



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:28 AM UTC

PDB ID : 6IY6 / pdb_00006iy6
Title : Crystal structure of human cytosolic aspartyl-tRNA synthetase (DRS) in complex with glutathion-S transferase (GST) domains from Aminoacyl tRNA synthetase complex-interacting multifunctional protein 2 (AIMP2) and glutamyl-prolyl-tRNA synthetase (EPRS)
Authors : Park, S.H.; Hahn, H.; Han, B.W.
Deposited on : 2018-12-13
Resolution : 3.60 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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

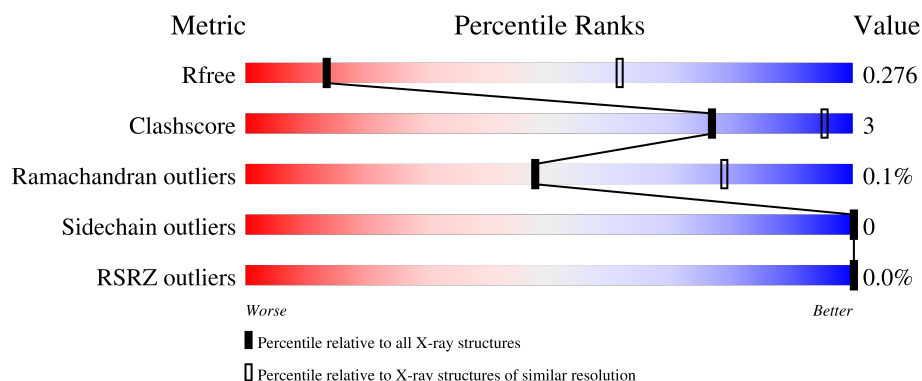
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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.



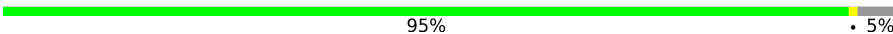
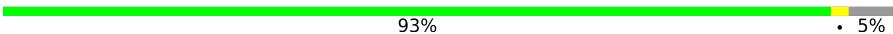
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	502	
1	B	502	
1	G	502	
1	H	502	

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Mol	Chain	Length	Quality of chain
2	C	215	 87% • 11%
2	D	215	 83% 6% 11%
2	I	215	 86% • 11%
2	J	215	 83% 7% 10%
3	E	165	 92% • 5%
3	F	165	 90% 5% 5%
3	K	165	 95% • 5%
3	L	165	 93% • 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24539 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 Aspartate-tRNA ligase, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3407	2165	600	622	20			
1	B	419	Total	C	N	O	S	0	0	0
			3390	2156	595	619	20			
1	G	417	Total	C	N	O	S	0	0	0
			3371	2145	589	617	20			
1	H	417	Total	C	N	O	S	0	0	0
			3371	2145	589	617	20			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P14868
A	1	GLY	-	expression tag	UNP P14868
A	2	SER	-	expression tag	UNP P14868
A	3	SER	-	expression tag	UNP P14868
A	4	HIS	-	expression tag	UNP P14868
A	5	HIS	-	expression tag	UNP P14868
A	6	HIS	-	expression tag	UNP P14868
A	7	HIS	-	expression tag	UNP P14868
A	8	HIS	-	expression tag	UNP P14868
A	9	HIS	-	expression tag	UNP P14868
A	10	SER	-	expression tag	UNP P14868
A	11	SER	-	expression tag	UNP P14868
A	12	GLY	-	expression tag	UNP P14868
A	13	LEU	-	expression tag	UNP P14868
A	14	VAL	-	expression tag	UNP P14868
A	15	PRO	-	expression tag	UNP P14868
A	16	ARG	-	expression tag	UNP P14868
A	17	GLY	-	expression tag	UNP P14868
A	18	SER	-	expression tag	UNP P14868
A	19	HIS	-	expression tag	UNP P14868
A	20	MET	-	expression tag	UNP P14868

