



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:38 am GMT

PDB ID : 2VGK  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

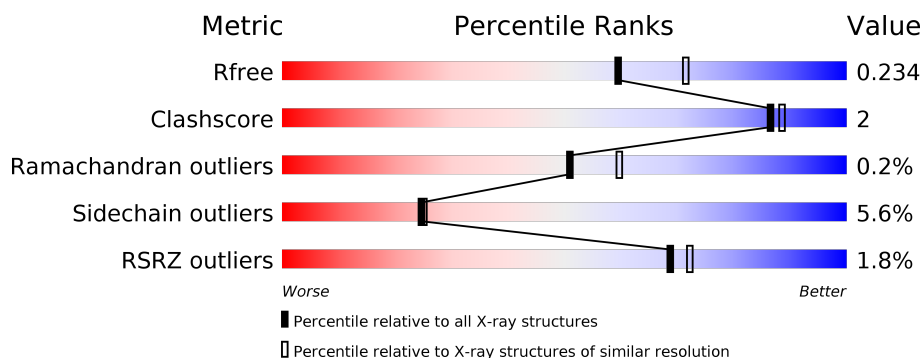
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>• •</div> </div> </div>
1	B	489	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• 5%</div> </div> </div>
1	C	489	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>• 5%</div> </div> </div>
1	D	489	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>• •</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	REZ	B	500	-	-	-	X
3	SO4	A	602	-	-	-	X
3	SO4	B	604	-	-	-	X
3	SO4	D	604	-	-	-	X
4	MG	D	611	-	-	-	X

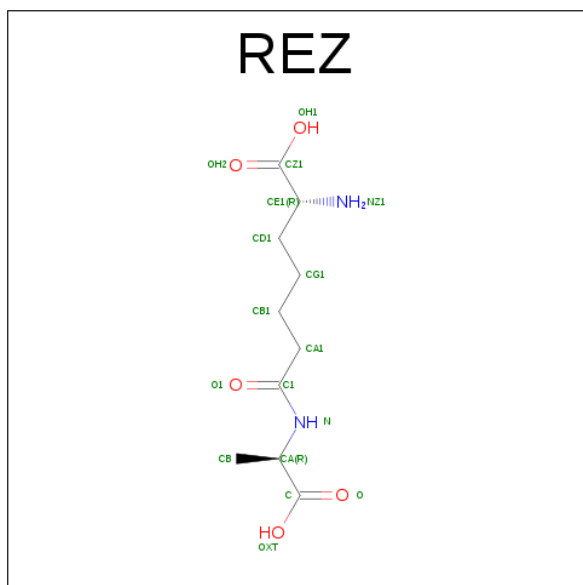


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-ALANYL-D-ALANINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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-OXOHEPTANOIC ACID (three-letter code: REZ) (formula: C<sub>10</sub>H<sub>18</sub>N<sub>2</sub>O<sub>5</sub>).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	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	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
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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

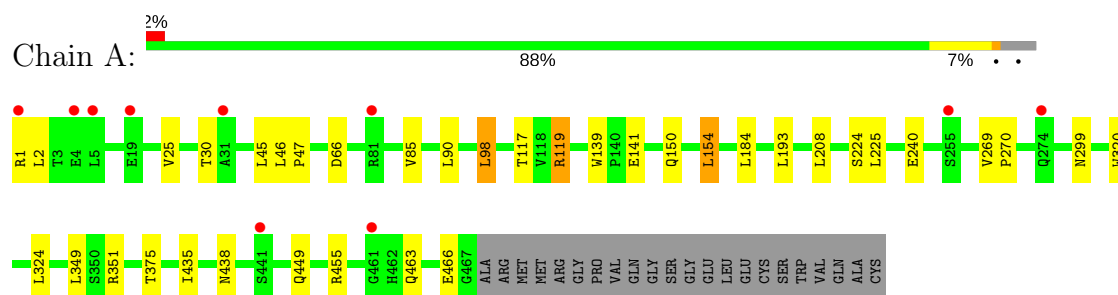
- Molecule 5 is water.

