Full wwPDB X-ray Structure Validation Report (i)

Mar 22, 2016 – 07:37 PM EDT

PDB ID	:	5AJ9
Title	:	G7 mutant of PAS, arylsulfatase from Pseudomonas Aeruginosa
Authors	:	Miton, C.M.; Fischer, G.; Jonas, S.; Mohammed, M.F.; Loo, B.v.; Kintses, B.; Hyvonen, M.; Tokuriki, N.; Hollfelder, F.
Deposited on	:	2015-02-20
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

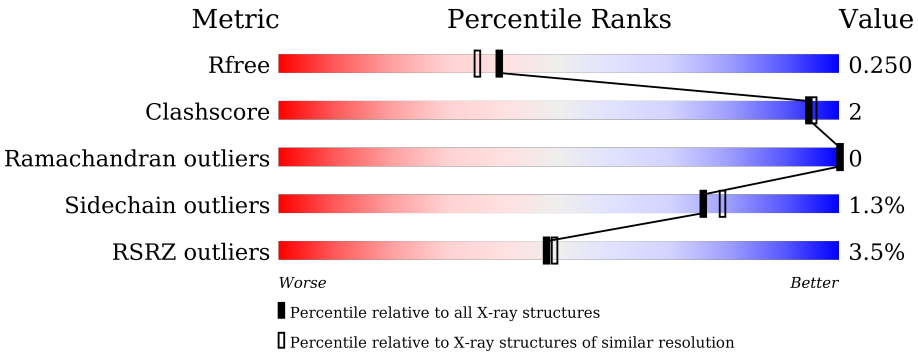
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 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))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% 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	3% 89% 8%
1	B	536	4% 92% 6%

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
1	DDZ	A	51	X	-	-	-
1	DDZ	B	51	X	-	-	-
4	SO4	B	1533	-	-	-	X
4	SO4	B	1534	-	-	-	X
5	MES	A	1537	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8848 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	526	Total	C	N	O	S	66	0	0
			4154	2643	731	772	8			
1	B	526	Total	C	N	O	S	64	2	0
			4173	2653	736	776	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	ALA	THR	ENGINEERED MUTATION	UNP U5R2L4
A	51	DDZ	CYS	ENGINEERED MUTATION	UNP U5R2L4
A	69	LEU	ILE	ENGINEERED MUTATION	UNP U5R2L4
A	72	VAL	MET	ENGINEERED MUTATION	UNP U5R2L4
A	337	ASP	GLY	ENGINEERED MUTATION	UNP U5R2L4
A	352	SER	ARG	ENGINEERED MUTATION	UNP U5R2L4
A	461	GLY	GLU	ENGINEERED MUTATION	UNP U5R2L4
A	523	ASP	GLU	ENGINEERED MUTATION	UNP U5R2L4
B	50	ALA	THR	ENGINEERED MUTATION	UNP U5R2L4
B	51	DDZ	CYS	ENGINEERED MUTATION	UNP U5R2L4
B	69	LEU	ILE	ENGINEERED MUTATION	UNP U5R2L4
B	72	VAL	MET	ENGINEERED MUTATION	UNP U5R2L4
B	337	ASP	GLY	ENGINEERED MUTATION	UNP U5R2L4
B	352	SER	ARG	ENGINEERED MUTATION	UNP U5R2L4
B	461	GLY	GLU	ENGINEERED MUTATION	UNP U5R2L4
B	523	ASP	GLU	ENGINEERED MUTATION	UNP U5R2L4

