



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:24 PM UTC

PDB ID : 5CHE / pdb_00005che
Title : Crystal structure of Arabidopsis glutamyl-tRNA reductase in complex with its regulatory proteins
Authors : Fang, Y.; Liu, L.
Deposited on : 2015-07-10
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

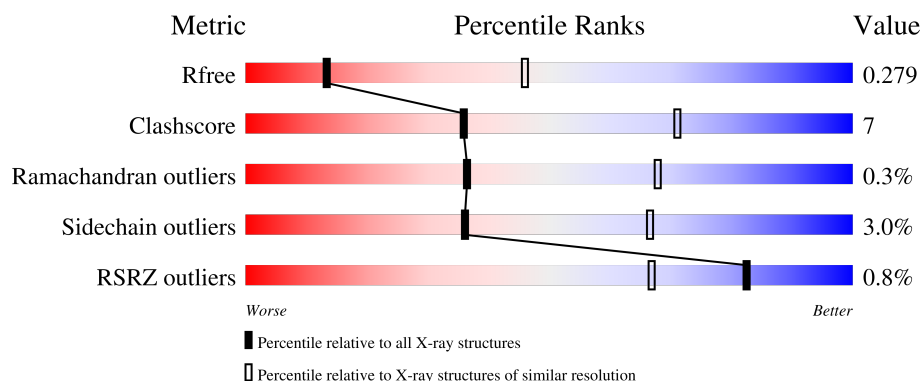
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	472	% 74% 16% • 10%
1	B	472	% 69% 19% • 10%
2	C	310	% 65% 14% • 19%
2	D	310	65% 14% • 19%
3	E	159	60% 14% • 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	159	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (54%), yellow (19%), and grey (26%).

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12371 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 Glutamyl-tRNA reductase 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	1	0
			3292	2055	591	621	25			
1	B	423	Total	C	N	O	S	0	0	0
			3243	2029	586	603	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	SER	-	expression tag	UNP P42804
B	72	SER	-	expression tag	UNP P42804

- Molecule 2 is a protein called Glutamyl-tRNA reductase-binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	250	Total	C	N	O	S	0	0	0
			1970	1246	335	376	13			
2	D	250	Total	C	N	O	S	0	1	0
			1992	1260	339	380	13			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	MET	-	initiating methionine	UNP Q9LU39
C	9	GLY	-	expression tag	UNP Q9LU39
C	10	SER	-	expression tag	UNP Q9LU39
C	11	SER	-	expression tag	UNP Q9LU39
C	12	HIS	-	expression tag	UNP Q9LU39
C	13	HIS	-	expression tag	UNP Q9LU39
C	14	HIS	-	expression tag	UNP Q9LU39
C	15	HIS	-	expression tag	UNP Q9LU39
C	16	HIS	-	expression tag	UNP Q9LU39
C	17	HIS	-	expression tag	UNP Q9LU39

