



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 02:21 PM UTC

PDB ID : 2GLS / pdb\_00002gls  
Title : REFINED ATOMIC MODEL OF GLUTAMINE SYNTHETASE AT 3.5  
ANGSTROMS RESOLUTION  
Authors : Eisenberg, D.; Almasy, R.J.; Yamashita, M.M.  
Deposited on : 1989-05-19  
Resolution : 3.50 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](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 : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

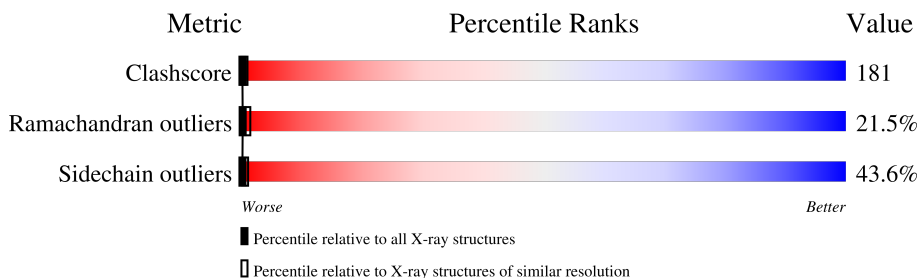
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)





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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	469	7% 35% 37% 21%
1	B	469	7% 35% 34% 24%
1	C	469	7% 33% 37% 23%
1	D	469	7% 31% 34% 28%
1	E	469	7% 30% 34% 29%
1	F	469	7% 31% 33% 29%
1	G	469	7% 33% 35% 24%
1	H	469	8% 41% 39% 12%

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Mol	Chain	Length	Quality of chain
1	I	469	
1	J	469	
1	K	469	
1	L	469	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 43692 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	468	3636	2301	624	691	20	0	0	0
1	B	468	3636	2301	624	691	20	0	0	0
1	C	468	3636	2301	624	691	20	0	0	0
1	D	468	3636	2301	624	691	20	0	0	0
1	E	468	3636	2301	624	691	20	0	0	0
1	F	468	3636	2301	624	691	20	0	0	0
1	G	468	3636	2301	624	691	20	0	0	0
1	H	468	3636	2301	624	691	20	0	0	0
1	I	468	3636	2301	624	691	20	0	0	0
1	J	468	3636	2301	624	691	20	0	0	0
1	K	468	3636	2301	624	691	20	0	0	0
1	L	468	3636	2301	624	691	20	0	0	0

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total 2	Mn 2	0	0
2	D	2	Total 2	Mn 2	0	0
2	E	2	Total 2	Mn 2	0	0
2	F	2	Total 2	Mn 2	0	0
2	G	2	Total 2	Mn 2	0	0
2	H	2	Total 2	Mn 2	0	0
2	I	2	Total 2	Mn 2	0	0
2	J	2	Total 2	Mn 2	0	0
2	K	2	Total 2	Mn 2	0	0
2	L	2	Total 2	Mn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	O 3	0	0
3	B	3	Total 3	O 3	0	0
3	C	3	Total 3	O 3	0	0
3	D	3	Total 3	O 3	0	0
3	E	3	Total 3	O 3	0	0
3	F	3	Total 3	O 3	0	0
3	G	3	Total 3	O 3	0	0
3	H	3	Total 3	O 3	0	0
3	I	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	3	Total O 3 3	0	0
3	K	3	Total O 3 3	0	0
3	L	3	Total O 3 3	0	0

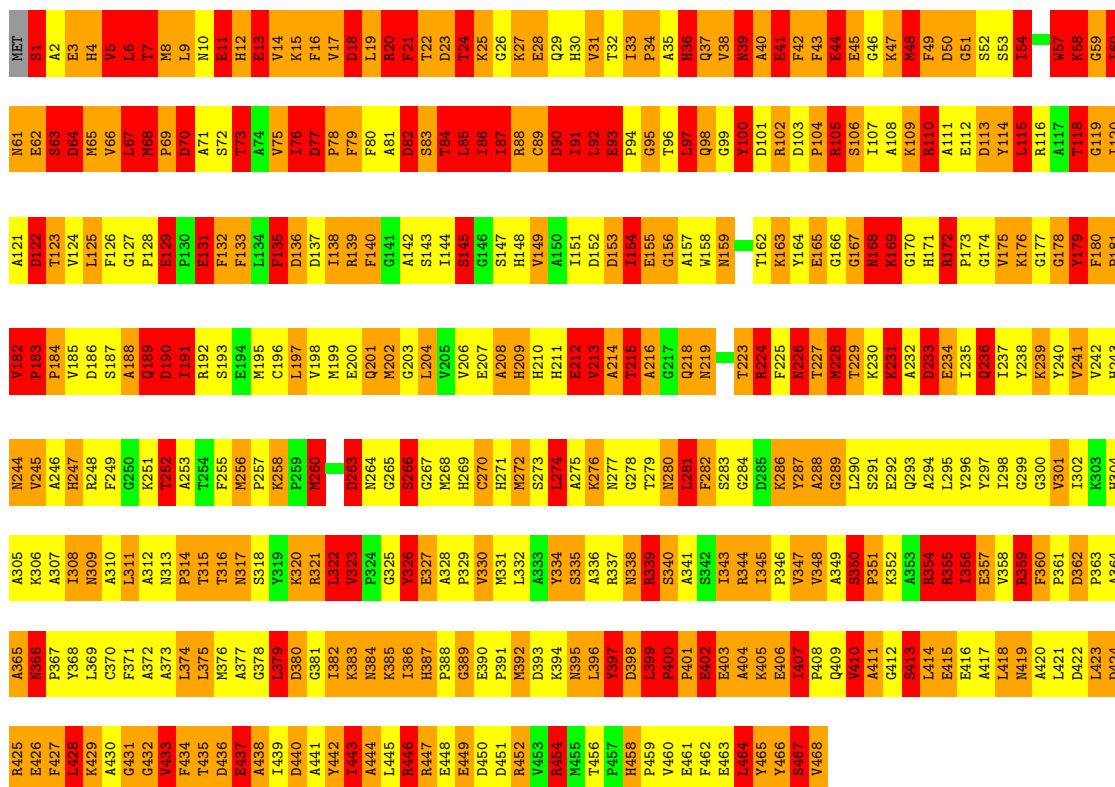
### 3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