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P14868
B	1	GLY	-	expression tag	UNP P14868
B	2	SER	-	expression tag	UNP P14868
B	3	SER	-	expression tag	UNP P14868
B	4	HIS	-	expression tag	UNP P14868
B	5	HIS	-	expression tag	UNP P14868
B	6	HIS	-	expression tag	UNP P14868
B	7	HIS	-	expression tag	UNP P14868
B	8	HIS	-	expression tag	UNP P14868
B	9	HIS	-	expression tag	UNP P14868
B	10	SER	-	expression tag	UNP P14868
B	11	SER	-	expression tag	UNP P14868
B	12	GLY	-	expression tag	UNP P14868
B	13	LEU	-	expression tag	UNP P14868
B	14	VAL	-	expression tag	UNP P14868
B	15	PRO	-	expression tag	UNP P14868
B	16	ARG	-	expression tag	UNP P14868
B	17	GLY	-	expression tag	UNP P14868
B	18	SER	-	expression tag	UNP P14868
B	19	HIS	-	expression tag	UNP P14868
B	20	MET	-	expression tag	UNP P14868
G	0	MET	-	initiating methionine	UNP P14868
G	1	GLY	-	expression tag	UNP P14868
G	2	SER	-	expression tag	UNP P14868
G	3	SER	-	expression tag	UNP P14868
G	4	HIS	-	expression tag	UNP P14868
G	5	HIS	-	expression tag	UNP P14868
G	6	HIS	-	expression tag	UNP P14868
G	7	HIS	-	expression tag	UNP P14868
G	8	HIS	-	expression tag	UNP P14868
G	9	HIS	-	expression tag	UNP P14868
G	10	SER	-	expression tag	UNP P14868
G	11	SER	-	expression tag	UNP P14868
G	12	GLY	-	expression tag	UNP P14868
G	13	LEU	-	expression tag	UNP P14868
G	14	VAL	-	expression tag	UNP P14868
G	15	PRO	-	expression tag	UNP P14868
G	16	ARG	-	expression tag	UNP P14868
G	17	GLY	-	expression tag	UNP P14868
G	18	SER	-	expression tag	UNP P14868
G	19	HIS	-	expression tag	UNP P14868
G	20	MET	-	expression tag	UNP P14868

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Chain	Residue	Modelled	Actual	Comment	Reference
H	0	MET	-	initiating methionine	UNP P14868
H	1	GLY	-	expression tag	UNP P14868
H	2	SER	-	expression tag	UNP P14868
H	3	SER	-	expression tag	UNP P14868
H	4	HIS	-	expression tag	UNP P14868
H	5	HIS	-	expression tag	UNP P14868
H	6	HIS	-	expression tag	UNP P14868
H	7	HIS	-	expression tag	UNP P14868
H	8	HIS	-	expression tag	UNP P14868
H	9	HIS	-	expression tag	UNP P14868
H	10	SER	-	expression tag	UNP P14868
H	11	SER	-	expression tag	UNP P14868
H	12	GLY	-	expression tag	UNP P14868
H	13	LEU	-	expression tag	UNP P14868
H	14	VAL	-	expression tag	UNP P14868
H	15	PRO	-	expression tag	UNP P14868
H	16	ARG	-	expression tag	UNP P14868
H	17	GLY	-	expression tag	UNP P14868
H	18	SER	-	expression tag	UNP P14868
H	19	HIS	-	expression tag	UNP P14868
H	20	MET	-	expression tag	UNP P14868

- Molecule 2 is a protein called Aminoacyl tRNA synthase complex-interacting multifunctional protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	192	Total	C	N	O	S	0	0	0
			1499	968	258	265	8			
2	D	192	Total	C	N	O	S	0	0	0
			1499	968	258	265	8			
2	I	192	Total	C	N	O	S	0	0	0
			1499	968	258	265	8			
2	J	193	Total	C	N	O	S	0	0	0
			1508	973	259	268	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	114	MET	-	initiating methionine	UNP Q13155
C	321	LEU	-	expression tag	UNP Q13155
C	322	GLU	-	expression tag	UNP Q13155
C	323	HIS	-	expression tag	UNP Q13155

