



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:27 PM GMT

PDB ID : 4LNK
Title : B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: structure of GS-glutamate-AMPPCP complex
Authors : Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.
Deposited on : 2013-07-11
Resolution : 2.87 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

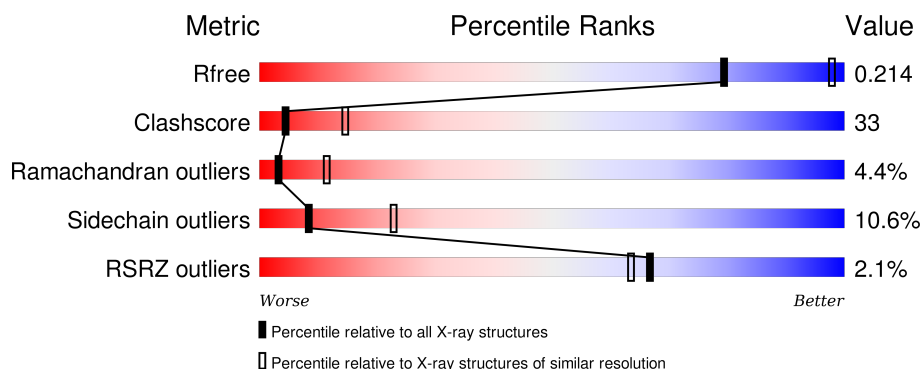
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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.



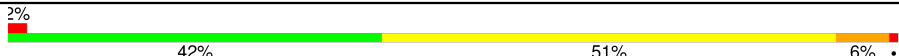
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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 $\leq 5\%$. 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	443	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>43%</div> <div>9%</div> </div> </div>
1	B	443	<div> <div>2%</div> <div> <div></div> <div>44%</div> <div>50%</div> <div>6%</div> </div> </div>
1	C	443	<div> <div>2%</div> <div> <div></div> <div>44%</div> <div>47%</div> <div>9%</div> </div> </div>
1	D	443	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>43%</div> <div>10%</div> </div> </div>
1	E	443	<div> <div>3%</div> <div> <div></div> <div>47%</div> <div>43%</div> <div>10%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	443	

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
2	GLU	B	501	-	-	-	X
2	GLU	C	501	-	-	X	X
2	GLU	D	501	-	-	X	X
2	GLU	E	501	-	-	-	X
2	GLU	F	501	-	-	-	X
3	ADP	A	502	-	-	-	X
3	ADP	D	502	-	-	-	X
3	ADP	E	502	-	-	-	X
4	MG	B	503	-	-	-	X
4	MG	C	503	-	-	-	X
4	MG	D	503	-	-	-	X
5	SO4	A	506	-	-	-	X

2 Entry composition [i](#)

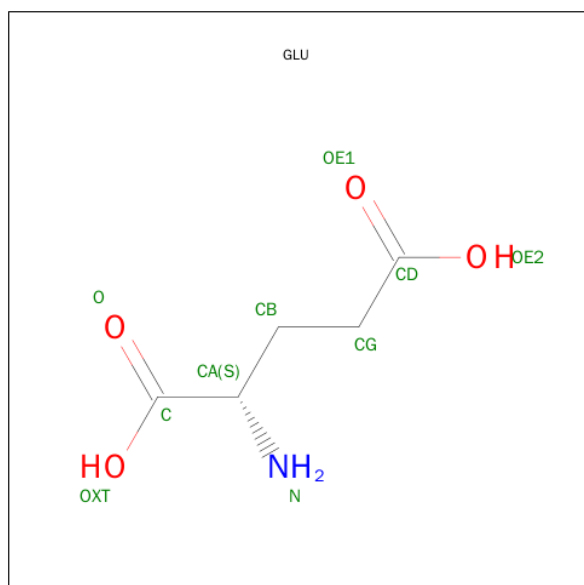
There are 6 unique types of molecules in this entry. The entry contains 21514 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase.