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	SER	-	expression tag	UNP Q9LU39
C	19	SER	-	expression tag	UNP Q9LU39
C	20	GLY	-	expression tag	UNP Q9LU39
C	21	LEU	-	expression tag	UNP Q9LU39
C	22	VAL	-	expression tag	UNP Q9LU39
C	23	PRO	-	expression tag	UNP Q9LU39
C	24	ARG	-	expression tag	UNP Q9LU39
C	25	GLY	-	expression tag	UNP Q9LU39
C	26	SER	-	expression tag	UNP Q9LU39
C	27	HIS	-	expression tag	UNP Q9LU39
C	28	MET	-	expression tag	UNP Q9LU39
C	29	ALA	-	expression tag	UNP Q9LU39
C	30	SER	-	expression tag	UNP Q9LU39
C	31	MET	-	expression tag	UNP Q9LU39
C	32	THR	-	expression tag	UNP Q9LU39
C	33	GLY	-	expression tag	UNP Q9LU39
C	34	GLY	-	expression tag	UNP Q9LU39
C	35	GLN	-	expression tag	UNP Q9LU39
C	36	GLN	-	expression tag	UNP Q9LU39
C	37	MET	-	expression tag	UNP Q9LU39
C	38	GLY	-	expression tag	UNP Q9LU39
C	39	ARG	-	expression tag	UNP Q9LU39
C	40	GLY	-	expression tag	UNP Q9LU39
C	41	SER	-	expression tag	UNP Q9LU39
D	8	MET	-	initiating methionine	UNP Q9LU39
D	9	GLY	-	expression tag	UNP Q9LU39
D	10	SER	-	expression tag	UNP Q9LU39
D	11	SER	-	expression tag	UNP Q9LU39
D	12	HIS	-	expression tag	UNP Q9LU39
D	13	HIS	-	expression tag	UNP Q9LU39
D	14	HIS	-	expression tag	UNP Q9LU39
D	15	HIS	-	expression tag	UNP Q9LU39
D	16	HIS	-	expression tag	UNP Q9LU39
D	17	HIS	-	expression tag	UNP Q9LU39
D	18	SER	-	expression tag	UNP Q9LU39
D	19	SER	-	expression tag	UNP Q9LU39
D	20	GLY	-	expression tag	UNP Q9LU39
D	21	LEU	-	expression tag	UNP Q9LU39
D	22	VAL	-	expression tag	UNP Q9LU39
D	23	PRO	-	expression tag	UNP Q9LU39
D	24	ARG	-	expression tag	UNP Q9LU39
D	25	GLY	-	expression tag	UNP Q9LU39

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	26	SER	-	expression tag	UNP Q9LU39
D	27	HIS	-	expression tag	UNP Q9LU39
D	28	MET	-	expression tag	UNP Q9LU39
D	29	ALA	-	expression tag	UNP Q9LU39
D	30	SER	-	expression tag	UNP Q9LU39
D	31	MET	-	expression tag	UNP Q9LU39
D	32	THR	-	expression tag	UNP Q9LU39
D	33	GLY	-	expression tag	UNP Q9LU39
D	34	GLY	-	expression tag	UNP Q9LU39
D	35	GLN	-	expression tag	UNP Q9LU39
D	36	GLN	-	expression tag	UNP Q9LU39
D	37	MET	-	expression tag	UNP Q9LU39
D	38	GLY	-	expression tag	UNP Q9LU39
D	39	ARG	-	expression tag	UNP Q9LU39
D	40	GLY	-	expression tag	UNP Q9LU39
D	41	SER	-	expression tag	UNP Q9LU39