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

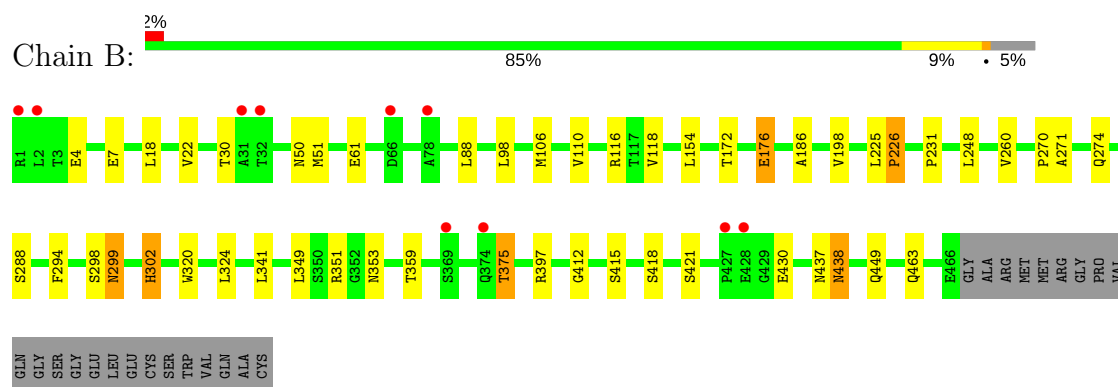
### 3 Residue-property plots [i](#)

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

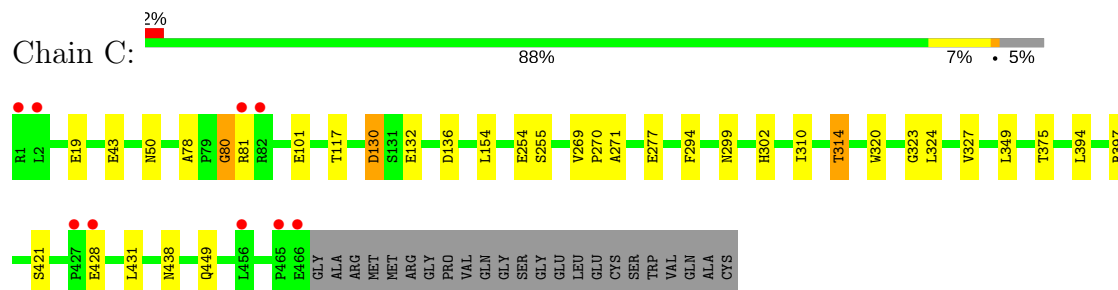
#### • Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



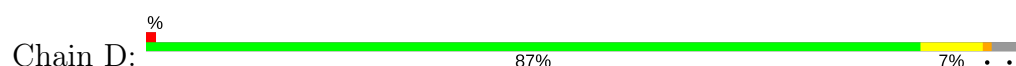
#### • Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

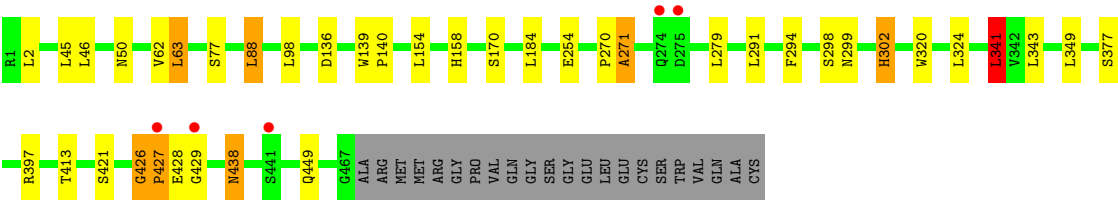


#### • Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE



#### • 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, $\alpha$ , $\beta$ , $\gamma$	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) 99.2 (15.71-2.25)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.230 , 0.286 0.233 , 0.234	Depositor DCC
$R_{free}$ test set	4949 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.032 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: REZ, MG, 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	0.49	1/3412 (0.0%)	0.63	2/4668 (0.0%)
1	B	0.47	0/3403	0.62	0/4656
1	C	0.49	0/3403	0.62	0/4656
1	D	0.50	0/3412	0.65	1/4668 (0.0%)
All	All	0.49	1/13630 (0.0%)	0.63	3/18648 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	GLU	C-N	-5.38	1.23	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	LEU	CA-CB-CG	6.03	129.17	115.30
1	D	341	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	46	LEU	CA-CB-CG	5.07	126.96	115.30

