



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:51 AM GMT

PDB ID : 3GA9  
Title : Crystal structure of Bacillus anthracis transpeptidase enzyme CapD, crystal form II  
Authors : Zhang, R.; Wu, R.; Richter, S.; Anderson, V.J.; Missiakas, D.; Joachimiak, A.; The Great Lakes Regional Center of Excellence (GLRCE)  
Deposited on : 2009-02-16  
Resolution : 2.30 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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

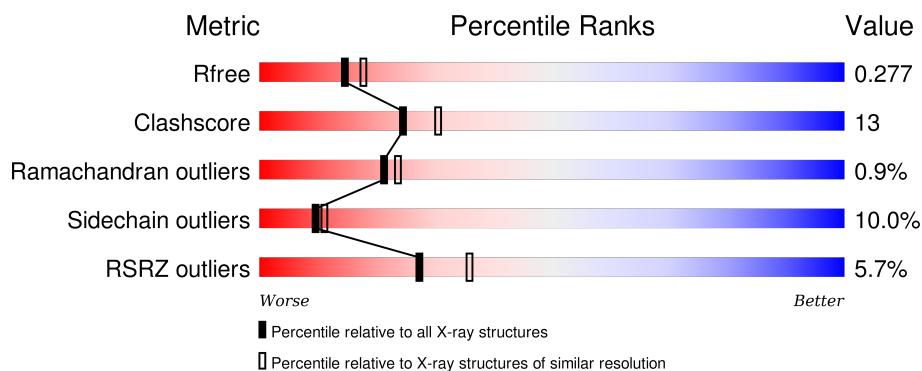
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 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	L	323	<div> <div>5%</div> <div>68%</div> <div>17%</div> <div>• 11%</div> </div>
2	S	177	<div> <div>6%</div> <div>60%</div> <div>32%</div> <div>•• 6%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLU	S	2	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3605 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.

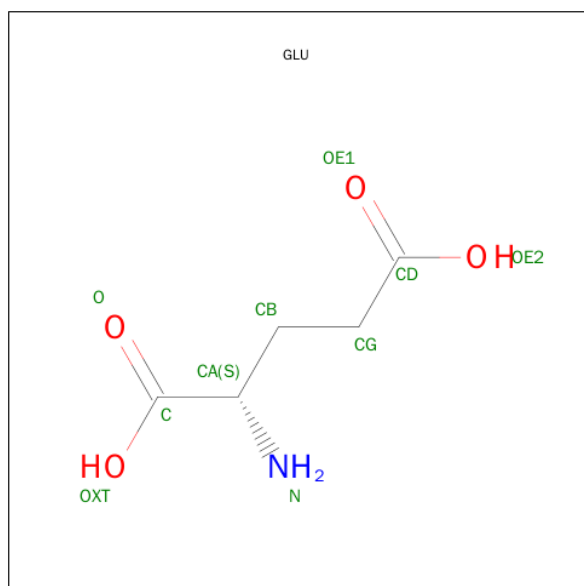
- Molecule 1 is a protein called Capsule biosynthesis protein capD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	286	Total	C	N	O	Se	0	0	0
			2208	1411	364	421	12			

- Molecule 2 is a protein called Capsule biosynthesis protein capD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	167	Total	C	N	O	Se	0	0	0
			1299	816	232	250	1			

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	S	1	Total	C	N	O	0	0
			9	5	1	3		
3	S	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	58	Total 58	O 58	0	0
4	S	21	Total 21	O 21	0	0

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.

- Chain L:
- 
- 5% 68% 17% 11%
- 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 215 216 217 218 219 220 221 222 223 224 225 226 227 228 229 230 231 232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 267 268 269 270 271 272 273 274 275 276 277 278 279 280 281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300
- PHE ASN LYS ILE ASP VAL GLN LYS ILE ASP MSE GLY K46 G47 T48 Y49 L57 E61 K64 V73 L88 M99 D105 K106 E107 I110 T116 P117 Y118 F119 T120 G121 N122 Q123 P125 H126 I127 I139 Y143 G149 Q152
- N157 V165 D166 D167 S168 L169 T170 M171 R172 K177 P178 D183 K184 L185 Y189 E193 P194 I195 I196 T197 Q214 K245 Y256 M257 G258 D259 D260 V261 L273 L274 D275 H276 K278 L279 A280 E281 K282 K283 E284 V285 V286 K287 H291 T292 Y295 F299

