wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 09:43 AM EDT

PDB ID	:	4LNO
Title	:	B. subtilis glutamine synthetase structures reveal large active site conformational changes and basis for isoenzyme specific regulation: form two of GS-1
Authors	:	Schumacher, M.A.; Chinnam, N.; Tonthat, N.; Fisher, S.; Wray, L.
Deposited on	:	2013-07-11
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

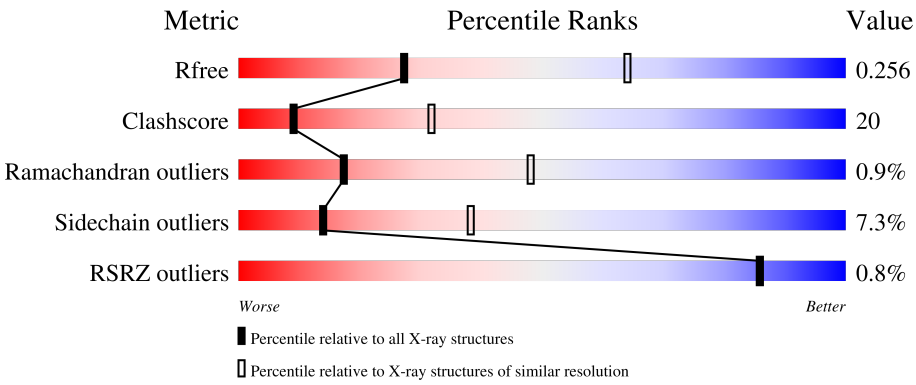
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	443	.% 65% 30% .
1	B	443	58% 37% .
1	C	443	.% 61% 35% .
1	D	443	.% 62% 33% 5%
1	E	443	.% 59% 37% .

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Mol	Chain	Length	Quality of chain
1	F	443	% 58% 36% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21993 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.

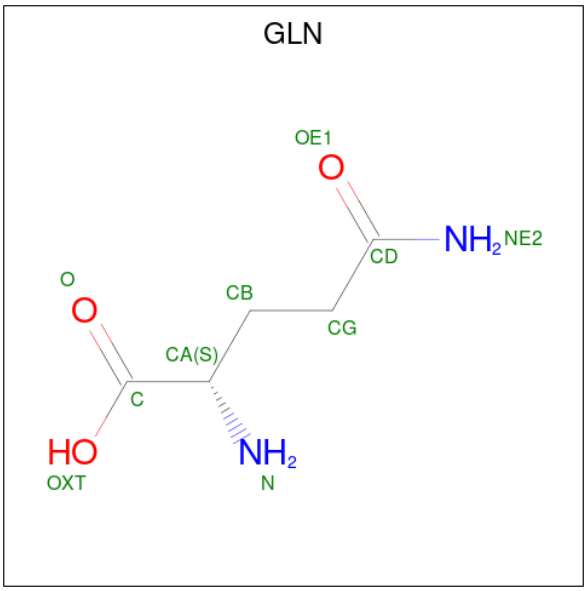
- Molecule 1 is a protein called Glutamine synthetase.

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



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

- Molecule 4 is water.

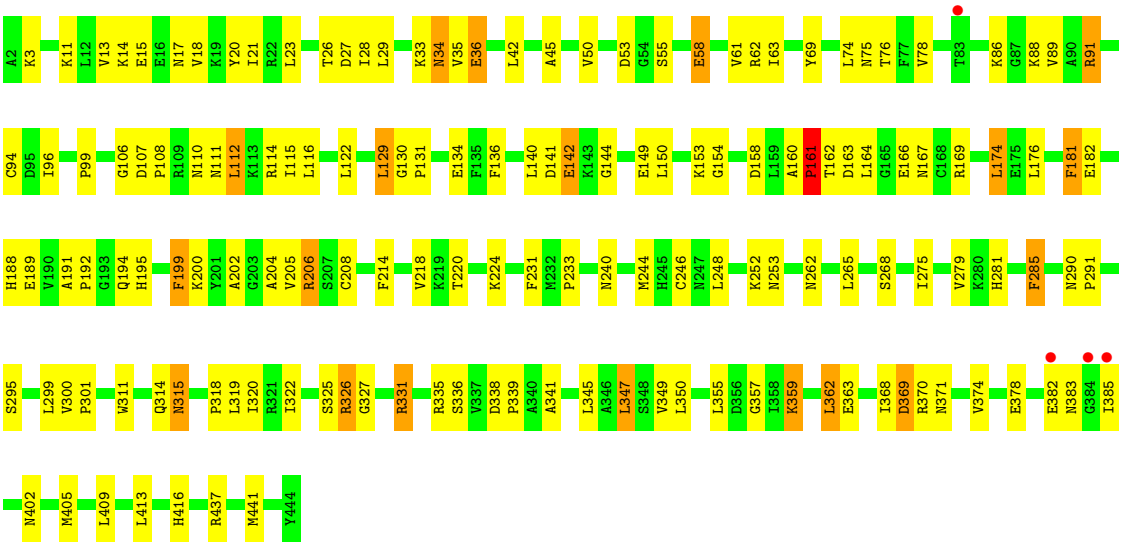
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	122	122	122	0	0
4	B	117	117	117	0	0
4	C	123	123	123	0	0
4	D	114	114	114	0	0
4	E	134	134	134	0	0
4	F	103	103	103	0	0

