



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 05:28 PM EDT

PDB ID : 3G9K  
Title : Crystal structure of Bacillus anthracis transpeptidase enzyme CapD  
Authors : Zhang, R.; Wu, R.; Richter, S.; Anderson, V.J.; Missiakas, D.; Joachimiak, A.  
Deposited on : 2009-02-13  
Resolution : 1.79 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

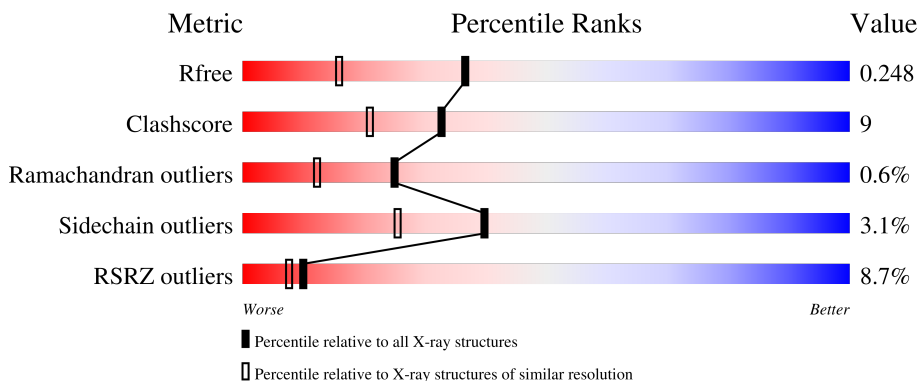
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	D	323	 5% 74% 12% 13%
1	L	323	 4% 80% 7% 13%
2	F	177	 11% 73% 16% 5% 6%
2	S	177	 15% 74% 18% 6% 6%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7489 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.

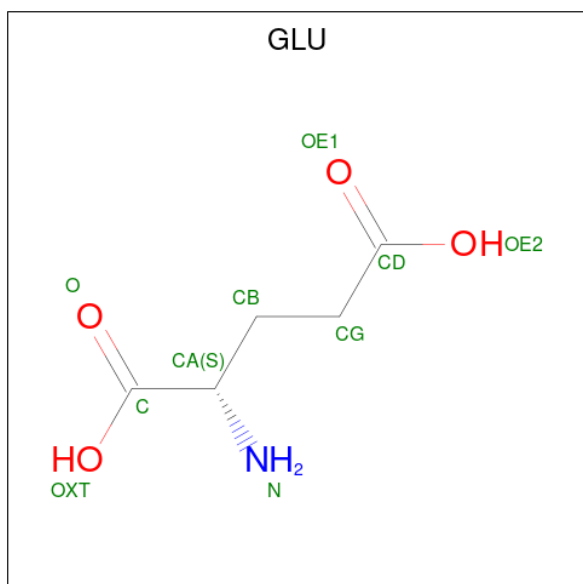
- Molecule 1 is a protein called Capsule biosynthesis protein capD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	L	280	Total 2160	C 1381	N 355	O 412	Se 12	0	0	0
1	D	280	Total 2163	C 1385	N 355	O 412	Se 11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	S	166	Total 1301	C 817	N 235	O 248	Se 1	0	1	0
2	F	166	Total 1291	C 813	N 231	O 246	Se 1	0	0	0

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



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		

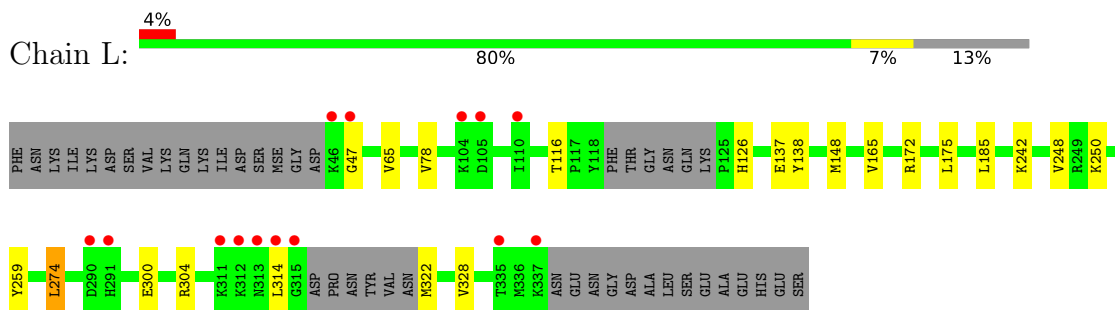
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	190	Total	O	0	0
			190	190		
4	S	72	Total	O	0	0
			72	72		
4	D	186	Total	O	0	0
			186	186		
4	F	107	Total	O	0	0
			107	107		