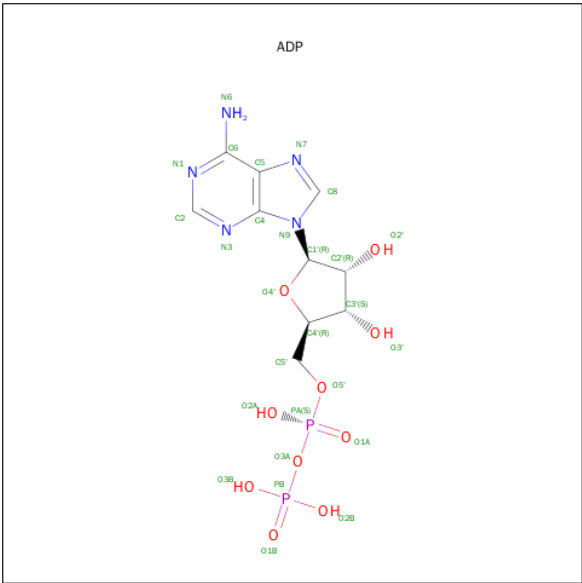
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	B	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	C	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	D	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	E	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			
1	F	443	Total	C	N	O	S	0	0	0
			3535	2259	590	670	16			

- Molecule 2 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			9	5	1	3		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		
2	E	1	Total	C	N	O	0	0
			10	5	1	4		
2	F	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0

Continued on next page...

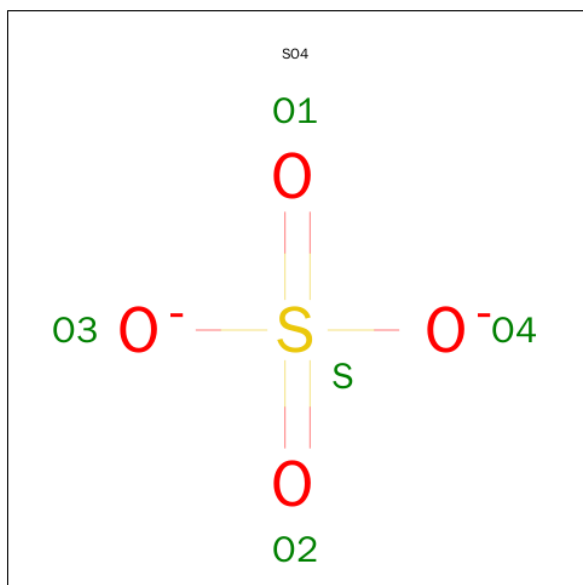
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

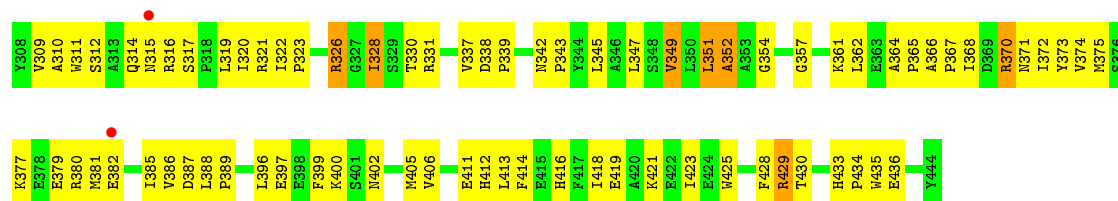
Continued on next page...

Continued from previous page...

