



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:29 PM UTC

PDB ID : 3ELQ / pdb_00003elq
Title : Crystal structure of a bacterial arylsulfate sulfotransferase
Authors : Malojcic, G.; Owen, R.L.; Grimshaw, J.P.; Glockshuber, R.
Deposited on : 2008-09-23
Resolution : 2.00 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

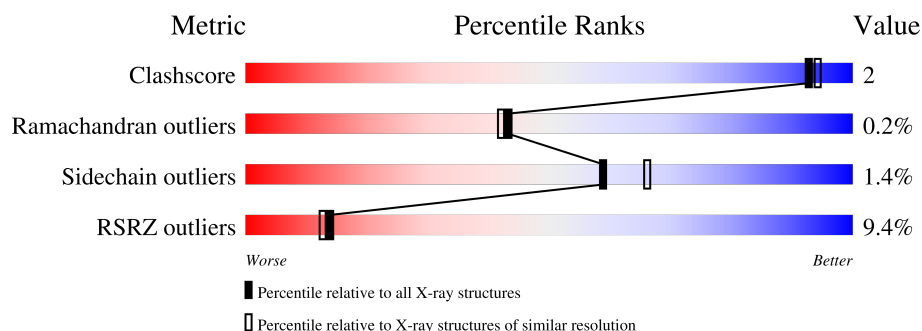
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	571	
1	B	571	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	2001	-	-	X	-
3	CL	B	5010	-	-	X	-

2 Entry composition [i](#)

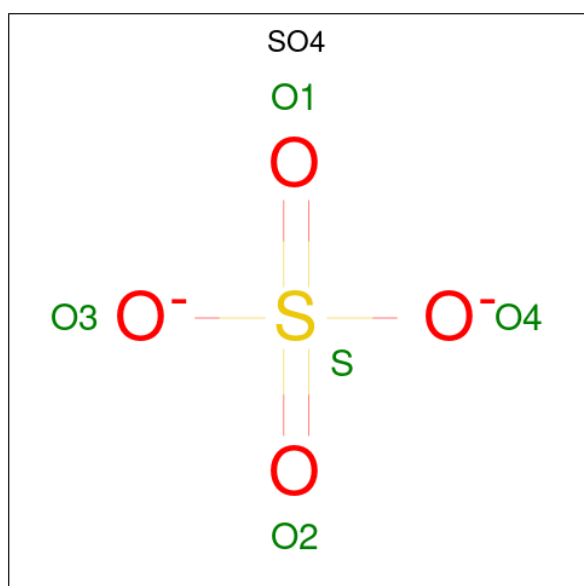
There are 4 unique types of molecules in this entry. The entry contains 9997 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Arylsulfate sulfotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	3	0
			4457	2833	762	852	10			
1	B	566	Total	C	N	O	S	0	2	0
			4467	2840	764	853	10			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Cl 3 3	0	0
3	B	5	Total Cl 5 5	0	0

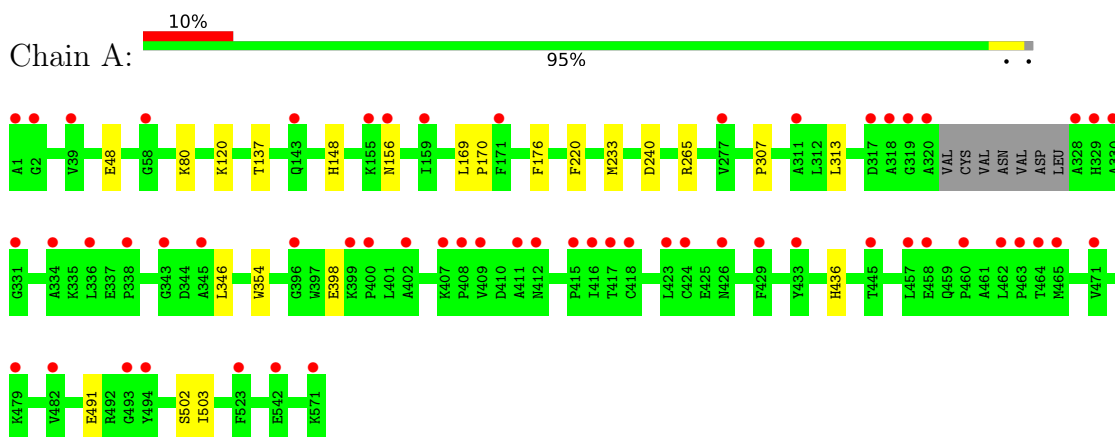
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	509	Total O 509 509	0	0
4	B	501	Total O 501 501	0	0

