



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 28, 2026 – 01:38 PM UTC

PDB ID : 2VGK / pdb_00002vgk
Title : Crystal structure of Actinomadura R39 DD-peptidase complexed with a peptidoglycan-mimetic cephalosporin
Authors : Sauvage, E.; kerff, F.; Herman, R.; Charlier, P.
Deposited on : 2007-11-14
Resolution : 2.25 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 ⓘ 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

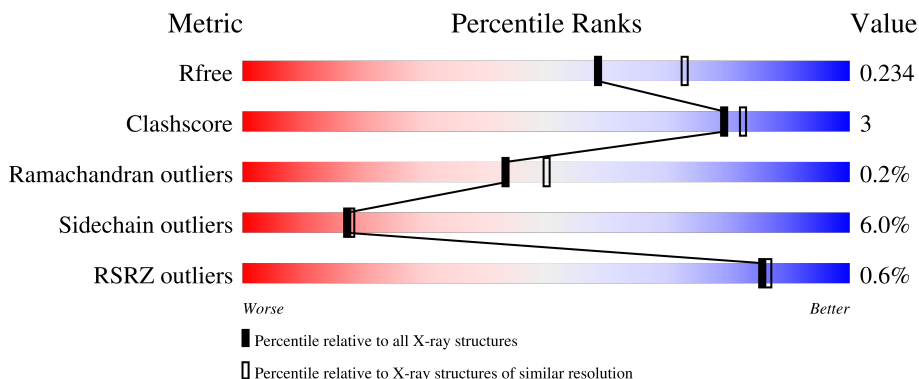
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	489	 87% 8% .
1	B	489	 % 84% 10% . 5%
1	C	489	 86% 9% . 5%
1	D	489	 % 87% 8% . .

2 Entry composition [i](#)

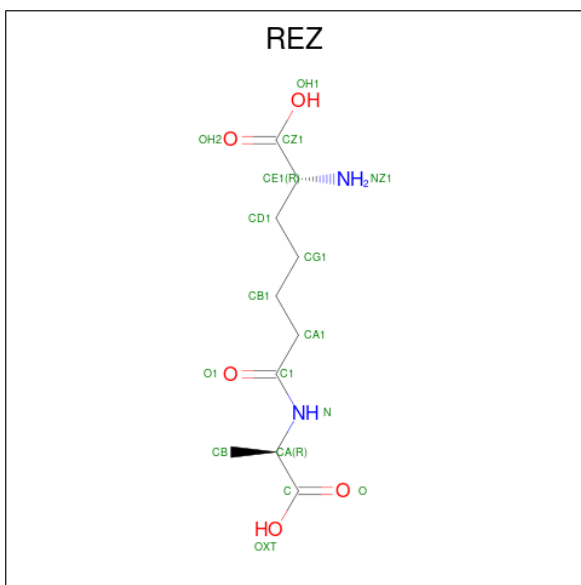
There are 5 unique types of molecules in this entry. The entry contains 14044 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-ALANYL-D-ALANINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	467	Total 3353	C 2076	N 565	O 706	S 6	0	0	1
1	B	466	Total 3344	C 2071	N 564	O 703	S 6	0	0	1
1	C	466	Total 3344	C 2071	N 564	O 703	S 6	0	0	1
1	D	467	Total 3353	C 2076	N 565	O 706	S 6	0	0	1

- Molecule 2 is (2R)-2-AMINO-7-[[[(1R)-1-CARBOXYETHYL]AMINO]-7-OXOHEPTANOI
C ACID (CCD ID: REZ) (formula: C₁₀H₁₈N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 17	C 10	N 2	O 5	0	0
2	B	1	Total 17	C 10	N 2	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	17	10	2	5	0	0

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



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

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		

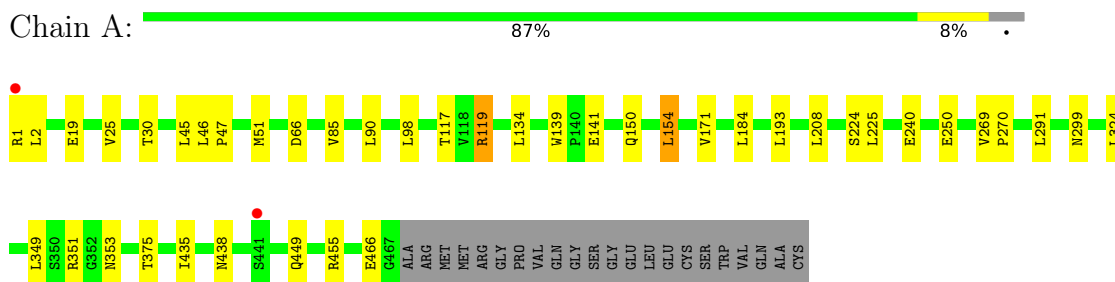
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	111	Total	O	0	0
			111	111		
5	C	123	Total	O	0	0
			123	123		
5	D	146	Total	O	0	0
			146	146		

