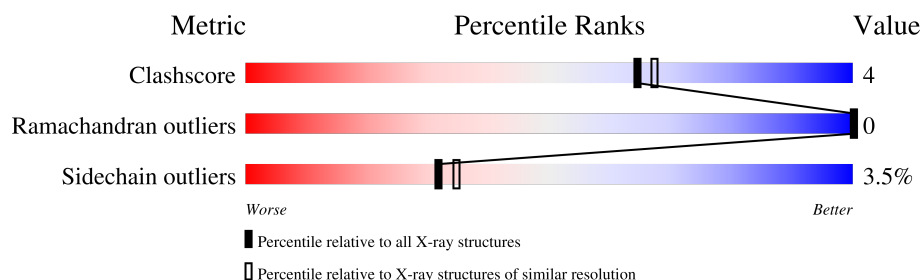
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	
2	P	5	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1593 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			

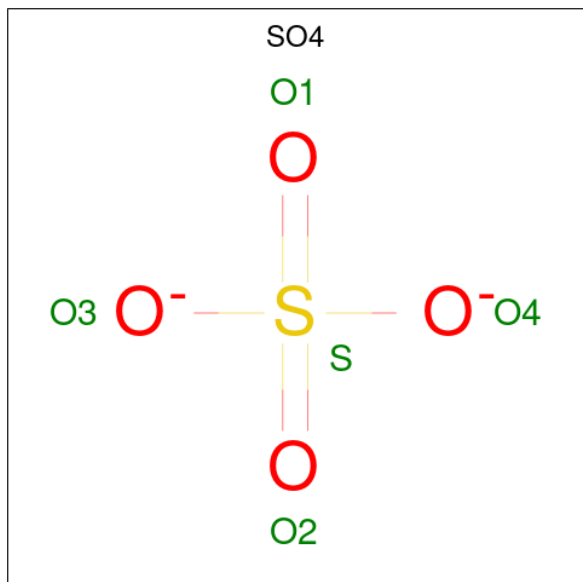
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a protein called METHOXYSUCCINYL-ALA-ALA-PRO-NORLEUCINE 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.

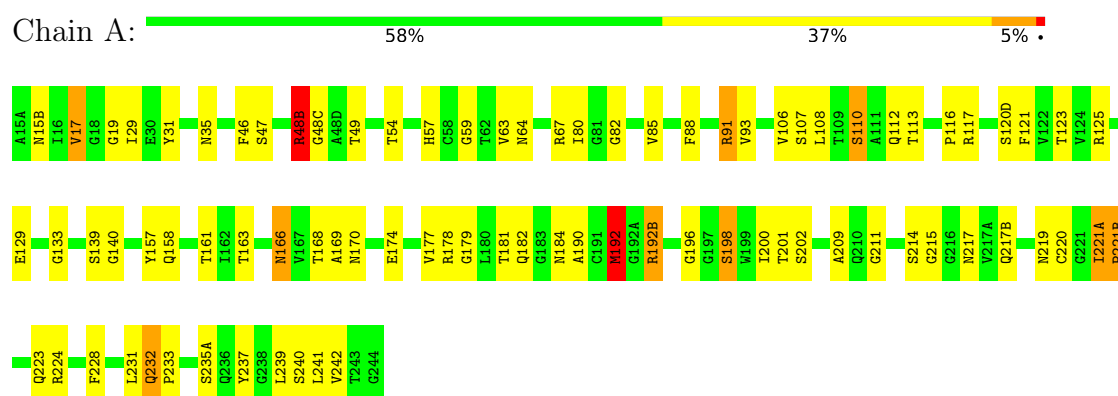
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	171	Total	O	0	0
			171	171		
4	P	3	Total	O	0	0
			3	3		

3 Residue-property plots

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-NORLEUCINE 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	66.33Å 66.33Å 80.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.132 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1593	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: SO4, BNO

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	1.51	5/1406 (0.4%)	2.62	103/1906 (5.4%)
2	P	1.04	0/17	3.06	2/23 (8.7%)
All	All	1.51	5/1423 (0.4%)	2.63	105/1929 (5.4%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	GLY	N-CA	7.52	1.53	1.45
1	A	163	THR	CA-CB	5.81	1.62	1.54
1	A	215	GLY	N-CA	5.59	1.52	1.45
1	A	117	ARG	N-CA	5.41	1.52	1.45
1	A	168	THR	CA-CB	5.36	1.61	1.53