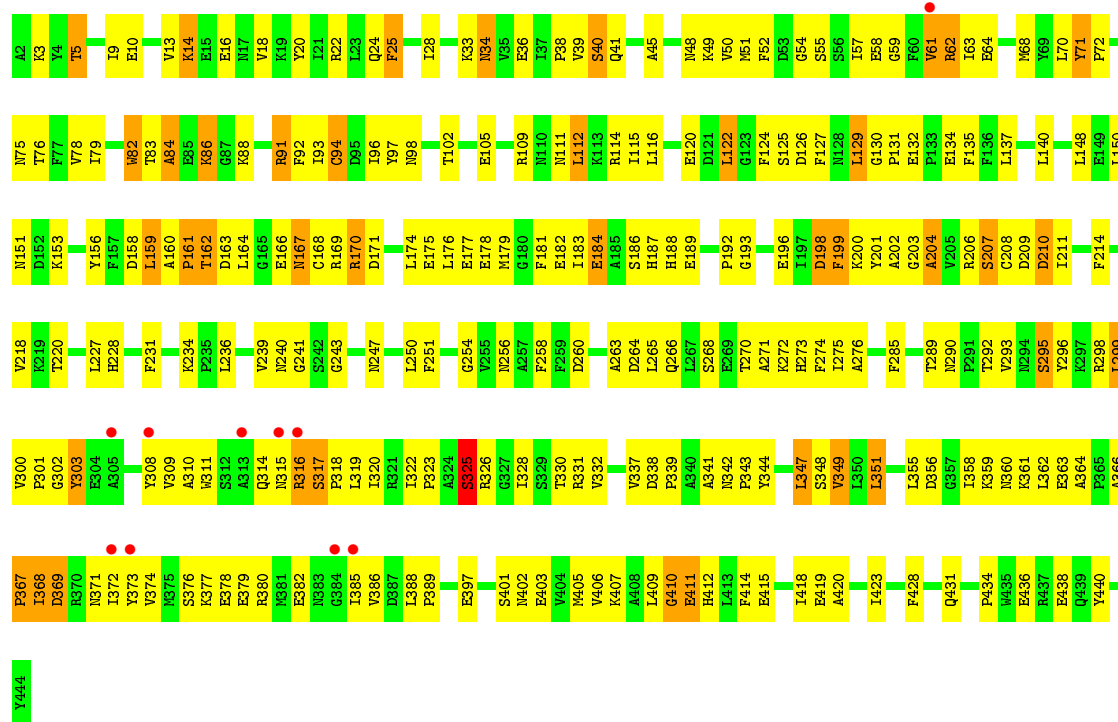
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

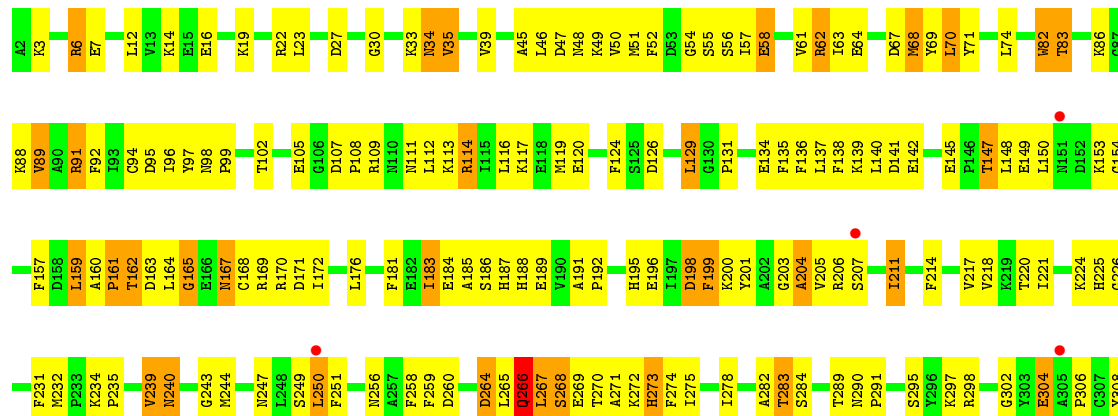
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O	0	0
			12	12		
6	B	7	Total	O	0	0
			7	7		
6	C	6	Total	O	0	0
			6	6		
6	D	10	Total	O	0	0
			10	10		
6	E	11	Total	O	0	0
			11	11		
6	F	11	Total	O	0	0
			11	11		