- Molecule 3 is a protein called Protein FLUORESCENT IN BLUE LIGHT, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	119	Total	C	N	O	S	0	1	0
			951	599	160	190	2			
3	F	117	Total	C	N	O	S	0	0	0
			917	579	157	179	2			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	159	MET	-	initiating methionine	UNP Q940U6
E	160	LYS	-	expression tag	UNP Q940U6
E	161	TYR	-	expression tag	UNP Q940U6
E	162	LEU	-	expression tag	UNP Q940U6
E	163	LEU	-	expression tag	UNP Q940U6
E	164	PRO	-	expression tag	UNP Q940U6
E	165	THR	-	expression tag	UNP Q940U6
E	166	ALA	-	expression tag	UNP Q940U6
E	167	ALA	-	expression tag	UNP Q940U6
E	168	ALA	-	expression tag	UNP Q940U6
E	169	GLY	-	expression tag	UNP Q940U6
E	170	LEU	-	expression tag	UNP Q940U6
E	171	LEU	-	expression tag	UNP Q940U6
E	172	LEU	-	expression tag	UNP Q940U6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	173	LEU	-	expression tag	UNP Q940U6
E	174	ALA	-	expression tag	UNP Q940U6
E	175	ALA	-	expression tag	UNP Q940U6
E	176	GLN	-	expression tag	UNP Q940U6
E	177	PRO	-	expression tag	UNP Q940U6
E	178	ALA	-	expression tag	UNP Q940U6
E	179	MET	-	expression tag	UNP Q940U6
E	180	ALA	-	expression tag	UNP Q940U6
E	181	MET	-	expression tag	UNP Q940U6
E	182	ASP	-	expression tag	UNP Q940U6
E	183	ILE	-	expression tag	UNP Q940U6
E	184	GLY	-	expression tag	UNP Q940U6
E	185	ILE	-	expression tag	UNP Q940U6
E	186	ASN	-	expression tag	UNP Q940U6
E	187	SER	-	expression tag	UNP Q940U6
E	188	ASP	-	expression tag	UNP Q940U6
E	189	PRO	-	expression tag	UNP Q940U6
E	190	HIS	-	expression tag	UNP Q940U6
E	191	HIS	-	expression tag	UNP Q940U6
E	192	HIS	-	expression tag	UNP Q940U6
E	193	HIS	-	expression tag	UNP Q940U6
E	194	HIS	-	expression tag	UNP Q940U6
E	195	HIS	-	expression tag	UNP Q940U6
F	159	MET	-	initiating methionine	UNP Q940U6
F	160	LYS	-	expression tag	UNP Q940U6
F	161	TYR	-	expression tag	UNP Q940U6
F	162	LEU	-	expression tag	UNP Q940U6
F	163	LEU	-	expression tag	UNP Q940U6
F	164	PRO	-	expression tag	UNP Q940U6
F	165	THR	-	expression tag	UNP Q940U6
F	166	ALA	-	expression tag	UNP Q940U6
F	167	ALA	-	expression tag	UNP Q940U6
F	168	ALA	-	expression tag	UNP Q940U6
F	169	GLY	-	expression tag	UNP Q940U6
F	170	LEU	-	expression tag	UNP Q940U6
F	171	LEU	-	expression tag	UNP Q940U6
F	172	LEU	-	expression tag	UNP Q940U6
F	173	LEU	-	expression tag	UNP Q940U6
F	174	ALA	-	expression tag	UNP Q940U6
F	175	ALA	-	expression tag	UNP Q940U6
F	176	GLN	-	expression tag	UNP Q940U6
F	177	PRO	-	expression tag	UNP Q940U6

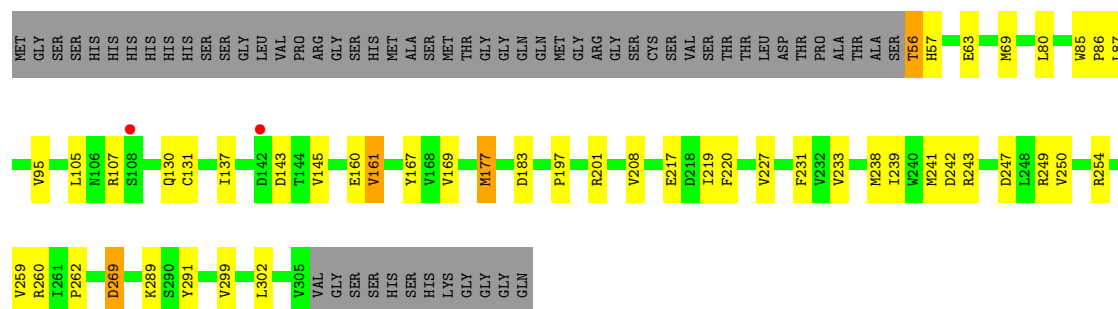
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	178	ALA	-	expression tag	UNP Q940U6
F	179	MET	-	expression tag	UNP Q940U6
F	180	ALA	-	expression tag	UNP Q940U6
F	181	MET	-	expression tag	UNP Q940U6
F	182	ASP	-	expression tag	UNP Q940U6
F	183	ILE	-	expression tag	UNP Q940U6
F	184	GLY	-	expression tag	UNP Q940U6
F	185	ILE	-	expression tag	UNP Q940U6
F	186	ASN	-	expression tag	UNP Q940U6
F	187	SER	-	expression tag	UNP Q940U6
F	188	ASP	-	expression tag	UNP Q940U6
F	189	PRO	-	expression tag	UNP Q940U6
F	190	HIS	-	expression tag	UNP Q940U6
F	191	HIS	-	expression tag	UNP Q940U6
F	192	HIS	-	expression tag	UNP Q940U6
F	193	HIS	-	expression tag	UNP Q940U6
F	194	HIS	-	expression tag	UNP Q940U6
F	195	HIS	-	expression tag	UNP Q940U6