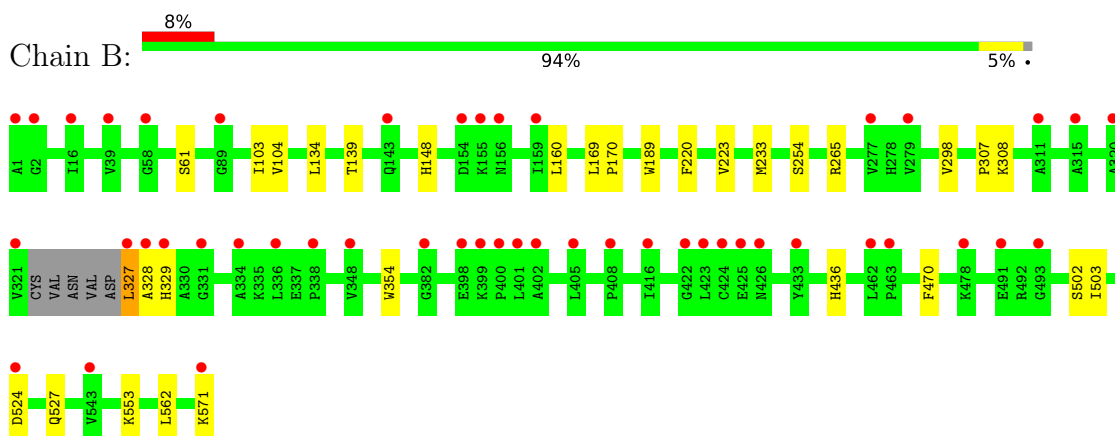
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: Arylsulfate sulfotransferase



• Molecule 1: Arylsulfate sulfotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	181.73Å 181.73Å 100.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.90 – 2.00 33.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.90-2.00) 97.1 (33.90-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.207 , 0.248 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9997	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.59	0/4576	0.73	0/6210
1	B	0.58	0/4583	0.73	1/6221 (0.0%)
All	All	0.59	0/9159	0.73	1/12431 (0.0%)

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	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	329	HIS	N-CA-C	-6.06	102.64	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	328	ALA	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	4457	0	4305	10	0
1	B	4467	0	4324	16	1
2	A	30	0	0	2	0
2	B	25	0	0	1	0
3	A	3	0	0	0	0
3	B	5	0	0	2	0
4	A	509	0	0	1	0
4	B	501	0	0	3	0
All	All	9997	0	8629	27	1

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 2.

All (27) 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)
3:B:5010:CL:CL	4:B:5444:HOH:O	2.52	0.64
1:B:308:LYS:NZ	3:B:5010:CL:CL	2.69	0.63
1:B:327:LEU:N	4:B:5510:HOH:O	2.38	0.56
1:B:220:PHE:CE2	1:B:233:MET:HE3	2.40	0.56
1:A:313:LEU:HD22	1:A:346:LEU:HD22	1.91	0.51
1:B:436:HIS:NE2	2:B:2002:SO4:S	2.68	0.51
1:A:169:LEU:N	1:A:170:PRO:CD	2.74	0.51
1:A:220:PHE:CE2	1:A:233:MET:HE3	2.47	0.49
1:B:169:LEU:N	1:B:170:PRO:CD	2.75	0.49
1:A:307:PRO:HA	1:A:354:TRP:CE3	2.48	0.49
1:B:307:PRO:HA	1:B:354:TRP:CE3	2.48	0.48
1:A:436:HIS:NE2	2:A:2001:SO4:S	2.72	0.48
1:B:134:LEU:C	1:B:134:LEU:HD23	2.38	0.48
1:A:436:HIS:NE2	2:A:2001:SO4:O2	2.47	0.47
1:B:61:SER:OG	1:B:571:LYS:OXT	2.28	0.47
1:B:524:ASP:HB3	1:B:527:GLN:HB2	1.98	0.45
1:A:120:LYS:NZ	4:A:5438:HOH:O	2.46	0.45
1:B:571:LYS:NZ	4:B:5465:HOH:O	2.49	0.44
1:A:137:THR:HG23	1:A:176:PHE:HB3	1.99	0.44
1:B:134:LEU:HD22	1:B:562:LEU:HD13	2.00	0.44
1:B:470:PHE:N	1:B:470:PHE:CD1	2.86	0.43
1:B:223:VAL:HG13	1:B:254:SER:HB3	1.99	0.43
1:A:240:ASP:OD1	1:A:240:ASP:C	2.61	0.42
1:A:48:GLU:H	1:A:48:GLU:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ILE:HG23	1:B:189:TRP:CE2	2.54	0.41
1:B:103:ILE:HG23	1:B:189:TRP:CD2	2.56	0.41
1:B:139:THR:OG1	1:B:553:LYS:NZ	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:CG2	1:B:104:VAL:CG2[5_555]	2.19	0.01