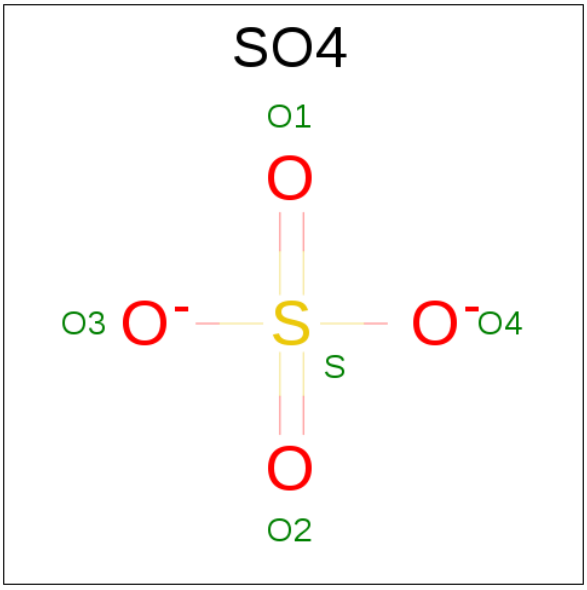
- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	7	Total	Cl	0	0
			7	7		
2	A	3	Total	Cl	0	0
			3	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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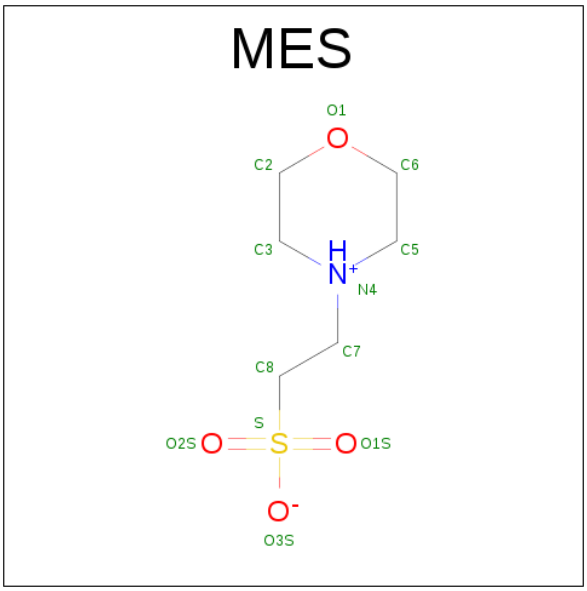
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 12 6 1 4 1	0	0
5	B	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 6 is water.

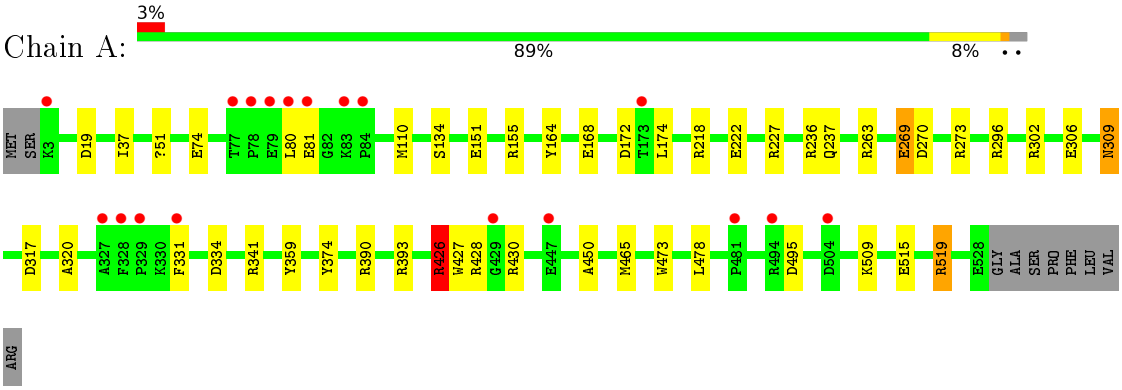
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	218	Total O 218 218	0	0
6	B	202	Total O 202 202	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

