Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 02:33 am GMT

PDB ID	:	8OOW
Title	:	Glutamine synthetase from Methermicoccus shengliensis at a resolution of 2.64 A
Authors	:	Mueller, M.-C.; Lemaire, O.N.; Wagner, T.
Deposited on	:	2023-04-06
Resolution	:	2.64 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

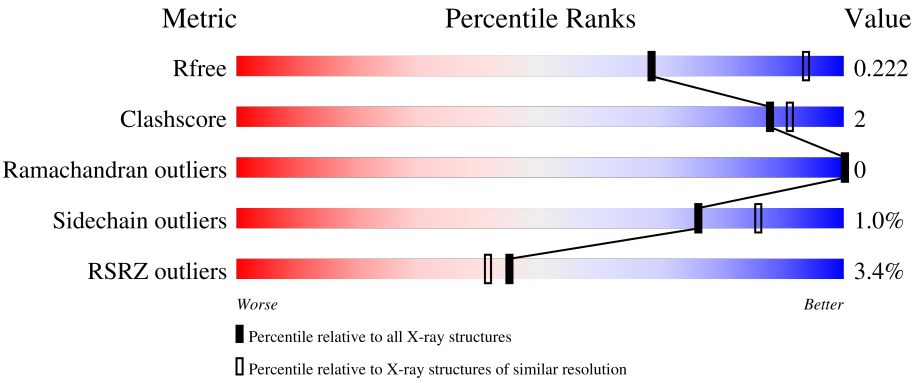
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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.



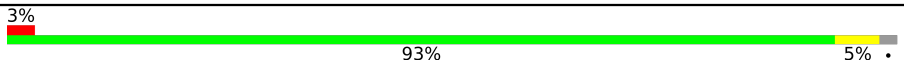
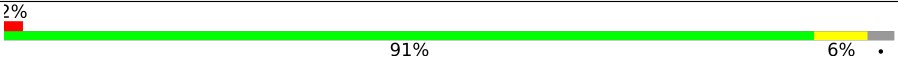
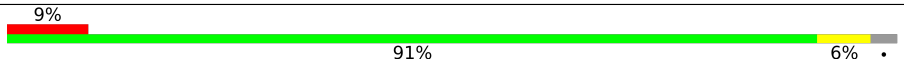
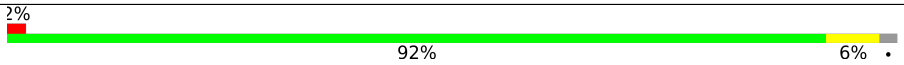
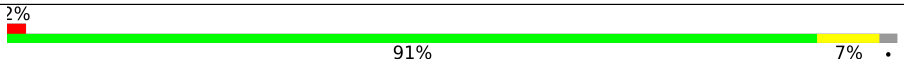
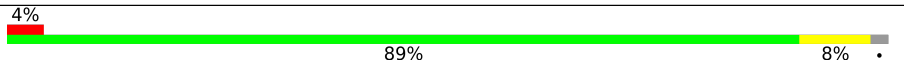
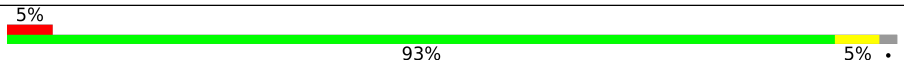
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	442	2% 91% 6% ·
1	B	442	2% 93% 5% ·
1	C	442	2% 91% 6% ·
1	D	442	4% 93% 5% ·
1	E	442	4% 94% · ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	442	
1	G	442	
1	H	442	
1	I	442	
1	J	442	
1	K	442	
1	L	442	

2 Entry composition (i)

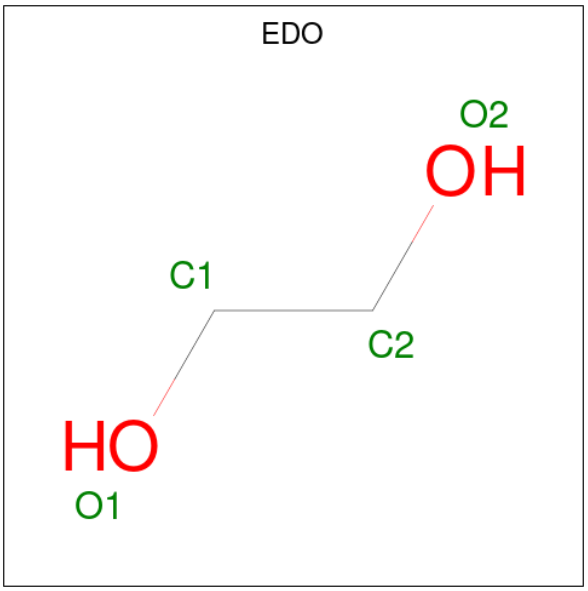
There are 5 unique types of molecules in this entry. The entry contains 40963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	431	Total	C	N	O	S	0	0	0
			3401	2170	577	639	15			
1	B	434	Total	C	N	O	S	0	0	0
			3416	2178	578	645	15			
1	C	430	Total	C	N	O	S	0	0	0
			3389	2164	573	637	15			
1	D	434	Total	C	N	O	S	0	0	0
			3416	2178	578	645	15			
1	E	431	Total	C	N	O	S	0	0	0
			3395	2167	574	639	15			
1	F	432	Total	C	N	O	S	0	0	0
			3399	2169	575	640	15			
1	G	430	Total	C	N	O	S	0	0	0
			3391	2165	573	638	15			
1	H	430	Total	C	N	O	S	0	0	0
			3391	2165	573	638	15			
1	I	432	Total	C	N	O	S	0	0	0
			3399	2169	575	640	15			
1	J	433	Total	C	N	O	S	0	0	0
			3403	2171	576	641	15			
1	K	431	Total	C	N	O	S	0	0	0
			3395	2167	574	639	15			
1	L	435	Total	C	N	O	S	0	0	0
			3426	2183	582	646	15			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