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.

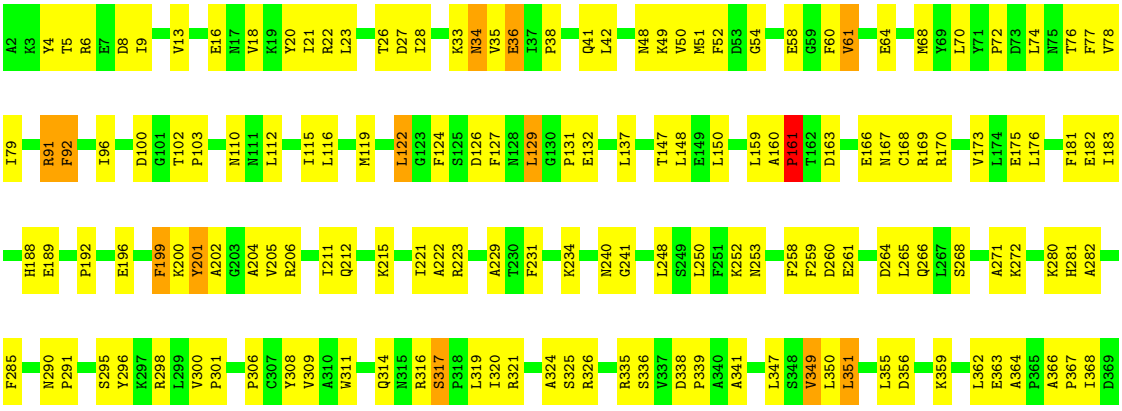
- Molecule 1: Glutamine synthetase

Chain A:



- Molecule 1: Glutamine synthetase

Chain B:



R370 N371 I372 Y373 K377 R380 M381 E382 I385 T391 L392 A393 E394 A395 L396 S401 N402 M405 V406 L413 F414 E415 E419 I423 E424 W425 D426 R429 T430 P434 E438 M441 S442 Q443 Y444

• Molecule 1: Glutamine synthetase

Chain C: % 61% 35% •

A2 R6 I9 E16 K19 Y20 I21 R22 F25 T26 D27 I28 K33 N34 V35 E36 L46 D47 N48 K49 V50 S55 S56 I57 E58 G59 F60 V61 R62 E65 S66 D67 P72 D73 L74 I79 T83 A84 E85 K86 G87 K88 V89 A90 R91 F92 I96

Y97 N98 T102 E105 N110 N111 L112 K113 R114 I115 L116 M119 F124 F127 N128 L129 G130 P131 E134 L140 D141 E142 D152 Y156 F157 D158 L159 A160 E166 R169 I172 L176 E177 E178 M179 G180 F181 E182 I183 H188 E189 V190 F199

G203 A204 C208 V217 V218 I221 H225 H228 P233 K234 P235 L236 V239 N240 L248 S249 K252 N253 F258 N262 A263 D264 L265 T270 A271 K272 I278 A282 T283 S284 F285 P291 Y296 K297 R298 L299 V300 P301 G302 Y303 P306 C307 Y308

V309 A310 W311 N315 R316 S317 P318 L319 I320 R326 G327 I328 S329 T330 R331 R335 S336 V337 D338 P339 A340 A341 N342 P343 L347 S348 V349 L350 L351 L355 D356 G357 I358 K359 N360 K361 L362 E363 A364 P367 I368 D369 R370 N371 I372 Y373 S376 K377 E378 E379 R380 M381