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 ⓘ

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	12	0
1	B	3344	0	3195	23	0
1	C	3344	0	3195	13	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	65	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 (65) 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
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
1:D:341:LEU:HD13	1:D:343:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:THR:HG23	5:D:2134:HOH:O	1.96	0.64
1:B:172:THR:HG22	1:B:231:PRO:HB3	1.81	0.62
1:B:288:SER:HB2	1:B:375:THR:HG21	1.82	0.61
1:B:397:ARG:HH12	1:B:449:GLN:HE21	1.47	0.61
1:C:323:GLY:O	1:C:327:VAL:HG23	2.02	0.60
1:D:426:GLY:C	1:D:428:GLU:H	2.05	0.59
1:D:270:PRO:O	1:D:271:ALA:HB3	2.02	0.59
1:D:294:PHE:HB2	1:D:302:HIS:CD2	2.37	0.58
1:D:426:GLY:C	1:D:428:GLU:N	2.56	0.58
1:C:294:PHE:HB2	1:C:302:HIS:CD2	2.39	0.56
1:C:130:ASP:HB3	1:C:132:GLU:H	1.69	0.56
1:D:88:LEU:HD21	1:D:279:LEU:HD12	1.88	0.55
1:D:270:PRO:O	1:D:271:ALA:CB	2.56	0.54
1:B:51:MET:HE2	1:B:353:ASN:HB3	1.91	0.52
1:D:158:HIS:HD2	5:D:2059:HOH:O	1.92	0.51
1:C:78:ALA:HB2	1:C:277:GLU:OE2	2.12	0.50
1:B:294:PHE:HB2	1:B:302:HIS:HD2	1.77	0.50
1:B:299:ASN:HD22	1:B:302:HIS:H	1.60	0.49
1:A:208:LEU:HD22	1:A:225:LEU:HD13	1.95	0.49
1:A:47:PRO:HD2	5:A:2088:HOH:O	2.11	0.49
1:D:45:LEU:HD22	1:D:438:ASN:HB2	1.94	0.49
1:C:270:PRO:O	1:C:271:ALA:HB3	2.12	0.49
1:A:139:TRP:HB3	1:A:141:GLU:OE1	2.13	0.48
1:A:184:LEU:HD21	1:A:193:LEU:HD13	1.96	0.48
1:C:310:ILE:O	1:C:314:THR:HB	2.13	0.48
1:C:50:ASN:ND2	1:C:421:SER:OG	2.47	0.48
1:A:85:VAL:O	1:A:119:ARG:HB2	2.14	0.47
1:B:397:ARG:HH12	1:B:449:GLN:NE2	2.10	0.47
1:B:61:GLU:HG2	5:B:2079:HOH:O	2.14	0.47
1:C:101:GLU:HG2	5:C:2032:HOH:O	2.13	0.47
1:D:397:ARG:HH12	1:D:449:GLN:HE21	1.62	0.46
1:D:62:VAL:HG12	1:D:63:LEU:HD13	1.98	0.46
1:A:25:VAL:HG22	1:A:435:ILE:HG23	1.98	0.46
1:A:351:ARG:NH2	5:A:2089:HOH:O	2.49	0.45
1:C:397:ARG:HH12	1:C:449:GLN:HE21	1.65	0.45
1:B:270:PRO:O	1:B:271:ALA:HB3	2.17	0.44
1:A:150:GLN:HE22	1:A:240:GLU:H	1.66	0.44
1:A:45:LEU:HD22	1:A:438:ASN:HB2	1.99	0.44
1:A:449:GLN:NE2	5:A:2107:HOH:O	2.50	0.44
1:B:437:ASN:C	1:B:438:ASN:HD22	2.21	0.44
1:B:341:LEU:HG	1:B:359:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ASN:ND2	1:D:421:SER:OG	2.52	0.43
1:B:351:ARG:NH2	1:B:415:SER:O	2.51	0.43
1:B:118:VAL:HB	1:B:260:VAL:HA	2.00	0.43
1:B:397:ARG:NH1	1:B:449:GLN:HE21	2.16	0.43
1:C:269:VAL:HA	1:C:270:PRO:HD3	1.89	0.42
1:C:80:GLY:HA3	5:C:2026:HOH:O	2.19	0.42
1:D:426:GLY:HA2	1:D:427:PRO:HD2	1.92	0.42
1:B:186:ALA:HB1	1:B:248:LEU:HD21	2.01	0.42
1:B:225:LEU:HA	1:B:226:PRO:HD3	1.84	0.42
1:B:412:GLY:O	1:B:418:SER:HA	2.20	0.42
1:A:90:LEU:HG	1:A:154:LEU:HD11	2.01	0.42
1:A:269:VAL:HA	1:A:270:PRO:HD3	1.86	0.42
1:B:351:ARG:HH22	1:B:415:SER:CB	2.27	0.42
1:B:106:MET:O	1:B:110:VAL:HG23	2.20	0.41
1:B:50:ASN:ND2	1:B:421:SER:OG	2.53	0.41
1:C:294:PHE:CD2	1:C:302:HIS:HB2	2.54	0.41
1:B:176:GLU:H	1:B:176:GLU:HG2	1.52	0.41
1:D:139:TRP:HA	1:D:140:PRO:HD3	1.99	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	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%)	38	42
1	D	465/489 (95%)	442 (95%)	21 (4%)	2 (0%)	38	42
All	All	1858/1956 (95%)	1775 (96%)	79 (4%)	4 (0%)	51	60

