



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1HDH / pdb_00001hdh
Title : Arylsulfatase from *Pseudomonas aeruginosa*
Authors : Boltes, I.; Czapinska, H.; Kahnert, A.; von Buelow, R.; Dirks, T.; Schmidt, B.; von Figura, K.; Kertesz, M.A.; Uson, I.
Deposited on : 2000-11-16
Resolution : 1.30 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

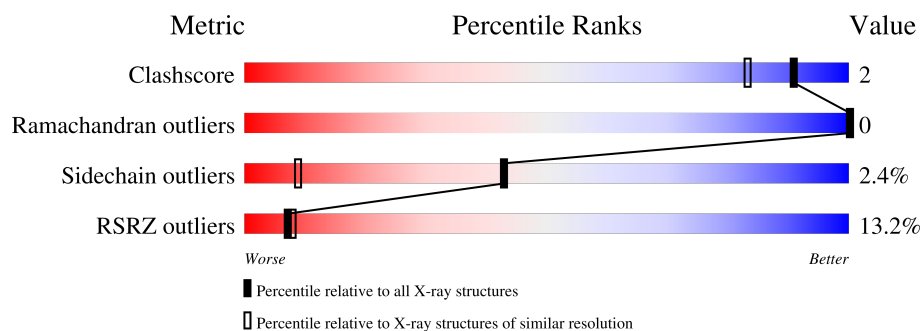
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	536	11% 89% 8% ..
1	B	536	15% 90% 8% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9041 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 Arylsulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	5	0
			4095	2613	720	753	9			
1	B	525	Total	C	N	O	S	0	7	0
			4094	2610	719	756	9			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

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



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	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	B	1	Total O S 5 4 1	0	0

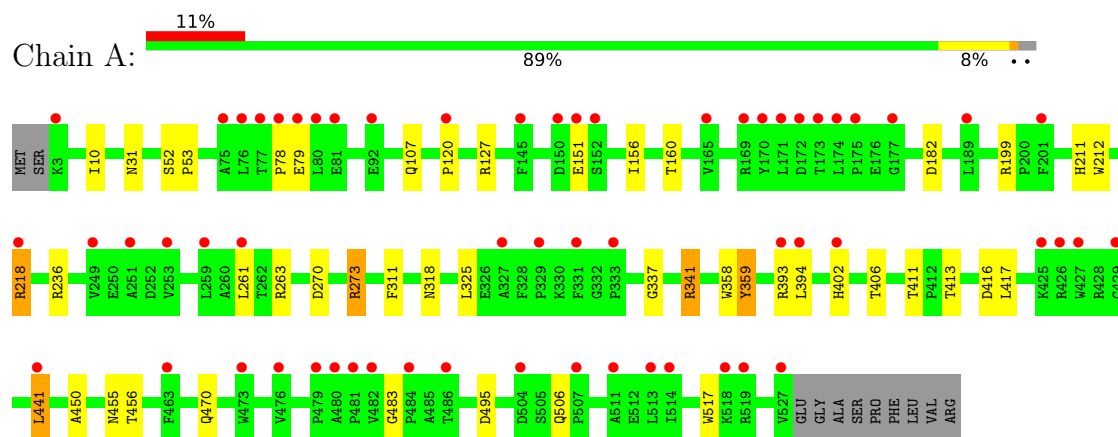
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	412	Total O 412 412	0	0
4	B	398	Total O 398 398	0	0