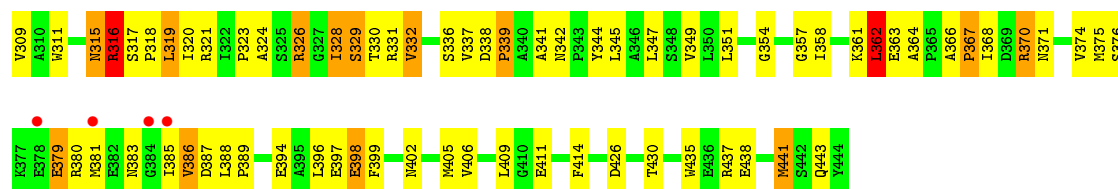


• Molecule 1: Glutamine synthetase

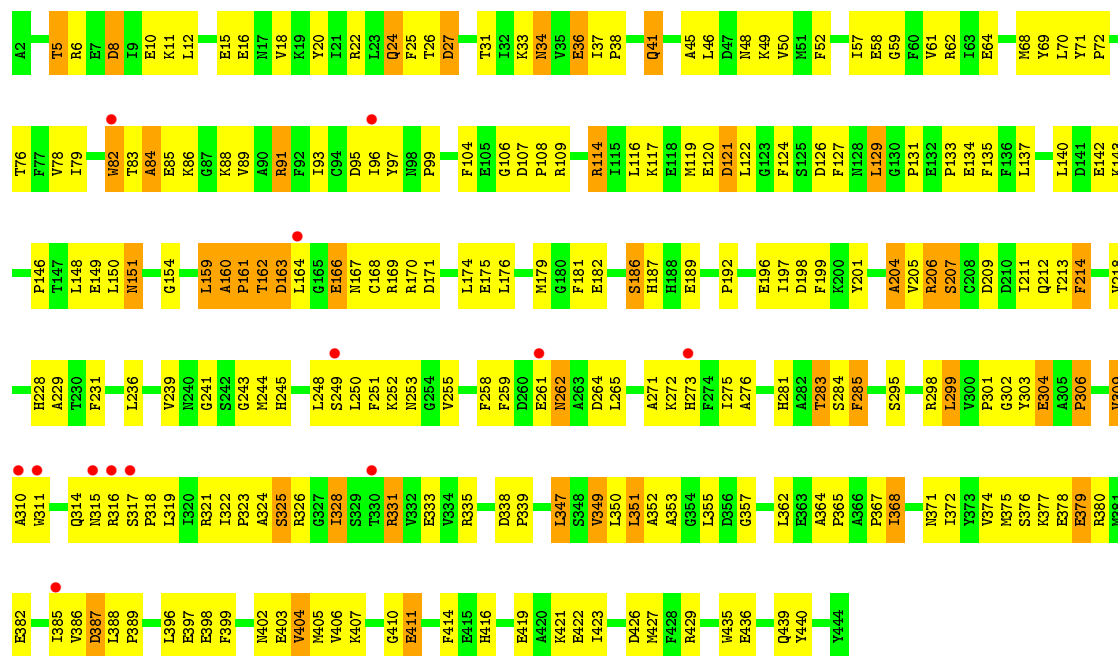


• Molecule 1: Glutamine synthetase

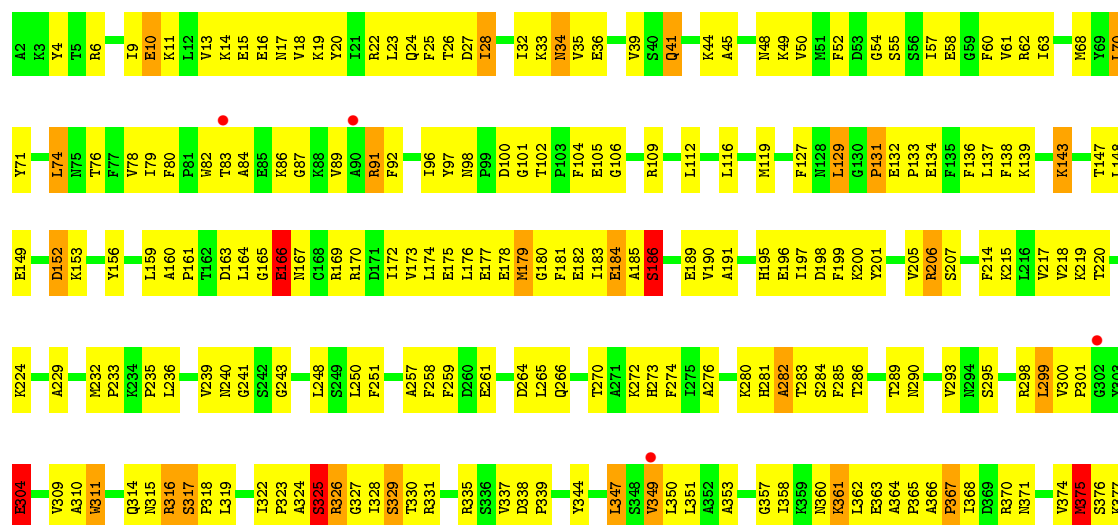




• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



E378	E379	M381	N383	G384	V386	D387	L388	P389	L396	F399	K400	S401	N402	E403	V404	M405	V406	K407	A408	L409	G410	E411	H412	L413	F414	E419	A420	K421	E422	I423	E424	W425	D426	M427	F428	Q431	P434	W435	E436	R437	E438	Q439	Y440	M441	Y444
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.50Å 240.86Å 207.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	120.06 – 2.87 120.07 – 2.87	Depositor EDS
% Data completeness (in resolution range)	91.8 (120.06-2.87) 91.5 (120.07-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.195 , 0.236 0.194 , 0.214	Depositor DCC
R_{free} test set	9598 reflections (15.18%)	DCC
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.2	EDS
Estimated twinning fraction	0.278 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.250 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.207 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
Reported twinning fraction	0.278 for -1/2*h+1/2*k,3/2*h+1/2*k,-l	Depositor
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 72956 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21514	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.84 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.5001e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SO4, ADP

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	0.50	0/3618	0.64	0/4895
1	B	0.50	0/3618	0.64	0/4895
1	C	0.49	0/3618	0.64	0/4895