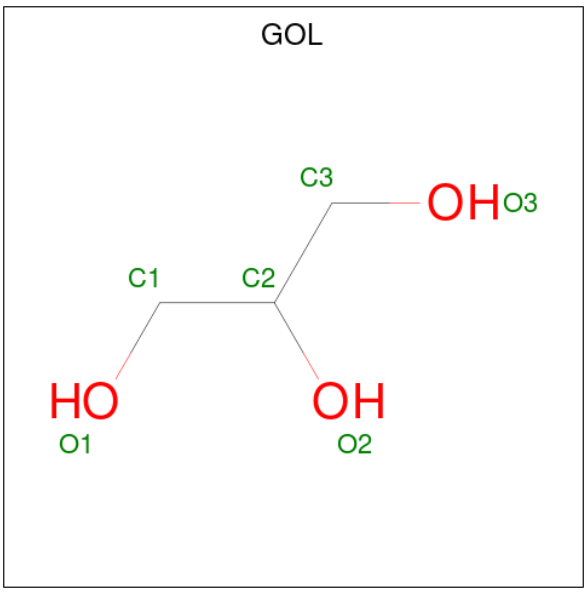


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

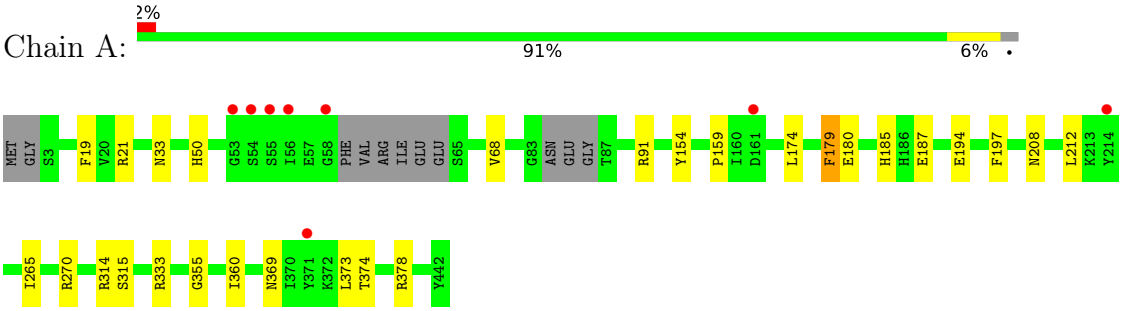
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	8	Total O 8 8	0	0
5	B	8	Total O 8 8	0	0
5	C	8	Total O 8 8	0	0
5	D	8	Total O 8 8	0	0
5	E	4	Total O 4 4	0	0
5	F	5	Total O 5 5	0	0
5	G	4	Total O 4 4	0	0
5	H	2	Total O 2 2	0	0
5	I	4	Total O 4 4	0	0
5	J	6	Total O 6 6	0	0
5	K	6	Total O 6 6	0	0
5	L	3	Total O 3 3	0	0

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.

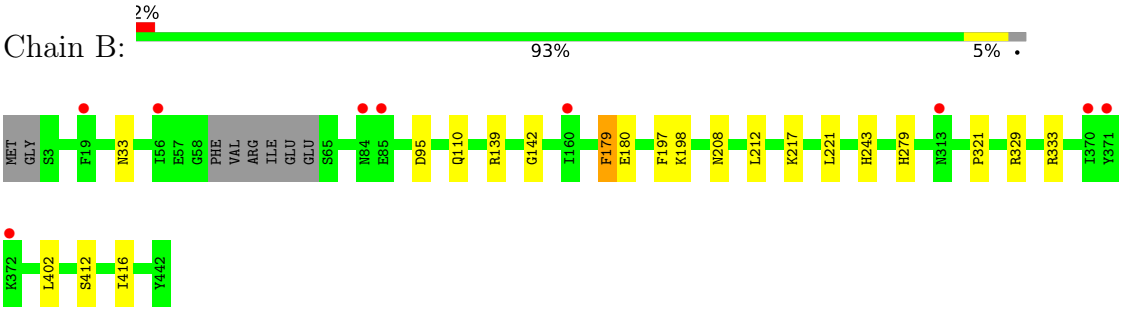
• Molecule 1: Glutamine synthetase

Chain A:



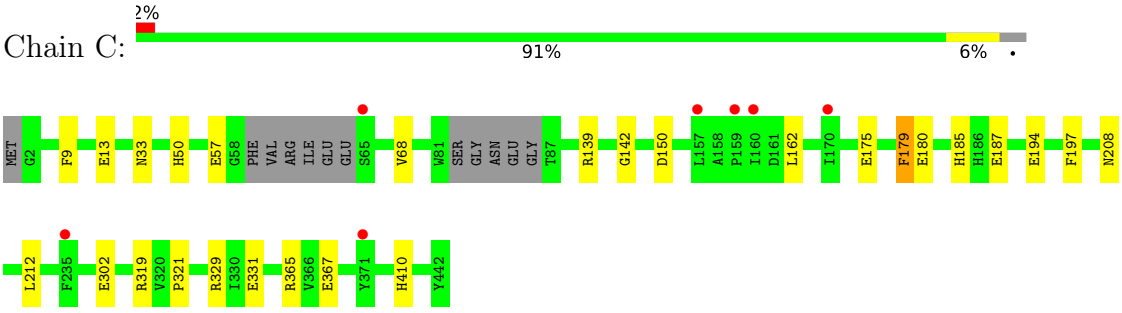
• Molecule 1: Glutamine synthetase

Chain B:



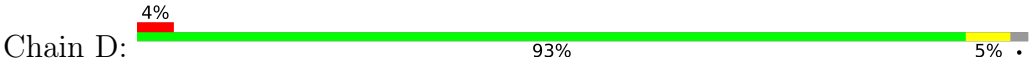
• Molecule 1: Glutamine synthetase

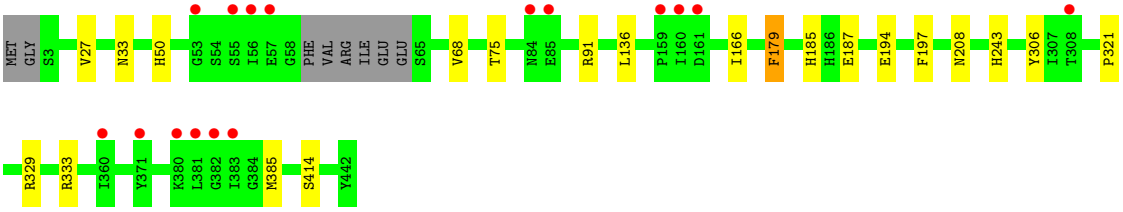
Chain C:



• Molecule 1: Glutamine synthetase

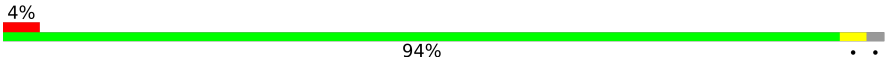
Chain D:

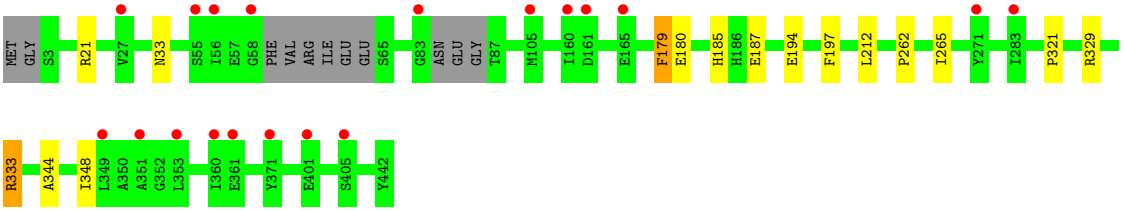




• Molecule 1: Glutamine synthetase

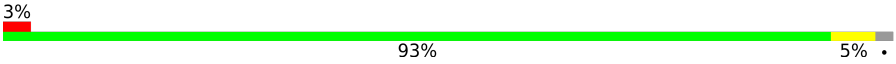
Chain E:

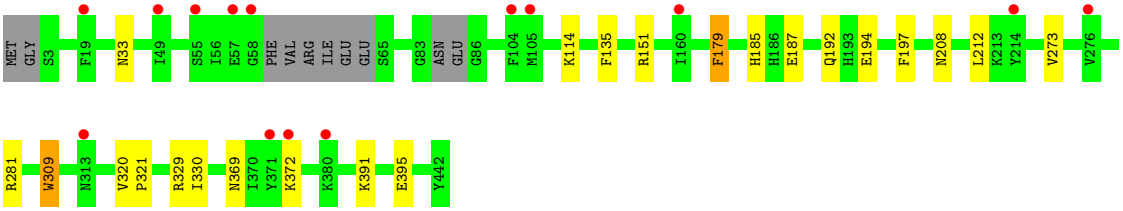




• Molecule 1: Glutamine synthetase

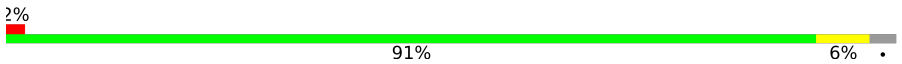
Chain F:

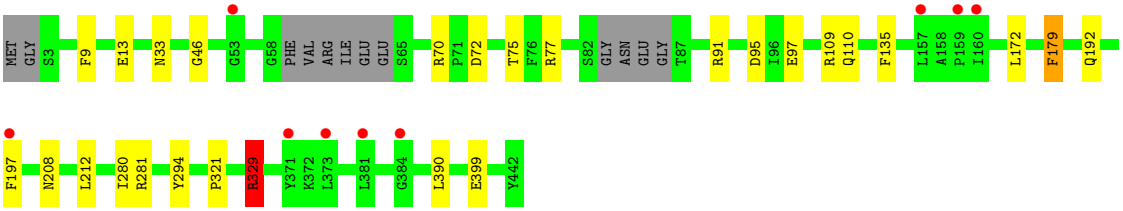




• Molecule 1: Glutamine synthetase

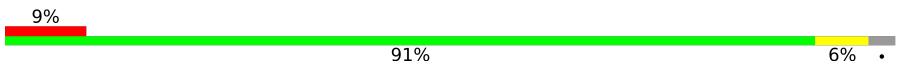
Chain G:

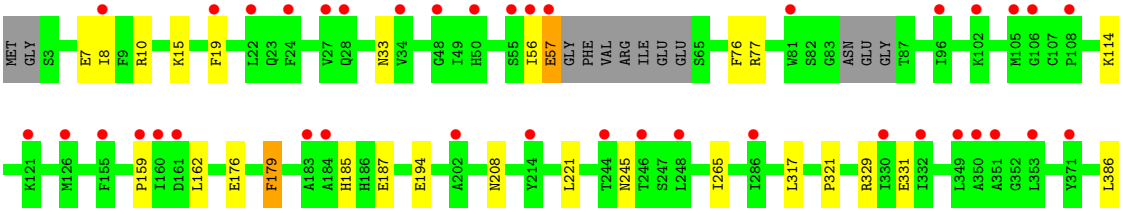




• Molecule 1: Glutamine synthetase

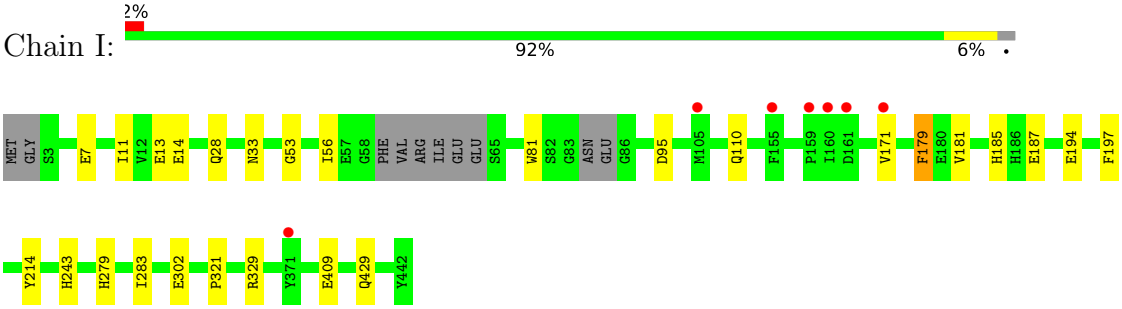
Chain H:





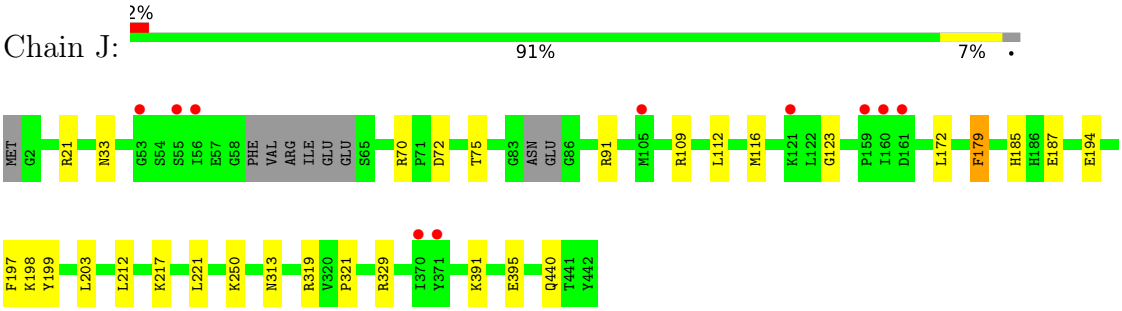
• Molecule 1: Glutamine synthetase

Chain I:



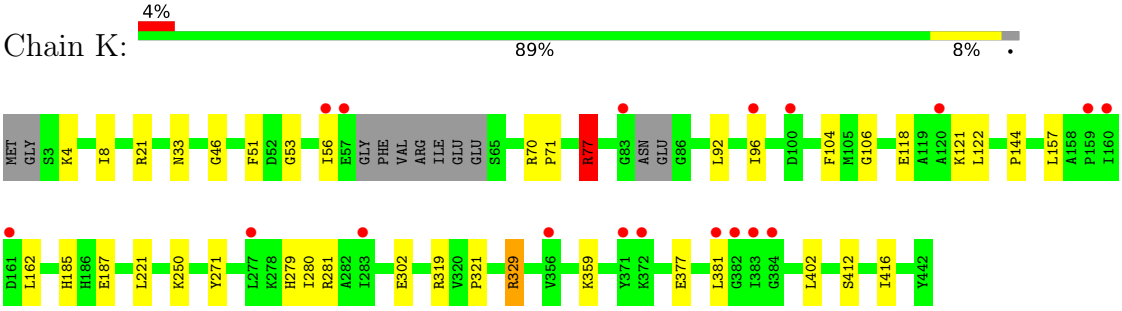
• Molecule 1: Glutamine synthetase

Chain J:



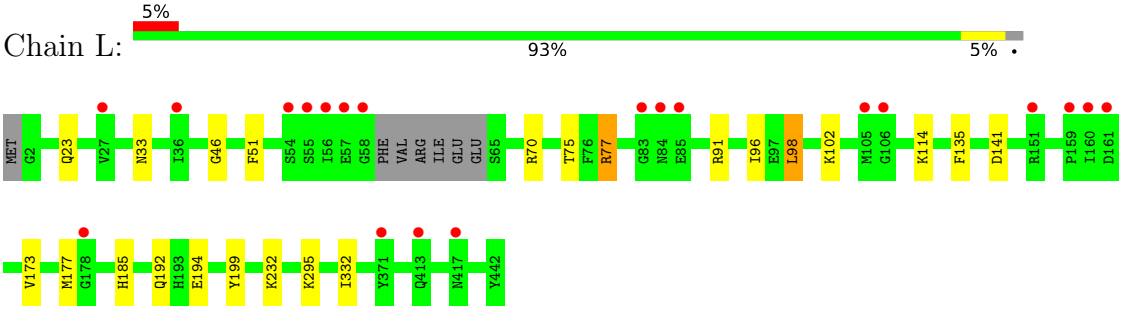
• Molecule 1: Glutamine synthetase

Chain K:



• Molecule 1: Glutamine synthetase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	130.92Å 195.65Å 133.44Å 90.00° 94.71° 90.00°	Depositor
Resolution (Å)	62.96 – 2.64 130.48 – 2.64	Depositor EDS
% Data completeness (in resolution range)	62.8 (62.96-2.64) 62.8 (130.48-2.64)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.191 , 0.225 0.191 , 0.222	Depositor DCC
R_{free} test set	6185 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 27.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	40963	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, EDO, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.37	0/3479	0.55	0/4713
1	B	0.35	0/3495	0.54	0/4737
1	C	0.35	0/3467	0.54	0/4698
1	D	0.36	0/3495	0.54	0/4737
1	E	0.36	0/3473	0.54	0/4706
1	F	0.37	0/3477	0.55	0/4711
1	G	0.38	0/3469	0.55	0/4701
1	H	0.40	0/3469	0.56	0/4701
1	I	0.37	0/3477	0.56	0/4711
1	J	0.37	0/3481	0.56	0/4716
1	K	0.37	0/3473	0.55	0/4706
1	L	0.37	0/3505	0.55	0/4749
All	All	0.37	0/41760	0.55	0/56586