I385 V386 D387 A390 T391 L392 L396 E397 K400 S401 N402 E403 V404 M405 V406 K407 L413 E419 I423 Q431 P434 E438 M441 S442 Q443 Y444

• Molecule 1: Glutamine synthetase

Chain D: % 62% 33% 5%

A2 R6 I9 E10 K11 L12 V13 K14 E15 V18 K19 Y20 I21 D27 I28 N34 V35 E36 L42 L46 K49 G54 S55 S56 I57 E58 G59 F60 V61 R62 I63 E64 E65 S66 D67 M68 L74 T83 A84 E85 K86 V89 A90 R91 F92 I96 Y97

P103 F104 N110 N111 R114 I115 L116 K117 E118 M119 E120 D121 L122 G123 F127 N128 L129 G130 P131 E134 F135 F136 L137 F138 K139 E142 L150 N151 D152 K153 G154 G155 Y156 F157 D158 L159 A160 P161 T162 D163 L164 C168 R169 R170 D171 I172 L176 F181 E182 I183

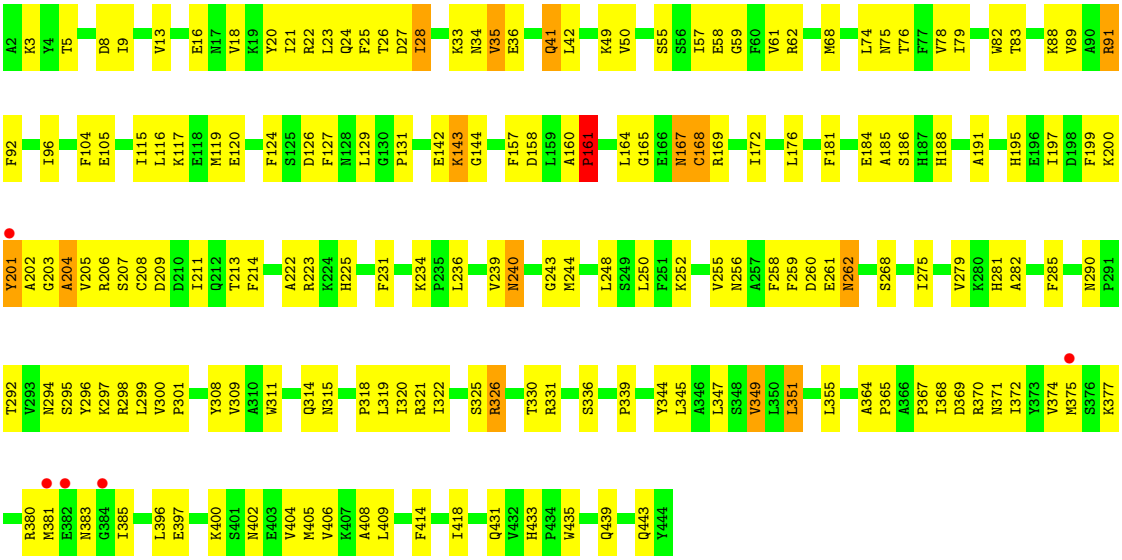
E184 A185 H188 P192 G193 Q194 F199 K200 Y201 A202 G203 A204 V205 R206 S207 C208 T213 R223 A229 T230 F231 M232 P233 K234 P235 N240 H245 S249 K252 N256 A257 F258 F259 D260 A263 H273 F274 I275 A276 G277 I278 V279 K280 T283 R298

L299 V300 P301 Y308 V309 A310 W311 Q314 N315 R316 S317 P318 L319 I320 R321 I322 P323 A324 S325 I328 R331 V332 R335 D338 P339 P343 Y344 L345 L351 G354 L355 D356 G357 I358 K359 L362 E363 P367 I368 D369 R370 N371 I372 Y373 V374 M375 S376 K377 E378

E379 R380 M381 E382 N383 G384 I385 V386 D387 L388 P389 V406 K407 A408 L409 L413 F414 F417 I418 E419 E422 I423 M427 Q431 Y444