1	D	0.47	0/3618	0.64	0/4895
1	E	0.50	0/3618	0.64	1/4895 (0.0%)
1	F	0.50	0/3618	0.66	0/4895
All	All	0.49	0/21708	0.64	1/29370 (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	E	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	160	ALA	C-N-CD	-5.41	108.69	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	160	ALA	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	3535	0	3466	226	0
1	B	3535	0	3466	242	0
1	C	3535	0	3466	231	0
1	D	3535	0	3466	227	0
1	E	3535	0	3466	267	0
1	F	3535	0	3466	255	0
2	A	10	0	5	0	0
2	B	9	0	5	0	0
2	C	10	0	5	4	0
2	D	10	0	5	4	0
2	E	10	0	5	3	0
2	F	9	0	5	1	0
3	A	27	0	12	3	0
3	B	27	0	12	3	0
3	C	27	0	12	5	0
3	D	27	0	12	1	0
3	E	27	0	12	4	0
3	F	27	0	12	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	10	0	0	0	0
5	E	5	0	0	1	0
6	A	12	0	0	0	0
6	B	7	0	0	0	0
6	C	6	0	0	1	0
6	D	10	0	0	1	0
6	E	11	0	0	0	0
6	F	11	0	0	0	0
All	All	21514	0	20898	1379	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 33.

The worst 5 of 1379 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:F:55:SER:HB2	1:F:62:ARG:HG3	1.32	1.10
1:C:182:GLU:HG3	1:C:200:LYS:HG3	1.32	1.08
1:C:162:THR:HG21	1:D:220:THR:OG1	1.54	1.07
1:D:328:ILE:HD13	1:D:328:ILE:H	1.14	1.05
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.40	1.03

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	441/443 (100%)	362 (82%)	57 (13%)	22 (5%)	3	8
1	B	441/443 (100%)	348 (79%)	76 (17%)	17 (4%)	4	14
1	C	441/443 (100%)	359 (81%)	60 (14%)	22 (5%)	3	8
1	D	441/443 (100%)	360 (82%)	59 (13%)	22 (5%)	3	8
1	E	441/443 (100%)	364 (82%)	61 (14%)	16 (4%)	4	16
1	F	441/443 (100%)	369 (84%)	55 (12%)	17 (4%)	4	14
All	All	2646/2658 (100%)	2162 (82%)	368 (14%)	116 (4%)	3	11