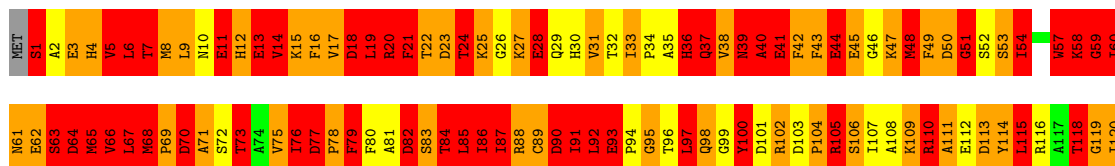
- Molecule 1: GLUTAMINE SYNTHETASE

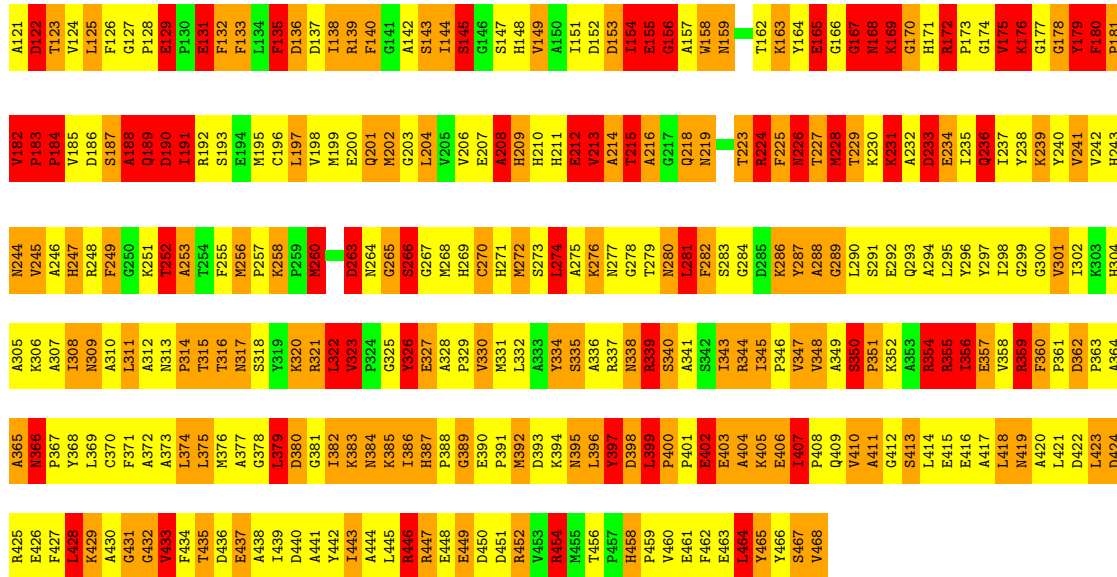
Chain A: 



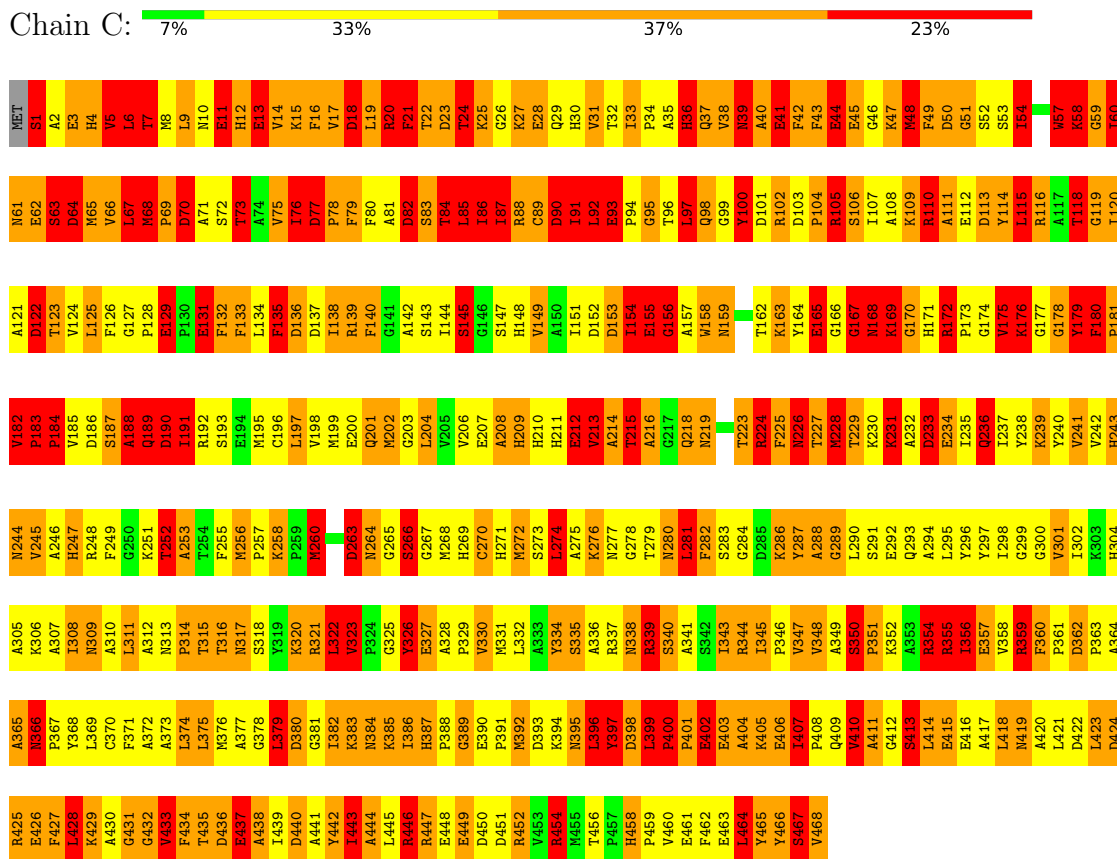
- Molecule 1: GLUTAMINE SYNTHETASE

Chain B: 





• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE



MET	S1	M61	A121	V182	N244	A305	A365	R425
S1	E2	E62	D122	P163	V245	K306	R366	E426
A2	S63	S63	T123	P184	A246	A307	P367	F427
E3	D64	D64	V124	V185	H247	I308	Y368	L428
H4	M65	M65	L125	P186	R248	N309	K369	K429
V5	V66	V66	F126	S187	F249	A310	C370	A430
L6	L67	L67	G127	A188	G250	L311	F371	G431
T7	M68	M68	P128	Q189	K251	A312	A372	G432
M8	P69	P69	E129	D190	K252	N313	A373	V433
L9	D70	D70	F130	I191	T253	P314	L374	F434
N10	A71	A71	E131	N192	A254	T315	L375	T435
E11	S72	S72	F132	S193	T254	T316	K376	D436
H12	T73	T73	F133	F194	M255	N317	A377	E437
E13	A74	A74	L134	M195	P257	S318	G378	A438
V14	V75	V75	F135	C196	K258	Y319	L379	L439
K15	I76	I76	L136	L197	D259	K320	D380	D440
F16	D77	D77	M137	V198	M260	R321	G381	A441
V17	P78	P78	I138	M199	K261	L322	I382	Y442
D18	F79	F79	R139	E200	D263	V323	K383	L443
L19	F80	F80	F140	Q201	N264	P324	N384	A444
R20	A81	A81	G141	M202	G265	G325	K385	L445
F21	D82	D82	A142	G203	S266	Y326	I386	R446
T22	S83	S83	S143	L204	G267	E327	H387	R447
D23	T84	T84	I144	L204	M268	A328	P388	E448
T24	L85	L85	S145	V206	H269	P329	G389	E449
K25	I86	I86	G146	E207	C270	V330	E390	D450
G26	I87	I87	S147	A208	H271	N331	P391	D451
K27	R88	R88	H148	H209	M272	L332	M392	R452
E28	C89	C89	V149	H210	S273	A333	D393	V453
Q29	D90	D90	A150	H211	L274	Y334	K394	R454
H30	I91	I91	I151	F212	A275	S335	N395	V455
L92	L92	L92	D152	V213	K276	A336	L396	T456
V31	E93	E93	M153	A214	N277	R337	P397	F457
T32	P94	P94	I154	T215	G278	N338	D398	H458
I33	G95	G95	E155	A216	T279	R339	L399	P459
A35	T96	T96	G156	G217	M280	P400	V460	V460
H36	L97	L97	A157	Q218	L281	A341	P401	E461
Q37	O88	O88	M158	M219	F282	S342	E402	F462
V38	G99	G99	M159	T223	S283	I343	A403	E463
N39	Y100	Y100	T162	T223	K284	R344	A404	L464
A40	D101	D101	K163	R224	D285	I345	K405	Y465
E41	R102	R102	K163	F225	K286	P346	E406	Y466
F42	D103	D103	Y164	M226	Y287	V347	I407	S467
F43	P104	P104	E165	T227	A288	V348	P408	V468
E44	R105	R105	G166	M228	C289	A349	Q409	
E45	S106	S106	G167	T229	L290	S350	V410	
G46	I107	I107	M168	K230	S291	P351	A411	
K47	A108	A108	K169	K231	E292	K352	C412	
M48	K109	K109	G170	A232	Q293	A353	S413	
F49	R110	R110	H171	D233	A294	R354	L414	
D50	A111	A111	R172	E234	L295	R355	E415	
G51	E112	E112	P173	I235	Y296	I356	E416	
S52	D113	D113	G174	Q236	Y297	E357	A417	
S53	Y114	Y114	V175	I237	I298	V358	L418	
I54	K115	K115	K176	G299	G299	N419	N419	
M57	R116	R116	G177	K239	G300	F360	A420	
K58	A117	A117	G178	Y240	R381	P361	L421	
G59	T118	T118	Y179	V241	I302	D362	D422	
I60	F180	F180	F180	H243	K303	P363	L423	
	P181	P181	P181		H304	A364	D424	

• Molecule 1: GLUTAMINE SYNTHETASE



MET	S1	M61	A121	V182	N244	A305	A365	R425
S1	E2	E62	D122	P163	V245	K306	R366	E426
A2	S63	S63	T123	P184	A246	A307	P367	F427
E3	D64	D64	V124	V185	H247	I308	Y368	L428
H4	M65	M65	L125	P186	R248	N309	K369	K429
V5	V66	V66	F126	S187	F249	A310	C370	A430
L6	L67	L67	G127	A188	G250	L311	F371	G431
T7	M68	M68	P128	Q189	K251	A312	A372	G432
M8	P69	P69	E129	D190	K252	N313	A373	V433
L9	D70	D70	F130	I191	T253	P314	L374	F434
N10	A71	A71	E131	N192	A254	T315	L375	T435
E11	S72	S72	F132	S193	T254	T316	K376	D436
H12	T73	T73	F133	F194	M255	N317	A377	E437
E13	A74	A74	L134	M195	P257	S318	G378	A438
V14	V75	V75	F135	C196	K258	Y319	L379	L439
K15	I76	I76	L136	L197	D259	K320	D380	D440
F16	D77	D77	M137	V198	M260	R321	G381	A441
V17	P78	P78	I138	M199	K261	L322	I382	Y442
D18	F79	F79	R139	E200	D263	V323	K383	L443
L19	F80	F80	F140	Q201	N264	P324	N384	A444
R20	A81	A81	G141	M202	G265	G325	K385	L445
F21	D82	D82	A142	G203	S266	Y326	I386	R446
T22	S83	S83	S143	L204	G267	E327	H387	R447
D23	T84	T84	I144	L204	M268	A328	P388	E448
T24	L85	L85	S145	V206	H269	P329	G389	E449
K25	I86	I86	G146	E207	C270	V330	E390	D450
G26	I87	I87	S147	A208	H271	N331	P391	D451
K27	R88	R88	H148	H209	M272	L332	M392	R452
E28	C89	C89	V149	H210	S273	A333	D393	V453
Q29	D90	D90	A150	H211	L274	Y334	K394	R454
H30	I91	I91	I151	F212	A275	S335	N395	V455
L92	L92	L92	D152	V213	K276	A336	L396	T456
V31	E93	E93	M153	A214	N277	R337	P397	F457
T32	P94	P94	I154	T215	G278	N338	D398	H458
I33	G95	G95	E155	A216	T279	R339	L399	P459
A35	T96	T96	G156	G217	M280	P400	V460	V460
H36	L97	L97	A157	Q218	L281	A341	P401	E461
Q37	O88	O88	M158	M219	F282	S342	E402	F462
V38	G99	G99	M159	T223	S283	I343	A403	E463
N39	Y100	Y100	T162	T223	K284	R344	A404	L464
A40	D101	D101	K163	R224	D285	I345	K405	Y465
E41	R102	R102	K163	F225	K286	P346	E406	Y466
F42	D103	D103	Y164	M226	Y287	V347	I407	S467
F43	P104	P104	E165	T227	A288	V348	P408	V468
E44	R105	R105	G166	M228	C289	A349	Q409	
E45	S106	S106	G167	T229	L290	S350	V410	
G46	I107	I107	M168	K230	S291	P351	A411	
K47	A108	A108	K169	K231	E292	K352	C412	
M48	K109	K109	G170	A232	Q293	A353	S413	
F49	R110	R110	H171	D233	A294	R354	L414	
D50	A111	A111	R172	E234	L295	R355	E415	
G51	E112	E112	P173	I235	Y296	I356	E416	
S52	D113	D113	G174	Q236	Y297	E357	A417	
S53	Y114	Y114	V175	I237	I298	V358	L418	
I54	K115	K115	K176	G299	G299	N419	N419	
M57	R116	R116	G177	K239	G300	F360	A420	
K58	A117	A117	G178	Y240	R381	P361	L421	
G59	T118	T118	Y179	V241	I302	D362	D422	
I60	F180	F180	F180	H243	K303	P363	L423	
	P181	P181	P181		H304	A364	D424	

