



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 02:50 PM GMT

PDB ID : 2D3B
Title : Crystal Structure of the Maize Glutamine Synthetase complexed with
AMPPNP and Methionine sulfoximine
Authors : Unno, H.; Uchida, T.; Sugawara, H.; Kurisu, G.; Sugiyama, T.; Yamaya, T.;
Sakakibara, H.; Hase, T.; Kusunoki, M.
Deposited on : 2005-09-26
Resolution : 3.50 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

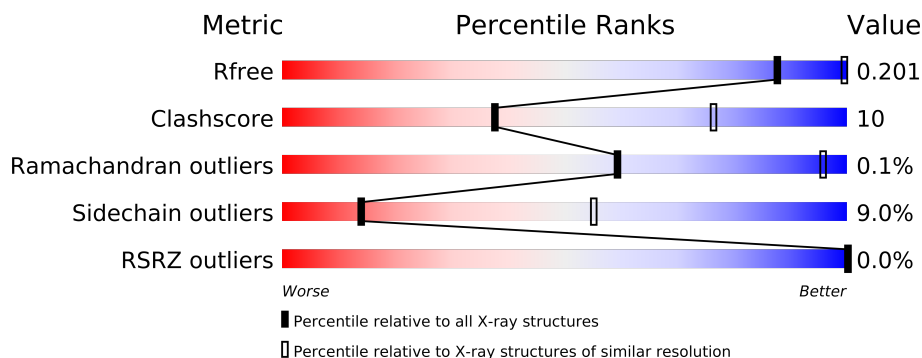
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
R_{free}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	356	
1	B	356	
1	C	356	
1	D	356	
1	E	356	
1	F	356	
1	G	356	
1	H	356	
1	I	356	
1	J	356	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28277 atoms, of which 0 are hydrogen and 0 are deuterium.

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	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	B	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	C	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	D	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	E	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	F	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	G	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	H	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	I	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	J	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

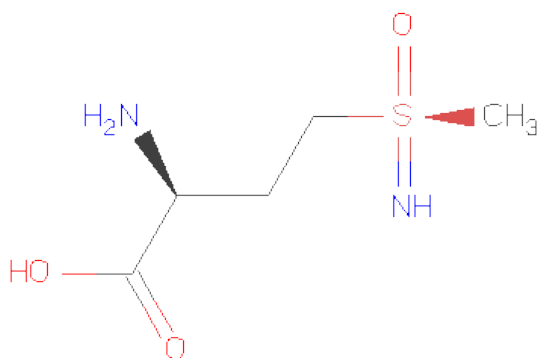
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	3	Total	Mn	0	0
			3	3		
2	J	3	Total	Mn	0	0
			3	3		
2	D	3	Total	Mn	0	0
			3	3		
2	E	3	Total	Mn	0	0
			3	3		

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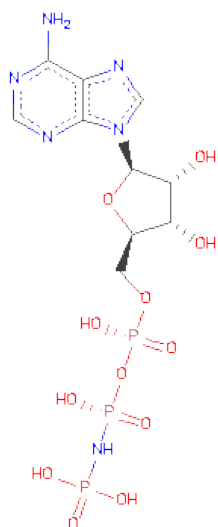
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	3	Total 3	Mn 3	0	0
2	B	3	Total 3	Mn 3	0	0
2	I	3	Total 3	Mn 3	0	0
2	C	3	Total 3	Mn 3	0	0
2	A	3	Total 3	Mn 3	0	0
2	F	3	Total 3	Mn 3	0	0

- Molecule 3 is (2S)-2-AMINO-4-(METHYLSULFONIMIDOYL)BUTANOICACID (three-letter code: MSL) (formula: C₅H₁₂N₂O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	10	Total 110	C 50	N 20	O 30	S 10	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONICACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	36	Total	O	0	0
			36	36		