- [illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.70 Å 72.00 Å 128.85 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.74 – 2.30 44.74 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.74-2.30) 97.8 (44.74-2.28)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.27 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.252 0.213 , 0.277	Depositor DCC
$R_{free}$ test set	1022 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 20609 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	L	0.77	0/2239	0.74	0/2995
2	S	0.78	0/1320	0.78	0/1775
All	All	0.77	0/3559	0.75	0/4770

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	L	2208	0	2243	56	0
2	S	1299	0	1299	50	0
3	S	19	0	14	0	0
4	L	58	0	0	2	0
4	S	21	0	0	3	0
All	All	3605	0	3556	91	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 13.

All (91) 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:L:257:MSE:HE2	1:L:281:GLU:HB2	1.22	1.07
1:L:123:GLN:HG2	1:L:126:HIS:HE1	1.08	1.05
1:L:123:GLN:HG2	1:L:126:HIS:CE1	1.99	0.97
1:L:313:ASN:OD1	1:L:327:MSE:HE3	1.64	0.97
1:L:116:THR:HB	2:S:403:PRO:O	1.65	0.96
2:S:431:ASN:HD22	2:S:431:ASN:C	1.65	0.96
1:L:257:MSE:CE	1:L:281:GLU:HB2	2.05	0.87
1:L:257:MSE:HE2	1:L:281:GLU:CB	2.06	0.83
2:S:508:ARG:HA	2:S:509:ASP:HB3	1.59	0.83
1:L:124:LYS:HB2	1:L:125:PRO:HD2	1.62	0.81
1:L:48:THR:HG21	2:S:510:ASN:HB2	1.62	0.79
2:S:431:ASN:ND2	2:S:431:ASN:C	2.37	0.71
1:L:172:ARG:NH1	4:L:361:HOH:O	2.26	0.69
2:S:501:GLN:HE22	2:S:522:GLY:HA3	1.61	0.66
1:L:257:MSE:HE3	2:S:446:HIS:NE2	2.13	0.64
2:S:470:GLU:O	2:S:490:LYS:HE3	1.98	0.64
2:S:465:ASN:HA	2:S:486:LEU:HD23	1.81	0.62
1:L:301:GLU:HA	1:L:304:ARG:NH1	2.16	0.61
1:L:124:LYS:HB2	1:L:125:PRO:CD	2.26	0.61
1:L:123:GLN:CG	1:L:126:HIS:HE1	1.99	0.59
1:L:273:LEU:HD23	2:S:414:THR:HG21	1.85	0.58
1:L:106:LYS:HE2	1:L:143:TYR:HE1	1.69	0.57
1:L:279:LEU:O	1:L:283:LYS:HG2	2.04	0.57
2:S:402:GLU:HG3	2:S:403:PRO:HD2	1.87	0.57
2:S:448:LYS:HG2	2:S:448:LYS:O	2.05	0.57
2:S:448:LYS:O	2:S:448:LYS:CG	2.53	0.56
1:L:313:ASN:HD22	1:L:313:ASN:N	2.03	0.55
2:S:368:THR:HG22	2:S:413:PRO:HG3	1.89	0.55
1:L:170:THR:HB	1:L:195:ILE:O	2.06	0.55
1:L:314:LEU:HD22	2:S:408:ARG:HE	1.73	0.54
2:S:492:VAL:HG23	4:S:68:HOH:O	2.08	0.54
1:L:119:PHE:CZ	1:L:124:LYS:HB3	2.44	0.53
2:S:452:GLN:OE1	2:S:515:ALA:HA	2.09	0.53
2:S:354:HIS:HD2	2:S:368:THR:HB	1.72	0.53
1:L:153:GLN:HE21	1:L:157:ASN:HD21	1.56	0.52
1:L:48:THR:CG2	2:S:510:ASN:HD22	2.23	0.52