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	563/571 (99%)	545 (97%)	17 (3%)	1 (0%)	43	42
1	B	564/571 (99%)	543 (96%)	20 (4%)	1 (0%)	43	42
All	All	1127/1142 (99%)	1088 (96%)	37 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	502	SER
1	A	502	SER

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	471/483 (98%)	463 (98%)	8 (2%)	53	60
1	B	472/483 (98%)	466 (99%)	6 (1%)	61	68
All	All	943/966 (98%)	929 (98%)	14 (2%)	59	64

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	148	HIS
1	A	156[A]	ASN
1	A	156[B]	ASN
1	A	265	ARG
1	A	398	GLU
1	A	491	GLU
1	A	503	ILE
1	B	148	HIS
1	B	160	LEU
1	B	265	ARG
1	B	298	VAL
1	B	327	LEU
1	B	503	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	106	ASN
1	A	527	GLN
1	B	99	HIS
1	B	224	GLN
1	B	270	ASN
1	B	435	GLN
1	B	527	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 for Mogul analysis.

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	SO4	A	2009	-	4,4,4	0.25	0	6,6,6	0.29	0
2	SO4	B	2010	-	4,4,4	0.27	0	6,6,6	0.16	0
2	SO4	A	2004	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	B	2002	-	4,4,4	0.26	0	6,6,6	0.45	0
2	SO4	A	2006	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	B	2008	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	A	2001	-	4,4,4	0.21	0	6,6,6	0.33	0
2	SO4	B	2003	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	B	2011	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	A	2007	-	4,4,4	0.30	0	6,6,6	0.12	0
2	SO4	A	2005	-	4,4,4	0.25	0	6,6,6	0.26	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2002	SO4	1	0
2	A	2001	SO4	2	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