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	A	0	2
1	E	0	1
1	F	0	2
1	G	0	2
1	H	0	1
1	J	0	2
1	K	0	3
1	L	0	1
All	All	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
1	A	270	ARG	Sidechain
1	E	333	ARG	Sidechain
1	F	151	ARG	Sidechain
1	F	281	ARG	Sidechain
1	G	329	ARG	Sidechain
1	G	77	ARG	Sidechain
1	H	77	ARG	Sidechain
1	J	21	ARG	Sidechain
1	J	70	ARG	Sidechain
1	K	319	ARG	Sidechain
1	K	329	ARG	Sidechain
1	K	77	ARG	Sidechain
1	L	77	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3401	0	3369	17	0
1	B	3416	0	3374	14	0
1	C	3389	0	3353	18	0
1	D	3416	0	3374	12	0
1	E	3395	0	3358	9	0
1	F	3399	0	3361	10	0
1	G	3391	0	3355	16	0
1	H	3391	0	3355	16	0
1	I	3399	0	3361	12	0
1	J	3403	0	3364	17	0
1	K	3395	0	3358	23	0
1	L	3426	0	3388	10	0
2	A	8	0	12	0	0
2	B	20	0	30	0	0
2	D	12	0	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	4	0	6	0	0
2	L	8	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	F	12	0	16	0	0
5	A	8	0	0	0	0
5	B	8	0	0	0	0
5	C	8	0	0	1	0
5	D	8	0	0	0	0
5	E	4	0	0	0	0
5	F	5	0	0	0	0
5	G	4	0	0	0	0
5	H	2	0	0	0	0
5	I	4	0	0	0	0
5	J	6	0	0	0	0
5	K	6	0	0	0	0
5	L	3	0	0	0	0
All	All	40963	0	40464	165	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 (165) 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:K:77:ARG:NH1	1:K:77:ARG:HG2	2.17	0.59
1:H:159:PRO:HG3	1:J:217:LYS:HB3	1.88	0.56
1:B:221:LEU:O	1:B:221:LEU:HD23	2.05	0.56
1:J:72:ASP:OD2	1:J:109:ARG:NH2	2.39	0.55
1:K:21:ARG:HH11	1:K:21:ARG:HG2	1.72	0.55
1:A:265:ILE:O	1:A:265:ILE:HG13	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:GLU:OE1	1:C:410:HIS:HE1	1.90	0.55
1:I:53:GLY:O	1:I:56:ILE:HG22	2.07	0.55
1:B:95:ASP:HB3	1:B:110:GLN:HE22	1.72	0.54
1:K:4:LYS:O	1:K:8:ILE:HG12	2.08	0.54
1:C:365:ARG:HD2	1:C:367:GLU:OE2	2.07	0.54
1:A:179:PHE:CZ	1:A:208:ASN:HB3	2.43	0.54
1:E:197:PHE:CZ	1:E:212:LEU:HD22	2.44	0.53
1:K:302:GLU:O	1:K:302:GLU:HG2	2.08	0.52
1:A:179:PHE:HZ	1:A:197:PHE:CE2	2.25	0.52
1:G:46:GLY:O	1:G:70:ARG:NH1	2.42	0.52
1:H:162:LEU:HD23	1:J:221:LEU:HD21	1.91	0.52
1:F:197:PHE:CZ	1:F:212:LEU:HD22	2.45	0.52
1:G:9:PHE:O	1:G:13:GLU:OE1	2.28	0.52
1:H:245:ASN:OD1	1:H:331:GLU:HG3	2.10	0.52
1:B:179:PHE:CZ	1:B:208:ASN:HB3	2.45	0.52
1:E:344:ALA:O	1:E:348:ILE:HD12	2.10	0.51
1:E:265:ILE:O	1:E:265:ILE:HG13	2.09	0.51
1:L:232:LYS:HD3	1:L:295:LYS:O	2.10	0.51
1:D:179:PHE:HZ	1:D:197:PHE:CE2	2.28	0.51
1:K:122:LEU:O	1:K:250:LYS:HE2	2.10	0.51
1:C:139:ARG:NH2	1:C:142:GLY:O	2.42	0.51
1:B:412:SER:O	1:B:416:ILE:HD12	2.10	0.51
1:C:50:HIS:CD2	1:C:68:VAL:HG12	2.46	0.51
1:L:135:PHE:CE1	1:L:192:GLN:HB2	2.46	0.50
1:C:179:PHE:HD1	1:C:180:GLU:N	2.08	0.50
1:G:72:ASP:OD2	1:G:109:ARG:NH2	2.45	0.50
1:H:7:GLU:HA	1:H:10:ARG:NH1	2.26	0.50
1:K:279:HIS:NE2	1:K:402:LEU:HD23	2.27	0.50
1:L:46:GLY:O	1:L:70:ARG:NH1	2.45	0.50
1:K:53:GLY:O	1:K:56:ILE:HG22	2.11	0.50
1:L:75:THR:O	1:L:91:ARG:NH1	2.45	0.49
1:B:139:ARG:NH1	1:B:142:GLY:O	2.45	0.49
1:K:46:GLY:O	1:K:70:ARG:NH1	2.44	0.49
1:A:355:GLY:HA2	1:A:360:ILE:HD12	1.94	0.49
1:C:197:PHE:CZ	1:C:212:LEU:HD22	2.48	0.49
1:F:320:VAL:HG22	1:F:330:ILE:HG22	1.95	0.49
1:K:221:LEU:HD23	1:K:221:LEU:O	2.11	0.49
1:A:197:PHE:CZ	1:A:212:LEU:HD22	2.47	0.49
1:F:185:HIS:HE1	1:F:187:GLU:OE1	1.96	0.49
1:B:197:PHE:CZ	1:B:212:LEU:HD22	2.48	0.49
1:I:214:TYR:CE1	1:K:157:LEU:HD22	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:112:LEU:O	1:J:116:MET:HG3	2.13	0.48
1:J:391:LYS:O	1:J:395:GLU:HG2	2.14	0.48
1:G:197:PHE:CZ	1:G:212:LEU:HD22	2.48	0.48
1:H:321:PRO:HD2	1:H:329:ARG:O	2.13	0.48
1:I:279:HIS:O	1:I:283:ILE:HD12	2.14	0.48
1:F:369:ASN:OD1	1:F:372:LYS:HD3	2.12	0.48
1:K:321:PRO:HD2	1:K:329:ARG:O	2.14	0.47
1:B:179:PHE:HZ	1:B:197:PHE:CE2	2.32	0.47
1:I:243:HIS:HE1	1:I:302:GLU:OE2	1.96	0.47
1:K:412:SER:O	1:K:416:ILE:HD12	2.15	0.47
1:C:179:PHE:HZ	1:C:197:PHE:CE2	2.33	0.47
1:D:306:TYR:CE1	1:D:385:MET:SD	3.08	0.47
1:J:185:HIS:NE2	1:J:194:GLU:OE1	2.46	0.47
1:K:377:GLU:O	1:K:381:LEU:HD12	2.15	0.47
1:J:197:PHE:CZ	1:J:212:LEU:HD22	2.50	0.46
1:A:185:HIS:NE2	1:A:194:GLU:OE1	2.45	0.46
1:A:159:PRO:HG3	1:B:217:LYS:HB3	1.97	0.46
1:H:221:LEU:HD23	1:H:221:LEU:O	2.16	0.46
1:J:440:GLN:HE21	1:K:144:PRO:HG3	1.80	0.46
1:K:104:PHE:CZ	1:K:106:GLY:HA3	2.51	0.46
1:A:179:PHE:HD1	1:A:180:GLU:N	2.13	0.46
1:K:271:TYR:CD2	1:K:359:LYS:HA	2.51	0.46
1:G:321:PRO:HD2	1:G:329:ARG:O	2.16	0.46
1:E:185:HIS:NE2	1:E:194:GLU:OE1	2.44	0.46
1:E:262:PRO:O	1:E:265:ILE:HG12	2.15	0.45
1:C:9:PHE:O	1:C:13:GLU:HG2	2.16	0.45
1:L:98:LEU:HD12	1:L:102:LYS:O	2.16	0.45
1:A:369:ASN:O	1:A:373:LEU:HG	2.16	0.45
1:B:179:PHE:HD1	1:B:180:GLU:N	2.15	0.45
1:L:173:VAL:O	1:L:177:MET:HG3	2.17	0.45
1:D:185:HIS:NE2	1:D:194:GLU:OE1	2.45	0.45
1:F:135:PHE:CE1	1:F:192:GLN:HB2	2.51	0.45
1:H:317:LEU:HD11	1:H:386:LEU:HD11	1.97	0.45
1:K:118:GLU:O	1:K:121:LYS:HB2	2.17	0.45
1:L:51:PHE:CZ	1:L:96:ILE:HD12	2.52	0.45
1:L:332:ILE:N	1:L:332:ILE:HD12	2.32	0.45