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Chain	Residue	Modelled	Actual	Comment	Reference
C	324	HIS	-	expression tag	UNP Q13155
C	325	HIS	-	expression tag	UNP Q13155
C	326	HIS	-	expression tag	UNP Q13155
C	327	HIS	-	expression tag	UNP Q13155
C	328	HIS	-	expression tag	UNP Q13155
D	114	MET	-	initiating methionine	UNP Q13155
D	321	LEU	-	expression tag	UNP Q13155
D	322	GLU	-	expression tag	UNP Q13155
D	323	HIS	-	expression tag	UNP Q13155
D	324	HIS	-	expression tag	UNP Q13155
D	325	HIS	-	expression tag	UNP Q13155
D	326	HIS	-	expression tag	UNP Q13155
D	327	HIS	-	expression tag	UNP Q13155
D	328	HIS	-	expression tag	UNP Q13155
I	114	MET	-	initiating methionine	UNP Q13155
I	321	LEU	-	expression tag	UNP Q13155
I	322	GLU	-	expression tag	UNP Q13155
I	323	HIS	-	expression tag	UNP Q13155
I	324	HIS	-	expression tag	UNP Q13155
I	325	HIS	-	expression tag	UNP Q13155
I	326	HIS	-	expression tag	UNP Q13155
I	327	HIS	-	expression tag	UNP Q13155
I	328	HIS	-	expression tag	UNP Q13155
J	114	MET	-	initiating methionine	UNP Q13155
J	321	LEU	-	expression tag	UNP Q13155
J	322	GLU	-	expression tag	UNP Q13155
J	323	HIS	-	expression tag	UNP Q13155
J	324	HIS	-	expression tag	UNP Q13155
J	325	HIS	-	expression tag	UNP Q13155
J	326	HIS	-	expression tag	UNP Q13155
J	327	HIS	-	expression tag	UNP Q13155
J	328	HIS	-	expression tag	UNP Q13155

- Molecule 3 is a protein called Bifunctional glutamate/proline--tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	157	Total	C	N	O	S	0	0	0
			1224	777	206	237	4			
3	F	157	Total	C	N	O	S	0	0	0
			1224	777	206	237	4			
3	K	157	Total	C	N	O	S	0	0	0
			1224	777	206	237	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	157	Total	C	N	O	S	0	0	0
			1224	777	206	237	4			

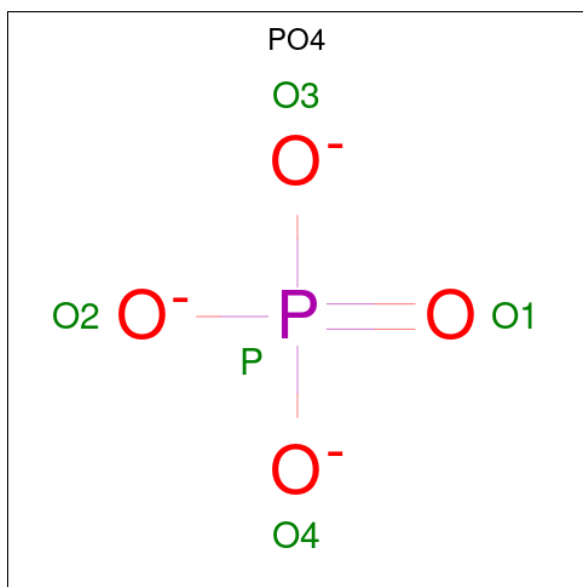
There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	158	LEU	-	expression tag	UNP P07814
E	159	GLU	-	expression tag	UNP P07814
E	160	HIS	-	expression tag	UNP P07814
E	161	HIS	-	expression tag	UNP P07814
E	162	HIS	-	expression tag	UNP P07814
E	163	HIS	-	expression tag	UNP P07814
E	164	HIS	-	expression tag	UNP P07814
E	165	HIS	-	expression tag	UNP P07814
F	158	LEU	-	expression tag	UNP P07814
F	159	GLU	-	expression tag	UNP P07814
F	160	HIS	-	expression tag	UNP P07814
F	161	HIS	-	expression tag	UNP P07814
F	162	HIS	-	expression tag	UNP P07814
F	163	HIS	-	expression tag	UNP P07814
F	164	HIS	-	expression tag	UNP P07814
F	165	HIS	-	expression tag	UNP P07814
K	158	LEU	-	expression tag	UNP P07814
K	159	GLU	-	expression tag	UNP P07814
K	160	HIS	-	expression tag	UNP P07814
K	161	HIS	-	expression tag	UNP P07814
K	162	HIS	-	expression tag	UNP P07814
K	163	HIS	-	expression tag	UNP P07814
K	164	HIS	-	expression tag	UNP P07814
K	165	HIS	-	expression tag	UNP P07814
L	158	LEU	-	expression tag	UNP P07814
L	159	GLU	-	expression tag	UNP P07814
L	160	HIS	-	expression tag	UNP P07814
L	161	HIS	-	expression tag	UNP P07814
L	162	HIS	-	expression tag	UNP P07814
L	163	HIS	-	expression tag	UNP P07814
L	164	HIS	-	expression tag	UNP P07814
L	165	HIS	-	expression tag	UNP P07814