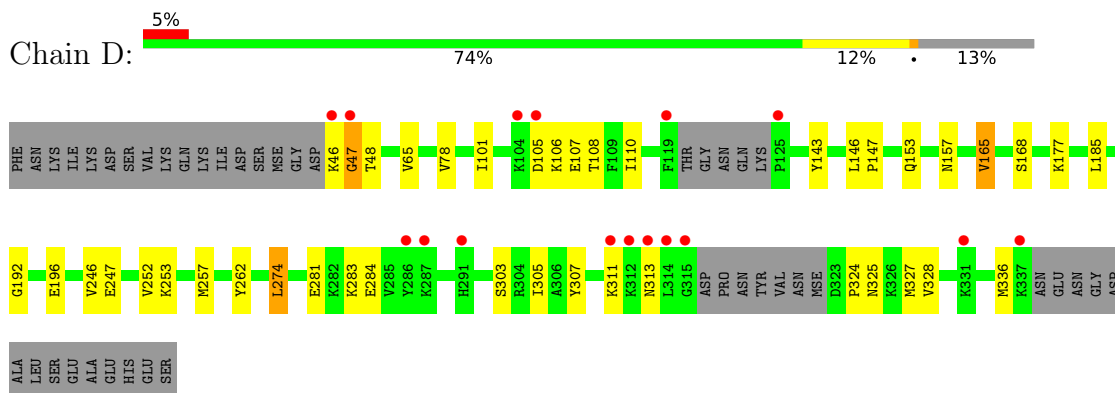
### 3 Residue-property plots [i](#)

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.

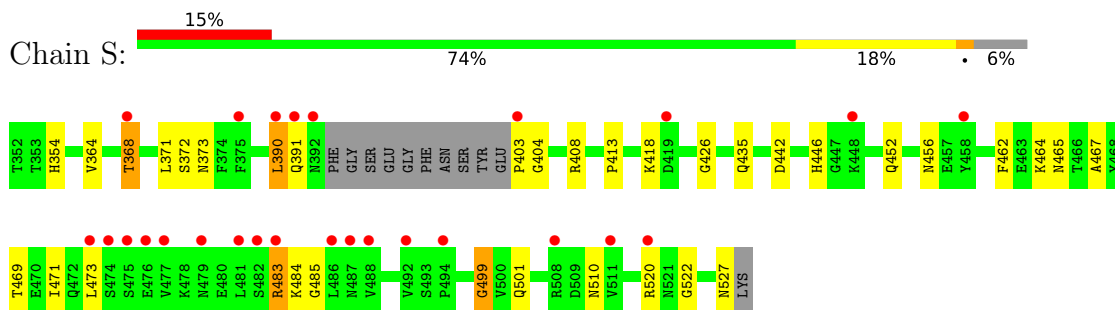
- Molecule 1: Capsule biosynthesis protein capD



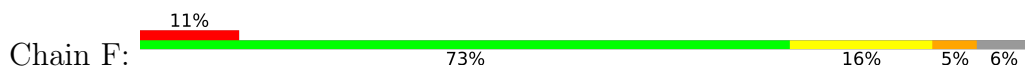
- Molecule 1: Capsule biosynthesis protein capD