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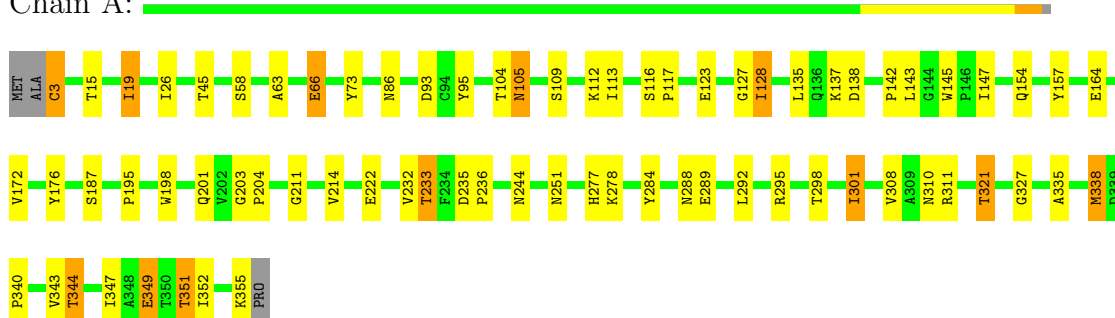
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	40	Total 40	O 40	0	0
5	D	42	Total 42	O 42	0	0
5	E	41	Total 41	O 41	0	0
5	F	39	Total 39	O 39	0	0
5	G	40	Total 40	O 40	0	0
5	H	32	Total 32	O 32	0	0
5	I	37	Total 37	O 37	0	0
5	J	38	Total 38	O 38	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

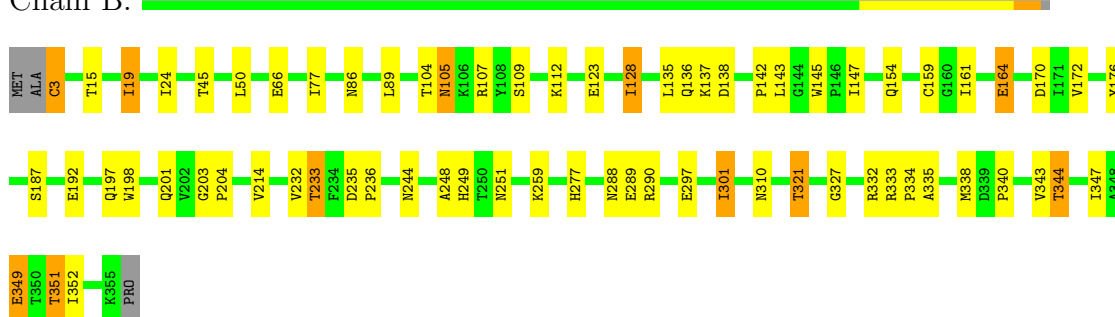
- Molecule 1: glutamine synthetase

Chain A:



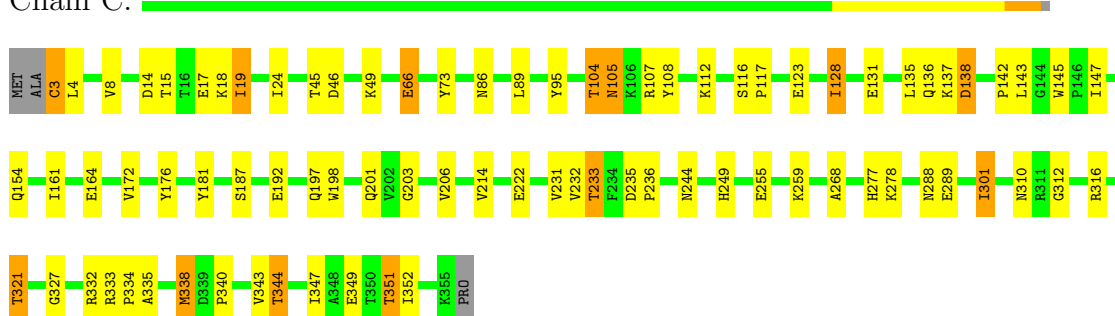
- Molecule 1: glutamine synthetase

Chain B:



- Molecule 1: glutamine synthetase

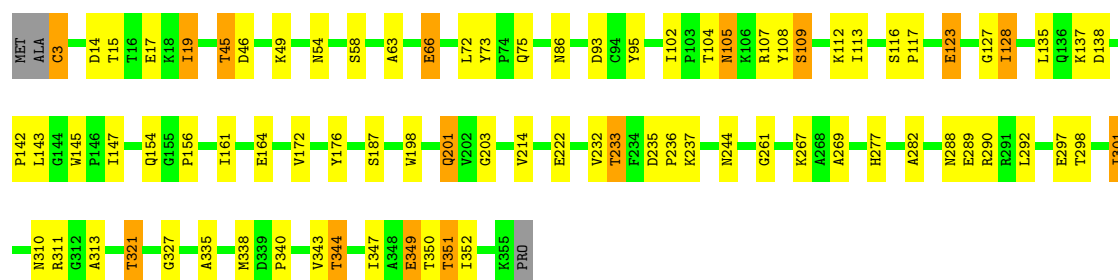
Chain C:



- Molecule 1: glutamine synthetase

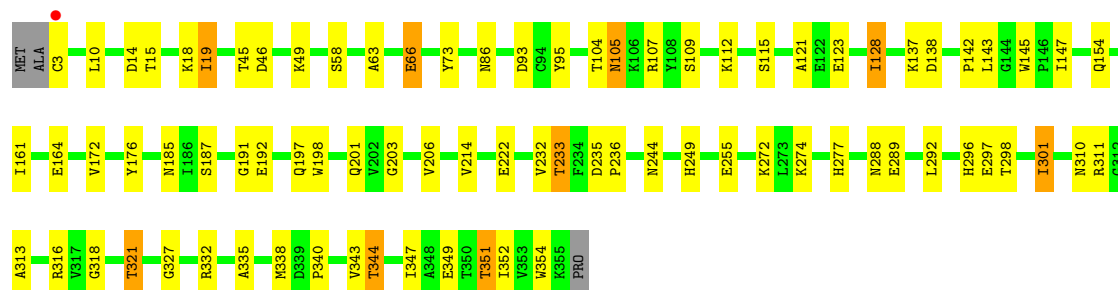
Chain D:





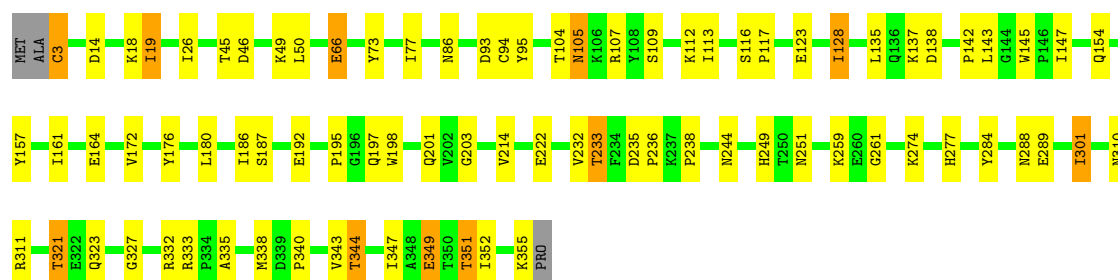
- Molecule 1: glutamine synthetase

Chain E:



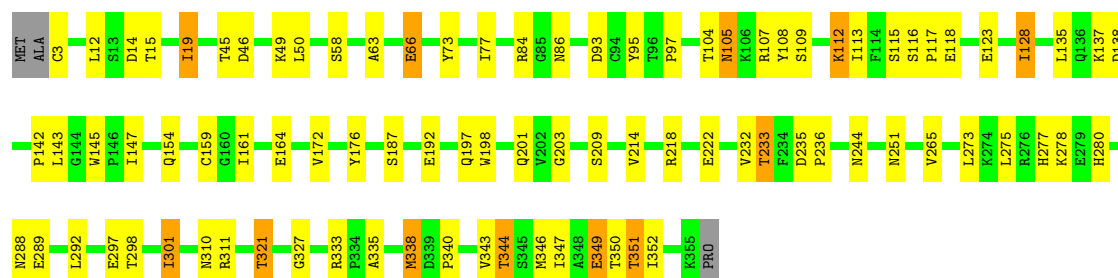
- Molecule 1: glutamine synthetase

Chain F:



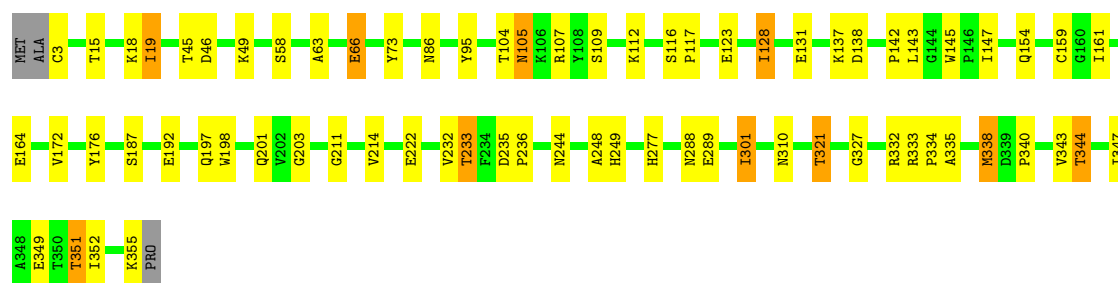
- Molecule 1: glutamine synthetase

Chain G:



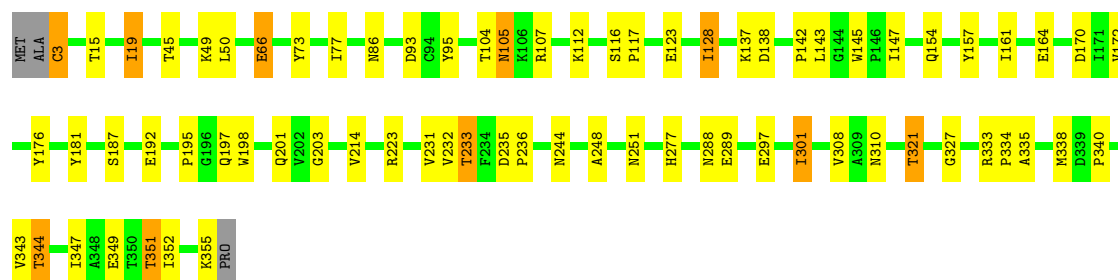
- Molecule 1: glutamine synthetase

Chain H:



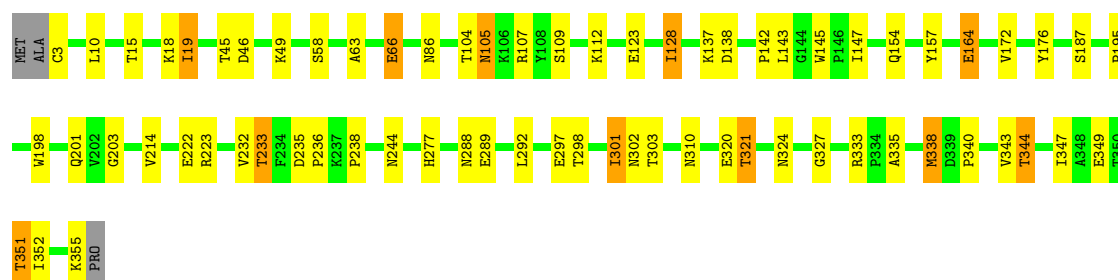
- Molecule 1: glutamine synthetase

Chain I:



- Molecule 1: glutamine synthetase

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.88Å 190.94Å 117.90Å 90.00° 101.23° 90.00°	Depositor
Resolution (Å)	33.50 – 3.50 33.50 – 3.50	Depositor EDS
% Data completeness (in resolution range)	83.1 (33.50-3.50) 83.1 (33.50-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.166 , 0.209 0.161 , 0.201	Depositor DCC
R_{free} test set	2227 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	86.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 15.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43542 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28277	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MSL, ANP, 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	0.67	0/2819	0.70	0/3834
1	B	0.69	1/2819 (0.0%)	0.70	0/3834
1	C	0.67	0/2819	0.70	0/3834
1	D	0.75	0/2819	0.72	0/3834
1	E	0.71	0/2819	0.70	0/3834
1	F	0.73	0/2819	0.72	0/3834
1	G	0.74	1/2819 (0.0%)	0.71	1/3834 (0.0%)
1	H	0.70	1/2819 (0.0%)	0.70	0/3834
1	I	0.66	0/2819	0.69	0/3834
1	J	0.67	0/2819	0.70	0/3834
All	All	0.70	3/28190 (0.0%)	0.70	1/38340 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	CYS	CB-SG	-5.96	1.72	1.81
1	H	159	CYS	CB-SG	-5.62	1.72	1.81
1	G	159	CYS	CB-SG	-5.14	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	218	ARG	NE-CZ-NH2	-5.24	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2745	0	2653	48	0
1	B	2745	0	2653	49	0
1	C	2745	0	2653	59	0
1	D	2745	0	2653	73	0
1	E	2745	0	2653	57	0
1	F	2745	0	2653	64	0
1	G	2745	0	2653	63	0
1	H	2745	0	2653	45	0
1	I	2745	0	2653	48	0
1	J	2745	0	2653	43	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
3	C	110	0	100	37	0
4	A	31	0	10	7	0
4	B	31	0	11	3	0
4	C	31	0	10	4	0
4	D	31	0	11	6	0
4	E	31	0	11	6	0
4	F	31	0	11	4	0
4	G	31	0	10	4	0
4	H	31	0	10	3	0
4	I	31	0	10	3	0
4	J	31	0	10	3	0
5	A	32	0	0	7	0
5	B	36	0	0	11	0
5	C	40	0	0	12	0
5	D	42	0	0	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	41	0	0	14	0
5	F	39	0	0	12	0
5	G	40	0	0	19	0
5	H	32	0	0	9	0
5	I	37	0	0	7	0
5	J	38	0	0	11	0
All	All	28277	0	26734	546	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

The worst 5 of 546 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:12:LEU:HD23	5:G:6047:HOH:O	1.47	1.11
3:C:5010:MSL:NE	4:H:6008:ANP:PG	2.25	1.09
1:E:354:TRP:HA	5:E:6026:HOH:O	1.56	1.05
1:G:346:MET:SD	5:G:6041:HOH:O	2.14	1.03
1:E:255:GLU:HG2	5:E:6019:HOH:O	1.58	1.02

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	351/356 (99%)	331 (94%)	20 (6%)	0	100	100
1	B	351/356 (99%)	331 (94%)	20 (6%)	0	100	100
1	C	351/356 (99%)	334 (95%)	16 (5%)	1 (0%)	50	92
1	D	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	E	351/356 (99%)	328 (93%)	23 (7%)	0	100	100
1	F	351/356 (99%)	331 (94%)	20 (6%)	0	100	100
1	G	351/356 (99%)	332 (95%)	18 (5%)	1 (0%)	50	92

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	I	351/356 (99%)	330 (94%)	21 (6%)	0	100	100
1	J	351/356 (99%)	332 (95%)	19 (5%)	0	100	100
All	All	3510/3560 (99%)	3316 (94%)	192 (6%)	2 (0%)	59	96