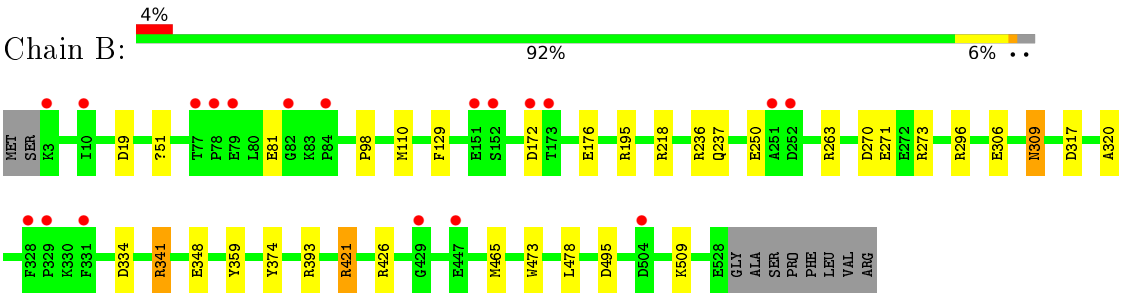
- Molecule 1: ARYLSULFATASE

Chain A:



- Molecule 1: ARYLSULFATASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	184.40Å 66.50Å 89.44Å 90.00° 93.84° 90.00°	Depositor
Resolution (Å)	91.99 – 2.00 29.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.4 (91.99-2.00) 92.5 (29.30-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.201 , 0.248 0.208 , 0.250	Depositor DCC
R_{free} test set	3461 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 67876 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8848	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, CA, SO4, MES, CL

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	0.97	8/4262 (0.2%)	1.01	29/5798 (0.5%)
1	B	1.00	9/4281 (0.2%)	1.11	23/5823 (0.4%)
All	All	0.98	17/8543 (0.2%)	1.06	52/11621 (0.4%)

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	1	1
1	B	1	0
All	All	2	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	GLU	CB-CG	21.58	1.93	1.52
1	B	341	ARG	NE-CZ	18.51	1.57	1.33
1	A	172	ASP	CB-CG	18.17	1.90	1.51
1	B	341	ARG	CZ-NH2	-17.25	1.10	1.33
1	B	341	ARG	CZ-NH1	14.50	1.51	1.33
1	B	393	ARG	CD-NE	-13.37	1.23	1.46
1	B	250	GLU	CB-CG	-11.91	1.29	1.52
1	B	426	ARG	CB-CG	10.09	1.79	1.52
1	A	80	LEU	CB-CG	-7.74	1.30	1.52
1	A	168	GLU	CB-CG	-7.09	1.38	1.52
1	A	331	PHE	CB-CG	-6.39	1.40	1.51
1	A	393	ARG	CG-CD	-5.70	1.37	1.51
1	A	269	GLU	CG-CD	-5.67	1.43	1.51
1	B	172	ASP	CB-CG	5.27	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	348	GLU	CB-CG	5.18	1.62	1.52
1	A	222	GLU	CB-CG	-5.14	1.42	1.52
1	B	218	ARG	CD-NE	-5.14	1.37	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	341	ARG	NE-CZ-NH1	-32.44	104.08	120.30
1	B	341	ARG	NE-CZ-NH2	18.94	129.77	120.30
1	B	236	ARG	NE-CZ-NH1	13.55	127.08	120.30
1	B	236	ARG	NE-CZ-NH2	-12.59	114.01	120.30
1	A	218	ARG	CG-CD-NE	12.21	137.43	111.80
1	A	331	PHE	CB-CG-CD2	10.60	128.22	120.80
1	B	341	ARG	CD-NE-CZ	10.18	137.85	123.60
1	B	421	ARG	CD-NE-CZ	10.15	137.81	123.60
1	A	331	PHE	CB-CG-CD1	-10.03	113.78	120.80
1	A	519	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	A	269	GLU	CG-CD-OE1	-9.50	99.31	118.30
1	B	176	GLU	N-CA-CB	-7.76	96.63	110.60
1	A	273	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	218	ARG	CB-CG-CD	7.34	130.68	111.60
1	B	81	GLU	CA-CB-CG	7.33	129.52	113.40
1	B	273	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	218	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	236	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	172	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	341	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	236	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	426	ARG	CA-CB-CG	-6.54	99.01	113.40
1	A	269	GLU	CG-CD-OE2	6.38	131.06	118.30
1	B	393	ARG	CG-CD-NE	6.36	125.16	111.80
1	B	317	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	331	PHE	CA-CB-CG	6.16	128.68	113.90
1	A	519	ARG	CB-CG-CD	6.15	127.58	111.60
1	B	341	ARG	NH1-CZ-NH2	6.08	126.09	119.40
1	A	19	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	317	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	172	ASP	CB-CG-OD1	5.79	123.52	118.30
1	A	390	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	236	ARG	CD-NE-CZ	5.64	131.50	123.60
1	A	302	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	426	ARG	NE-CZ-NH1	5.58	123.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	263	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	222	GLU	CA-CB-CG	5.54	125.59	113.40
1	B	195	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	263	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	430	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	19	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	81	GLU	CA-CB-CG	-5.31	101.72	113.40
1	B	495	ASP	CB-CG-OD1	5.27	123.05	118.30
1	B	176	GLU	CB-CA-C	-5.25	99.91	110.40
1	B	271	GLU	CG-CD-OE1	-5.24	107.83	118.30
1	B	271	GLU	CG-CD-OE2	5.23	128.76	118.30
1	A	334	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	495	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	296	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	227	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	218	ARG	CD-NE-CZ	5.03	130.64	123.60
1	A	296	ARG	NE-CZ-NH1	5.02	122.81	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	51	DDZ	CA
1	B	51	DDZ	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	GLU	Sidechain