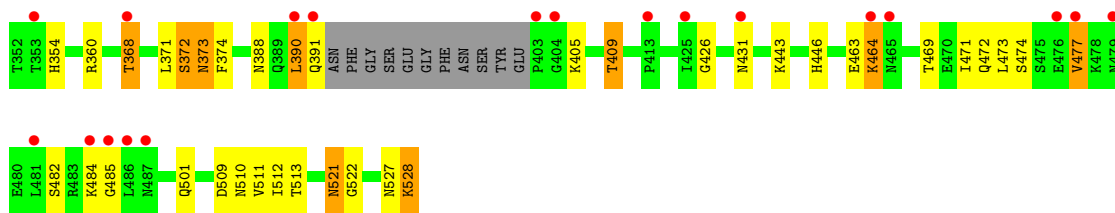


- Molecule 2: Capsule biosynthesis protein capD



- Molecule 2: Capsule biosynthesis protein capD





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.67Å 120.62Å 77.38Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	40.69 – 1.79 40.69 – 1.79	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.69-1.79) 97.6 (40.69-1.79)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.242 0.202 , 0.248	Depositor DCC
$R_{free}$ test set	4413 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtrriage
Anisotropy	0.641	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7489	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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 [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	D	0.80	0/2193	0.73	0/2932
1	L	0.72	0/2189	0.69	0/2926
2	F	0.86	0/1312	0.82	0/1762
2	S	0.81	0/1322	0.76	1/1776 (0.1%)
All	All	0.79	0/7016	0.74	1/9396 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	373	ASN	N-CA-C	-5.40	96.41	111.00

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	D	2163	0	2197	38	0
1	L	2160	0	2197	14	0
2	F	1291	0	1301	50	0
2	S	1301	0	1306	33	0
3	S	19	0	14	1	0
4	D	186	0	0	2	0
4	F	107	0	0	12	0
4	L	190	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	72	0	0	4	0
All	All	7489	0	7015	121	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 9.