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	84	ARG
1	C	138	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/290 (99%)	261 (91%)	27 (9%)	13	52
1	B	288/290 (99%)	264 (92%)	24 (8%)	16	59
1	C	288/290 (99%)	262 (91%)	26 (9%)	14	55
1	D	288/290 (99%)	262 (91%)	26 (9%)	14	55
1	E	288/290 (99%)	262 (91%)	26 (9%)	14	55
1	F	288/290 (99%)	262 (91%)	26 (9%)	14	55
1	G	288/290 (99%)	262 (91%)	26 (9%)	14	55
1	H	288/290 (99%)	262 (91%)	26 (9%)	14	55
1	I	288/290 (99%)	264 (92%)	24 (8%)	16	59
1	J	288/290 (99%)	261 (91%)	27 (9%)	13	52
All	All	2880/2900 (99%)	2622 (91%)	258 (9%)	14	55

5 of 258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	147	ILE
1	F	201	GLN

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Mol	Chain	Res	Type
1	J	109	SER
1	E	232	VAL
1	F	19	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	288	ASN
1	F	277	HIS
1	J	154	GLN
1	E	296	HIS
1	F	190	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 50 ligands modelled in this entry, 30 are monoatomic - leaving 20 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	$\# Z > 2$
4	ANP	A	6001	2	33,33,33	3.05	13 (39%)	51,52,52	4.35	25 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ANP	B	6002	2	33,33,33	2.98	14 (42%)	51,52,52	4.91	25 (49%)
3	MSL	C	5001	2	10,10,10	3.03	2 (20%)	14,14,14	2.11	4 (28%)
3	MSL	C	5002	2	10,10,10	3.33	1 (10%)	14,14,14	5.21	7 (50%)
3	MSL	C	5003	2	10,10,10	3.24	1 (10%)	14,14,14	2.61	5 (35%)
3	MSL	C	5004	2	10,10,10	3.39	1 (10%)	14,14,14	2.69	3 (21%)
3	MSL	C	5005	2	10,10,10	3.04	1 (10%)	14,14,14	2.82	4 (28%)
3	MSL	C	5006	2	10,10,10	3.39	2 (20%)	14,14,14	2.20	4 (28%)
3	MSL	C	5007	2	10,10,10	3.15	2 (20%)	14,14,14	4.03	7 (50%)
3	MSL	C	5008	2	10,10,10	3.42	1 (10%)	14,14,14	2.93	2 (14%)
3	MSL	C	5009	2	10,10,10	2.98	1 (10%)	14,14,14	2.14	4 (28%)
3	MSL	C	5010	2	10,10,10	3.29	1 (10%)	14,14,14	3.41	7 (50%)
4	ANP	C	6003	2	33,33,33	2.83	12 (36%)	51,52,52	4.95	22 (43%)
4	ANP	D	6004	2	33,33,33	3.18	12 (36%)	51,52,52	4.26	23 (45%)
4	ANP	E	6005	2	33,33,33	3.33	13 (39%)	51,52,52	4.84	25 (49%)
4	ANP	F	6006	2	33,33,33	3.18	16 (48%)	51,52,52	4.10	22 (43%)
4	ANP	G	6007	2	33,33,33	2.86	11 (33%)	51,52,52	4.10	24 (47%)
4	ANP	H	6008	2	33,33,33	2.80	15 (45%)	51,52,52	4.79	23 (45%)
4	ANP	I	6009	2	33,33,33	2.90	12 (36%)	51,52,52	3.96	22 (43%)
4	ANP	J	6010	2	33,33,33	3.53	12 (36%)	51,52,52	4.68	28 (54%)