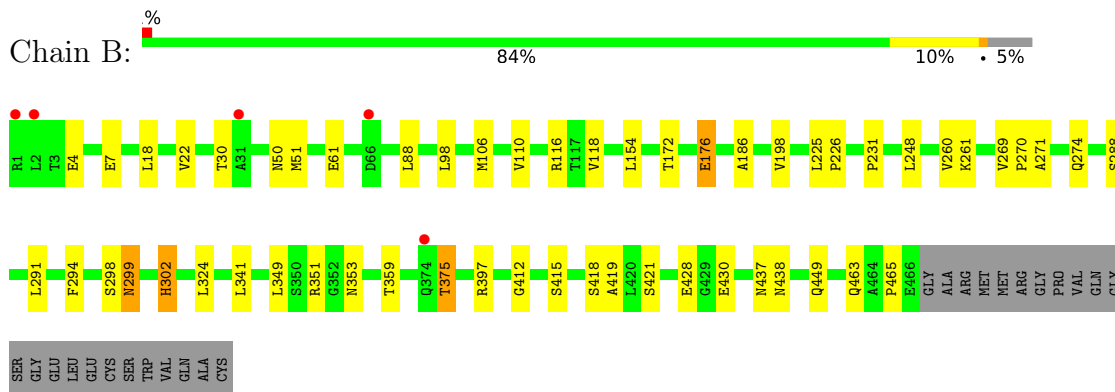
3 Residue-property plots [i](#)

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.

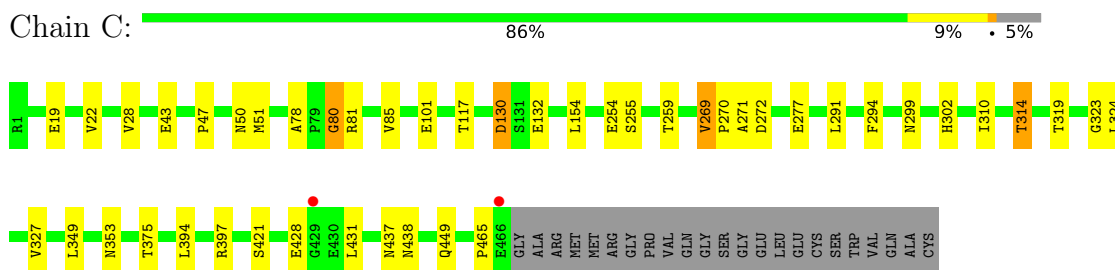
- Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



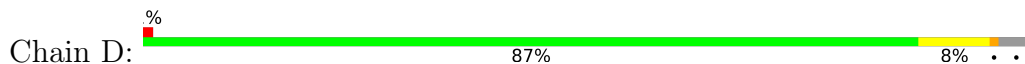
- Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

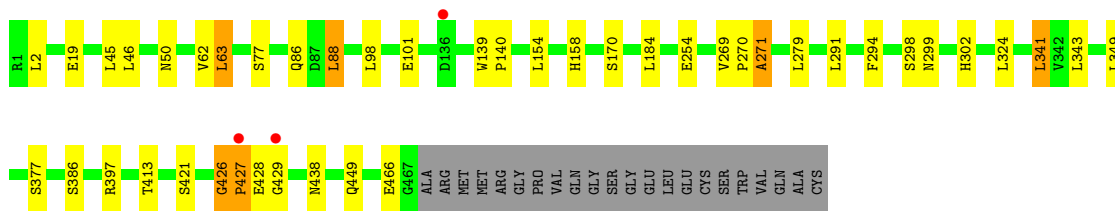


- Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



- Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.14Å 93.35Å 109.10Å 90.00° 94.98° 90.00°	Depositor
Resolution (Å)	15.71 – 2.25 15.71 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.71-2.25) 99.3 (15.71-2.25)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.25Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.286 0.233 , 0.234	Depositor DCC
R_{free} test set	4953 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtrriage
Anisotropy	0.148	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.032 for l,-k,h	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14044	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: REZ, SO4, MG