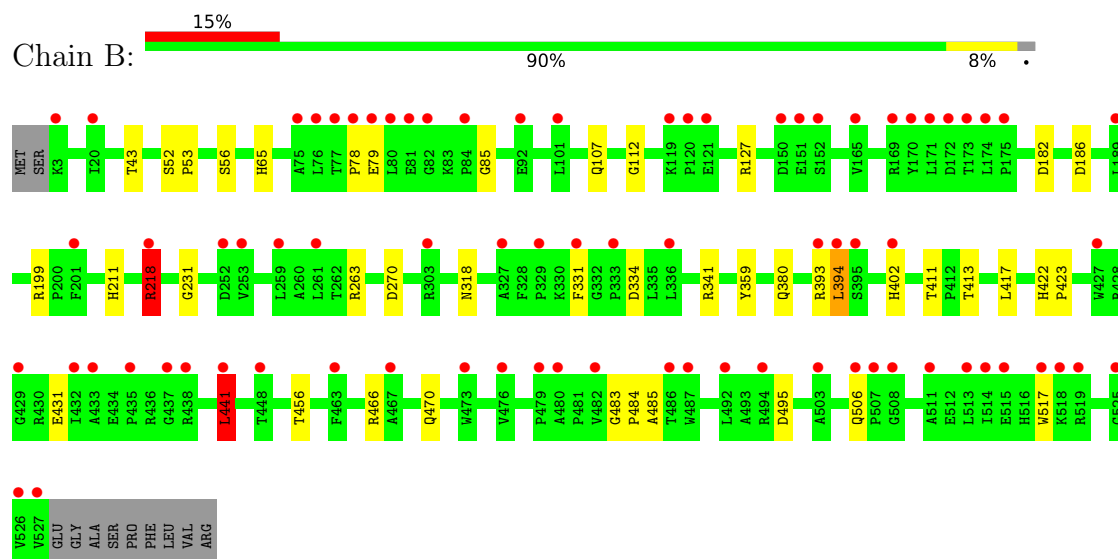
3 Residue-property plots [i](#)

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 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: Arylsulfatase



• Molecule 1: Arylsulfatase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.92Å 67.29Å 89.70Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	20.00 – 1.30 20.00 – 1.30	Depositor EDS
% Data completeness (in resolution range)	93.1 (20.00-1.30) 93.0 (20.00-1.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 1.30Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.200 , 0.229 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	10.7	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9041	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DDZ, SO4, CA

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	0.70	0/4223	1.39	25/5751 (0.4%)
1	B	0.71	0/4233	1.38	19/5767 (0.3%)
All	All	0.70	0/8456	1.39	44/11518 (0.4%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ARG	CD-NE-CZ	11.17	140.04	124.40
1	B	211	HIS	CA-CB-CG	8.48	122.28	113.80
1	B	263	ARG	CD-NE-CZ	8.00	135.60	124.40
1	A	341[A]	ARG	CD-NE-CZ	7.99	135.58	124.40
1	A	341[B]	ARG	CD-NE-CZ	7.99	135.58	124.40
1	A	107	GLN	OE1-CD-NE2	7.79	130.39	122.60
1	A	495	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	393	ARG	CA-C-O	7.66	128.78	119.97
1	A	127	ARG	CD-NE-CZ	7.21	134.49	124.40
1	B	495	ASP	CA-CB-CG	7.19	119.79	112.60
1	A	199	ARG	O-C-N	7.12	127.92	121.80
1	A	236	ARG	NE-CZ-NH1	6.98	128.48	121.50
1	B	393	ARG	CA-C-O	6.79	127.61	120.42
1	A	416	ASP	CA-CB-CG	6.73	119.33	112.60
1	A	211	HIS	CA-CB-CG	6.62	120.42	113.80
1	B	380	GLN	OE1-CD-NE2	6.59	129.19	122.60
1	A	182	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	311	PHE	CA-CB-CG	6.08	119.88	113.80
1	A	151	GLU	CA-C-N	6.07	130.86	120.72
1	A	151	GLU	C-N-CA	6.07	130.86	120.72
1	B	218	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	A	10	ILE	CA-C-O	-5.93	114.19	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ILE	O-C-N	5.91	129.39	123.18
1	B	56	SER	CA-C-N	5.70	128.19	120.44
1	B	56	SER	C-N-CA	5.70	128.19	120.44
1	B	107	GLN	OE1-CD-NE2	5.67	128.27	122.60
1	B	331	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	31	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	517	TRP	CA-C-O	5.41	126.29	120.55
1	B	127	ARG	CD-NE-CZ	5.36	131.91	124.40
1	A	359	TYR	CA-CB-CG	5.36	123.55	113.90
1	B	231	GLY	O-C-N	5.35	127.12	121.77
1	A	455	ASN	CA-CB-CG	-5.33	107.28	112.60
1	A	160	THR	O-C-N	-5.31	116.37	121.05
1	A	261	LEU	CA-C-O	5.27	125.45	119.18
1	B	394	LEU	O-C-N	-5.19	116.56	122.89
1	B	483	GLY	O-C-N	5.18	126.95	121.77
1	B	199	ARG	O-C-N	5.16	126.23	121.80
1	A	483	GLY	O-C-N	5.15	126.92	121.77
1	B	186	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	431	GLU	O-C-N	5.10	129.01	123.04
1	A	263	ARG	CD-NE-CZ	5.09	131.53	124.40
1	B	182	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	441	LEU	N-CA-C	5.03	116.84	111.36