All (121) 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)
2:F:469:THR:HG22	2:F:471:ILE:O	1.41	1.20
2:F:511:VAL:HG13	2:F:528:LYS:HD2	1.30	1.12
1:D:257:MSE:HE3	2:F:446:HIS:NE2	1.64	1.11
2:F:521:ASN:O	2:F:521:ASN:ND2	1.86	1.05
2:F:469:THR:CG2	2:F:471:ILE:O	2.05	1.03
2:F:409:THR:HG21	4:F:94:HOH:O	1.58	1.02
2:F:354:HIS:HD2	2:F:368:THR:HG22	1.26	0.97
2:F:521:ASN:HB2	4:F:269:HOH:O	1.64	0.96
1:D:47:GLY:O	2:F:527:ASN:ND2	1.99	0.95
2:F:511:VAL:CG1	2:F:528:LYS:HD2	1.97	0.95
2:F:354:HIS:CD2	2:F:368:THR:HG22	2.05	0.91
3:S:2:GLU:HG2	4:S:539:HOH:O	1.75	0.87
2:S:354:HIS:HD2	2:S:368:THR:HG22	1.37	0.86
1:D:257:MSE:HE2	1:D:281:GLU:HG3	1.56	0.86
2:S:469:THR:HG22	2:S:471:ILE:O	1.78	0.84
2:F:368:THR:HG21	4:F:28:HOH:O	1.76	0.83
2:F:373:ASN:H	2:F:388:ASN:HD21	1.26	0.83
2:S:435:GLN:HE22	2:S:462:PHE:H	1.28	0.81
2:S:354:HIS:CD2	2:S:368:THR:HG22	2.17	0.79
2:F:354:HIS:HD2	2:F:368:THR:CG2	1.96	0.78
2:S:368:THR:HG21	4:S:6:HOH:O	1.84	0.78
1:D:257:MSE:CE	2:F:446:HIS:NE2	2.46	0.77
1:D:305:ILE:HG22	1:D:336:MSE:HE2	1.67	0.77
2:S:469:THR:CG2	2:S:471:ILE:O	2.35	0.74
1:D:65:VAL:HG21	1:D:78:VAL:HG21	1.69	0.74
2:S:354:HIS:HD2	2:S:368:THR:CG2	2.03	0.72
2:F:513:THR:HG22	2:F:528:LYS:HZ1	1.56	0.71
2:S:501:GLN:HE22	2:S:522:GLY:HA3	1.54	0.71
2:F:513:THR:HG22	2:F:528:LYS:NZ	2.05	0.71
2:F:527:ASN:O	2:F:528:LYS:C	2.29	0.70
2:S:484:LYS:N	2:S:485:GLY:HA2	2.07	0.69
1:D:257:MSE:CE	1:D:281:GLU:HG3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:373:ASN:HD22	2:F:374:PHE:H	1.41	0.69
1:D:257:MSE:CE	2:F:446:HIS:CE1	2.79	0.66
2:F:501:GLN:HE22	2:F:522:GLY:HA3	1.62	0.64
1:L:116:THR:HB	2:S:403:PRO:O	1.99	0.62
2:F:484:LYS:N	2:F:485:GLY:HA2	2.15	0.62
1:D:257:MSE:HE3	2:F:446:HIS:CE1	2.33	0.61
1:D:48:THR:HG22	4:F:252:HOH:O	2.00	0.61
2:F:513:THR:CG2	2:F:528:LYS:NZ	2.63	0.61
1:D:48:THR:HG23	4:F:30:HOH:O	2.01	0.60
2:F:521:ASN:HD22	2:F:521:ASN:C	1.97	0.59
1:L:138:TYR:OH	1:L:248:VAL:HG21	2.03	0.59
2:F:513:THR:CG2	2:F:528:LYS:HZ3	2.15	0.58
1:L:259:TYR:CE2	2:S:418:LYS:HE3	2.40	0.57
2:F:511:VAL:HG13	2:F:528:LYS:CD	2.21	0.55
1:D:153:GLN:HE21	1:D:157:ASN:HD21	1.52	0.55
1:D:257:MSE:HE1	2:F:446:HIS:CE1	2.41	0.55
2:F:472:GLN:HG2	4:F:547:HOH:O	2.07	0.54
2:F:474:SER:OG	2:F:477:VAL:HG22	2.06	0.54
1:D:257:MSE:HE2	1:D:281:GLU:CG	2.36	0.54
2:S:483:ARG:CZ	2:S:483:ARG:HB2	2.37	0.53
2:S:442:ASP:O	2:S:446:HIS:HD2	1.91	0.53
2:F:509:ASP:CB	4:F:554:HOH:O	2.56	0.53
1:L:47:GLY:O	2:S:527:ASN:ND2	2.41	0.53
2:F:513:THR:HG23	2:F:528:LYS:HZ3	1.72	0.53
1:D:65:VAL:CG2	1:D:78:VAL:HG21	2.37	0.52
2:F:354:HIS:CE1	2:F:426:GLY:HA3	2.44	0.52
2:S:418:LYS:NZ	4:S:547:HOH:O	2.36	0.51
1:D:253:LYS:H	1:D:325:ASN:ND2	2.09	0.51
1:D:153:GLN:HE21	1:D:157:ASN:ND2	2.08	0.51
2:F:469:THR:HG21	2:F:471:ILE:O	2.05	0.50
1:L:314:LEU:HD22	2:S:408:ARG:NH1	2.27	0.50
2:S:484:LYS:H	2:S:485:GLY:HA2	1.77	0.50
2:S:435:GLN:HE22	2:S:462:PHE:N	2.03	0.49
1:L:300:GLU:OE1	1:L:304:ARG:NH1	2.45	0.49
1:L:65:VAL:HG21	1:L:78:VAL:HG21	1.95	0.49
2:S:391:GLN:NE2	4:S:542:HOH:O	2.47	0.48
2:S:499:GLY:HA3	2:S:520[A]:ARG:HG3	1.96	0.48
2:F:463:GLU:HG3	2:F:464:LYS:HD2	1.94	0.48
1:D:305:ILE:CG2	1:D:336:MSE:HE2	2.41	0.48
1:L:274:LEU:HD13	1:L:328:VAL:HB	1.96	0.48
2:F:528:LYS:NZ	4:F:337:HOH:O	2.08	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:172:ARG:HH12	1:L:175:LEU:HD12	1.79	0.48
1:D:105:ASP:O	1:D:106:LYS:HB2	2.14	0.47
1:D:252:VAL:HG22	1:D:324:PRO:HB2	1.96	0.47
4:D:548:HOH:O	2:F:443:LYS:HG2	2.13	0.47
2:F:509:ASP:HB3	4:F:554:HOH:O	2.13	0.47
1:D:177:LYS:NZ	1:D:192:GLY:O	2.39	0.47
2:F:373:ASN:H	2:F:388:ASN:ND2	2.05	0.47
2:F:469:THR:HG21	2:F:473:LEU:HG	1.97	0.46
1:L:137:GLU:HA	1:L:148:MSE:HE2	1.97	0.46
2:F:512:ILE:O	2:F:528:LYS:HE2	2.15	0.46
2:S:371:LEU:O	2:S:372:SER:HB2	2.14	0.46
1:D:48:THR:HG21	2:F:510:ASN:ND2	2.31	0.45
2:S:462:PHE:CE2	2:S:467:ALA:HB2	2.52	0.45
1:D:313:ASN:OD1	1:D:327:MSE:HE3	2.16	0.45
2:F:472:GLN:CG	4:F:547:HOH:O	2.64	0.45
2:S:435:GLN:NE2	2:S:462:PHE:H	2.05	0.45
1:D:48:THR:CG2	2:F:510:ASN:HD21	2.31	0.45
2:F:390:LEU:O	2:F:391:GLN:C	2.54	0.45
1:D:108:THR:HG21	1:D:143:TYR:OH	2.17	0.44
1:D:146:LEU:HB3	1:D:147:PRO:HD2	1.99	0.44
2:S:469:THR:HG21	2:S:473:LEU:HG	2.00	0.44
1:D:48:THR:CG2	4:F:30:HOH:O	2.62	0.44
2:S:464:LYS:HB3	2:S:465:ASN:H	1.60	0.44
2:F:371:LEU:O	2:F:372:SER:HB2	2.18	0.44
1:L:126:HIS:CE1	2:S:391:GLN:HE21	2.36	0.43
1:D:274:LEU:HD13	1:D:328:VAL:HB	2.00	0.43
1:D:101:ILE:HD12	1:D:110:ILE:HD11	1.99	0.43
1:L:314:LEU:CD2	2:S:408:ARG:NH1	2.82	0.43
1:D:303:SER:O	1:D:307:TYR:HD2	2.01	0.43
2:F:373:ASN:HD22	2:F:374:PHE:N	2.10	0.43
2:S:452:GLN:HE21	2:S:456:ASN:ND2	2.17	0.43
1:D:253:LYS:H	1:D:325:ASN:HD21	1.66	0.43
2:S:469:THR:HG21	2:S:471:ILE:O	2.16	0.42
1:D:107:GLU:HG2	1:D:262:TYR:CE2	2.54	0.42
1:D:46:LYS:HG2	2:F:360:ARG:HE	1.85	0.42
2:S:368:THR:HG23	2:S:413:PRO:HD3	2.01	0.41
1:D:283:LYS:O	1:D:283:LYS:CG	2.68	0.41
2:S:354:HIS:CE1	2:S:426:GLY:HA3	2.56	0.41
1:D:246:VAL:HG12	1:D:247:GLU:N	2.36	0.41
2:S:390:LEU:HD13	2:S:390:LEU:HA	1.90	0.41
2:S:442:ASP:O	2:S:446:HIS:CD2	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:VAL:HG22	1:D:196:GLU:O	2.21	0.41
1:D:46:LYS:N	1:D:47:GLY:HA2	2.35	0.41
1:L:242:LYS:NZ	4:L:465:HOH:O	2.53	0.41
2:F:431:ASN:HA	4:F:538:HOH:O	2.21	0.41
2:F:482:SER:O	2:F:485:GLY:HA2	2.21	0.40
1:L:137:GLU:HA	1:L:148:MSE:CE	2.51	0.40
1:D:311:LYS:HB3	4:D:508:HOH:O	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	D	274/323 (85%)	267 (97%)	6 (2%)	1 (0%)	34 21
1	L	274/323 (85%)	272 (99%)	2 (1%)	0	100 100
2	F	162/177 (92%)	153 (94%)	7 (4%)	2 (1%)	13 3
2	S	163/177 (92%)	155 (95%)	6 (4%)	2 (1%)	13 3
All	All	873/1000 (87%)	847 (97%)	21 (2%)	5 (1%)	25 12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	372	SER
2	F	405	LYS
2	S	404	GLY
1	D	47	GLY
2	S	499	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	D	232/257 (90%)	227 (98%)	5 (2%)	52	39
1	L	232/257 (90%)	227 (98%)	5 (2%)	52	39
2	F	141/149 (95%)	133 (94%)	8 (6%)	20	8
2	S	142/149 (95%)	137 (96%)	5 (4%)	36	21
All	All	747/812 (92%)	724 (97%)	23 (3%)	40	25