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	4154	0	4013	18	1
1	B	4173	0	4029	9	1
2	A	3	0	0	0	0
2	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	35	0	0	1	0
4	B	30	0	0	1	0
5	A	12	0	13	2	0
5	B	12	0	13	1	0
6	A	218	0	0	2	0
6	B	202	0	0	0	0
All	All	8848	0	8068	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)
1:B:51:DDZ:O	4:B:1530:SO4:O2	2.09	0.70
1:A:450:ALA:HB1	6:A:2189:HOH:O	1.94	0.66
1:A:237:GLN:HE22	5:A:1537:MES:HN4	1.47	0.62
1:B:473:TRP:CD1	1:B:509:LYS:HE3	2.41	0.55
1:A:473:TRP:CD1	1:A:509:LYS:HE3	2.43	0.54
1:A:37:ILE:HD11	6:A:2009:HOH:O	2.06	0.54
1:A:51:DDZ:O	4:A:1530:SO4:O3	2.27	0.51
1:A:320:ALA:O	1:A:374:TYR:HB2	2.11	0.51
1:B:320:ALA:O	1:B:374:TYR:HB2	2.11	0.51
1:A:427:TRP:CH2	1:A:428:ARG:HD2	2.46	0.50
1:A:237:GLN:NE2	5:A:1537:MES:HN4	2.08	0.49
1:B:465:MET:HE2	1:B:478:LEU:HA	1.98	0.46
1:A:465:MET:HE1	1:A:478:LEU:HD22	1.99	0.44
1:A:515:GLU:HB3	1:A:519:ARG:NH2	2.31	0.44
1:A:519:ARG:CG	1:A:519:ARG:HH11	2.30	0.44
1:A:465:MET:HE2	1:A:478:LEU:HA	1.99	0.43
1:A:465:MET:CE	1:A:478:LEU:HD22	2.48	0.43
1:A:74:GLU:O	1:A:155:ARG:NH2	2.51	0.42
1:B:98:PRO:HG3	1:B:129:PHE:CE1	2.54	0.42
1:B:465:MET:CE	1:B:478:LEU:HD22	2.49	0.42
1:B:306:GLU:OE1	1:B:309:ASN:ND2	2.52	0.42
1:A:134:SER:O	1:A:164:TYR:HA	2.20	0.41
1:A:306:GLU:OE1	1:A:309:ASN:ND2	2.54	0.41
1:A:426:ARG:HH11	1:A:426:ARG:CG	2.33	0.41
1:B:237:GLN:NE2	5:B:1536:MES:H32	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.92	0.40
1:B:465:MET:HE1	1:B:478:LEU:HD22	2.03	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:A:151:GLU:OE2	1:B:341:ARG:NH1[3_555]	2.18	0.02