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 ⓘ

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%)	323 (95%)	16 (5%)	30	34
1	B	338/356 (95%)	317 (94%)	21 (6%)	21	20
1	C	338/356 (95%)	320 (95%)	18 (5%)	26	28
1	D	339/356 (95%)	318 (94%)	21 (6%)	21	20
All	All	1354/1424 (95%)	1278 (94%)	76 (6%)	25	25

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ARG
1	A	2	LEU
1	A	30	THR
1	A	66	ASP
1	A	98	LEU
1	A	117	THR
1	A	119	ARG
1	A	154	LEU
1	A	224	SER
1	A	299	ASN
1	A	320	TRP
1	A	324	LEU
1	A	349	LEU
1	A	375	THR
1	A	455	ARG
1	A	463	GLN
1	B	18	LEU
1	B	22	VAL

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Mol	Chain	Res	Type
1	B	30	THR
1	B	88	LEU
1	B	98	LEU
1	B	116	ARG
1	B	154	LEU
1	B	176	GLU
1	B	198	VAL
1	B	226	PRO
1	B	274	GLN
1	B	298	SER
1	B	299	ASN
1	B	302	HIS
1	B	320	TRP
1	B	324	LEU
1	B	349	LEU
1	B	375	THR
1	B	430	GLU
1	B	438	ASN
1	B	463	GLN
1	C	19	GLU
1	C	43	GLU
1	C	81	ARG
1	C	117	THR
1	C	136	ASP
1	C	154	LEU
1	C	254	GLU
1	C	255	SER
1	C	299	ASN
1	C	314	THR
1	C	320	TRP
1	C	324	LEU
1	C	349	LEU
1	C	375	THR
1	C	394	LEU
1	C	428	GLU
1	C	431	LEU
1	C	438	ASN
1	D	2	LEU
1	D	46	LEU
1	D	63	LEU
1	D	77	SER
1	D	88	LEU

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Mol	Chain	Res	Type
1	D	98	LEU
1	D	136	ASP
1	D	154	LEU
1	D	170	SER
1	D	184	LEU
1	D	254	GLU
1	D	291	LEU
1	D	298	SER
1	D	299	ASN
1	D	302	HIS
1	D	320	TRP
1	D	324	LEU
1	D	341	LEU
1	D	349	LEU
1	D	377	SER
1	D	438	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	50	ASN
1	A	150	GLN
1	A	299	ASN
1	A	312	GLN
1	A	437	ASN
1	A	449	GLN
1	A	463	GLN
1	B	50	ASN
1	B	150	GLN
1	B	158	HIS
1	B	274	GLN
1	B	299	ASN
1	B	302	HIS
1	B	396	ASN
1	B	449	GLN
1	C	50	ASN
1	C	299	ASN
1	C	302	HIS
1	C	366	GLN
1	C	437	ASN
1	C	449	GLN