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		
5	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		
6	D	2	Total	O	0	0
			2	2		
6	G	2	Total	O	0	0
			2	2		
6	H	2	Total	O	0	0
			2	2		
6	I	2	Total	O	0	0
			2	2		
6	J	2	Total	O	0	0
			2	2		

- Molecule 1: Aspartate-tRNA ligase, cytoplasmic

R273	ALA	PRO	GLU	GLY	MET
R281	HIS	GLU	ALA	SER	GLY
H288	ASN	SER	GLY	HIS	HIS
M303	THR	ASN	GLU	HIS	HIS
E304	HIS	ARG	GLY	HIS	HIS
E305	THR	ALA	THR	SER	SER
I306	THR	VAL	VAL	GLY	GLY
A307	THR	ASN	ASN	VAL	LEU
D308	THR	THR	THR	VAL	VAL
T309	THR	R179	ASP	PRO	PRO
M354	THR	R183	THR	ARG	GLY
K383	THR	F196	THR	SER	GLY
I390	THR	L210	THR	HIS	HIS
D457	THR	K213	THR	MET	MET
R460	THR	I223	THR	ALA	ALA
F461	THR	S225	ALA	GLU	GLU
G462	THR	ALA	ALA	GLY	Q84
H466	THR	ALA	SER	GLY	Q83
M491	THR	ALA	GLY	GLY	Q82
P493	THR	ALA	ALA	ALA	R81
R494	THR	ASN	ASN	ASN	R85
D495	THR	VAL	VAL	ASN	V91
PRO	THR	PHE	PHE	THR	A92
ARG	THR	THR	VAL	THR	H86
LEU	THR	SER	VAL	SER	V123
THR	THR	TYR	TYR	TYR	I127
PRO	THR	LYS	LYS	PHE	V139
		ASN	ASN	ASN	I142
		ALA	ALA	ALA	V143
		TYR	TYR	TYR	V144
		LEU	LEU	LEU	L154
		A247	ALA	GLN	GLN
		L252	THR	LEU	LEU
		I258	THR	ASP	ASP
		E263	THR	ALA	ALA
		K264	THR	VAL	VAL

- Molecule 1: Aspartate-tRNA ligase, cytoplasmic

[illegible]

- Molecule 1: Aspartate-tRNA ligase, cytoplasmic

PRO	GLU	ALA	GLU	GLY	GLU	GLU	GLU	GLY	ARG	ALA	SER	SER	THR	VAL	ASN	GLN	ASP	GLN	THR	R179	R180	F196	T209	T220	P221	K222	I223	I224	S225	ALA	ALA	SER	GLU	GLY	GLY	ALA	ASN	VAL	PHE	THR	VAL	ASN	ASN	ASN	TYR	PHE	LYS	THR	VAL	SER	TYR	LEU	ALA	GLN	S249	I258	F272	ARG	ALA
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	VAL	VAL	LEU	PRO	ARG	GLY	SER	HIS	MET	ALA	GLU	D23	R28	R65	S69	R70	F77	L78	R81	R82	O83	O84	L90	T91	A92	H96	V123	I127	I142	I154	GLN	LEU	ASP	ASP	ALA	VAL	ASP										



- Molecule 3: Bifunctional glutamate/proline--tRNA ligase

Chain F: 90% 5% 5%



- Molecule 3: Bifunctional glutamate/proline--tRNA ligase

Chain K: 95% • 5%



- Molecule 3: Bifunctional glutamate/proline--tRNA ligase

Chain L: 93% • 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	108.07Å 108.07Å 815.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-3.60) 98.9 (30.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.237 , 0.275 0.240 , 0.276	Depositor DCC
R_{free} test set	3084 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	113.5	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 146.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.398 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24539	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ZN, PO4