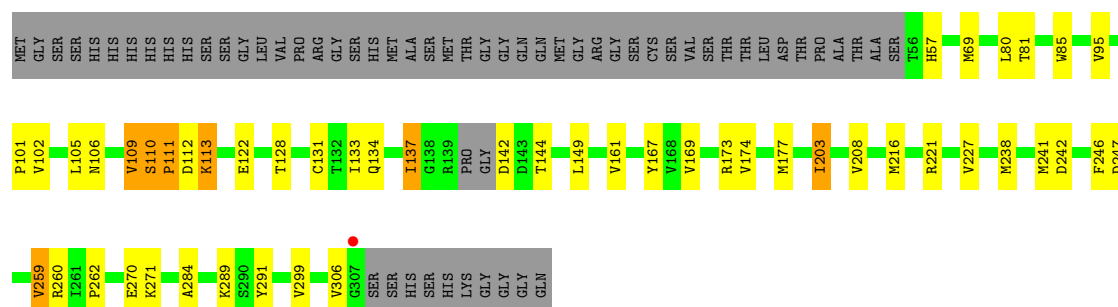
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	2	Total O 2 2	0	0
4	C	2	Total O 2 2	0	0



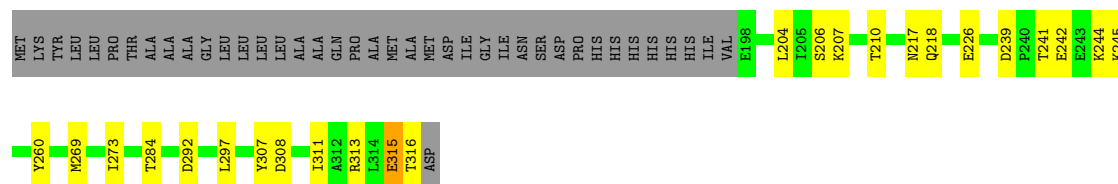
- Molecule 2: Glutamyl-tRNA reductase-binding protein, chloroplastic

Chain D: 65% 14% 19%



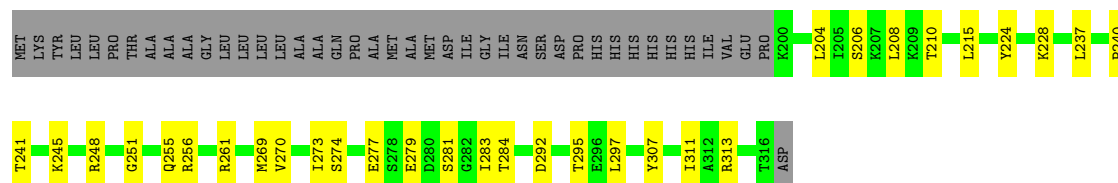
- Molecule 3: Protein FLUORESCENT IN BLUE LIGHT, chloroplastic

Chain E: 60% 14% 25%



- Molecule 3: Protein FLUORESCENT IN BLUE LIGHT, chloroplastic

Chain F: 54% 19% 26%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.99Å 53.21Å 203.76Å 90.00° 108.36° 90.00°	Depositor
Resolution (Å)	39.27 – 3.20 39.27 – 3.20	Depositor EDS
% Data completeness (in resolution range)	87.2 (39.27-3.20) 87.3 (39.27-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.223 , 0.278 0.224 , 0.279	Depositor DCC
R_{free} test set	1636 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	58.7	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 9.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12371	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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

