wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 11:45 PM EDT

PDB ID	:	1R1P
Title	:	Structural Basis for Differential Recognition of Tyrosine Phosphorylated Sites in the Linker for Activation of T cells (LAT) by the Adaptor Protein Gads
Authors	:	Cho, S.; Mariuzza, R.A.
Deposited on	:	2003-09-24
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

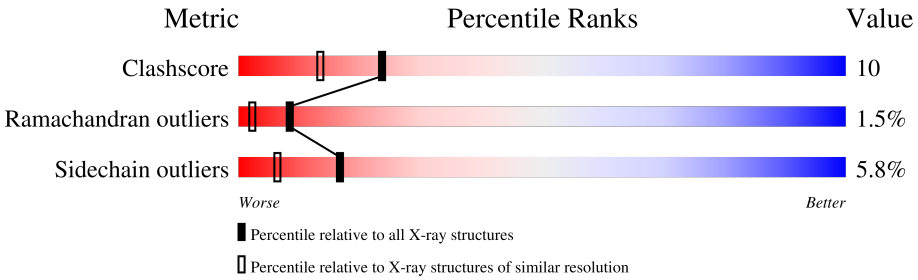
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	100	79% 11% • • 5%
1	B	100	76% 18% • •
1	C	100	86% 8% 5% •
1	D	100	80% 10% • • 5%
2	E	7	71% 14% 14%
2	F	7	43% 14% 43%
2	G	7	57% 29% 14%
2	H	7	57% 43%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3916 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 GRB2-related adaptor protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	0	0
			800	514	138	146	2			
1	B	100	Total	C	N	O	S	0	0	0
			837	538	143	154	2			
1	C	100	Total	C	N	O	S	0	0	0
			837	538	143	154	2			
1	D	95	Total	C	N	O	S	0	0	0
			800	514	138	146	2			

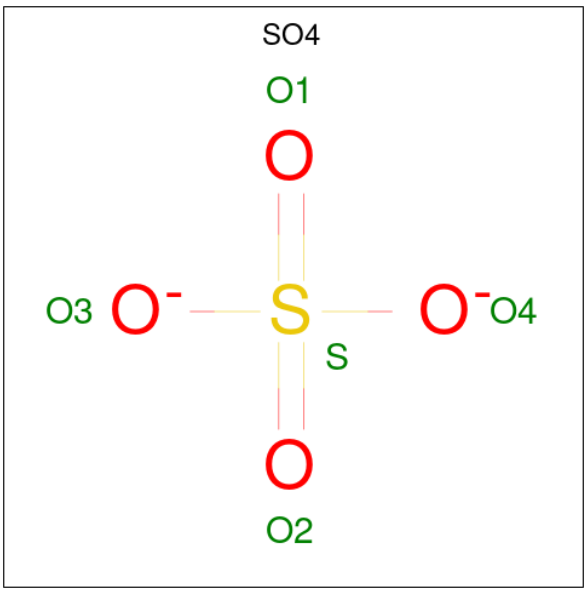
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLY	-	cloning artifact	UNP O89100
A	51	SER	-	cloning artifact	UNP O89100
B	50	GLY	-	cloning artifact	UNP O89100
B	51	SER	-	cloning artifact	UNP O89100
C	50	GLY	-	cloning artifact	UNP O89100
C	51	SER	-	cloning artifact	UNP O89100
D	50	GLY	-	cloning artifact	UNP O89100
D	51	SER	-	cloning artifact	UNP O89100

- Molecule 2 is a protein called LAT pY171 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	0
			58	33	7	17	1			
2	F	7	Total	C	N	O	P	0	0	0
			58	33	7	17	1			
2	G	7	Total	C	N	O	P	0	0	0
			58	33	7	17	1			
2	H	7	Total	C	N	O	P	0	0	0
			58	33	7	17	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	94	Total O 94 94	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	78	Total O 78 78	0	0
4	C	96	Total O 96 96	0	0
4	D	71	Total O 71 71	0	0
4	E	7	Total O 7 7	0	0
4	F	4	Total O 4 4	0	0
4	G	6	Total O 6 6	0	0
4	H	4	Total O 4 4	0	0

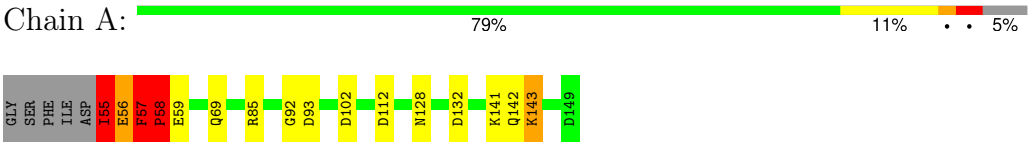
3 Residue-property plots (i)

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.