● Molecule 1: GLUTAMINE SYNTHETASE



MET	S1	A2	E3	H4	V5	L6	T7	M8	L9	N10	E11	H12	E13	V14	K15	F16	V17	D18	L19	R20	S21	T22	D23	T24	K25	G26	R27	R28	E29	Q29	H30	V31	T32	I33	P34	A35	H36	O37	V38	N39	Y100	A40	E41	R42	D43	F43	F44	E44	E45	G46	K47	M48	F49	D50	G51	S52	S53	L54	M57	K58	G59	I60	
N61	E62	S63	D64	M65	V66	L67	M68	P69	D70	A71	S72	T73	A74	V75	F76	D77	P78	F79	F80	A81	D82	S83	T84	L85	L86	K87	G88	R88	C89	E90	D90	I91	L92	E93	P94	G95	T96	L97	O88	G99	Y100	D101	R102	E103	F104	R105	S106	I107	G108	K109	M110	A111	E112	D113	Y114	L115	A117	T118	G119	I120			
A121	D122	T123	V124	F125	G126	P127	E128	P129	P130	A131	F132	F133	L134	F135	C136	D137	L138	M139	F140	G141	A142	S143	I144	S145	G146	S147	H148	V149	E150	D90	I91	D152	E153	A154	E155	G156	A157	M158	M159	S160	S161	T162	K163	Y164	E165	G166	G167	T229	K230	K231	K169	G170	H171	R172	P173	G174	Y236	I237	Y238	K239	Y240	V241	F180
P181	V182	P183	P184	D185	V186	S187	A188	Q189	D190	I191	R192	F193	L194	M195	C196	L197	V198	M199	E200	Q201	M202	G203	L204	V205	G206	E207	A208	H209	E210	H210	H211	E212	V213	A214	T215	A216	G217	Q218	M219	T223	R224	F225	M226	T227	M228	T229	K230	K231	K169	A232	D233	E234	I235	Y236	I237	Y238	K239	Y240	V241	F242			
H243	N244	V245	A246	H247	R248	F249	G250	K251	A252	A253	F254	F255	M256	P257	K258	P259	M260	D261	N264	G265	S266	G267	V268	H269	C270	H271	H272	H273	S274	S275	G276	G277	N278	G279	M280	L281	F282	S283	G284	G285	D286	K287	Y287	A288	G289	L290	S291	K352	Q293	A294	L295	Y296	E297	V298	V359	P361	D362	P363					
H304	A305	K306	A307	I308	M309	C310	L311	A312	N313	P314	T315	T316	N317	S318	Y319	K320	R321	L322	V323	P324	G325	Y326	E327	A328	P329	V330	N331	A332	A333	D334	Y335	S336	A337	L338	R339	M340	A341	S342	I343	R344	I345	K346	P347	V348	A349	S350	P351	K352	Q353	R354	K355	E356	A417	V358	G299	F360	P361	D362	P363				
A364	A365	R366	P367	I368	L369	C370	F371	A372	A373	L374	L375	M376	A377	G378	L379	D380	G381	L382	K383	N384	K385	L386	H387	A388	E389	D390	D451	R452	V453	V454	R455	T456	H457	H458	L399	M280	A341	E402	E403	A404	K405	E406	I407	P408	Q409	V410	A411	K412	G413	L414	E415	A417	N419	F360	L421	D422	L423						
D424	R425	E426	F427	K428	A429	A430	G431	G432	V433	F434	T435	D436	E437	A438	L439	D440	A441	Y442	L443	A444	L445	R446	R447	E448	E449	D450	D451	R452	V453	V454	R455	T456	H457	H458	L399	M280	A341	E402	E403	A404	K405	E406	I407	P408	Q409	V410	A411	K412	G413	L414	E415	A417	N419	F360	L421	D422	L423						