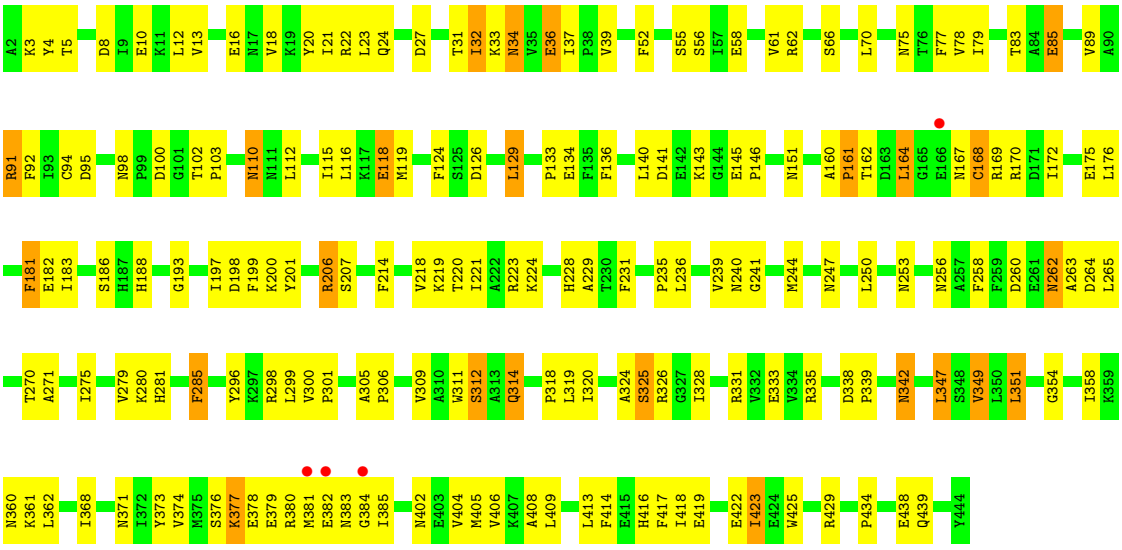
• Molecule 1: Glutamine synthetase

Chain E: % 59% 37% •



- Molecule 1: Glutamine synthetase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.86Å 138.94Å 144.73Å 90.00° 125.17° 90.00°	Depositor
Resolution (Å)	71.68 – 2.90 71.68 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.68-2.90) 99.8 (71.68-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.196 , 0.256 0.195 , 0.256	Depositor DCC
R_{free} test set	4572 reflections (6.08%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21993	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/3618	0.61	0/4895
1	B	0.44	0/3618	0.61	0/4895
1	C	0.46	0/3618	0.62	0/4895
1	D	0.44	0/3618	0.61	0/4895
1	E	0.43	0/3618	0.62	0/4895
1	F	0.44	0/3618	0.61	0/4895
All	All	0.44	0/21708	0.61	0/29370

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	B	0	1
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	296	TYR	Sidechain
1	C	296	TYR	Sidechain
1	E	296	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	F	296	TYR	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	3535	0	3466	130	0
1	B	3535	0	3466	146	0
1	C	3535	0	3466	138	0
1	D	3535	0	3466	147	0
1	E	3535	0	3466	153	0
1	F	3535	0	3466	166	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	9	0	7	2	0
3	B	9	0	7	1	0
3	C	10	0	7	2	0
3	D	10	0	7	1	0
3	E	10	0	7	0	0
3	F	10	0	7	2	0
4	A	122	0	0	6	0
4	B	117	0	0	6	0
4	C	123	0	0	10	0
4	D	114	0	0	7	0
4	E	134	0	0	8	0
4	F	103	0	0	4	0
All	All	21993	0	20838	847	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 20.

The worst 5 of 847 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:E:160:ALA:HB1	1:E:161:PRO:HD2	1.29	1.10
1:C:328:ILE:HD13	1:C:328:ILE:H	1.11	1.09
1:D:160:ALA:HB1	1:D:161:PRO:HD2	1.38	1.05
1:D:160:ALA:HB3	1:D:169:ARG:HH22	1.22	1.03
1:D:63:ILE:HG22	1:D:64:GLU:HG3	1.43	0.95

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%)	397 (90%)	39 (9%)	5 (1%)	14	42
1	B	441/443 (100%)	412 (93%)	25 (6%)	4 (1%)	17	48
1	C	441/443 (100%)	404 (92%)	36 (8%)	1 (0%)	47	78
1	D	441/443 (100%)	403 (91%)	33 (8%)	5 (1%)	14	42
1	E	441/443 (100%)	401 (91%)	35 (8%)	5 (1%)	14	42
1	F	441/443 (100%)	418 (95%)	20 (4%)	3 (1%)	22	54
All	All	2646/2658 (100%)	2435 (92%)	188 (7%)	23 (1%)	17	48

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO
1	B	161	PRO
1	D	161	PRO
1	E	143	LYS
1	E	161	PRO