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Mol	Chain	Res	Type
1	D	50	ASN
1	D	86	GLN
1	D	150	GLN
1	D	158	HIS
1	D	299	ASN
1	D	302	HIS
1	D	437	ASN
1	D	449	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
2	REZ	A	500	-	8,16,16	0.20	0	9,20,20	1.63	1 (11%)
3	SO4	A	600	-	4,4,4	0.17	0	6,6,6	0.30	0
3	SO4	A	601	-	4,4,4	0.21	0	6,6,6	0.43	0
3	SO4	A	602	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	A	603	-	4,4,4	0.17	0	6,6,6	0.14	0
3	SO4	A	604	-	4,4,4	0.19	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	REZ	B	500	-	8,16,16	0.33	0	9,20,20	1.20	1 (11%)
3	SO4	B	600	-	4,4,4	0.18	0	6,6,6	0.24	0
3	SO4	B	601	-	4,4,4	0.15	0	6,6,6	0.13	0
3	SO4	B	602	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	B	603	-	4,4,4	0.15	0	6,6,6	0.19	0
3	SO4	B	604	-	4,4,4	0.16	0	6,6,6	0.10	0
2	REZ	C	500	-	8,16,16	0.30	0	9,20,20	1.26	1 (11%)
3	SO4	C	600	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	C	601	-	4,4,4	0.15	0	6,6,6	0.33	0
3	SO4	C	602	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	C	603	-	4,4,4	0.27	0	6,6,6	0.30	0
3	SO4	C	604	-	4,4,4	0.15	0	6,6,6	0.24	0
3	SO4	D	600	-	4,4,4	0.09	0	6,6,6	0.31	0
3	SO4	D	601	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	D	602	-	4,4,4	0.20	0	6,6,6	0.14	0
3	SO4	D	603	-	4,4,4	0.14	0	6,6,6	0.22	0
3	SO4	D	604	-	4,4,4	0.21	0	6,6,6	0.14	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	A	500	-	-	0/11/19/19	0/0/0/0
3	SO4	A	600	-	-	0/0/0/0	0/0/0/0
3	SO4	A	601	-	-	0/0/0/0	0/0/0/0
3	SO4	A	602	-	-	0/0/0/0	0/0/0/0
3	SO4	A	603	-	-	0/0/0/0	0/0/0/0
3	SO4	A	604	-	-	0/0/0/0	0/0/0/0
2	REZ	B	500	-	-	0/11/19/19	0/0/0/0
3	SO4	B	600	-	-	0/0/0/0	0/0/0/0
3	SO4	B	601	-	-	0/0/0/0	0/0/0/0
3	SO4	B	602	-	-	0/0/0/0	0/0/0/0
3	SO4	B	603	-	-	0/0/0/0	0/0/0/0
3	SO4	B	604	-	-	0/0/0/0	0/0/0/0
2	REZ	C	500	-	-	0/11/19/19	0/0/0/0
3	SO4	C	600	-	-	0/0/0/0	0/0/0/0
3	SO4	C	601	-	-	0/0/0/0	0/0/0/0
3	SO4	C	602	-	-	0/0/0/0	0/0/0/0
3	SO4	C	603	-	-	0/0/0/0	0/0/0/0
3	SO4	C	604	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	D	600	-	-	0/0/0/0	0/0/0/0
3	SO4	D	601	-	-	0/0/0/0	0/0/0/0
3	SO4	D	602	-	-	0/0/0/0	0/0/0/0
3	SO4	D	603	-	-	0/0/0/0	0/0/0/0
3	SO4	D	604	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	REZ	CA-N-C1	2.22	126.13	122.89
2	B	500	REZ	CA-N-C1	2.34	126.31	122.89
2	A	500	REZ	CA-N-C1	3.65	128.21	122.89