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY
1	A	190	VAL
1	A	325	SER
1	B	316	ARG
1	C	84	ALA

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	382/382 (100%)	342 (90%)	40 (10%)	8	23
1	B	382/382 (100%)	349 (91%)	33 (9%)	13	35
1	C	382/382 (100%)	341 (89%)	41 (11%)	8	22
1	D	382/382 (100%)	334 (87%)	48 (13%)	5	15
1	E	382/382 (100%)	340 (89%)	42 (11%)	8	21
1	F	382/382 (100%)	342 (90%)	40 (10%)	8	23
All	All	2292/2292 (100%)	2048 (89%)	244 (11%)	8	23

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	363	GLU
1	D	199	PHE
1	F	206	ARG
1	C	431	GLN
1	D	82	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	110	ASN
1	C	167	ASN
1	E	416	HIS
1	B	315	ASN
1	E	314	GLN

5.3.3 RNA ⓘ

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, 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	$\# Z > 2$
2	GLU	A	501	4	3,9,9	0.40	0	2,11,11	0.11	0
3	ADP	A	502	-	22,29,29	1.25	3 (13%)	27,45,45	1.68	4 (14%)
5	SO4	A	505	-	4,4,4	0.10	0	6,6,6	0.16	0
5	SO4	A	506	-	4,4,4	0.14	0	6,6,6	0.25	0
2	GLU	B	501	4	4,8,9	0.65	0	3,9,11	0.83	0
3	ADP	B	502	-	22,29,29	1.10	2 (9%)	27,45,45	1.69	3 (11%)
2	GLU	C	501	4	3,9,9	0.34	0	2,11,11	0.16	0
3	ADP	C	502	-	22,29,29	1.10	2 (9%)	27,45,45	1.68	2 (7%)
2	GLU	D	501	4	3,9,9	0.42	0	2,11,11	0.16	0
3	ADP	D	502	-	22,29,29	1.27	2 (9%)	27,45,45	1.77	3 (11%)
2	GLU	E	501	4	3,9,9	0.38	0	2,11,11	0.20	0
3	ADP	E	502	-	22,29,29	1.06	1 (4%)	27,45,45	1.92	4 (14%)
5	SO4	E	505	-	4,4,4	0.21	0	6,6,6	0.14	0
2	GLU	F	501	-	4,8,9	0.85	0	3,9,11	1.17	1 (33%)
3	ADP	F	502	-	22,29,29	1.12	2 (9%)	27,45,45	1.84	4 (14%)

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	GLU	A	501	4	-	0/3/9/9	0/0/0/0
3	ADP	A	502	-	-	0/12/32/32	0/3/3/3
5	SO4	A	505	-	-	0/0/0/0	0/0/0/0
5	SO4	A	506	-	-	0/0/0/0	0/0/0/0
2	GLU	B	501	4	-	0/3/7/9	0/0/0/0
3	ADP	B	502	-	-	0/12/32/32	0/3/3/3
2	GLU	C	501	4	-	0/3/9/9	0/0/0/0
3	ADP	C	502	-	-	0/12/32/32	0/3/3/3
2	GLU	D	501	4	-	0/3/9/9	0/0/0/0
3	ADP	D	502	-	-	0/12/32/32	0/3/3/3
2	GLU	E	501	4	-	0/3/9/9	0/0/0/0
3	ADP	E	502	-	-	0/12/32/32	0/3/3/3
5	SO4	E	505	-	-	0/0/0/0	0/0/0/0
2	GLU	F	501	-	-	0/3/7/9	0/0/0/0
3	ADP	F	502	-	-	0/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ADP	O4'-C1'	2.06	1.43	1.41
3	A	502	ADP	C2-N3	2.07	1.35	1.32
3	C	502	ADP	O4'-C1'	2.24	1.44	1.41
3	D	502	ADP	O4'-C1'	2.69	1.44	1.41
3	F	502	ADP	O4'-C1'	2.76	1.44	1.41