● Molecule 1: GLUTAMINE SYNTHETASE



MET	S1	A2	E3	H4	V5	L6	T7	M8	L9	N10	E11	H12	E13	V14	K15	F16	V17	D18	L19	R20	S21	T22	D23	T24	K25	G26	R27	R28	E29	Q29	H30	V31	T32	I33	P34	A35	H36	O37	V38	N39	Y100	A40	E41	R42	D43	F43	F44	E44	E45	G46	K47	M48	F49	D50	G51	S52	S53	L54	M57	K58	G59	I60		
N61	E62	S63	D64	M65	V66	L67	M68	P69	D70	A71	S72	T73	A74	V75	F76	D77	P78	F79	F80	A81	D82	S83	T84	L85	L86	K87	G88	R88	C89	E90	D90	I91	L92	E93	P94	G95	T96	L97	O88	G99	Y100	D101	R102	E103	F104	R105	S106	I107	G108	K109	M110	A111	E112	D113	Y114	L115	A117	T118	G119	I120				
A121	D122	T123	V124	F125	G126	P127	E128	P129	P130	A131	F132	F133	L134	F135	C136	D137	L138	M139	F140	G141	A142	S143	I144	S145	G146	S147	H148	V149	E150	D90	I91	D152	E153	A154	E155	G156	A157	M158	M159	S160	S161	T162	K163	Y164	E165	G166	G167	T229	K230	K231	K169	G170	H171	R172	P173	G174	Y236	I237	Y238	K239	Y240	V241	F180	P181
V182	P183	P184	D185	V186	S187	A188	Q189	D190	I191	R192	F193	L194	M195	C196	L197	V198	M199	E200	Q201	M202	G203	L204	V205	G206	E207	A208	H209	E210	H210	H211	E212	V213	A214	T215	A216	G217	Q218	M219	T223	R224	F225	M226	T227	M228	T229	K230	K231	K169	A232	D233	E234	I235	Y236	I237	Y238	K239	Y240	V241	F180	H243				
N244	V245	A246	H247	R248	F249	G250	K251	A252	A253	F254	F255	M256	P257	K258	P259	M260	D261	N264	G265	S266	G267	V268	H269	C270	H271	H272	H273	S274	S275	G276	G277	N278	G279	M280	L281	F282	S283	G284	G285	D286	K287	Y287	A288	G289	L290	S291	K352	Q293	A294	L295	Y296	E297	V298	V359	P361	D362	P363	H304						
A305	K306	A307	I308	M309	C310	L311	A312	N313	P314	T315	T316	N317	S318	Y319	K320	R321	L322	V323	P324	G325	Y326	E327	A328	P329	V330	N331	A332	A333	D334	Y335	S336	A337	L338	R339	M340	A341	S342	I343	R344	I345	K346	P347	V348	A349	S350	P351	K352	Q353	R354	K355	E356	A417	V358	G299	F360	P361	D362	P363						
A365	P367	Y368	L369	M309	C370	F371	A372	A373	L374	L375	M376	A377	G378	L379	D380	G381	L382	K383	N384	K385	L386	H387	A388	E389	D390	D451	R452	V453	V454	R455	T456	H457	H458	L399	M280	A341	E402	E403	A404	K405	E406	I407	P408	Q409	V410	A411	K412	G413	L414	E415	A417	N419	F360	L421	D422	L423	D424							



K306	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468
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• Molecule 1: GLUTAMINE SYNTHETASE