1:C:321:PRO:HD2	1:C:329:ARG:O	2.17	0.45
1:H:56:ILE:HG22	1:H:57:GLU:OE2	2.16	0.45
1:C:185:HIS:NE2	1:C:194:GLU:OE1	2.46	0.45
1:G:135:PHE:CE1	1:G:192:GLN:HB2	2.52	0.45
1:K:279:HIS:CD2	1:K:402:LEU:HD23	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:185:HIS:NE2	1:L:194:GLU:OE1	2.47	0.44
1:D:27:VAL:HG21	1:D:414:SER:OG	2.17	0.44
1:D:321:PRO:HG2	1:D:329:ARG:NH1	2.32	0.44
1:A:50:HIS:CD2	1:A:68:VAL:HG22	2.52	0.44
1:B:321:PRO:HG2	1:B:329:ARG:NH1	2.32	0.44
1:I:185:HIS:NE2	1:I:194:GLU:OE1	2.48	0.44
1:I:321:PRO:HG2	1:I:329:ARG:NH1	2.33	0.44
1:C:319:ARG:O	1:C:321:PRO:HD3	2.17	0.44
1:A:50:HIS:NE2	1:A:68:VAL:HG22	2.33	0.44
1:G:179:PHE:HZ	1:G:197:PHE:CE2	2.36	0.44
1:K:77:ARG:HG2	1:K:77:ARG:HH11	1.83	0.44
1:G:70:ARG:HG3	1:G:97:GLU:OE2	2.18	0.43
1:G:110:GLN:HE21	1:G:110:GLN:HB3	1.61	0.43
1:J:179:PHE:HZ	1:J:197:PHE:CE2	2.36	0.43
1:J:199:TYR:OH	1:J:329:ARG:NE	2.51	0.43
1:C:302:GLU:O	1:C:302:GLU:HG2	2.19	0.43
1:E:321:PRO:HG2	1:E:329:ARG:NH1	2.33	0.43
1:D:179:PHE:CE2	1:D:208:ASN:HB3	2.52	0.43
1:G:294:TYR:CE2	1:G:390:LEU:HA	2.53	0.43
1:J:75:THR:O	1:J:91:ARG:NH1	2.52	0.43
1:D:50:HIS:CD2	1:D:68:VAL:HG22	2.54	0.43
1:G:280:ILE:HG23	1:G:281:ARG:N	2.34	0.43
1:A:159:PRO:CG	1:B:217:LYS:HB3	2.49	0.43
1:F:185:HIS:NE2	1:F:194:GLU:OE1	2.48	0.43
1:D:185:HIS:HE1	1:D:187:GLU:OE2	2.01	0.43
1:I:7:GLU:O	1:I:11:ILE:HG13	2.19	0.43
1:D:179:PHE:CZ	1:D:208:ASN:HB3	2.54	0.42
1:I:179:PHE:HZ	1:I:197:PHE:CE2	2.37	0.42
1:K:280:ILE:HG23	1:K:281:ARG:N	2.34	0.42
1:D:243:HIS:ND1	1:D:333:ARG:HG2	2.34	0.42
1:H:176:GLU:O	1:H:176:GLU:HG3	2.19	0.42
1:J:319:ARG:O	1:J:321:PRO:HD3	2.19	0.42
1:L:23:GLN:NE2	1:L:91:ARG:HD3	2.34	0.42
1:E:179:PHE:HD1	1:E:180:GLU:N	2.18	0.42
1:F:179:PHE:CZ	1:F:208:ASN:HB3	2.55	0.42
1:A:174:LEU:HD22	1:A:179:PHE:CD2	2.55	0.42
1:E:185:HIS:HE1	1:E:187:GLU:OE2	2.03	0.42
1:D:75:THR:O	1:D:91:ARG:NH1	2.53	0.42
1:B:243:HIS:CE1	1:B:333:ARG:HB3	2.55	0.42
1:F:391:LYS:O	1:F:395:GLU:HG3	2.19	0.42
1:C:185:HIS:HE1	1:C:187:GLU:OE2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ARG:NH1	5:C:601:HOH:O	2.50	0.41
1:C:179:PHE:CE2	1:C:208:ASN:HB3	2.55	0.41
1:H:162:LEU:CD2	1:J:221:LEU:HD21	2.50	0.41
1:F:321:PRO:HD2	1:F:329:ARG:O	2.20	0.41
1:C:150:ASP:HB3	1:C:162:LEU:HB2	2.02	0.41
1:H:185:HIS:NE2	1:H:194:GLU:OE1	2.48	0.41
1:C:175:GLU:HA	1:C:179:PHE:O	2.21	0.41
1:G:95:ASP:HB3	1:G:110:GLN:OE1	2.20	0.41
1:I:185:HIS:HE1	1:I:187:GLU:OE2	2.03	0.41
1:A:374:THR:O	1:A:378:ARG:HG3	2.21	0.41
1:H:179:PHE:CZ	1:H:208:ASN:HB3	2.54	0.41
1:J:185:HIS:HE1	1:J:187:GLU:OE2	2.03	0.41
1:B:180:GLU:HB2	1:B:198:LYS:HE3	2.02	0.41
1:B:279:HIS:NE2	1:B:402:LEU:HD23	2.36	0.41
1:G:172:LEU:HD13	1:H:19:PHE:CE2	2.55	0.41
1:A:19:PHE:CE2	1:J:172:LEU:HD13	2.56	0.41
1:A:315:SER:HB2	1:A:333:ARG:NH2	2.35	0.41
1:E:21:ARG:NH1	1:E:21:ARG:HG2	2.35	0.41
1:H:265:ILE:O	1:H:265:ILE:HD12	2.21	0.41
1:G:75:THR:HB	1:G:91:ARG:HH12	1.86	0.41
1:H:185:HIS:HE1	1:H:187:GLU:OE2	2.03	0.41
1:J:109:ARG:NH1	1:J:203:LEU:HD21	2.36	0.41
1:F:273:VAL:HG11	1:F:309:TRP:CE3	2.57	0.40
1:G:179:PHE:CE2	1:G:208:ASN:HB3	2.55	0.40
1:I:95:ASP:HB3	1:I:110:GLN:OE1	2.21	0.40
1:K:51:PHE:CZ	1:K:96:ILE:HD12	2.56	0.40
1:G:172:LEU:HD12	1:G:172:LEU:HA	1.90	0.40
1:H:8:ILE:HG12	1:H:76:PHE:CG	2.56	0.40
1:I:171:VAL:HG13	1:I:181:VAL:HG11	2.03	0.40
1:J:123:GLY:O	1:J:250:LYS:HA	2.20	0.40
1:K:185:HIS:HE1	1:K:187:GLU:OE2	2.04	0.40
1:C:319:ARG:NH1	1:C:331:GLU:OE1	2.49	0.40
1:D:136:LEU:HD21	1:D:166:ILE:HG21	2.04	0.40
1:I:13:GLU:HG2	1:I:14:GLU:N	2.36	0.40
1:K:71:PRO:HB3	1:K:92:LEU:HG	2.04	0.40
1:A:185:HIS:HE1	1:A:187:GLU:OE2	2.04	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	A	425/442 (96%)	418 (98%)	7 (2%)	0	100	100
1	B	430/442 (97%)	422 (98%)	8 (2%)	0	100	100
1	C	424/442 (96%)	416 (98%)	8 (2%)	0	100	100
1	D	430/442 (97%)	422 (98%)	8 (2%)	0	100	100
1	E	425/442 (96%)	417 (98%)	8 (2%)	0	100	100
1	F	426/442 (96%)	419 (98%)	7 (2%)	0	100	100
1	G	424/442 (96%)	416 (98%)	8 (2%)	0	100	100
1	H	424/442 (96%)	415 (98%)	9 (2%)	0	100	100
1	I	426/442 (96%)	419 (98%)	7 (2%)	0	100	100
1	J	427/442 (97%)	415 (97%)	12 (3%)	0	100	100
1	K	425/442 (96%)	418 (98%)	7 (2%)	0	100	100
1	L	431/442 (98%)	425 (99%)	6 (1%)	0	100	100
All	All	5117/5304 (96%)	5022 (98%)	95 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/376 (98%)	362 (99%)	5 (1%)	67	80
1	B	368/376 (98%)	366 (100%)	2 (0%)	88	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	365/376 (97%)	363 (100%)	2 (0%)	88 94
1	D	368/376 (98%)	366 (100%)	2 (0%)	88 94
1	E	366/376 (97%)	363 (99%)	3 (1%)	81 89
1	F	366/376 (97%)	362 (99%)	4 (1%)	73 85
1	G	366/376 (97%)	362 (99%)	4 (1%)	73 85
1	H	366/376 (97%)	361 (99%)	5 (1%)	67 80
1	I	366/376 (97%)	360 (98%)	6 (2%)	62 78
1	J	366/376 (97%)	362 (99%)	4 (1%)	73 85
1	K	366/376 (97%)	363 (99%)	3 (1%)	81 89
1	L	369/376 (98%)	363 (98%)	6 (2%)	62 78
All	All	4399/4512 (98%)	4353 (99%)	46 (1%)	76 86