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
4	ANP	A	6001	2	2/2/7/8	1/18/38/38	0/1/3/3
4	ANP	B	6002	2	2/2/7/8	2/18/38/38	0/1/3/3
3	MSL	C	5001	2	-	1/10/10/10	0/0/0/0
3	MSL	C	5002	2	-	1/10/10/10	0/0/0/0
3	MSL	C	5003	2	-	1/10/10/10	0/0/0/0
3	MSL	C	5004	2	-	1/10/10/10	0/0/0/0
3	MSL	C	5005	2	-	1/10/10/10	0/0/0/0
3	MSL	C	5006	2	-	1/10/10/10	0/0/0/0
3	MSL	C	5007	2	-	1/10/10/10	0/0/0/0
3	MSL	C	5008	2	-	1/10/10/10	0/0/0/0
3	MSL	C	5009	2	-	1/10/10/10	0/0/0/0
3	MSL	C	5010	2	-	1/10/10/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ANP	C	6003	2	2/2/7/8	1/18/38/38	0/1/3/3
4	ANP	D	6004	2	2/2/7/8	1/18/38/38	0/1/3/3
4	ANP	E	6005	2	2/2/7/8	1/18/38/38	0/1/3/3
4	ANP	F	6006	2	2/2/7/8	1/18/38/38	0/1/3/3
4	ANP	G	6007	2	2/2/7/8	1/18/38/38	0/1/3/3
4	ANP	H	6008	2	2/2/7/8	0/18/38/38	0/1/3/3
4	ANP	I	6009	2	2/2/7/8	1/18/38/38	0/1/3/3
4	ANP	J	6010	2	2/2/7/8	1/18/38/38	0/1/3/3

The worst 5 of 143 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	6010	ANP	PG-N3B	15.47	1.77	1.64
3	C	5008	MSL	CG-SD	-10.47	1.67	1.79
3	C	5004	MSL	CG-SD	-10.39	1.67	1.79
4	E	6005	ANP	PG-N3B	10.38	1.73	1.64
3	C	5002	MSL	CG-SD	-10.12	1.67	1.79

The worst 5 of 286 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	6002	ANP	O4'-C1'-N9	22.95	129.79	108.44
4	J	6010	ANP	O4'-C1'-N9	22.76	129.61	108.44
4	C	6003	ANP	O4'-C1'-N9	21.73	128.66	108.44
4	H	6008	ANP	O4'-C1'-N9	20.85	127.83	108.44
4	E	6005	ANP	O4'-C1'-N9	20.19	127.22	108.44

5 of 20 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	J	6010	ANP	C4'
4	J	6010	ANP	C1'
4	E	6005	ANP	C4'
4	E	6005	ANP	C1'
4	D	6004	ANP	C4'

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	5002	MSL	CB-CG-SD-NE

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Mol	Chain	Res	Type	Atoms
3	C	5003	MSL	CB-CG-SD-NE
3	C	5005	MSL	CB-CG-SD-NE
3	C	5007	MSL	CB-CG-SD-NE
3	C	5008	MSL	CB-CG-SD-NE