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48(B)	ARG	NE-CZ-NH2	-19.44	101.70	119.20
1	A	48(B)	ARG	NE-CZ-NH1	19.01	140.51	121.50
1	A	110	SER	N-CA-CB	-12.68	88.76	110.32
1	A	67	ARG	NE-CZ-NH1	12.38	133.88	121.50
1	A	192(B)	ARG	NE-CZ-NH2	-11.58	108.78	119.20
1	A	91	ARG	CD-NE-CZ	11.23	140.12	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	3	ALA	O-C-N	10.52	129.35	121.88
1	A	184	ASN	OD1-CG-ND2	-10.41	112.19	122.60
1	A	67	ARG	NE-CZ-NH2	-9.57	110.58	119.20
1	A	88	PHE	CA-C-O	-9.31	110.10	120.81
1	A	228	PHE	CA-CB-CG	9.05	122.85	113.80
1	A	35	ASN	OD1-CG-ND2	8.95	131.55	122.60
1	A	217(B)	GLN	OE1-CD-NE2	-8.67	113.93	122.60
1	A	110	SER	CB-CA-C	-8.60	92.18	110.32
1	A	116	PRO	CA-C-O	-8.26	115.20	121.31
1	A	107	SER	CA-CB-OG	-8.22	94.65	111.10
1	A	121	PHE	CA-C-O	-8.16	111.59	121.06
1	A	221(A)	ILE	N-CA-CB	7.76	117.19	111.83
1	A	57	HIS	CA-C-O	-7.71	109.03	119.05
1	A	85	VAL	CA-C-O	-7.51	112.29	118.90
1	A	15(B)	ASN	OD1-CG-ND2	-7.49	115.11	122.60
1	A	64	ASN	CA-C-O	-7.47	109.22	119.16
1	A	161	THR	CA-CB-OG1	-7.43	98.46	109.60
1	A	177	VAL	N-CA-CB	7.41	121.27	111.64
1	A	170	ASN	CA-CB-CG	-7.37	105.23	112.60
1	A	241	LEU	CA-C-O	-7.22	113.07	121.16
1	A	112	GLN	OE1-CD-NE2	-7.10	115.50	122.60
1	A	220	CYS	CA-C-O	-7.09	110.52	119.31
1	A	120(D)	SER	N-CA-CB	-7.05	98.01	110.14
1	A	169	ALA	N-CA-C	-6.78	98.68	109.59
1	A	54	THR	CA-C-O	-6.71	114.23	121.14
1	A	190	ALA	N-CA-C	-6.71	99.60	110.20
1	A	196	GLY	CA-C-O	-6.70	112.30	119.27
1	A	15(B)	ASN	CB-CG-ND2	6.63	126.35	116.40
1	A	221(B)	PRO	CB-CA-C	6.63	119.67	110.98
1	A	157	TYR	CA-C-O	-6.59	113.31	120.36
1	A	198	SER	CA-C-O	-6.59	113.78	121.16
1	A	106	VAL	CA-C-O	-6.56	113.53	120.48
1	A	93	VAL	CA-C-O	-6.52	113.68	120.27
1	A	166	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	A	163	THR	O-C-N	6.42	130.25	122.48
1	A	113	THR	CA-CB-OG1	-6.42	99.97	109.60
1	A	88	PHE	O-C-N	6.42	130.83	122.93
1	A	63	VAL	CA-C-O	-6.41	113.79	121.28
1	A	224	ARG	CA-C-O	-6.28	113.82	121.36
1	A	133	GLY	CA-C-O	-6.27	112.75	119.27
1	A	182	GLN	CB-CG-CD	-6.18	102.09	112.60
1	A	139	SER	N-CA-CB	-6.15	99.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ARG	CA-C-O	-6.10	113.97	121.78
1	A	49	THR	CA-CB-OG1	-6.05	100.53	109.60
2	P	4	ALA	CB-CA-C	-6.05	101.43	110.50
1	A	168	THR	CA-CB-OG1	-6.01	100.58	109.60
1	A	242	VAL	N-CA-CB	-5.98	104.19	111.00
1	A	201	THR	CA-CB-OG1	-5.97	100.64	109.60
1	A	217	ASN	CB-CG-ND2	-5.94	107.49	116.40
1	A	158	GLN	CA-C-O	-5.90	114.20	121.11
1	A	31	TYR	N-CA-C	-5.88	100.14	109.07
1	A	200	ILE	CA-C-O	-5.82	115.63	121.45
1	A	64	ASN	CB-CG-ND2	5.80	125.11	116.40
1	A	196	GLY	N-CA-C	-5.79	108.19	115.08
1	A	198	SER	O-C-N	5.79	129.96	122.89
1	A	46	PHE	CA-CB-CG	-5.78	108.02	113.80
1	A	125	ARG	NH1-CZ-NH2	5.77	126.80	119.30
1	A	240	SER	CA-CB-OG	-5.76	99.59	111.10
1	A	129	GLU	CA-C-O	-5.74	114.15	120.69
1	A	224	ARG	O-C-N	5.67	129.42	123.06
1	A	123	THR	CA-CB-OG1	-5.67	101.09	109.60
1	A	214	SER	CA-C-N	-5.66	112.52	120.56
1	A	214	SER	C-N-CA	-5.66	112.52	120.56
1	A	232	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	A	125	ARG	NE-CZ-NH1	-5.62	115.89	121.50
1	A	17	VAL	N-CA-CB	-5.61	102.23	111.44
1	A	59	GLY	CA-C-O	-5.59	115.14	121.68
1	A	202	SER	CA-CB-OG	-5.59	99.92	111.10
1	A	174	GLU	CG-CD-OE2	-5.57	105.58	118.40
1	A	31	TYR	CA-C-O	-5.54	115.34	121.33
1	A	219	ASN	N-CA-C	-5.53	105.22	112.41
1	A	108	LEU	N-CA-CB	-5.50	101.94	110.46
1	A	80	ILE	O-C-N	5.49	128.89	123.18
1	A	235(A)	SER	CA-C-O	-5.47	114.17	120.24
1	A	242	VAL	CA-C-O	-5.46	114.26	120.65
1	A	107	SER	N-CA-CB	5.41	119.09	110.16
1	A	82	GLY	CA-C-O	-5.38	112.98	119.00
1	A	211	GLY	O-C-N	5.36	129.27	123.96
1	A	215	GLY	O-C-N	5.36	129.78	123.62
1	A	47	SER	CB-CA-C	-5.32	100.55	109.65
1	A	200	ILE	O-C-N	5.31	128.61	122.82
1	A	196	GLY	O-C-N	5.31	128.99	122.46
1	A	48(C)	GLY	N-CA-C	-5.30	102.27	111.50
1	A	237	TYR	O-C-N	5.30	128.56	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48(B)	ARG	CD-NE-CZ	5.30	131.82	124.40
1	A	19	GLY	O-C-N	5.25	128.58	122.65
1	A	170	ASN	CA-C-O	-5.24	116.20	122.13
1	A	209	ALA	N-CA-CB	-5.23	102.06	109.85
1	A	192	MET	CA-C-O	-5.22	115.64	121.23
1	A	157	TYR	O-C-N	5.21	129.16	123.22
1	A	121	PHE	O-C-N	5.20	129.30	123.27
1	A	184	ASN	CB-CG-OD1	5.18	131.16	120.80
1	A	192(B)	ARG	CD-NE-CZ	-5.16	117.17	124.40
1	A	181	THR	CA-CB-OG1	-5.16	101.87	109.60
1	A	214	SER	O-C-N	5.13	128.59	121.92
1	A	217(B)	GLN	CG-CD-NE2	5.12	124.08	116.40
1	A	231	LEU	N-CA-CB	-5.08	102.64	110.16
1	A	112	GLN	CG-CD-OE1	5.07	130.93	120.80
1	A	35	ASN	N-CA-CB	-5.02	104.50	112.08