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	1.01	0/3473	1.43	0/4680
1	B	1.00	0/3456	1.43	0/4658
1	G	1.01	0/3437	1.43	0/4633
1	H	1.01	0/3437	1.43	0/4633
2	C	1.02	0/1531	1.54	0/2076
2	D	1.02	0/1531	1.55	0/2076
2	I	1.02	0/1531	1.54	0/2076
2	J	1.01	0/1540	1.54	1/2088 (0.0%)
3	E	1.02	0/1248	1.58	0/1698
3	F	1.03	0/1248	1.58	0/1698
3	K	1.03	0/1248	1.58	0/1698
3	L	1.03	0/1248	1.59	0/1698
All	All	1.01	0/24928	1.49	1/33712 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	270	ALA	N-CA-C	-5.69	105.16	111.36

There are no chirality outliers.

There are no planarity outliers.

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	3407	0	3419	46	0
1	B	3390	0	3401	23	1
1	G	3371	0	3380	27	0
1	H	3371	0	3380	27	0
2	C	1499	0	1539	20	0
2	D	1499	0	1539	11	0
2	I	1499	0	1539	6	0
2	J	1508	0	1545	11	1
3	E	1224	0	1212	3	0
3	F	1224	0	1212	7	0
3	K	1224	0	1212	1	0
3	L	1224	0	1212	3	0
4	A	1	0	0	0	0
4	H	1	0	0	0	0
5	A	35	0	0	0	0
5	B	25	0	0	0	0
5	G	15	0	0	0	0
5	H	10	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
All	All	24539	0	24590	142	1

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 3.

The worst 5 of 142 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:A:65:ARG:NH2	1:B:462:GLY:O	1.94	0.99
1:A:383:LYS:HD3	2:C:119:LEU:HD13	1.43	0.97
1:A:383:LYS:HZ3	2:C:119:LEU:HD22	1.27	0.97
1:A:383:LYS:CE	2:C:119:LEU:HD13	1.97	0.94
1:G:494:ARG:HG2	1:H:223:ILE:HD13	1.47	0.93

All (1) 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:B:24:TYR:OH	2:J:257:ARG:NH1[1_445]	2.04	0.16

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	413/502 (82%)	384 (93%)	29 (7%)	0	100	100
1	B	411/502 (82%)	382 (93%)	28 (7%)	1 (0%)	43	72
1	G	409/502 (82%)	382 (93%)	27 (7%)	0	100	100
1	H	409/502 (82%)	380 (93%)	28 (7%)	1 (0%)	43	72
2	C	186/215 (86%)	178 (96%)	8 (4%)	0	100	100
2	D	186/215 (86%)	177 (95%)	9 (5%)	0	100	100
2	I	186/215 (86%)	177 (95%)	9 (5%)	0	100	100
2	J	187/215 (87%)	179 (96%)	8 (4%)	0	100	100
3	E	155/165 (94%)	150 (97%)	5 (3%)	0	100	100
3	F	155/165 (94%)	150 (97%)	5 (3%)	0	100	100
3	K	155/165 (94%)	150 (97%)	5 (3%)	0	100	100
3	L	155/165 (94%)	150 (97%)	5 (3%)	0	100	100
All	All	3007/3528 (85%)	2839 (94%)	166 (6%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	ARG
1	H	151	ARG