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	4095	0	3911	13	0
1	B	4094	0	3896	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
4	A	412	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	398	0	0	0	0
All	All	9041	0	7807	27	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 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)
1:A:417:LEU:HG	1:A:441:LEU:HD21	1.72	0.71
1:A:337:GLY:O	1:A:341[B]:ARG:HD3	1.92	0.68
1:B:417:LEU:HG	1:B:441:LEU:HD21	1.82	0.62
1:A:78:PRO:HG2	1:A:79:GLU:OE2	2.03	0.57
1:B:78:PRO:HG2	1:B:79:GLU:OE2	2.05	0.56
1:B:413:THR:HG23	1:B:441:LEU:HD23	1.89	0.55
1:B:218:ARG:H	1:B:218:ARG:NE	2.07	0.53
1:A:450:ALA:HB1	4:A:2327:HOH:O	2.09	0.52
1:A:417:LEU:CG	1:A:441:LEU:HD21	2.40	0.51
1:B:65:HIS:O	1:B:85:GLY:HA3	2.10	0.50
1:B:466:ARG:HD3	1:B:517:TRP:CZ2	2.48	0.48
1:B:218:ARG:H	1:B:218:ARG:CD	2.26	0.48
1:A:52:SER:OG	1:A:53:PRO:HD3	2.13	0.48
1:B:52:SER:OG	1:B:53:PRO:HD3	2.16	0.45
1:A:456:THR:O	1:A:470:GLN:HA	2.16	0.45
1:A:413:THR:HG23	1:A:441:LEU:HD23	1.99	0.45
1:B:456:THR:O	1:B:470:GLN:HA	2.16	0.45
1:A:156:ILE:HD11	1:A:212:TRP:CH2	2.52	0.44
1:A:218:ARG:NE	1:A:218:ARG:H	2.14	0.44
1:A:273:ARG:NH2	4:A:2219:HOH:O	2.51	0.43
1:A:325:LEU:HD12	1:A:358:TRP:CE3	2.53	0.43
1:A:218:ARG:H	1:A:218:ARG:CD	2.32	0.43
1:B:43:THR:OG1	1:B:402:HIS:HD2	2.02	0.42
1:B:334:ASP:OD2	1:B:341[B]:ARG:NH2	2.49	0.41
1:B:484:PRO:O	1:B:485:ALA:HB3	2.22	0.40
1:B:422:HIS:CG	1:B:423:PRO:HD2	2.56	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	526/536 (98%)	512 (97%)	14 (3%)	0	100	100
1	B	528/536 (98%)	514 (97%)	14 (3%)	0	100	100
All	All	1054/1072 (98%)	1026 (97%)	28 (3%)	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	402/429 (94%)	391 (97%)	11 (3%)	39	7
1	B	404/429 (94%)	396 (98%)	8 (2%)	48	12
All	All	806/858 (94%)	787 (98%)	19 (2%)	43	9