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	564/571 (98%)	0.99	58 (10%)	12 11	26, 41, 61, 80	3 (0%)
1	B	566/571 (99%)	0.95	48 (8%)	16 15	27, 41, 61, 81	2 (0%)
All	All	1130/1142 (98%)	0.97	106 (9%)	14 13	26, 41, 61, 81	5 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	LEU	6.9
1	B	1	ALA	5.7
1	A	328	ALA	5.2
1	A	320	ALA	4.8
1	B	416	ILE	4.2
1	A	494	TYR	4.2
1	A	1	ALA	4.2
1	A	523	PHE	4.2
1	B	321	VAL	4.2
1	B	154	ASP	4.1
1	B	155	LYS	4.0
1	B	328	ALA	3.9
1	A	542	GLU	3.8
1	A	418	CYS	3.7
1	A	336	LEU	3.6
1	B	320	ALA	3.6
1	A	416	ILE	3.5
1	A	426	ASN	3.5
1	A	329	HIS	3.5
1	B	543	VAL	3.4
1	A	334	ALA	3.4
1	B	143	GLN	3.4
1	A	571	LYS	3.4
1	B	329	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	423	LEU	3.3
1	A	429	PHE	3.3
1	B	493	GLY	3.0
1	A	330	ALA	3.0
1	B	425	GLU	3.0
1	B	331	GLY	3.0
1	B	401	LEU	3.0
1	A	2	GLY	2.9
1	A	396	GLY	2.9
1	B	2	GLY	2.9
1	A	479	LYS	2.9
1	B	402	ALA	2.9
1	A	462	LEU	2.9
1	B	334	ALA	2.9
1	A	155	LYS	2.8
1	B	422	GLY	2.8
1	B	463	PRO	2.8
1	A	424	CYS	2.8
1	A	58	GLY	2.7
1	A	331	GLY	2.7
1	B	462	LEU	2.7
1	B	408	PRO	2.7
1	A	412	ASN	2.7
1	B	424	CYS	2.7
1	A	471	VAL	2.7
1	A	318	ALA	2.7
1	A	463	PRO	2.7
1	A	345	ALA	2.6
1	A	417	THR	2.6
1	A	338	PRO	2.6
1	A	400	PRO	2.6
1	A	143	GLN	2.6
1	A	409	VAL	2.6
1	A	408	PRO	2.5
1	A	423	LEU	2.5
1	A	465	MET	2.5
1	B	279	VAL	2.5
1	A	411	ALA	2.5
1	B	311	ALA	2.5
1	B	400	PRO	2.5
1	A	460	PRO	2.5
1	B	405	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	493	GLY	2.5
1	B	156	ASN	2.5
1	A	277	VAL	2.4
1	B	159	ILE	2.5
1	A	445	THR	2.4
1	A	415	PRO	2.4
1	B	491	GLU	2.4
1	B	338	PRO	2.4
1	A	399	LYS	2.4
1	B	315	ALA	2.4
1	A	407	LYS	2.3
1	B	16	ILE	2.3
1	A	464	THR	2.3
1	A	156[A]	ASN	2.3
1	A	319	GLY	2.3
1	A	402	ALA	2.3
1	B	89	GLY	2.3
1	A	457	LEU	2.3
1	B	398	GLU	2.2
1	A	39	VAL	2.2
1	B	571	LYS	2.2
1	B	39	VAL	2.2
1	A	433	TYR	2.2
1	B	399	LYS	2.2
1	A	159	ILE	2.2
1	A	171	PHE	2.2
1	B	348	VAL	2.2
1	A	343	GLY	2.2
1	B	426	ASN	2.2
1	B	277	VAL	2.1
1	B	433	TYR	2.1
1	B	478	LYS	2.1
1	B	382	GLY	2.1
1	A	311	ALA	2.1
1	A	458	GLU	2.0
1	B	336	LEU	2.0
1	A	482	VAL	2.0
1	A	317	ASP	2.0
1	B	524	ASP	2.0
1	B	58	GLY	2.0

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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	2011	5/5	0.47	0.19	93,93,94,94	0
2	SO4	B	2010	5/5	0.63	0.15	87,88,88,88	0
2	SO4	A	2009	5/5	0.70	0.17	84,85,86,87	0
2	SO4	A	2007	5/5	0.73	0.14	87,88,88,89	0
2	SO4	A	2005	5/5	0.76	0.15	83,83,83,84	0
2	SO4	B	2008	5/5	0.78	0.13	80,80,80,80	0
2	SO4	A	2004	5/5	0.80	0.10	106,106,106,107	0
3	CL	B	5009	1/1	0.84	0.25	81,81,81,81	0
3	CL	B	5007	1/1	0.86	0.20	69,69,69,69	0
2	SO4	A	2006	5/5	0.88	0.11	63,63,63,64	0
2	SO4	B	2003	5/5	0.89	0.10	66,67,67,67	0
3	CL	A	5008	1/1	0.90	0.13	58,58,58,58	0
3	CL	A	5004	1/1	0.91	0.13	66,66,66,66	0
3	CL	B	5010	1/1	0.93	0.10	50,50,50,50	0
3	CL	B	5006	1/1	0.94	0.09	40,40,40,40	0
2	SO4	A	2001	5/5	0.95	0.11	43,43,44,45	0
2	SO4	B	2002	5/5	0.95	0.10	42,43,44,46	0
3	CL	B	5001	1/1	0.96	0.09	45,45,45,45	0
3	CL	A	5002	1/1	0.98	0.05	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.