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	0.50	1/3338 (0.0%)	0.92	7/4501 (0.2%)
1	B	0.54	2/3283 (0.1%)	0.98	14/4423 (0.3%)
2	C	0.43	0/2013	0.79	1/2731 (0.0%)
2	D	0.47	0/2034	0.87	5/2755 (0.2%)
3	E	0.43	0/967	0.85	4/1294 (0.3%)
3	F	0.38	0/929	0.80	0/1243
All	All	0.48	3/12564 (0.0%)	0.90	31/16947 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	ASN	CA-C	-7.94	1.45	1.52
1	A	502	ASP	CA-C	-6.34	1.45	1.53
1	B	280	ARG	N-CA	5.20	1.53	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	ASP	N-CA-C	-16.10	86.98	108.24
1	A	186	TYR	N-CA-C	13.53	130.67	112.68
1	B	188	LYS	N-CA-C	-12.99	97.12	113.23
2	D	306	VAL	N-CA-C	11.96	124.55	111.88
1	B	280	ARG	N-CA-C	10.87	124.60	111.02
2	D	110	SER	CA-C-N	10.77	130.44	119.56
2	D	110	SER	C-N-CA	10.77	130.44	119.56
1	B	188	LYS	N-CA-CB	-9.84	95.08	110.44
1	B	187	ASN	CB-CA-C	9.68	130.39	117.23
1	A	228	PHE	N-CA-C	-9.29	96.59	110.24
1	B	223	GLN	N-CA-C	8.95	123.63	108.23
1	B	271	LEU	CA-C-N	7.67	128.13	119.92
1	B	271	LEU	C-N-CA	7.67	128.13	119.92
1	B	474	LYS	N-CA-C	7.14	118.75	110.97
1	B	322	MET	CA-C-N	7.00	127.97	120.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	MET	C-N-CA	7.00	127.97	120.83
1	A	501	CYS	N-CA-C	-6.76	98.38	108.99
3	E	315	GLU	N-CA-C	6.61	118.14	111.07
2	D	111	PRO	N-CA-C	6.55	122.04	113.86
1	A	287	GLY	N-CA-C	-6.53	104.95	112.79
1	B	222	GLY	N-CA-C	6.46	127.03	115.80
1	A	117	ILE	N-CA-C	5.91	113.73	107.76
1	A	390	VAL	N-CA-C	-5.53	104.92	113.16
3	E	239	ASP	CA-C-N	5.42	125.06	119.05
3	E	239	ASP	C-N-CA	5.42	125.06	119.05
1	B	186	TYR	CB-CA-C	-5.39	98.67	109.35
1	B	279	ALA	CA-C-N	5.25	130.77	122.78
1	B	279	ALA	C-N-CA	5.25	130.77	122.78
2	D	306	VAL	CB-CA-C	-5.23	105.20	112.36
3	E	218	GLN	N-CA-C	5.05	119.08	111.81
2	C	269	ASP	N-CA-C	5.03	114.93	108.34

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	3292	0	3363	44	0
1	B	3243	0	3309	55	0
2	C	1970	0	1928	30	0
2	D	1992	0	1955	30	0
3	E	951	0	959	15	0
3	F	917	0	926	18	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
4	C	2	0	0	1	0
All	All	12371	0	12440	182	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 7.