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	165	VAL
1	L	185	LEU
1	L	250	LYS
1	L	274	LEU
1	L	322	MSE
2	S	364	VAL
2	S	368	THR
2	S	390	LEU
2	S	483	ARG
2	S	510	ASN
1	D	165	VAL
1	D	168	SER
1	D	185	LEU
1	D	274	LEU
1	D	284	GLU
2	F	368	THR
2	F	373	ASN
2	F	390	LEU
2	F	409	THR
2	F	464	LYS
2	F	477	VAL
2	F	521	ASN
2	F	528	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	157	ASN
2	S	354	HIS
2	S	388	ASN
2	S	435	GLN
2	S	446	HIS
2	S	456	ASN
2	S	501	GLN
1	D	157	ASN
1	D	325	ASN
2	F	354	HIS
2	F	373	ASN
2	F	388	ASN
2	F	456	ASN
2	F	501	GLN
2	F	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 monosaccharides 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	7,8,9	0.88	0	4,9,11	1.09	0
3	GLU	S	2	3	8,9,9	0.91	0	10,11,11	1.54	2 (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
3	GLU	S	1	3	-	2/6/7/9	-
3	GLU	S	2	3	-	3/9/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	2	GLU	OXT-C-CA	3.15	124.10	113.38
3	S	2	GLU	OXT-C-O	-3.03	117.20	124.09