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	0.68	1/3412 (0.0%)	0.90	0/4668
1	B	0.67	1/3403 (0.0%)	0.91	3/4656 (0.1%)
1	C	0.68	1/3403 (0.0%)	0.94	2/4656 (0.0%)
1	D	0.71	1/3412 (0.0%)	0.97	3/4668 (0.1%)
All	All	0.68	4/13630 (0.0%)	0.93	8/18648 (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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	GLU	C-N	-7.13	1.23	1.33
1	B	465	PRO	C-N	-6.71	1.24	1.33
1	D	466	GLU	C-N	-6.56	1.24	1.33
1	C	465	PRO	C-N	-6.28	1.24	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	VAL	CA-C-N	7.42	129.12	119.84
1	B	269	VAL	C-N-CA	7.42	129.12	119.84
1	C	269	VAL	CA-C-N	6.87	128.43	119.84
1	C	269	VAL	C-N-CA	6.87	128.43	119.84
1	D	269	VAL	CA-C-N	6.80	128.34	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	426	GLY	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	3353	0	3201	13	0
1	B	3344	0	3195	23	0
1	C	3344	0	3195	18	0
1	D	3353	0	3201	17	0
2	A	17	0	16	0	0
2	B	17	0	16	0	0
2	C	17	0	16	0	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
3	C	25	0	0	0	0
3	D	25	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	115	0	0	3	0
5	B	111	0	0	1	0
5	C	123	0	0	2	0
5	D	146	0	0	3	0
All	All	14044	0	12840	71	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 3.

The worst 5 of 71 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:D:429:GLY:HA2	5:D:2137:HOH:O	1.70	0.90
1:B:351:ARG:HH22	1:B:415:SER:HB2	1.53	0.73
1:D:294:PHE:HB2	1:D:302:HIS:HD2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:GLU:O	1:B:7:GLU:HG2	1.90	0.70
1:C:294:PHE:HB2	1:C:302:HIS:HD2	1.57	0.68

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	465/489 (95%)	444 (96%)	21 (4%)	0	100	100
1	B	464/489 (95%)	446 (96%)	18 (4%)	0	100	100
1	C	464/489 (95%)	443 (96%)	19 (4%)	2 (0%)	30	31
1	D	465/489 (95%)	442 (95%)	21 (4%)	2 (0%)	30	31
All	All	1858/1956 (95%)	1775 (96%)	79 (4%)	4 (0%)	43	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	271	ALA
1	D	427	PRO
1	C	130	ASP
1	C	80	GLY

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	339/356 (95%)	319 (94%)	20 (6%)	18	18
1	B	338/356 (95%)	317 (94%)	21 (6%)	16	16
1	C	338/356 (95%)	318 (94%)	20 (6%)	18	18
1	D	339/356 (95%)	319 (94%)	20 (6%)	18	18
All	All	1354/1424 (95%)	1273 (94%)	81 (6%)	17	18

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	375	THR
1	D	170	SER
1	C	428	GLU
1	D	77	SER
1	D	298	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	449	GLN
1	D	302	HIS
1	C	299	ASN
1	D	437	ASN
1	D	50	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](#)