2:S:368:THR:CG2	2:S:413:PRO:HG3	2.41	0.51
1:L:120:THR:HB	4:L:355:HOH:O	2.11	0.51
2:S:425:ILE:HG13	2:S:502:ALA:HB2	1.91	0.50
2:S:470:GLU:OE2	2:S:519:ARG:NE	2.44	0.49
1:L:123:GLN:HB3	1:L:124:LYS:O	2.12	0.49
1:L:49:TYR:CZ	2:S:527:ASN:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:285:VAL:HG22	1:L:295:TYR:CD1	2.48	0.49
1:L:124:LYS:HE3	1:L:125:PRO:O	2.12	0.48
1:L:153:GLN:HE21	1:L:157:ASN:ND2	2.12	0.48
1:L:259:TYR:CZ	2:S:418:LYS:HE3	2.49	0.48
2:S:427:SER:HB2	2:S:500:VAL:HG22	1.96	0.48
2:S:508:ARG:O	2:S:508:ARG:HG2	2.14	0.48
1:L:256:TYR:O	1:L:259:TYR:HB2	2.14	0.47
1:L:177:LYS:HB3	1:L:178:PRO:HD3	1.96	0.47
2:S:412:ALA:O	2:S:414:THR:HG23	2.15	0.47
1:L:127:ILE:HD11	2:S:379:LYS:HD2	1.96	0.47
1:L:301:GLU:HG2	1:L:304:ARG:HH12	1.80	0.47
1:L:123:GLN:CG	1:L:126:HIS:CE1	2.85	0.46
1:L:99:MSE:SE	1:L:139:ILE:HD13	2.66	0.46
1:L:48:THR:HG23	4:S:72:HOH:O	2.15	0.46
2:S:354:HIS:HD2	2:S:368:THR:CG2	2.29	0.46
1:L:48:THR:HG22	2:S:510:ASN:HD22	1.80	0.46
1:L:276:MSE:SE	2:S:434:PRO:HB2	2.65	0.45
2:S:460:PHE:HA	2:S:468:TYR:O	2.16	0.45
1:L:256:TYR:CE2	2:S:445:THR:HG21	2.52	0.45
2:S:438:THR:HB	2:S:439:PRO:HD3	1.97	0.45
2:S:464:LYS:O	2:S:465:ASN:HB2	2.17	0.45
2:S:416:LEU:HB2	2:S:423:ILE:HB	1.98	0.45
1:L:110:ILE:HG13	1:L:139:ILE:HG12	1.99	0.45
2:S:451:LEU:HD22	2:S:504:ILE:HD11	1.98	0.45
1:L:285:VAL:O	1:L:285:VAL:HG22	2.16	0.44
2:S:354:HIS:CD2	2:S:368:THR:HB	2.52	0.44
1:L:73:VAL:HG21	1:L:143:TYR:O	2.17	0.44
2:S:354:HIS:HD2	2:S:368:THR:HG22	1.82	0.44
1:L:166:ASP:OD2	1:L:168:SER:OG	2.25	0.44
1:L:189:TYR:HA	1:L:193:GLU:O	2.18	0.44
1:L:122:ASN:OD1	1:L:122:ASN:N	2.50	0.43
1:L:285:VAL:HG22	1:L:295:TYR:CE1	2.52	0.43
2:S:468:TYR:HA	2:S:489:LYS:O	2.18	0.43
1:L:283:LYS:H	1:L:283:LYS:HG2	1.70	0.42
2:S:352:THR:HB	2:S:428:PRO:HB3	2.00	0.42
1:L:285:VAL:CG2	1:L:285:VAL:O	2.68	0.42
1:L:259:TYR:CD2	2:S:418:LYS:HG3	2.55	0.42
2:S:508:ARG:HA	2:S:509:ASP:CB	2.36	0.41
2:S:417:LYS:CG	2:S:422:THR:HG23	2.51	0.41
2:S:405:LYS:HG3	4:S:55:HOH:O	2.20	0.41
1:L:117:PRO:HG2	1:L:124:LYS:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:521:ASN:O	2:S:521:ASN:CG	2.59	0.41
2:S:508:ARG:CG	2:S:508:ARG:O	2.69	0.41
1:L:261:VAL:HG12	2:S:416:LEU:HD12	2.03	0.41
1:L:257:MSE:CE	2:S:446:HIS:CE1	3.04	0.40
2:S:475:SER:O	2:S:476:GLU:C	2.59	0.40
1:L:149:GLY:HA2	1:L:214:GLN:HG3	2.02	0.40
1:L:170:THR:HG21	1:L:197:THR:OG1	2.21	0.40
1:L:57:LEU:O	1:L:61:GLU:HG2	2.20	0.40