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	PRO
1	A	218	ARG
1	A	270	ASP
1	A	318	ASN
1	A	359	TYR
1	A	394	LEU
1	A	402	HIS
1	A	406	THR

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Mol	Chain	Res	Type
1	A	411	THR
1	A	441	LEU
1	A	506	GLN
1	B	218	ARG
1	B	270	ASP
1	B	318	ASN
1	B	359	TYR
1	B	394	LEU
1	B	411	THR
1	B	441	LEU
1	B	506	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	A	349	ASN
1	A	506	GLN
1	B	89	HIS
1	B	349	ASN
1	B	402	HIS
1	B	506	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
1	DDZ	A	51	2,1	4,6,7	0.57	0	3,7,9	1.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	DDZ	B	51	2,1	4,6,7	0.34	0	3,7,9	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
1	DDZ	A	51	2,1	-	0/2/6/8	-
1	DDZ	B	51	2,1	-	0/2/6/8	-

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](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
3	SO4	B	1531	-	4,4,4	0.47	0	6,6,6	0.20	0
3	SO4	A	1529	2	4,4,4	0.62	0	6,6,6	0.18	0
3	SO4	A	1530	-	4,4,4	0.54	0	6,6,6	0.08	0
3	SO4	A	1532	-	4,4,4	0.54	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	1532	-	4,4,4	0.54	0	6,6,6	0.08	0
3	SO4	B	1529	2	4,4,4	0.69	0	6,6,6	0.26	0
3	SO4	A	1531	-	4,4,4	0.58	0	6,6,6	0.13	0
3	SO4	B	1530	-	4,4,4	0.52	0	6,6,6	0.05	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