MET	S1	A2	E3	H4	V5	L6	T7	M8	L9	N10	E11	H12	E13	V14	K15	R16	F17	V18	D19	E20	R21	F22	T23	S24	H25	L26	K27	R28	E29	D30	H31	S32	T33	F34	V35	L36	K37	R38	E39	D40	H41	S42	T43	F44	V45	L46	K47	R48	E49	D50	H51	S52	T53	F54	V55	L56	K57	R58	E59	D60	H61	S62	T63	F64	V65	L66	K67	R68	E69	D70	H71	S72	T73	F74	V75	L76	K77	R78	E79	D80	H81	S82	T83	F84	V85	L86	K87	R88	E89	D90	H91	S92	T93	F94	V95	L96	K97	R98	E99	D100	H101	S102	T103	F104	V105	L106	K107	R108	E109	D110	H111	S112	T113	F114	V115	L116	K117	R118	E119	D120	H121	S122	T123	F124	V125	L126	K127	R128	E129	D130	H131	S132	T133	F134	V135	L136	K137	R138	E139	D140	H141	S142	T143	F144	V145	L146	K147	R148	E149	D150	H151	S152	T153	F154	V155	L156	K157	R158	E159	D160	H161	S162	T163	F164	V165	L166	K167	R168	E169	D170	H171	S172	T173	F174	V175	L176	K177	R178	E179	D180	H181	S182	T183	F184	V185	L186	K187	R188	E189	D190	H191	S192	T193	F194	V195	L196	K197	R198	E199	D200	H201	S202	T203	F204	V205	L206	K207	R208	E209	D210	H211	S212	T213	F214	V215	L216	K217	R218	E219	D220	H221	S222	T223	F224	V225	L226	K227	R228	E229	D230	H231	S232	T233	F234	V235	L236	K237	R238	E239	D240	H241	S242	T243	F244	V245	L246	K247	R248	E249	D250	H251	S252	T253	F254	V255	L256	K257	R258	E259	D260	H261	S262	T263	F264	V265	L266	K267	R268	E269	D270	H271	S272	T273	F274	V275	L276	K277	R278	E279	D280	H281	S282	T283	F284	V285	L286	K287	R288	E289	D290	H291	S292	T293	F294	V295	L296	K297	R298	E299	D300	H301	S302	T303	F304	V305	L306	K307	R308	E309	D310	H311	S312	T313	F314	V315	L316	K317	R318	E319	D320	H321	S322	T323	F324	V325	L326	K327	R328	E329	D330	H331	S332	T333	F334	V335	L336	K337	R338	E339	D340	H341	S342	T343	F344	V345	L346	K347	R348	E349	D350	H351	S352	T353	F354	V355	L356	K357	R358	E359	D360	H361	S362	T363	F364	V365	L366	K367	R368	E369	D370	H371	S372	T373	F374	V375	L376	K377	R378	E379	D380	H381	S382	T383	F384	V385	L386	K387	R388	E389	D390	H391	S392	T393	F394	V395	L396	K397	R398	E399	D400	H401	S402	T403	F404	V405	L406	K407	R408	E409	D410	H411	S412	T413	F414	V415	L416	K417	R418	E419	D420	H421	S422	T423	F424	V425	L426	K427	R428	E429	D430	H431	S432	T433	F434	V435	L436	K437	R438	E439	D440	H441	S442	T443	F444	V445	L446	K447	R448	E449	D450	H451	S452	T453	F454	V455	L456	K457	R458	E459	D460	H461	S462	T463	F464	V465	L466	K467	R468	E469	D470	H471	S472	T473	F474	V475	L476	K477	R478	E479	D480	H481	S482	T483	F484	V485	L486	K487	R488	E489	D490	H491	S492	T493	F494	V495	L496	K497	R498	E499	D500	H501	S502	T503	F504	V505	L506	K507	R508	E509	D510	H511	S512	T513	F514	V515	L516	K517	R518	E519	D520	H521	S522	T523	F524	V525	L526	K527	R528	E529	D530	H531	S532	T533	F534	V535	L536	K537	R538	E539	D540	H541	S542	T543	F544	V545	L546	K547	R548	E549	D550	H551	S552	T553	F554	V555	L556	K557	R558	E559	D560	H561	S562	T563	F564	V565	L566	K567	R568	E569	D570	H571	S572	T573	F574	V575	L576	K577	R578	E579	D580	H581	S582	T583	F584	V585	L586	K587	R588	E589	D590	H591	S592	T593	F594	V595	L596	K597	R598	E599	D600	H601	S602	T603	F604	V605	L606	K607	R608	E609	D610	H611	S612	T613	F614	V615	L616	K617	R618	E619	D620	H621	S622	T623	F624	V625	L626	K627	R628	E629	D630	H631	S632	T633	F634	V635	L636	K637	R638	E639	D640	H641	S642	T643	F644	V645	L646	K647	R648	E649	D650	H651	S652	T653	F654	V655	L656	K657	R658	E659	D660	H661	S662	T663	F664	V665	L666	K667	R668	E669	D670	H671	S672	T673	F674	V675	L676	K677	R678	E679	D680	H681	S682	T683	F684	V685	L686	K687	R688	E689	D690	H691	S692	T693	F694	V695	L696	K697	R698	E699	D700	H701	S702	T703	F704	V705	L706	K707	R708	E709	D710	H711	S712	T713	F714	V715	L716	K717	R718	E719	D720	H721	S722	T723	F724	V725	L726	K727	R728	E729	D730	H731	S732	T733	F734	V735	L736	K737	R738	E739	D740	H741	S742	T743	F744	V745	L746	K747	R748	E749	D750	H751	S752	T753	F754	V755	L756	K757	R758	E759	D760	H761	S762	T763	F764	V765	L766	K767	R768	E769	D770	H771	S772	T773	F774	V775	L776	K777	R778	E779	D780	H781	S782	T783	F784	V785	L786	K787	R788	E789	D790	H791	S792	T793	F794	V795	L796	K797	R798	E799	D800	H801	S802	T803	F804	V805	L806	K807	R808	E809	D810	H811	S812	T813	F814	V815	L816	K817	R818	E819	D820	H821	S822	T823	F824	V825	L826	K827	R828	E829	D830	H831	S832	T833	F834	V835	L836	K837	R838	E839	D840	H841	S842	T843	F844	V845	L846	K847	R848	E849	D850	H851	S852	T853	F854	V855	L856	K857	R858	E859	D860	H861	S862	T863	F864	V865	L866	K867	R868	E869	D870	H871	S872	T873	F874	V875	L876	K877	R878	E879	D880	H881	S882	T883	F884	V885	L886	K887	R888	E889	D890	H891	S892	T893	F894	V895	L896	K897	R898	E899	D900	H901	S902	T903	F904	V905	L906	K907	R908	E909	D910	H911	S912	T913	F914	V915	L916	K917	R918	E919	D920	H921	S922	T923	F924	V925	L926	K927	R928	E929	D930	H931	S932	T933	F934	V935	L936	K937	R938	E939	D940	H941	S942	T943	F944	V945	L946	K947	R948	E949	D950	H951	S952	T953	F954	V955	L956	K957	R958	E959	D960	H961	S962	T963	F964	V965	L966	K967	R968	E969	D970	H971	S972	T973	F974	V975	L976	K977	R978	E979	D980	H981	S982	T983	F984	V985	L986	K987	R988	E989	D990	H991	S992	T993	F994	V995	L996	K997	R998	E999	D1000	H1001	S1002	T1003	F1004	V1005	L1006	K1007	R1008	E1009	D1010	H1011	S1012	T1013	F1014	V1015	L1016	K1017	R1018	E1019	D1020	H1021	S1022	T1023	F1024	V1025	L1026	K1027	R1028	E1029	D1030	H1031	S1032	T1033	F1034	V1035	L1036	K1037	R1038	E1039	D1040	H1041	S1042	T1043	F1044	V1045	L1046	K1047	R1048	E1049	D1050	H1051	S1052	T1053	F1054	V1055	L1056	K1057	R1058	E1059	D1060	H1061	S1062	T1063	F1064	V1065	L1066	K1067	R1068	E1069	D1070	H1071	S1072	T1073	F1074	V1075	L1076	K1077	R1078	E1079	D1080	H1081	S1082	T1083	F1084	V1085	L1086	K1087	R1088	E1089	D1090	H1091	S1092	T1093	F1094	V1095	L1096	K1097	R1098	E1099	D1100	H1101	S1102	T1103	F1104	V1105	L1106	K1107	R1108	E1109	D1110	H1111	S1112	T1113	F1114	V1115	L1116	K1117	R1118	E1119	D1120	H1121	S1122	T1123	F1124	V1125	L1126	K1127	R1128	E1129	D1130	H1131	S1132	T1133	F1134	V1135	L1136	K1137	R1138	E1139	D1140	H1141	S1142	T1143	F1144	V1145	L1146	K1147	R1148	E1149	D1150	H1151	S1152	T1153	F1154	V1155	L1156	K1157	R1158	E1159	D1160	H1161	S1162	T1163	F1164	V1165	L1166	K1167	R1168	E1169	D1170	H1171	S1172	T1173	F1174	V1175	L1176	K1177	R1178	E1179	D1180	H1181	S1182	T1183	F1184	V1185	L1186	K1187	R1188	E1189	D1190	H1191	S1192	T1193	F1194	V1195	L1196	K1197	R1198	E1199	D1200	H1201	S1202	T1203	F1204	V1205	L1206	K1207	R1208	E1209	D1210	H1211	S1212	T1213	F1214	V1215	L1216	K1217	R1218	E1219	D1220	H1221	S1222	T1223	F1224	V1225	L1226	K1227	R1228	E1229	D1230	H1231	S1232	T1233	F1234	V1235	L1236	K1237	R1238	E1239	D1240	H1241	S1242	T1243	F1244	V1245	L1246	K1247	R1248	E1249	D1250	H1251	S1252	T1253	F1254	V1255	L1256	K1257	R1258	E1259	D1260	H1261	S1262	T1263	F1264	V1265	L1266	K1267	R1268	E1269	D1270	H1271	S1272	T1273	F1274	V1275	L1276	K1277	R1278	E1279	D1280	H1281	S1282	T1283	F1284	V1285	L1286	K1287	R1288	E1289	D1290	H1291	S1292	T1293	F1294	V1295	L1296	K1297	R1298	E1299	D1300	H1301	S1302	T1303	F1304	V1305	L1306	K1307	R1308	E1309	D1310	H1311	S1312	T1313	F1314	V1315	L1316	K1317	R1318	E1319	D1320	H1321	S1322	T1323	F1324	V1325	L1326	K1327	R1328	E1329	D1330	H1331	S1332	T1333	F1334	V1335	L1336	K1337	R1338	E1339	D1340	H1341	S1342	T1343	F1344	V1345	L1346	K1347	R1348	E1349	D1350	H1351	S1352	T1353	F1354	V1355	L1356	K1357	R1358	E1359	D1360	H1361	S1362	T1363	F1364	V1365	L1366	K1367	R1368	E1369	D1370	H1371
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N244	A305	A365	R425
V245	K306	R366	E426
A246	A307	P367	F427
H247	I308	Y368	L428
R248	N309	L369	K429
F249	A310	C370	A430
G250	L311	F371	G431
K251	A312	A372	G432
T252	N313	A373	V433
A253	P314	L374	F434
T254	L315	L375	T435
F255	T316	M376	D436
M256	N317	A377	E437
P257	S318	G378	A438
K258	Y319	L379	I439
P259	K320	D380	D440
M260	R321	G381	A441
G261	L322	I382	Y442
R262	V323	K383	I443
G263	F324	K384	A444
G264	G325	K385	L445
G265	Y326	I386	R446
S266	E327	H387	R447
G267	A328	P388	E448
M268	P329	G389	E449
H269	V330	E390	D450
C270	M331	P391	D451
H271	L332	M392	R452
M272	S333	K393	V453
S273	Y334	K394	R454
L274	R335	N395	M455
L275	A336	L396	T456
A276	K276	Y397	P457
K277	N277	D398	H458
G278	N338	G398	P459
T279	R339	L399	V460
N280	S340	P400	G461
L281	A341	P401	E462
L282	S342	E402	F463
S283	I343	E403	E464
G284	R344	A404	L464
D285	I345	K405	Y465
K286	P346	E406	Y466
Y287	V347	I407	S467
Y288	V348	P408	V468
G289	A349	Q409	
L290	S350	V410	
S291	P351	A411	
E292	K352	G412	
Q293	A353	S413	
A294	R354	L414	
L295	K355	E415	
Y296	L356	E416	
Y297	E357	A417	
I298	V358	L418	
G299	R359	L419	
G300	F360	A420	
K301	P361	L421	
I302	D362	D422	
K303	P363	L423	
H304	A364	D424	