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	S	2	GLU	C-CA-CB-CG
3	S	2	GLU	OXT-C-CA-N
3	S	2	GLU	O-C-CA-N
3	S	1	GLU	OE2-CD-CG-CB
3	S	1	GLU	OE1-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	2	GLU	1	0

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

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 [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, 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	D	269/323 (83%)	0.30	16 (5%) 22 17	14, 25, 44, 58	0
1	L	268/323 (82%)	0.42	14 (5%) 27 22	14, 25, 43, 64	0
2	F	165/177 (93%)	0.76	19 (11%) 4 3	14, 24, 50, 56	0
2	S	165/177 (93%)	0.81	26 (15%) 2 1	14, 25, 55, 62	0
All	All	867/1000 (86%)	0.52	75 (8%) 10 8	14, 25, 49, 64	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	403	PRO	8.5
2	F	404	GLY	8.4
1	L	314	LEU	7.7
1	L	315	GLY	7.2
1	L	337	LYS	5.9
1	L	46	LYS	5.5
1	D	314	LEU	5.4
1	L	313	ASN	5.4
2	S	477	VAL	5.2
1	D	315	GLY	5.1
1	D	312	LYS	4.9
2	S	403	PRO	4.6
2	S	483	ARG	4.5
2	S	479	ASN	4.4
1	L	312	LYS	4.4
1	D	46	LYS	4.2
2	S	492	VAL	4.1
2	F	477	VAL	4.1
2	F	486	LEU	3.9
1	D	313	ASN	3.9
2	S	487	ASN	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	286	TYR	3.9
2	S	494	PRO	3.8
2	S	486	LEU	3.8
2	F	465	ASN	3.6
2	S	482	SER	3.4
1	D	105	ASP	3.3
2	F	487	ASN	3.3
2	S	391	GLN	3.2
1	L	291	HIS	3.2
2	S	488	VAL	3.1
1	D	337	LYS	3.1
1	D	291	HIS	3.1
2	S	448	LYS	3.0
1	D	104	LYS	3.0
2	S	392	ASN	3.0
2	S	508	ARG	3.0
2	S	511	VAL	3.0
1	L	311	LYS	2.8
1	L	290	ASP	2.8
1	D	47	GLY	2.8
1	D	119	PHE	2.8
1	L	47	GLY	2.7
2	F	481	LEU	2.7
2	S	476	GLU	2.7
2	F	476	GLU	2.5
2	F	431	ASN	2.5
2	S	473	LEU	2.5
2	F	391	GLN	2.5
1	D	287	LYS	2.5
2	F	484	LYS	2.5
2	S	390	LEU	2.5
2	F	353	THR	2.4
1	L	335	THR	2.4
1	L	110	ILE	2.3
2	S	481	LEU	2.3
2	S	458	TYR	2.3
2	S	474	SER	2.3
2	S	375	PHE	2.3
1	L	104	LYS	2.3
1	D	331	LYS	2.2
1	D	125	PRO	2.2
2	S	368	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	S	475	SER	2.2
2	F	485	GLY	2.2
1	D	311	LYS	2.2
2	S	419	ASP	2.2
2	F	479	ASN	2.1
1	L	105	ASP	2.1
2	F	390	LEU	2.1
2	F	413	PRO	2.1
2	F	464	LYS	2.0
2	F	425	ILE	2.0
2	S	520[A]	ARG	2.0
2	F	368	THR	2.0

## 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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	GLU	S	1	9/10	0.53	0.29	50,51,52,56	0
3	GLU	S	2	10/10	0.77	0.19	38,48,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.