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	91	ARG
1	A	154	TYR
1	A	179	PHE
1	A	314	ARG
1	B	33	ASN
1	B	179	PHE
1	C	33	ASN
1	C	179	PHE
1	D	33	ASN
1	D	179	PHE
1	E	33	ASN
1	E	179	PHE
1	E	333	ARG
1	F	33	ASN
1	F	114	LYS
1	F	179	PHE
1	F	309	TRP
1	G	33	ASN
1	G	179	PHE
1	G	329	ARG
1	G	399	GLU
1	H	15	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	33	ASN
1	H	57	GLU
1	H	114	LYS
1	H	179	PHE
1	I	28	GLN
1	I	33	ASN
1	I	81	TRP
1	I	179	PHE
1	I	409	GLU
1	I	429	GLN
1	J	33	ASN
1	J	179	PHE
1	J	198	LYS
1	J	313	ASN
1	K	33	ASN
1	K	77	ARG
1	K	162	LEU
1	L	33	ASN
1	L	77	ARG
1	L	98	LEU
1	L	114	LYS
1	L	141	ASP
1	L	199	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	23	GLN
1	B	110	GLN
1	B	440	GLN
1	C	410	HIS
1	F	193	HIS
1	H	149	GLN
1	H	193	HIS
1	I	243	HIS
1	I	429	GLN
1	J	440	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 monosaccharides 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	EDO	L	501	-	3,3,3	0.59	0	2,2,2	0.27	0
2	EDO	A	502	-	3,3,3	0.59	0	2,2,2	0.28	0
2	EDO	B	502	-	3,3,3	0.63	0	2,2,2	0.17	0
2	EDO	D	502	-	3,3,3	0.62	0	2,2,2	0.33	0
4	GOL	F	501	-	5,5,5	0.14	0	5,5,5	0.48	0
2	EDO	L	502	-	3,3,3	0.51	0	2,2,2	0.38	0
2	EDO	A	501	-	3,3,3	0.49	0	2,2,2	0.40	0
2	EDO	B	501	-	3,3,3	0.54	0	2,2,2	0.33	0
4	GOL	F	502	-	5,5,5	0.06	0	5,5,5	0.28	0
2	EDO	I	501	-	3,3,3	0.60	0	2,2,2	0.26	0
2	EDO	D	503	-	3,3,3	0.64	0	2,2,2	0.10	0
2	EDO	B	503	-	3,3,3	0.64	0	2,2,2	0.32	0
2	EDO	B	505	-	3,3,3	0.54	0	2,2,2	0.37	0
2	EDO	B	504	-	3,3,3	0.07	0	2,2,2	0.18	0
2	EDO	D	501	-	3,3,3	0.63	0	2,2,2	0.23	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	EDO	L	501	-	-	0/1/1/1	-
2	EDO	A	502	-	-	1/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
2	EDO	D	502	-	-	1/1/1/1	-
4	GOL	F	501	-	-	2/4/4/4	-
2	EDO	L	502	-	-	0/1/1/1	-
2	EDO	A	501	-	-	1/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
4	GOL	F	502	-	-	2/4/4/4	-
2	EDO	I	501	-	-	0/1/1/1	-
2	EDO	D	503	-	-	0/1/1/1	-
2	EDO	B	503	-	-	1/1/1/1	-
2	EDO	B	505	-	-	0/1/1/1	-
2	EDO	B	504	-	-	1/1/1/1	-
2	EDO	D	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	502	GOL	O1-C1-C2-C3
4	F	501	GOL	O1-C1-C2-C3
2	B	503	EDO	O1-C1-C2-O2
2	D	501	EDO	O1-C1-C2-O2
4	F	502	GOL	O1-C1-C2-O2
4	F	501	GOL	O1-C1-C2-O2
2	A	501	EDO	O1-C1-C2-O2
2	A	502	EDO	O1-C1-C2-O2
2	B	504	EDO	O1-C1-C2-O2
2	B	501	EDO	O1-C1-C2-O2
2	D	502	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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^{th} 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	431/442 (97%)	0.15	8 (1%) 66 64	31, 60, 108, 147	0
1	B	434/442 (98%)	0.03	9 (2%) 63 60	28, 60, 109, 169	0
1	C	430/442 (97%)	0.01	7 (1%) 72 69	30, 63, 102, 134	0
1	D	434/442 (98%)	0.14	16 (3%) 41 38	31, 61, 114, 178	0
1	E	431/442 (97%)	0.13	19 (4%) 34 31	32, 65, 106, 149	0
1	F	432/442 (97%)	0.11	14 (3%) 47 44	33, 68, 110, 164	0
1	G	430/442 (97%)	0.14	9 (2%) 63 60	37, 74, 112, 169	0
1	H	430/442 (97%)	0.34	39 (9%) 9 7	47, 89, 135, 171	0
1	I	432/442 (97%)	-0.03	7 (1%) 72 69	45, 76, 115, 141	0
1	J	433/442 (97%)	0.13	10 (2%) 60 57	31, 67, 110, 154	0
1	K	431/442 (97%)	0.20	18 (4%) 36 33	35, 68, 119, 168	0
1	L	435/442 (98%)	0.26	20 (4%) 32 28	40, 67, 119, 177	0
All	All	5183/5304 (97%)	0.13	176 (3%) 45 41	28, 68, 116, 178	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	56	ILE	8.4
1	L	55	SER	8.1
1	L	85	GLU	8.1
1	G	371	TYR	7.4
1	H	160	ILE	7.3
1	B	84	ASN	6.7
1	L	105	MET	6.7
1	H	161	ASP	6.6
1	B	85	GLU	6.4
1	G	160	ILE	6.3
1	K	56	ILE	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	160	ILE	5.7
1	J	370	ILE	5.6
1	L	57	GLU	5.6
1	L	160	ILE	5.5
1	K	160	ILE	5.3
1	D	56	ILE	4.9
1	A	371	TYR	4.9
1	A	56	ILE	4.8
1	H	55	SER	4.7
1	B	56	ILE	4.7
1	F	313	ASN	4.6
1	H	56	ILE	4.5
1	I	160	ILE	4.4
1	I	371	TYR	4.3
1	D	382	GLY	4.3
1	J	105	MET	4.3
1	H	96	ILE	4.3