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	L	282/323 (87%)	273 (97%)	7 (2%)	2 (1%)	26	31
2	S	163/177 (92%)	149 (91%)	12 (7%)	2 (1%)	16	16
All	All	445/500 (89%)	422 (95%)	19 (4%)	4 (1%)	21	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	124	LYS
1	L	284	GLU
2	S	403	PRO
2	S	372	SER

### 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	L	237/257 (92%)	214 (90%)	23 (10%)	10	12
2	S	142/149 (95%)	128 (90%)	14 (10%)	10	11
All	All	379/406 (93%)	342 (90%)	37 (10%)	9	11

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	46	LYS
1	L	64	LYS
1	L	88	LEU
1	L	107	GLU
1	L	110	ILE
1	L	120	THR
1	L	124	LYS
1	L	165	VAL
1	L	170	THR
1	L	172	ARG
1	L	183	ASP
1	L	185	LEU
1	L	245	LYS
1	L	261	VAL
1	L	274	LEU
1	L	278	LYS
1	L	285	VAL
1	L	292	THR
1	L	300	GLU
1	L	313	ASN
1	L	327	MSE
1	L	328	VAL
1	L	334	SER
2	S	361	ASP
2	S	368	THR
2	S	391	GLN
2	S	403	PRO
2	S	409	THR
2	S	414	THR
2	S	431	ASN
2	S	441	LEU
2	S	469	THR
2	S	471	ILE

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Mol	Chain	Res	Type
2	S	482	SER
2	S	491	LYS
2	S	506	ASP
2	S	521	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	68	ASN
1	L	126	HIS
1	L	157	ASN
1	L	313	ASN
1	L	325	ASN
2	S	354	HIS
2	S	392	ASN
2	S	431	ASN
2	S	435	GLN
2	S	456	ASN
2	S	465	ASN
2	S	501	GLN
2	S	510	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 carbohydrates in this entry.

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

2 ligands 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	$\# Z  > 2$
3	GLU	S	1	3	4,8,9	0.62	0	3,9,11	0.90	0
3	GLU	S	2	3	3,9,9	0.48	0	2,11,11	0.43	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
3	GLU	S	1	3	-	0/3/7/9	0/0/0/0
3	GLU	S	2	3	-	0/3/9/9	0/0/0/0

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, 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	L	274/323 (84%)	0.28	15 (5%) 29 37	34, 53, 83, 98	0
2	S	166/177 (93%)	0.45	10 (6%) 25 33	38, 58, 87, 94	0
All	All	440/500 (88%)	0.34	25 (5%) 27 36	34, 54, 85, 98	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	509	ASP	8.6
1	L	333	ILE	6.4
2	S	483	ARG	6.3
1	L	315	GLY	5.9
1	L	314	LEU	5.0
1	L	122	ASN	4.3
2	S	486	LEU	3.9
2	S	476	GLU	3.8
2	S	465	ASN	3.4
1	L	308	GLN	3.3
1	L	123	GLN	3.2
1	L	312	LYS	3.1
1	L	287	LYS	3.0
2	S	508	ARG	2.7
2	S	477	VAL	2.7
1	L	46	LYS	2.6
1	L	284	GLU	2.6
1	L	313	ASN	2.6
1	L	326	LYS	2.4
2	S	390	LEU	2.4
2	S	481	LEU	2.4
1	L	105	ASP	2.1
1	L	301	GLU	2.1
2	S	478	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	291	HIS	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	GLU	S	2	10/10	0.62	0.29	9.07	84,91,92,92	0
3	GLU	S	1	9/10	0.82	0.20	1.02	92,92,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.