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	522/536 (97%)	507 (97%)	15 (3%)	0	100	100
1	B	524/536 (98%)	508 (97%)	16 (3%)	0	100	100
All	All	1046/1072 (98%)	1015 (97%)	31 (3%)	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	419/428 (98%)	414 (99%)	5 (1%)	78	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	421/428 (98%)	415 (99%)	6 (1%)	74 77
All	All	840/856 (98%)	829 (99%)	11 (1%)	76 79

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	MET
1	A	270	ASP
1	A	309	ASN
1	A	359	TYR
1	A	426	ARG
1	B	110	MET
1	B	270	ASP
1	B	309	ASN
1	B	334	ASP
1	B	359	TYR
1	B	421	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	237	GLN
1	A	309	ASN
1	B	197	GLN
1	B	309	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)

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	1,3	4,6,7	27.09	3 (75%)	2,7,9	3.26	1 (50%)
1	DDZ	B	51	1,3	4,6,7	28.07	3 (75%)	2,7,9	3.23	2 (100%)

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	1,3	1/1/2/3	0/2/6/8	0/0/0/0
1	DDZ	B	51	1,3	1/1/2/3	0/2/6/8	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	51	DDZ	OG1-CB	-6.69	1.23	1.40
1	A	51	DDZ	OG1-CB	-6.39	1.24	1.40
1	B	51	DDZ	O-C	6.29	1.49	1.19
1	A	51	DDZ	O-C	6.29	1.49	1.19
1	A	51	DDZ	OG2-CB	53.44	2.79	1.40
1	B	51	DDZ	OG2-CB	55.37	2.84	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	DDZ	O-C-CA	-4.18	114.28	125.69
1	B	51	DDZ	O-C-CA	-4.05	114.61	125.69
1	B	51	DDZ	C-CA-N	-2.09	105.34	109.95

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	51	DDZ	CA
1	B	51	DDZ	CA

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	51	DDZ	1	0
1	B	51	DDZ	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
4	SO4	A	1530	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	A	1531	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	A	1532	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	A	1533	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	A	1534	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	A	1535	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	A	1536	-	4,4,4	0.32	0	6,6,6	0.07	0
5	MES	A	1537	-	12,12,12	2.16	1 (8%)	15,16,16	1.67	3 (20%)
4	SO4	B	1530	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	B	1531	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	B	1532	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	B	1533	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	B	1534	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	B	1535	-	4,4,4	0.32	0	6,6,6	0.06	0
5	MES	B	1536	-	12,12,12	2.18	1 (8%)	15,16,16	1.68	3 (20%)