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

Of 27 ligands modelled in this entry, 4 are monoatomic - leaving 23 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	D	602	-	4,4,4	0.28	0	6,6,6	0.11	0
2	REZ	B	500	-	15,16,16	0.81	0	17,20,20	1.07	1 (5%)
3	SO4	A	600	-	4,4,4	0.26	0	6,6,6	0.33	0
3	SO4	C	601	-	4,4,4	0.24	0	6,6,6	0.34	0
3	SO4	D	603	-	4,4,4	0.23	0	6,6,6	0.25	0
3	SO4	C	600	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	A	601	-	4,4,4	0.29	0	6,6,6	0.43	0
3	SO4	B	603	-	4,4,4	0.24	0	6,6,6	0.24	0
3	SO4	B	604	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	D	604	-	4,4,4	0.28	0	6,6,6	0.17	0
3	SO4	C	604	-	4,4,4	0.22	0	6,6,6	0.19	0
3	SO4	B	602	-	4,4,4	0.23	0	6,6,6	0.13	0
3	SO4	C	603	-	4,4,4	0.35	0	6,6,6	0.34	0
3	SO4	A	603	-	4,4,4	0.26	0	6,6,6	0.19	0
3	SO4	A	604	-	4,4,4	0.27	0	6,6,6	0.32	0
3	SO4	D	601	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	D	600	-	4,4,4	0.19	0	6,6,6	0.30	0
2	REZ	A	500	-	15,16,16	0.76	0	17,20,20	1.42	1 (5%)
3	SO4	B	600	-	4,4,4	0.27	0	6,6,6	0.23	0
3	SO4	A	602	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	C	602	-	4,4,4	0.23	0	6,6,6	0.10	0
2	REZ	C	500	-	15,16,16	0.79	0	17,20,20	1.23	1 (5%)
3	SO4	B	601	-	4,4,4	0.24	0	6,6,6	0.15	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	REZ	C	500	-	-	3/19/19/19	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	REZ	B	500	-	-	3/19/19/19	-
2	REZ	A	500	-	-	2/19/19/19	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	REZ	CA-N-C1	4.66	128.21	121.13
2	B	500	REZ	CA-N-C1	3.41	126.31	121.13
2	C	500	REZ	CA-N-C1	3.29	126.13	121.13

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	REZ	C-CA-N-C1
2	A	500	REZ	CB-CA-N-C1
2	B	500	REZ	C1-CA1-CB1-CG1
2	B	500	REZ	NZ1-CE1-CZ1-OH2
2	C	500	REZ	CG1-CD1-CE1-NZ1

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	467/489 (95%)	-0.23	2 (0%) 88 89	13, 25, 42, 68	0
1	B	466/489 (95%)	-0.22	5 (1%) 78 79	16, 27, 42, 59	0
1	C	466/489 (95%)	-0.27	2 (0%) 88 89	16, 25, 38, 57	0
1	D	467/489 (95%)	-0.32	3 (0%) 85 86	10, 22, 36, 50	0
All	All	1866/1956 (95%)	-0.26	12 (0%) 85 86	10, 25, 40, 68	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	427	PRO	3.6
1	B	2	LEU	2.9
1	D	136	ASP	2.5
1	C	466	GLU	2.4
1	D	429	GLY	2.3

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(\AA^2)	Q<0.9
3	SO4	B	602	5/5	0.75	0.19	115,115,115,115	0
3	SO4	C	602	5/5	0.75	0.17	91,91,91,91	0
3	SO4	B	604	5/5	0.77	0.16	92,92,92,92	0
3	SO4	D	602	5/5	0.81	0.12	62,63,64,64	0
2	REZ	B	500	17/17	0.83	0.11	33,35,40,40	0
3	SO4	A	602	5/5	0.86	0.11	80,81,81,81	0
3	SO4	D	604	5/5	0.87	0.12	53,53,54,54	0
3	SO4	A	604	5/5	0.88	0.10	60,60,60,60	0
2	REZ	C	500	17/17	0.88	0.09	29,30,34,34	0
3	SO4	B	600	5/5	0.89	0.11	52,53,53,53	0
2	REZ	A	500	17/17	0.90	0.08	26,28,32,33	0
3	SO4	C	604	5/5	0.90	0.13	48,48,49,49	0
3	SO4	A	603	5/5	0.93	0.13	56,56,56,56	0
3	SO4	A	601	5/5	0.94	0.07	31,32,33,34	0
3	SO4	D	603	5/5	0.96	0.08	37,37,38,38	0
3	SO4	C	600	5/5	0.96	0.09	55,56,56,56	0
4	MG	A	611	1/1	0.96	0.04	13,13,13,13	0
4	MG	D	611	1/1	0.96	0.14	2,2,2,2	0
3	SO4	D	601	5/5	0.97	0.06	35,37,37,37	0
3	SO4	A	600	5/5	0.97	0.06	29,30,30,31	0
3	SO4	C	601	5/5	0.97	0.07	30,31,31,32	0
3	SO4	B	603	5/5	0.97	0.09	30,31,31,32	0
4	MG	A	610	1/1	0.97	0.08	13,13,13,13	0
3	SO4	C	603	5/5	0.97	0.07	25,27,28,29	0
4	MG	D	610	1/1	0.97	0.10	18,18,18,18	0
3	SO4	B	601	5/5	0.97	0.10	38,38,39,39	0
3	SO4	D	600	5/5	0.99	0.04	17,18,18,19	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.