1	J	159	PRO	4.2
1	L	58	GLY	4.2
1	H	48	GLY	4.2
1	J	371	TYR	4.2
1	E	161	ASP	4.1
1	L	84	ASN	4.1
1	C	159	PRO	3.9
1	A	53	GLY	3.9
1	E	105	MET	3.8
1	K	356	VAL	3.8
1	D	381	LEU	3.8
1	H	350	ALA	3.8
1	H	105	MET	3.8
1	F	214	TYR	3.7
1	E	160	ILE	3.6
1	L	371	TYR	3.6
1	F	105	MET	3.6
1	H	126	MET	3.5
1	I	159	PRO	3.5
1	J	53	GLY	3.5
1	J	160	ILE	3.4
1	D	371	TYR	3.4
1	K	159	PRO	3.4
1	A	55	SER	3.3
1	H	106	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	34	VAL	3.3
1	D	159	PRO	3.3
1	L	151	ARG	3.3
1	D	161	ASP	3.2
1	E	360	ILE	3.2
1	H	244	THR	3.1
1	D	53	GLY	3.1
1	D	57	GLU	3.1
1	I	161	ASP	3.1
1	H	246	THR	3.1
1	C	371	TYR	3.1
1	G	373	LEU	3.1
1	L	106	GLY	3.1
1	G	53	GLY	3.0
1	F	372	LYS	3.0
1	A	58	GLY	3.0
1	F	371	TYR	3.0
1	H	214	TYR	3.0
1	H	22	LEU	3.0
1	F	58	GLY	3.0
1	G	159	PRO	3.0
1	H	183	ALA	2.9
1	H	330	ILE	2.9
1	J	56	ILE	2.9
1	D	85	GLU	2.9
1	D	84	ASN	2.9
1	K	381	LEU	2.8
1	E	351	ALA	2.8
1	H	27	VAL	2.8
1	J	55	SER	2.8
1	H	28	GLN	2.8
1	H	81	TRP	2.8
1	B	160	ILE	2.8
1	K	384	GLY	2.8
1	H	184	ALA	2.7
1	C	65	SER	2.7
1	E	405	SER	2.7
1	H	19	PHE	2.7
1	H	102	LYS	2.7
1	L	161	ASP	2.6
1	K	283	ILE	2.6
1	L	159	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	56	ILE	2.6
1	F	49	ILE	2.6
1	E	361	GLU	2.6
1	L	83	GLY	2.6
1	H	50	HIS	2.6
1	K	277	LEU	2.6
1	B	313	ASN	2.5
1	K	372	LYS	2.5
1	C	157	LEU	2.5
1	G	384	GLY	2.5
1	D	383	ILE	2.5
1	J	161	ASP	2.5
1	L	36	ILE	2.5
1	E	401	GLU	2.5
1	I	155	PHE	2.5
1	G	157	LEU	2.5
1	G	197	PHE	2.5
1	K	383	ILE	2.4
1	F	276	VAL	2.4
1	F	57	GLU	2.4
1	K	83	GLY	2.4
1	H	57	GLU	2.4
1	K	382	GLY	2.4
1	H	371	TYR	2.4
1	H	332	ILE	2.4
1	E	83	GLY	2.3
1	H	8	ILE	2.3
1	B	371	TYR	2.3
1	B	372	LYS	2.3
1	A	214	TYR	2.3
1	K	100	ASP	2.3
1	F	55	SER	2.3
1	E	165	GLU	2.3
1	H	159	PRO	2.3
1	H	155	PHE	2.3
1	K	120	ALA	2.3
1	D	160	ILE	2.3
1	F	104	PHE	2.3
1	B	370	ILE	2.3
1	E	58	GLY	2.3
1	H	108	PRO	2.2
1	J	121	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	55	SER	2.2
1	E	353	LEU	2.2
1	F	160	ILE	2.2
1	H	121	LYS	2.2
1	H	351	ALA	2.2
1	E	271	TYR	2.2
1	E	27	VAL	2.2
1	L	27	VAL	2.2
1	A	161	ASP	2.2
1	H	286	ILE	2.2
1	K	371	TYR	2.2
1	K	96	ILE	2.2
1	G	381	LEU	2.2
1	L	54	SER	2.2
1	H	202	ALA	2.2
1	F	19	PHE	2.2
1	H	248	LEU	2.1
1	B	19	PHE	2.1
1	D	380	LYS	2.1
1	H	24	PHE	2.1
1	H	349	LEU	2.1
1	H	353	LEU	2.1
1	L	413	GLN	2.1
1	C	235	PHE	2.1
1	C	170	ILE	2.1
1	D	360	ILE	2.1
1	A	54	SER	2.1
1	E	349	LEU	2.0
1	E	371	TYR	2.0
1	D	308	THR	2.0
1	E	55	SER	2.0
1	I	105	MET	2.0
1	F	380	LYS	2.0
1	K	161	ASP	2.0
1	L	178	GLY	2.0
1	I	171	VAL	2.0
1	E	283	ILE	2.0
1	K	57	GLU	2.0
1	L	417	ASN	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^{th} 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^2)	Q<0.9
2	EDO	B	504	4/4	0.78	0.29	50,59,100,107	0
4	GOL	F	501	6/6	0.79	0.37	47,62,69,82	0
2	EDO	L	502	4/4	0.80	0.19	63,77,83,84	0
2	EDO	D	503	4/4	0.81	0.21	46,48,54,65	0
2	EDO	L	501	4/4	0.83	0.23	51,52,57,68	0
2	EDO	I	501	4/4	0.84	0.42	59,70,76,83	0
4	GOL	F	502	6/6	0.84	0.19	74,89,98,101	0
3	MG	K	501	1/1	0.85	0.12	66,66,66,66	0
2	EDO	B	502	4/4	0.86	0.30	47,53,55,66	0
2	EDO	B	503	4/4	0.86	0.54	70,74,82,82	0
2	EDO	A	502	4/4	0.87	0.20	55,69,75,78	0
2	EDO	B	501	4/4	0.90	0.24	49,58,64,66	0
2	EDO	D	502	4/4	0.91	0.16	72,81,87,91	0
2	EDO	D	501	4/4	0.91	0.17	49,55,61,66	0
3	MG	C	501	1/1	0.92	0.07	67,67,67,67	0
3	MG	G	501	1/1	0.92	0.12	80,80,80,80	0
3	MG	H	501	1/1	0.92	0.08	82,82,82,82	0
2	EDO	B	505	4/4	0.94	0.24	48,50,69,82	0
2	EDO	A	501	4/4	0.94	0.16	62,62,67,84	0
3	MG	I	502	1/1	0.94	0.05	78,78,78,78	0
3	MG	D	504	1/1	0.95	0.04	55,55,55,55	0
3	MG	E	501	1/1	0.95	0.10	56,56,56,56	0
3	MG	F	503	1/1	0.96	0.10	54,54,54,54	0
3	MG	A	503	1/1	0.96	0.12	76,76,76,76	0
3	MG	J	501	1/1	0.96	0.10	54,54,54,54	0
3	MG	L	503	1/1	0.97	0.16	62,62,62,62	0
3	MG	B	506	1/1	0.98	0.16	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.