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
4	SO4	A	1530	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1531	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1532	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1533	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1534	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1535	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1536	-	-	0/0/0/0	0/0/0/0
5	MES	A	1537	-	-	0/6/14/14	0/1/1/1
4	SO4	B	1530	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1531	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1532	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1533	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1534	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1535	-	-	0/0/0/0	0/0/0/0
5	MES	B	1536	-	-	0/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1536	MES	C8-S	-7.28	1.66	1.77
5	A	1537	MES	C8-S	-7.20	1.66	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1537	MES	O3S-S-C8	2.16	109.48	104.99
5	B	1536	MES	O3S-S-C8	2.17	109.50	104.99
5	A	1537	MES	O2S-S-C8	3.66	109.45	106.87
5	B	1536	MES	O1S-S-C8	3.66	109.45	106.87
5	A	1537	MES	O1S-S-C8	3.66	109.46	106.87
5	B	1536	MES	O2S-S-C8	3.69	109.48	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1530	SO4	1	0
5	A	1537	MES	2	0
4	B	1530	SO4	1	0
5	B	1536	MES	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	525/536 (97%)	0.07	18 (3%) 49 50	15, 29, 51, 89	18 (3%)
1	B	525/536 (97%)	0.09	19 (3%) 46 48	15, 30, 52, 78	17 (3%)
All	All	1050/1072 (97%)	0.08	37 (3%) 48 49	15, 29, 51, 89	35 (3%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	PHE	6.5
1	A	329	PRO	5.4
1	A	80	LEU	4.3
1	B	504	ASP	4.1
1	A	77	THR	3.8
1	A	331	PHE	3.8
1	A	78	PRO	3.6
1	B	82	GLY	3.6
1	A	327	ALA	3.3
1	B	447	GLU	3.3
1	A	429	GLY	3.2
1	A	447	GLU	3.1
1	B	78	PRO	3.1
1	B	151	GLU	3.1
1	B	429	GLY	3.0
1	A	173	THR	2.9
1	A	3	LYS	2.9
1	B	79	GLU	2.9
1	B	84	PRO	2.7
1	B	331	PHE	2.6
1	B	152	SER	2.6
1	B	10	ILE	2.6
1	A	79	GLU	2.5
1	B	328	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	83	LYS	2.5
1	A	81	GLU	2.5
1	B	3	LYS	2.5
1	B	173	THR	2.4
1	B	252	ASP	2.4
1	A	481	PRO	2.3
1	B	329	PRO	2.3
1	A	494	ARG	2.2
1	B	251	ALA	2.2
1	A	504	ASP	2.1
1	A	84	PRO	2.1
1	B	77	THR	2.1
1	B	172	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	DDZ	A	51	7/8	0.92	0.11	-	21,25,29,33	0
1	DDZ	B	51	7/8	0.95	0.15	-	27,27,29,29	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	SO4	B	1533	5/5	0.88	0.18	3.14	42,49,69,70	0
4	SO4	B	1534	5/5	0.89	0.20	2.43	45,53,59,70	0
5	MES	A	1537	12/12	0.85	0.20	2.37	40,48,55,56	0
4	SO4	B	1532	5/5	0.91	0.24	1.75	65,65,69,70	0
4	SO4	A	1535	5/5	0.80	0.20	1.70	51,67,79,81	0
4	SO4	A	1534	5/5	0.91	0.14	1.24	57,60,71,75	0
5	MES	B	1536	12/12	0.90	0.16	0.87	37,44,51,52	0
4	SO4	A	1533	5/5	0.91	0.17	0.44	61,61,71,71	0
4	SO4	A	1530	5/5	0.94	0.11	-0.63	44,51,54,54	0
4	SO4	B	1530	5/5	0.94	0.13	-0.75	40,45,47,52	0
4	SO4	A	1531	5/5	0.97	0.09	-0.92	41,43,45,46	0
4	SO4	B	1531	5/5	0.98	0.09	-1.31	40,40,43,45	0
3	CA	B	1529	1/1	0.96	0.06	-4.39	28,28,28,28	0
3	CA	A	1529	1/1	0.98	0.06	-4.44	31,31,31,31	0
4	SO4	A	1532	5/5	0.86	0.20	-	43,55,67,73	0
2	CL	B	1452	1/1	0.97	0.04	-	57,57,57,57	0
2	CL	B	1539	1/1	0.86	0.09	-	70,70,70,70	0
4	SO4	B	1535	5/5	0.88	0.18	-	55,61,62,64	0
2	CL	A	1539	1/1	0.53	0.16	-	75,75,75,75	0
2	CL	A	1541	1/1	0.92	0.20	-	63,63,63,63	0
4	SO4	A	1536	5/5	0.92	0.25	-	75,83,88,93	0
2	CL	B	1538	1/1	0.95	0.07	-	51,51,51,51	0
2	CL	B	1537	1/1	0.93	0.11	-	75,75,75,75	0
2	CL	B	1543	1/1	0.91	0.04	-	63,63,63,63	0
2	CL	B	1540	1/1	0.89	0.24	-	66,66,66,66	0
2	CL	A	1538	1/1	0.90	0.07	-	65,65,65,65	0
2	CL	B	1541	1/1	0.87	0.12	-	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.