● Molecule 1: GLUTAMINE SYNTHETASE



ME1	M61	A121	V182	N244	A305	A365	R425
S1	E62	D122	P183	P184	K306	R366	E426
A2	S63	T123	L184	P185	A307	P367	F427
E3	D64	V124	V185	P186	I308	Y368	L428
H4	M65	L125	L186	S187	N309	L369	K429
V5	V66	F126	V187	S188	A310	C370	A430
L6	L67	G127	A188	Q189	L311	F371	G431
T7	M68	P128	Q190	L190	A312	A372	G432
M8	P69	E129	D191	L191	N313	A373	V433
L9	D70	F130	R192	L192	P314	L374	F434
N10	A71	E131	R193	S193	L315	L375	T435
E11	S72	F132	S194	F194	T316	M376	D436
H12	T73	F133	E195	M195	N317	A377	E437
E13	A74	L134	M196	C196	S318	G378	A438
V14	V75	F135	L197	L197	Y319	L379	I439
K15	T76	D136	L198	V198	K320	D380	D440
F16	D77	I137	V199	M199	R321	G381	A441
V17	P78	I138	E200	E200	L322	I382	Y442
D18	F79	R139	Q201	Q201	V323	K383	I443
L19	F80	F140	M202	M202	F324	K384	A444
R20	A81	G141	G203	G203	G325	K385	L445
F21	D82	A142	L204	L204	Y326	I386	R446
T22	S83	S143	V205	V205	E327	H387	R447
Q29	R90	A150	I144	I144	A328	P388	E448
H30	I91	I151	S145	S145	P329	G389	E449
H30	L92	D152	E207	E207	V330	E390	D450
V31	E93	G146	A208	A208	M331	P391	D451
T32	R94	H147	H209	H209	L332	M392	R452
R94	P94	H148	H210	H210	S333	K393	V453
S34	G95	V149	H211	H211	Y334	K394	R454
A35	T96	A150	H212	H212	S335	N395	M455
H36	G97	D151	Q212	Q212	A336	L396	T456
Q37	Q98	D152	V213	V213	K276	Y397	P457
V38	G99	M158	A214	A214	N277	D398	H458
N39	Y100	M159	T215	T215	N338	G398	P459
A40	D101	T162	R224	R224	R339	L399	V460
E41	R102	K163	F225	F225	S340	P400	G461
F42	D103	Y164	M226	M226	A341	P401	E462
F43	P104	E165	T227	T227	L281	R281	L281
E44	R105	G166	M228	M228	F282	F282	F282
E45	S106	G167	T229	T229	S283	S283	S283
G46	I107	M168	K230	K230	G284	G284	G284
K47	A108	K169	K231	K231	D285	D285	D285
M48	K109	G170	A232	A232	K286	K286	K286
F49	R110	H171	D233	D233	Y287	Y287	Y287
D50	A111	R172	E234	E234	A288	A288	A288
G51	P173	I235	L235	L235	G289	G289	G289
S52	D113	G174	Q236	Q236	L290	L290	L290
S53	Y114	F175	I237	I237	S291	S291	S291
L115	L115	K176	Y238	Y238	E292	E292	E292
I54	I54	G177	K239	K239	Q293	Q293	Q293
M57	A117	G178	Y240	Y240	A294	A294	A294
K58	T118	Y179	V241	V241	L295	L295	L295
G59	G119	F180	V242	V242	Y296	Y296	Y296
I60	I120	H243	H243	H243	I298	I298	I298

## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.50Å 134.50Å 200.10Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.258 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	43692	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

## 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:  
MN

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	1.95	101/3723 (2.7%)	2.88	368/5043 (7.3%)
1	B	1.95	103/3723 (2.8%)	2.88	365/5043 (7.2%)
1	C	1.95	101/3723 (2.7%)	2.88	371/5043 (7.4%)
1	D	1.95	104/3723 (2.8%)	2.89	368/5043 (7.3%)
1	E	1.95	106/3723 (2.8%)	2.89	368/5043 (7.3%)
1	F	1.95	102/3723 (2.7%)	2.88	372/5043 (7.4%)
1	G	1.95	104/3723 (2.8%)	2.88	375/5043 (7.4%)
1	H	1.95	102/3723 (2.7%)	2.88	369/5043 (7.3%)
1	I	1.95	102/3723 (2.7%)	2.88	370/5043 (7.3%)
1	J	1.95	102/3723 (2.7%)	2.88	368/5043 (7.3%)
1	K	1.95	103/3723 (2.8%)	2.88	370/5043 (7.3%)
1	L	1.95	105/3723 (2.8%)	2.89	367/5043 (7.3%)
All	All	1.95	1235/44676 (2.8%)	2.88	4431/60516 (7.3%)

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	1	3
1	B	1	3
1	C	1	3
1	D	1	3
1	E	1	3
1	F	1	3
1	G	1	3
1	H	1	3
1	I	1	3
1	J	1	3
1	K	1	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	1	3
All	All	12	36

The worst 5 of 1235 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	183	PRO	CA-C	-12.11	1.41	1.52
1	C	183	PRO	CA-C	-11.97	1.41	1.52
1	F	183	PRO	CA-C	-11.94	1.41	1.52
1	E	183	PRO	CA-C	-11.93	1.41	1.52
1	I	183	PRO	CA-C	-11.93	1.41	1.52

The worst 5 of 4431 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	88	ARG	CD-NE-CZ	27.75	163.25	124.40
1	B	88	ARG	CD-NE-CZ	27.73	163.23	124.40
1	G	88	ARG	CD-NE-CZ	27.73	163.22	124.40
1	J	88	ARG	CD-NE-CZ	27.71	163.20	124.40
1	F	88	ARG	CD-NE-CZ	27.70	163.18	124.40

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	315	THR	CA
1	B	315	THR	CA
1	C	315	THR	CA
1	D	315	THR	CA
1	E	315	THR	CA

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	339	ARG	Sidechain
1	A	355	ARG	Sidechain
1	B	224	ARG	Sidechain
1	B	339	ARG	Sidechain

## 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	3636	0	3542	1388	0
1	B	3636	0	3542	1390	2
1	C	3636	0	3542	1399	28
1	D	3636	0	3542	1410	2
1	E	3636	0	3542	1404	28
1	F	3636	0	3542	1388	0
1	G	3636	0	3542	1394	4
1	H	3636	0	3542	1391	28
1	I	3636	0	3542	1403	4
1	J	3636	0	3542	1405	0
1	K	3636	0	3542	1400	0
1	L	3636	0	3542	1392	28
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
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
All	All	43692	0	42504	15574	62

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 181.

The worst 5 of 15574 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:465:TYR:CD2	1:L:315:THR:CG2	1.94	1.50
1:B:315:THR:CG2	1:H:465:TYR:CD2	1.94	1.50
1:C:315:THR:CG2	1:I:465:TYR:CD2	1.94	1.50
1:E:465:TYR:CD2	1:K:315:THR:CG2	1.94	1.50
1:J:27:LYS:HZ3	1:J:239:LYS:NZ	1.07	1.49

The worst 5 of 62 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:GLU:CG	1:L:39:ASN:O[4_445]	0.34	1.86
1:C:11:GLU:OE2	1:E:40:ALA:N[4_444]	0.65	1.55
1:C:11:GLU:CD	1:E:40:ALA:N[4_444]	0.70	1.50
1:H:11:GLU:N	1:L:41:GLU:OE1[4_445]	0.72	1.48
1:H:10:ASN:C	1:L:41:GLU:OE1[4_445]	1.03	1.17

## 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	94/469 (20%)	44 (47%)	29 (31%)	21 (22%)	0 1
1	B	254/469 (54%)	141 (56%)	61 (24%)	52 (20%)	0 1
1	C	195/469 (42%)	99 (51%)	55 (28%)	41 (21%)	0 1
1	D	436/469 (93%)	229 (52%)	110 (25%)	97 (22%)	0 1
1	E	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0 1
1	F	466/469 (99%)	248 (53%)	118 (25%)	100 (22%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	H	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	I	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	J	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	K	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
1	L	466/469 (99%)	249 (53%)	117 (25%)	100 (22%)	0	1
All	All	4707/5628 (84%)	2504 (53%)	1192 (25%)	1011 (22%)	0	1

5 of 1011 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	400	PRO
1	A	401	PRO
1	A	413	SER
1	A	414	LEU

### 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	384/385 (100%)	216 (56%)	168 (44%)	0	0
1	B	384/385 (100%)	216 (56%)	168 (44%)	0	0
1	C	384/385 (100%)	216 (56%)	168 (44%)	0	0
1	D	384/385 (100%)	216 (56%)	168 (44%)	0	0
1	E	384/385 (100%)	216 (56%)	168 (44%)	0	0
1	F	384/385 (100%)	216 (56%)	168 (44%)	0	0
1	G	283/385 (74%)	156 (55%)	127 (45%)	0	0
1	I	199/385 (52%)	123 (62%)	76 (38%)	0	1
1	J	384/385 (100%)	216 (56%)	168 (44%)	0	0
1	K	384/385 (100%)	216 (56%)	168 (44%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	384/385 (100%)	216 (56%)	168 (44%)	0	0
All	All	3938/4235 (93%)	2223 (56%)	1715 (44%)	0	0

5 of 1715 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	209	HIS
1	I	260	MET
1	L	109	LYS
1	F	286	LYS
1	F	204	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 142 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	39	ASN
1	K	168	ASN
1	L	61	ASN
1	D	280	ASN
1	D	168	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 oligosaccharides in this entry.

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

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

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](#)

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.