There are no ring outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	353/356 (99%)	-0.39	0 100 100	55, 73, 96, 108	0
1	B	353/356 (99%)	-0.34	0 100 100	55, 73, 96, 108	0
1	C	353/356 (99%)	-0.41	0 100 100	55, 73, 96, 108	0
1	D	353/356 (99%)	-0.36	0 100 100	55, 73, 96, 108	0
1	E	353/356 (99%)	-0.38	1 (0%) 91 76	55, 73, 96, 108	0
1	F	353/356 (99%)	-0.38	0 100 100	55, 73, 96, 108	0
1	G	353/356 (99%)	-0.33	0 100 100	55, 73, 96, 108	0
1	H	353/356 (99%)	-0.35	0 100 100	55, 73, 96, 108	0
1	I	353/356 (99%)	-0.39	0 100 100	55, 73, 96, 108	0
1	J	353/356 (99%)	-0.39	0 100 100	55, 73, 96, 108	0
All	All	3530/3560 (99%)	-0.37	1 (0%) 100 100	55, 73, 96, 108	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	3	CYS	2.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ANP	F	6006	31/31	0.27	1.07	78,91,100,101	0
4	ANP	E	6005	31/31	0.25	1.06	79,95,105,106	0
4	ANP	C	6003	31/31	0.25	0.91	64,76,92,93	0
3	MSL	C	5003	11/11	0.22	0.81	63,64,66,66	0
4	ANP	G	6007	31/31	0.26	0.80	65,86,95,96	0
3	MSL	C	5007	11/11	0.21	0.74	62,68,77,77	0
4	ANP	D	6004	31/31	0.23	0.63	83,95,105,106	0
3	MSL	C	5008	11/11	0.21	0.60	63,65,66,67	0
3	MSL	C	5006	11/11	0.23	0.55	73,79,85,85	0
4	ANP	A	6001	31/31	0.21	0.48	60,76,82,82	0
3	MSL	C	5001	11/11	0.18	0.32	51,54,57,58	0
4	ANP	I	6009	31/31	0.21	0.32	69,78,84,85	0
3	MSL	C	5005	11/11	0.19	0.17	75,78,79,79	0
3	MSL	C	5002	11/11	0.19	-0.23	37,41,46,48	0
4	ANP	J	6010	31/31	0.19	-0.25	47,58,64,67	0
2	MN	A	1003	1/1	0.21	-0.25	57,57,57,57	0
3	MSL	C	5009	11/11	0.17	-0.28	53,56,64,65	0
2	MN	A	1001	1/1	0.23	-0.37	68,68,68,68	0
4	ANP	B	6002	31/31	0.20	-0.42	42,50,60,65	0
4	ANP	H	6008	31/31	0.19	-0.53	40,48,59,67	0
2	MN	H	1072	1/1	0.18	-0.58	57,57,57,57	0
3	MSL	C	5004	11/11	0.16	-0.59	71,73,75,77	0
3	MSL	C	5010	11/11	0.16	-0.68	38,42,49,49	0
2	MN	G	1062	1/1	0.21	-0.70	65,65,65,65	0
2	MN	I	1082	1/1	0.17	-0.76	67,67,67,67	0
2	MN	E	1041	1/1	0.23	-0.76	73,73,73,73	0
2	MN	G	1063	1/1	0.20	-0.87	63,63,63,63	0
2	MN	D	1033	1/1	0.19	-0.92	56,56,56,56	0
2	MN	E	1043	1/1	0.17	-1.00	61,61,61,61	0
2	MN	C	1022	1/1	0.17	-1.04	66,66,66,66	0
2	MN	C	1023	1/1	0.20	-1.05	63,63,63,63	0
2	MN	F	1051	1/1	0.18	-1.08	69,69,69,69	0
2	MN	H	1073	1/1	0.22	-1.09	48,48,48,48	0
2	MN	I	1081	1/1	0.21	-1.23	68,68,68,68	0
2	MN	A	1002	1/1	0.16	-1.26	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	D	1032	1/1	0.15	-1.27	70,70,70,70	0
2	MN	F	1053	1/1	0.14	-1.28	69,69,69,69	0
2	MN	H	1071	1/1	0.24	-1.30	57,57,57,57	0
2	MN	E	1042	1/1	0.15	-1.38	65,65,65,65	0
2	MN	F	1052	1/1	0.17	-1.48	70,70,70,70	0
2	MN	D	1031	1/1	0.15	-1.68	65,65,65,65	0
2	MN	I	1083	1/1	0.17	-1.80	62,62,62,62	0
2	MN	B	1013	1/1	0.16	-2.04	56,56,56,56	0
2	MN	G	1061	1/1	0.17	-2.28	66,66,66,66	0
2	MN	B	1012	1/1	0.17	-2.28	60,60,60,60	0
2	MN	J	1092	1/1	0.12	-2.32	62,62,62,62	0
2	MN	C	1021	1/1	0.17	-2.57	66,66,66,66	0
2	MN	J	1091	1/1	0.24	-2.71	62,62,62,62	0
2	MN	B	1011	1/1	0.19	-3.34	62,62,62,62	0
2	MN	J	1093	1/1	0.21	-4.62	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.