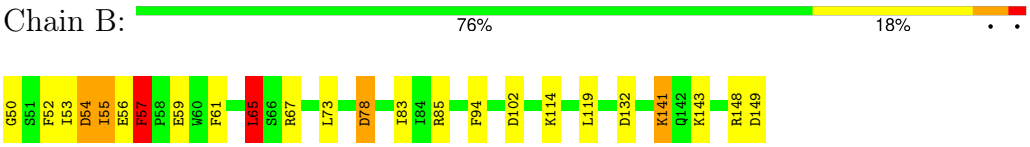
• Molecule 1: GRB2-related adaptor protein 2

Chain A:



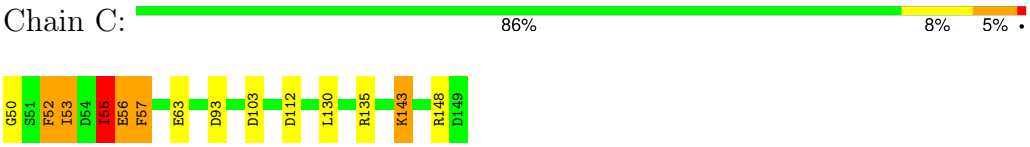
• Molecule 1: GRB2-related adaptor protein 2

Chain B:



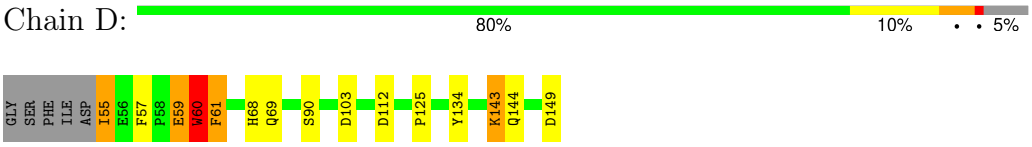
• Molecule 1: GRB2-related adaptor protein 2

Chain C:



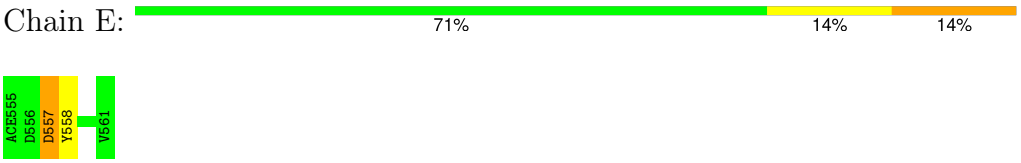
• Molecule 1: GRB2-related adaptor protein 2

Chain D:



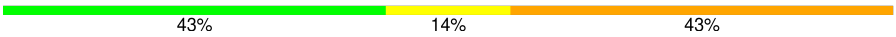
• Molecule 2: LAT pY171 peptide

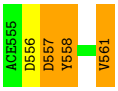
Chain E:



• Molecule 2: LAT pY171 peptide

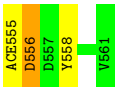
Chain F:





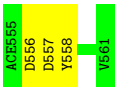
• Molecule 2: LAT pY171 peptide

Chain G:



• Molecule 2: LAT pY171 peptide

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	90.31Å 90.31Å 145.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.70 – 1.80	Depositor
% Data completeness (in resolution range)	93.7 (30.70-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.196 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3916	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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, PTR, ACE

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	1.24	1/822 (0.1%)	1.12	6/1104 (0.5%)
1	B	1.17	1/860 (0.1%)	1.26	12/1155 (1.0%)
1	C	1.25	3/860 (0.3%)	1.27	7/1155 (0.6%)
1	D	1.24	2/822 (0.2%)	1.11	5/1104 (0.5%)
2	E	1.54	0/38	1.56	2/49 (4.1%)
2	F	1.28	0/38	2.15	3/49 (6.1%)
2	G	1.47	0/38	1.46	0/49
2	H	1.23	0/38	1.97	2/49 (4.1%)
All	All	1.23	7/3516 (0.2%)	1.23	37/4714 (0.8%)

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	4
1	C	0	1
1	D	0	1
All	All	0	6

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	60	TRP	CB-CG	7.20	1.63	1.50
1	C	52	PHE	CB-CG	-6.54	1.40	1.51
1	A	143	LYS	CE-NZ	5.65	1.63	1.49
1	C	143	LYS	CD-CE	5.31	1.64	1.51
1	D	134	TYR	CE1-CZ	5.28	1.45	1.38

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	148	ARG	NE-CZ-NH1	12.06	126.33	120.30
1	C	148	ARG	NE-CZ-NH2	-11.93	114.33	120.30
1	B	78	ASP	CB-CG-OD2	10.41	127.67	118.30
1	C	103	ASP	CB-CG-OD2	9.34	126.71	118.30
1	B	102	ASP	CB-CG-OD2	8.88	126.29	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ILE	Peptide
1	A	56	GLU	Peptide
1	A	57	PHE	Peptide
1	A	58	PRO	Peptide
1	C	55	ILE	Peptide

5.2 Too-close contacts (i)

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	800	0	771	15	0
1	B	837	0	803	30	0
1	C	837	0	803	22	0
1	D	800	0	771	16	0
2	E	58	0	42	0	0
2	F	58	0	42	1	0
2	G	58	0	42	1	0
2	H	58	0	42	0	0
3	A	10	0	0	1	0
3	B	15	0	0	0	0
3	C	10	0	0	0	0
3	D	15	0	0	0	0
4	A	94	0	0	9	0
4	B	78	0	0	8	0
4	C	96	0	0	5	0
4	D	71	0	0	10	0
4	E	7	0	0	1	0
4	F	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	6	0	0	0	0
4	H	4	0	0	0	0
All	All	3916	0	3316	69	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 10.