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	382/382 (100%)	355 (93%)	27 (7%)	14	40
1	B	382/382 (100%)	352 (92%)	30 (8%)	12	34
1	C	382/382 (100%)	358 (94%)	24 (6%)	18	46
1	D	382/382 (100%)	352 (92%)	30 (8%)	12	34
1	E	382/382 (100%)	360 (94%)	22 (6%)	20	50
1	F	382/382 (100%)	349 (91%)	33 (9%)	10	30
All	All	2292/2292 (100%)	2126 (93%)	166 (7%)	14	39

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	91	ARG
1	F	126	ASP
1	E	167	ASN
1	E	381	MET
1	F	240	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	225	HIS
1	F	281	HIS
1	E	281	HIS
1	F	167	ASN
1	F	439	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
3	GLN	F	503	-	8,9,9	0.78	0	10,11,11	0.40	0
3	GLN	B	503	2	7,8,9	0.49	0	4,9,11	0.13	0
3	GLN	C	501	-	8,9,9	0.70	0	10,11,11	0.77	0
3	GLN	E	503	2	8,9,9	0.75	0	10,11,11	0.70	0
3	GLN	D	503	2	8,9,9	0.72	0	10,11,11	0.66	0
3	GLN	A	503	-	7,8,9	0.94	0	4,9,11	0.34	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	GLN	F	503	-	-	6/9/9/9	-
3	GLN	B	503	2	-	1/6/7/9	-
3	GLN	C	501	-	-	6/9/9/9	-
3	GLN	E	503	2	-	4/9/9/9	-
3	GLN	D	503	2	-	5/9/9/9	-
3	GLN	A	503	-	-	1/6/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	GLN	O-C-CA-CB
3	F	503	GLN	O-C-CA-N
3	F	503	GLN	N-CA-CB-CG
3	C	501	GLN	OXT-C-CA-N
3	D	503	GLN	OXT-C-CA-CB

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	503	GLN	2	0
3	B	503	GLN	1	0
3	C	501	GLN	2	0
3	D	503	GLN	1	0
3	A	503	GLN	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 (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, 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%)	-0.05	4 (0%)	84	84	19, 37, 66, 98	0
1	B	443/443 (100%)	-0.11	2 (0%)	91	91	18, 36, 61, 93	0
1	C	443/443 (100%)	-0.14	3 (0%)	87	87	19, 35, 62, 91	0
1	D	443/443 (100%)	-0.10	3 (0%)	87	87	19, 36, 62, 96	0
1	E	443/443 (100%)	-0.10	5 (1%)	80	80	14, 35, 63, 94	0
1	F	443/443 (100%)	-0.06	4 (0%)	84	84	19, 37, 66, 101	0
All	All	2658/2658 (100%)	-0.09	21 (0%)	86	86	14, 36, 64, 101	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	384	GLY	4.0
1	C	86	LYS	3.9
1	A	384	GLY	3.1
1	D	385	ILE	2.9
1	B	377	LYS	2.9

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, 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	B-factors(Å^2)	Q<0.9
2	MG	E	502	1/1	0.90	0.19	27,27,27,27	0
3	GLN	B	503	9/10	0.91	0.22	27,29,31,32	0
2	MG	A	501	1/1	0.92	0.17	12,12,12,12	0
3	GLN	A	503	9/10	0.93	0.26	28,32,33,35	0
2	MG	C	502	1/1	0.93	0.26	31,31,31,31	0
3	GLN	E	503	10/10	0.93	0.25	38,41,42,43	0
2	MG	A	502	1/1	0.94	0.18	17,17,17,17	0
3	GLN	F	503	10/10	0.95	0.17	28,32,34,36	0
3	GLN	C	501	10/10	0.96	0.19	25,27,29,34	0
3	GLN	D	503	10/10	0.97	0.21	34,36,39,42	0
2	MG	B	501	1/1	0.97	0.14	18,18,18,18	0
2	MG	E	501	1/1	0.97	0.14	20,20,20,20	0
2	MG	D	501	1/1	0.98	0.20	16,16,16,16	0
2	MG	D	502	1/1	0.98	0.17	14,14,14,14	0
2	MG	B	502	1/1	0.98	0.24	32,32,32,32	0
2	MG	C	503	1/1	0.98	0.18	13,13,13,13	0
2	MG	F	501	1/1	0.98	0.17	24,24,24,24	0
2	MG	F	502	1/1	0.98	0.12	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.