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	375/440 (85%)	375 (100%)	0	100	100
1	B	373/440 (85%)	373 (100%)	0	100	100
1	G	372/440 (84%)	372 (100%)	0	100	100
1	H	372/440 (84%)	372 (100%)	0	100	100
2	C	168/189 (89%)	168 (100%)	0	100	100
2	D	168/189 (89%)	168 (100%)	0	100	100
2	I	168/189 (89%)	168 (100%)	0	100	100
2	J	169/189 (89%)	169 (100%)	0	100	100
3	E	137/144 (95%)	137 (100%)	0	100	100
3	F	137/144 (95%)	137 (100%)	0	100	100
3	K	137/144 (95%)	137 (100%)	0	100	100
3	L	137/144 (95%)	137 (100%)	0	100	100
All	All	2713/3092 (88%)	2713 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	225	HIS
2	I	287	GLN
3	L	146	HIS
2	D	287	GLN
2	D	125	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\# Z > 2$
5	PO4	B	603	-	4,4,4	0.69	0	6,6,6	0.47	0
5	PO4	H	602	-	4,4,4	0.76	0	6,6,6	0.43	0
5	PO4	A	603	-	4,4,4	0.72	0	6,6,6	0.48	0
5	PO4	A	607	-	4,4,4	0.69	0	6,6,6	0.46	0
5	PO4	A	608	-	4,4,4	0.72	0	6,6,6	0.46	0
5	PO4	B	602	-	4,4,4	0.71	0	6,6,6	0.49	0
5	PO4	B	601	-	4,4,4	0.73	0	6,6,6	0.47	0
5	PO4	B	605	-	4,4,4	0.73	0	6,6,6	0.48	0
5	PO4	A	602	-	4,4,4	0.82	0	6,6,6	0.41	0
5	PO4	G	601	-	4,4,4	0.73	0	6,6,6	0.45	0
5	PO4	H	603	-	4,4,4	0.67	0	6,6,6	0.48	0
5	PO4	G	602	-	4,4,4	0.69	0	6,6,6	0.47	0
5	PO4	B	604	-	4,4,4	0.70	0	6,6,6	0.47	0
5	PO4	G	603	-	4,4,4	0.70	0	6,6,6	0.46	0
5	PO4	A	604	-	4,4,4	0.67	0	6,6,6	0.47	0
5	PO4	A	606	-	4,4,4	0.73	0	6,6,6	0.45	0
5	PO4	A	605	-	4,4,4	0.75	0	6,6,6	0.45	0

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](#)

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	421/502 (83%)	-0.82	0 100 100	100, 133, 178, 220	0
1	B	419/502 (83%)	-0.82	0 100 100	99, 134, 175, 219	0
1	G	417/502 (83%)	-0.77	0 100 100	100, 133, 180, 227	0
1	H	417/502 (83%)	-0.80	1 (0%) 91 80	100, 132, 177, 204	0
2	C	192/215 (89%)	-0.79	0 100 100	115, 156, 181, 196	0
2	D	192/215 (89%)	-0.82	0 100 100	111, 153, 180, 201	0
2	I	192/215 (89%)	-0.74	0 100 100	111, 150, 184, 192	0
2	J	193/215 (89%)	-0.76	0 100 100	110, 152, 186, 202	0
3	E	157/165 (95%)	-0.79	0 100 100	116, 152, 193, 210	0
3	F	157/165 (95%)	-0.82	0 100 100	119, 152, 185, 190	0
3	K	157/165 (95%)	-0.80	0 100 100	116, 155, 184, 196	0
3	L	157/165 (95%)	-0.67	0 100 100	118, 152, 185, 203	0
All	All	3071/3528 (87%)	-0.79	1 (0%) 100 100	99, 142, 182, 227	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	92	ALA	3.2

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 oligosaccharides 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. 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
5	PO4	A	603	5/5	0.94	0.08	189,199,203,206	0
5	PO4	A	607	5/5	0.94	0.16	191,194,195,200	0
5	PO4	B	603	5/5	0.94	0.06	188,189,192,195	0
5	PO4	A	606	5/5	0.95	0.06	197,199,201,204	0
5	PO4	G	603	5/5	0.95	0.07	179,180,183,184	0
5	PO4	B	605	5/5	0.96	0.05	199,204,204,207	0
5	PO4	G	602	5/5	0.96	0.07	185,187,189,190	0
5	PO4	A	602	5/5	0.96	0.07	133,135,140,141	0
5	PO4	B	604	5/5	0.97	0.08	157,157,160,167	0
5	PO4	A	605	5/5	0.97	0.13	168,173,182,183	0
5	PO4	B	602	5/5	0.97	0.24	157,164,166,169	0
5	PO4	A	604	5/5	0.97	0.06	165,165,168,173	0
5	PO4	H	602	5/5	0.97	0.05	135,140,141,142	0
5	PO4	A	608	5/5	0.98	0.04	205,211,212,213	0
5	PO4	B	601	5/5	0.98	0.06	138,143,146,146	0
5	PO4	G	601	5/5	0.98	0.04	136,140,142,144	0
5	PO4	H	603	5/5	0.98	0.04	176,177,180,183	0
4	ZN	H	601	1/1	0.99	0.10	144,144,144,144	0
4	ZN	A	601	1/1	0.99	0.07	136,136,136,136	0

6.5 Other polymers

There are no such residues in this entry.