The worst 5 of 69 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:B:59:GLU:HG2	4:B:576:HOH:O	1.59	1.02
1:D:55:ILE:HG13	4:D:570:HOH:O	1.66	0.96
1:B:55:ILE:HD13	4:C:555:HOH:O	1.70	0.91
4:A:556:HOH:O	1:C:57:PHE:HB3	1.71	0.88
1:D:59:GLU:HA	4:D:573:HOH:O	1.76	0.83

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	93/100 (93%)	90 (97%)	1 (1%)	2 (2%)	5 1
1	B	98/100 (98%)	94 (96%)	4 (4%)	0	100 100
1	C	98/100 (98%)	93 (95%)	3 (3%)	2 (2%)	6 1
1	D	93/100 (93%)	89 (96%)	3 (3%)	1 (1%)	12 3
2	E	4/7 (57%)	4 (100%)	0	0	100 100
2	F	4/7 (57%)	4 (100%)	0	0	100 100
2	G	4/7 (57%)	3 (75%)	0	1 (25%)	0 0
2	H	4/7 (57%)	4 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	398/428 (93%)	381 (96%)	11 (3%)	6 (2%)	8 2

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	PRO
1	C	53	ILE
1	D	60	TRP
2	G	556	ASP
1	A	57	PHE

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	88/92 (96%)	87 (99%)	1 (1%)	70 65
1	B	92/92 (100%)	83 (90%)	9 (10%)	6 1
1	C	92/92 (100%)	87 (95%)	5 (5%)	18 8
1	D	88/92 (96%)	83 (94%)	5 (6%)	17 7
2	E	5/5 (100%)	4 (80%)	1 (20%)	1 0
2	F	5/5 (100%)	4 (80%)	1 (20%)	1 0
2	G	5/5 (100%)	5 (100%)	0	100 100
2	H	5/5 (100%)	5 (100%)	0	100 100
All	All	380/388 (98%)	358 (94%)	22 (6%)	17 6

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	143	LYS
1	D	90	SER
1	D	59	GLU
1	D	125	PRO
1	B	114	LYS

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	62	HIS
1	A	72	ASN
1	C	72	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	H	558	2	15,16,17	2.01	3 (20%)	17,22,24	1.07	1 (5%)
2	PTR	G	558	2	15,16,17	1.84	4 (26%)	17,22,24	1.27	3 (17%)
2	PTR	E	558	2	15,16,17	1.48	1 (6%)	17,22,24	1.05	1 (5%)
2	PTR	F	558	2	15,16,17	1.96	1 (6%)	17,22,24	0.94	1 (5%)

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	H	558	2	-	0/10/11/13	0/1/1/1
2	PTR	G	558	2	-	1/10/11/13	0/1/1/1
2	PTR	E	558	2	-	2/10/11/13	0/1/1/1
2	PTR	F	558	2	-	0/10/11/13	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	558	PTR	OH-CZ	-6.77	1.25	1.40
2	H	558	PTR	OH-CZ	-5.17	1.29	1.40
2	G	558	PTR	OH-CZ	-4.99	1.29	1.40
2	E	558	PTR	OH-CZ	-4.78	1.29	1.40
2	H	558	PTR	P-OH	4.00	1.67	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	558	PTR	OH-P-O1P	-3.31	98.43	109.48
2	F	558	PTR	O2P-P-OH	2.47	112.61	105.32
2	G	558	PTR	O3P-P-O2P	2.29	116.40	107.80
2	G	558	PTR	O2P-P-OH	2.28	112.06	105.32
2	E	558	PTR	OH-CZ-CE1	2.21	125.83	119.22

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	558	PTR	O-C-CA-CB
2	E	558	PTR	CZ-OH-P-O2P
2	G	558	PTR	CZ-OH-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	558	PTR	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	SO4	C	507	-	4,4,4	0.13	0	6,6,6	0.54	0
3	SO4	D	506	-	4,4,4	0.28	0	6,6,6	0.54	0
3	SO4	B	504	-	4,4,4	0.50	0	6,6,6	1.33	1 (16%)
3	SO4	C	502	-	4,4,4	0.54	0	6,6,6	0.76	0
3	SO4	A	508	-	4,4,4	0.28	0	6,6,6	0.48	0
3	SO4	D	503	-	4,4,4	0.49	0	6,6,6	0.67	0
3	SO4	A	500	-	4,4,4	0.49	0	6,6,6	0.44	0
3	SO4	B	501	-	4,4,4	0.38	0	6,6,6	0.43	0
3	SO4	B	509	-	4,4,4	0.40	0	6,6,6	1.15	0
3	SO4	D	505	-	4,4,4	0.30	0	6,6,6	0.57	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	504	SO4	O4-S-O2	2.35	121.85	109.56

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	500	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.