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48(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	11	0
2	P	26	0	28	2	0
3	A	5	0	0	0	0
4	A	171	0	0	1	0
4	P	3	0	0	0	0
All	All	1593	0	1384	11	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 4.

All (11) 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:192:MET:HE3	2:P:1:BNO:HD2	1.56	0.85
1:A:166:ASN:HD22	1:A:179:GLY:HA2	1.52	0.74
1:A:48(B):ARG:HD2	4:A:353:HOH:O	2.07	0.52
1:A:166:ASN:ND2	1:A:179:GLY:HA2	2.25	0.47
1:A:221(B):PRO:HG2	1:A:223:GLN:NE2	2.31	0.45
1:A:192:MET:CE	2:P:1:BNO:HD2	2.36	0.43
1:A:17:VAL:O	1:A:29:ILE:HG12	2.19	0.43
1:A:48(B):ARG:HG3	1:A:239:LEU:HD23	2.00	0.43
1:A:221(A):ILE:HB	1:A:221(B):PRO:HD2	2.01	0.42
1:A:232:GLN:N	1:A:233:PRO:HD2	2.35	0.41
1:A:48(B):ARG:CG	1:A:239:LEU:HD23	2.52	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	196/198 (99%)	189 (96%)	7 (4%)	0	100	100
2	P	2/5 (40%)	2 (100%)	0	0	100	100
All	All	198/203 (98%)	191 (96%)	7 (4%)	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	141/141 (100%)	136 (96%)	5 (4%)	32	35
2	P	1/1 (100%)	1 (100%)	0	100	100
All	All	142/142 (100%)	137 (96%)	5 (4%)	32	35

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

Mol	Chain	Res	Type
1	A	91	ARG
1	A	110	SER
1	A	192	MET
1	A	192(B)	ARG
1	A	198	SER

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	64	ASN
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	BNO	P	1	2,1	3,8,8	0.37	0	2,9,9	0.79	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	BNO	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	1	BNO	2	0

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	0.54	0	6,6,6	0.78	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.

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.