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	467/489 (95%)	-0.21	10 (2%) 64 67	13, 25, 42, 68	0
1	B	466/489 (95%)	-0.18	10 (2%) 64 67	16, 27, 42, 59	0
1	C	466/489 (95%)	-0.21	9 (1%) 67 70	16, 25, 38, 57	0
1	D	467/489 (95%)	-0.30	5 (1%) 80 83	10, 22, 36, 50	0
All	All	1866/1956 (95%)	-0.23	34 (1%) 69 72	10, 25, 40, 68	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	ALA	5.5
1	C	466	GLU	5.0
1	B	427	PRO	4.9
1	A	1	ARG	4.3
1	B	374	GLN	4.1
1	A	31	ALA	3.9
1	A	4	GLU	3.9
1	A	441	SER	3.8
1	C	81	ARG	3.8
1	C	82	ARG	3.7
1	B	2	LEU	3.7
1	D	427	PRO	3.3
1	B	1	ARG	3.1
1	B	428	GLU	2.9
1	D	429	GLY	2.8
1	B	32	THR	2.8
1	D	274	GLN	2.6
1	A	274	GLN	2.6
1	C	2	LEU	2.6
1	A	5	LEU	2.5
1	C	465	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	275	ASP	2.4
1	C	456	LEU	2.4
1	A	19	GLU	2.4
1	A	255	SER	2.4
1	B	66	ASP	2.4
1	A	81	ARG	2.3
1	B	78	ALA	2.3
1	C	1	ARG	2.2
1	D	441	SER	2.2
1	C	428	GLU	2.1
1	B	369	SER	2.1
1	A	461	GLY	2.1
1	C	427	PRO	2.1

## 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 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	A	602	5/5	0.91	0.26	5.49	80,81,81,81	0
4	MG	D	611	1/1	0.98	0.20	4.71	2,2,2,2	0
3	SO4	B	604	5/5	0.92	0.22	2.41	92,92,92,92	0
2	REZ	B	500	17/17	0.82	0.17	2.14	33,35,40,40	0
3	SO4	D	604	5/5	0.95	0.20	2.07	53,53,54,54	0
3	SO4	C	600	5/5	0.97	0.13	1.54	55,56,56,56	0
2	REZ	C	500	17/17	0.90	0.14	1.34	29,30,34,34	0
2	REZ	A	500	17/17	0.91	0.13	0.56	26,28,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	D	610	1/1	0.99	0.09	-0.80	18,18,18,18	0
4	MG	A	610	1/1	0.98	0.08	-1.00	13,13,13,13	0
3	SO4	B	600	5/5	0.95	0.09	-1.26	52,53,53,53	0
3	SO4	D	600	5/5	0.99	0.07	-1.35	17,18,18,19	0
3	SO4	A	600	5/5	0.99	0.06	-4.19	29,30,30,31	0
4	MG	A	611	1/1	0.97	0.06	-5.06	13,13,13,13	0
3	SO4	A	603	5/5	0.95	0.21	-	56,56,56,56	0
3	SO4	A	601	5/5	0.95	0.10	-	31,32,33,34	0
3	SO4	A	604	5/5	0.95	0.14	-	60,60,60,60	0
3	SO4	D	602	5/5	0.92	0.17	-	62,63,64,64	0
3	SO4	B	601	5/5	0.98	0.22	-	38,38,39,39	0
3	SO4	C	601	5/5	0.98	0.14	-	30,31,31,32	0
3	SO4	B	602	5/5	0.80	0.39	-	115,115,115,115	0
3	SO4	C	602	5/5	0.90	0.39	-	91,91,91,91	0
3	SO4	B	603	5/5	0.98	0.15	-	30,31,31,32	0
3	SO4	D	603	5/5	0.97	0.14	-	37,37,38,38	0
3	SO4	D	601	5/5	0.98	0.12	-	35,37,37,37	0
3	SO4	C	604	5/5	0.97	0.20	-	48,48,49,49	0
3	SO4	C	603	5/5	0.98	0.12	-	25,27,28,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.