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	524/536 (97%)	0.97	60 (11%) 9 11	7, 13, 28, 58	7 (1%)
1	B	524/536 (97%)	1.03	78 (14%) 5 6	7, 13, 28, 58	10 (1%)
All	All	1048/1072 (97%)	1.00	138 (13%) 7 8	7, 13, 28, 58	17 (1%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	441	LEU	6.1
1	A	527	VAL	5.8
1	A	441	LEU	5.8
1	B	173	THR	5.2
1	A	394	LEU	5.1
1	B	394	LEU	5.1
1	B	527	VAL	5.1
1	B	81	GLU	4.9
1	B	175	PRO	4.5
1	B	482	VAL	4.5
1	A	78	PRO	4.4
1	B	171	LEU	4.4
1	A	175	PRO	4.4
1	A	81	GLU	4.3
1	A	482	VAL	4.3
1	B	76	LEU	4.2
1	A	171	LEU	4.0
1	A	511	ALA	4.0
1	A	173	THR	4.0
1	A	218	ARG	3.9
1	A	76	LEU	3.8
1	A	463	PHE	3.8
1	B	80	LEU	3.7
1	A	393	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	481	PRO	3.7
1	A	480	ALA	3.7
1	B	152	SER	3.6
1	B	174	LEU	3.6
1	B	480	ALA	3.5
1	B	513	LEU	3.5
1	A	152	SER	3.5
1	A	80	LEU	3.3
1	B	218	ARG	3.3
1	A	170	TYR	3.3
1	A	426	ARG	3.2
1	B	476	VAL	3.2
1	A	486	THR	3.2
1	B	77	THR	3.2
1	B	170	TYR	3.2
1	A	174	LEU	3.2
1	A	473	TRP	3.2
1	B	92[A]	GLU	3.1
1	A	261	LEU	3.1
1	A	92[A]	GLU	3.1
1	B	259	LEU	3.1
1	B	473	TRP	3.1
1	B	78	PRO	3.1
1	A	75	ALA	3.0
1	A	259	LEU	3.0
1	B	172	ASP	3.0
1	B	479	PRO	3.0
1	B	427	TRP	3.0
1	B	82	GLY	3.0
1	B	463	PHE	3.0
1	A	251	ALA	3.0
1	B	511	ALA	2.9
1	A	189	LEU	2.9
1	A	3	LYS	2.9
1	B	486	THR	2.8
1	A	169	ARG	2.8
1	B	514	ILE	2.8
1	A	329	PRO	2.8
1	A	120	PRO	2.7
1	A	507	PRO	2.7
1	A	327	ALA	2.7
1	B	151	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	402	HIS	2.7
1	B	331	PHE	2.6
1	A	77	THR	2.6
1	B	169	ARG	2.6
1	B	333	PRO	2.6
1	B	438	ARG	2.5
1	B	448	THR	2.5
1	B	75	ALA	2.5
1	B	79	GLU	2.5
1	A	513	LEU	2.5
1	A	165	VAL	2.5
1	A	479	PRO	2.5
1	A	504	ASP	2.5
1	B	507	PRO	2.5
1	B	3	LYS	2.5
1	A	150	ASP	2.5
1	B	435	PRO	2.5
1	A	429	GLY	2.4
1	A	331	PHE	2.4
1	B	121[A]	GLU	2.4
1	B	201	PHE	2.4
1	B	336	LEU	2.4
1	B	492	LEU	2.4
1	B	437	GLY	2.4
1	A	253	VAL	2.4
1	B	487	TRP	2.4
1	B	395	SER	2.4
1	A	484	PRO	2.4
1	B	189	LEU	2.4
1	A	79	GLU	2.4
1	B	329	PRO	2.4
1	B	508	GLY	2.4
1	B	150	ASP	2.3
1	B	494	ARG	2.3
1	B	519	ARG	2.3
1	B	119	LYS	2.3
1	B	518	LYS	2.3
1	B	253	VAL	2.3
1	A	427	TRP	2.3
1	B	503	ALA	2.3
1	B	303	ARG	2.3
1	A	151	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	519	ARG	2.2
1	B	429	GLY	2.2
1	B	165	VAL	2.2
1	B	327	ALA	2.2
1	A	177	GLY	2.2
1	A	476	VAL	2.2
1	B	506	GLN	2.2
1	A	333	PRO	2.2
1	B	84	PRO	2.2
1	B	393	ARG	2.1
1	B	402	HIS	2.1
1	A	145	PHE	2.1
1	B	252	ASP	2.1
1	B	432	ILE	2.1
1	B	433	ALA	2.1
1	B	517	TRP	2.1
1	A	514	ILE	2.1
1	B	20	ILE	2.1
1	A	249	VAL	2.1
1	B	526	VAL	2.1
1	B	120	PRO	2.1
1	B	101	LEU	2.1
1	B	261	LEU	2.1
1	A	201	PHE	2.1
1	B	467	ALA	2.1
1	A	518	LYS	2.1
1	B	525	GLY	2.0
1	A	425	LYS	2.0
1	B	515	GLU	2.0
1	A	172	ASP	2.0

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

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(Å ²)	Q<0.9
1	DDZ	A	51	7/8	0.94	0.08	9,11,12,16	0
1	DDZ	B	51	7/8	0.94	0.07	10,11,12,16	0

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
3	SO4	A	1532	5/5	0.57	0.29	31,33,39,53	5
3	SO4	B	1532	5/5	0.82	0.20	20,25,38,41	5
3	SO4	A	1530	5/5	0.89	0.14	24,28,36,50	0
3	SO4	B	1530	5/5	0.90	0.13	27,29,35,42	0
3	SO4	B	1529	5/5	0.92	0.17	13,17,18,21	0
3	SO4	A	1529	5/5	0.93	0.17	12,15,17,19	0
3	SO4	B	1531	5/5	0.96	0.09	17,18,19,28	0
3	SO4	A	1531	5/5	0.97	0.08	18,19,21,23	0
2	CA	A	1528	1/1	0.98	0.11	10,10,10,10	0
2	CA	B	1528	1/1	0.99	0.11	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.