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	502	ADP	N3-C2-N1	-7.16	123.41	128.89
3	F	502	ADP	N3-C2-N1	-6.96	123.57	128.89
3	C	502	ADP	N3-C2-N1	-6.90	123.61	128.89
3	D	502	ADP	N3-C2-N1	-6.07	124.25	128.89
3	B	502	ADP	N3-C2-N1	-5.79	124.46	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ADP	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	ADP	3	0
2	C	501	GLU	4	0
3	C	502	ADP	5	0
2	D	501	GLU	4	0
3	D	502	ADP	1	0
2	E	501	GLU	3	0
3	E	502	ADP	4	0
5	E	505	SO4	1	0
2	F	501	GLU	1	0
3	F	502	ADP	2	0

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, 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	443/443 (100%)	0.32	9 (2%) 68 65	43, 61, 97, 127	1 (0%)
1	B	443/443 (100%)	0.31	7 (1%) 74 73	42, 62, 95, 118	1 (0%)
1	C	443/443 (100%)	0.33	10 (2%) 64 60	45, 63, 94, 120	1 (0%)
1	D	443/443 (100%)	0.30	8 (1%) 71 69	45, 63, 98, 128	0
1	E	443/443 (100%)	0.33	13 (2%) 55 50	44, 61, 96, 122	1 (0%)
1	F	443/443 (100%)	0.27	8 (1%) 71 69	45, 63, 96, 136	2 (0%)
All	All	2658/2658 (100%)	0.31	55 (2%) 67 63	42, 62, 97, 136	6 (0%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	250	LEU	4.3
1	A	312	SER	4.2
1	D	381	MET	4.0
1	D	378	GLU	4.0
1	A	313	ALA	3.8

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GLU	F	501	9/10	0.67	0.55	6.56	55,68,71,72	0
3	ADP	A	502	27/27	0.66	0.42	4.72	83,106,152,159	0
4	MG	C	503	1/1	0.87	0.29	4.34	60,60,60,60	0
2	GLU	E	501	10/10	0.75	0.42	4.09	57,63,68,68	0
4	MG	D	503	1/1	0.89	0.26	3.78	49,49,49,49	0
2	GLU	C	501	10/10	0.80	0.44	3.62	57,62,68,68	0
5	SO4	A	506	5/5	0.84	0.28	3.56	73,74,82,90	0
2	GLU	B	501	9/10	0.79	0.47	3.22	65,71,75,76	0
4	MG	B	503	1/1	0.87	0.29	3.18	51,51,51,51	0
3	ADP	E	502	27/27	0.77	0.42	3.13	79,97,130,141	0
2	GLU	D	501	10/10	0.74	0.45	3.03	58,71,76,79	0
3	ADP	D	502	27/27	0.82	0.32	2.38	75,93,114,131	0
3	ADP	F	502	27/27	0.84	0.29	1.68	81,108,134,135	0
2	GLU	A	501	10/10	0.82	0.34	1.32	64,70,75,78	0
3	ADP	C	502	27/27	0.81	0.28	1.10	70,85,98,108	0
4	MG	F	503	1/1	0.96	0.23	1.09	59,59,59,59	0
4	MG	F	504	1/1	0.95	0.22	0.70	53,53,53,53	0
5	SO4	E	505	5/5	0.77	0.31	0.51	93,98,100,104	0
3	ADP	B	502	27/27	0.84	0.24	0.05	71,83,114,117	0
4	MG	E	504	1/1	0.92	0.17	-0.99	49,49,49,49	0
5	SO4	A	505	5/5	0.86	0.14	-1.24	90,93,99,108	0
4	MG	A	503	1/1	0.90	0.17	-1.76	64,64,64,64	0
4	MG	A	504	1/1	0.94	0.14	-2.74	50,50,50,50	0
4	MG	E	503	1/1	0.68	0.24	-	61,61,61,61	0
4	MG	C	504	1/1	0.85	0.38	-	51,51,51,51	0
4	MG	D	504	1/1	0.90	0.22	-	61,61,61,61	0
4	MG	B	504	1/1	0.92	0.22	-	64,64,64,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.