All (182) 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:B:252:ILE:HG22	1:B:418:LYS:HB3	1.61	0.80
1:A:271:LEU:HD11	1:A:276:ASN:HA	1.65	0.78
2:C:80:LEU:HD21	2:D:80:LEU:HD21	1.66	0.78
2:D:227:VAL:HG12	2:D:299:VAL:HB	1.67	0.77
2:D:238:MET:HE1	2:D:241:MET:HE3	1.68	0.75
2:C:238:MET:HE1	2:C:241:MET:HE3	1.68	0.74
3:F:215:LEU:O	3:F:256:ARG:NH1	2.21	0.73
1:A:504:SER:OG	1:A:505:ASP:N	2.22	0.73
1:A:475:LYS:HG3	1:A:478:ARG:HH21	1.54	0.72
1:A:450:ARG:NH1	3:E:292:ASP:OD2	2.24	0.71
1:A:496:MET:HB3	3:E:311:ILE:HD12	1.71	0.70
1:B:450:ARG:NH1	3:F:292:ASP:OD2	2.26	0.68
1:A:203:SER:HB3	1:A:204:LEU:HD23	1.75	0.68
2:C:183:ASP:OD1	2:D:106:ASN:ND2	2.26	0.68
3:F:204:LEU:HD12	3:F:237:LEU:HD12	1.76	0.67
1:B:291:LYS:HE3	1:B:314:ARG:HH12	1.60	0.67
2:D:69:MET:HB3	2:D:95:VAL:HG21	1.77	0.67
1:B:306:VAL:HG22	1:B:328:ILE:HD11	1.75	0.67
2:C:227:VAL:HG12	2:C:299:VAL:HB	1.76	0.66
2:C:69:MET:HB3	2:C:95:VAL:HG21	1.77	0.65
1:B:382:VAL:HA	1:B:383:PRO:C	2.20	0.65
1:A:310:ARG:HG2	1:A:332:LEU:HD21	1.78	0.65
1:A:115:LEU:HD13	1:A:171:SER:HB3	1.80	0.64
1:A:130:CYS:O	4:A:601:HOH:O	2.15	0.64
2:D:242:ASP:OD1	2:D:260:ARG:NH2	2.30	0.62
1:B:496:MET:HB3	3:F:311:ILE:HD12	1.82	0.62
3:F:261:ARG:HH21	3:F:297:LEU:HD13	1.64	0.61
1:B:457:ARG:HD2	1:B:485:ARG:HG2	1.82	0.61
1:B:252:ILE:HA	1:B:418:LYS:HD3	1.82	0.61
3:E:292:ASP:OD1	3:E:307:TYR:OH	2.18	0.60
3:E:284:THR:HG22	3:E:313:ARG:HE	1.66	0.60
2:D:101:PRO:HG2	2:D:169:VAL:HB	1.83	0.60
2:C:239:ILE:HD11	2:C:249:ARG:HB2	1.82	0.60
3:F:279:GLU:HG3	3:F:281:SER:H	1.67	0.59
1:B:349:THR:OG1	1:B:385:ASN:ND2	2.35	0.59
1:B:278:SER:OG	1:B:279:ALA:N	2.33	0.59
2:D:208:VAL:HG22	2:D:238:MET:HE2	1.85	0.59
1:B:366:GLN:HG2	1:B:395:THR:HG21	1.84	0.58
2:C:208:VAL:HG22	2:C:238:MET:HE2	1.85	0.58
1:B:188:LYS:HD3	1:B:434:GLU:HG3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:MET:HE3	1:A:149:ILE:HD11	1.86	0.57
1:A:188:LYS:HE2	1:A:434:GLU:HG2	1.86	0.57
1:B:145:ASN:OD1	1:B:146:ARG:NH1	2.38	0.57
3:F:248:ARG:HG3	3:F:270:VAL:HG11	1.86	0.57
2:D:109:VAL:HG13	2:D:167:TYR:HE1	1.70	0.57
1:A:460:GLU:OE2	1:B:490:ARG:NH1	2.33	0.56
3:E:307:TYR:O	3:E:311:ILE:HG12	2.06	0.56
3:E:260:TYR:HB2	3:E:297:LEU:HD21	1.88	0.55
1:B:277:VAL:HA	1:B:278:SER:HB3	1.87	0.54
2:C:269:ASP:OD1	2:C:269:ASP:N	2.40	0.54
2:D:238:MET:HE3	2:D:246:PHE:HB2	1.90	0.54
1:B:124:ARG:HB2	1:B:124:ARG:NH1	2.24	0.53
2:D:69:MET:HE2	2:D:131:CYS:SG	2.49	0.53
1:B:115:LEU:HD13	1:B:171:SER:HB3	1.89	0.53
2:C:69:MET:HE2	2:C:131:CYS:SG	2.49	0.53
2:D:203:ILE:HD13	2:D:270:GLU:HB2	1.90	0.53
2:C:160:GLU:HG3	2:C:161:VAL:H	1.72	0.53
1:B:408:VAL:HG12	1:B:409:ALA:H	1.74	0.53
1:B:134:HIS:ND1	1:B:162:GLU:OE2	2.42	0.52
1:A:275:SER:HB3	1:A:278:SER:HB3	1.92	0.52
1:B:340:SER:HA	1:B:375:ARG:HH12	1.75	0.52
1:A:97:ILE:O	1:A:186:TYR:O	2.27	0.52
1:B:381:SER:O	1:B:384:ARG:HA	2.09	0.52
2:C:231:PHE:HD1	2:C:254:ARG:HD2	1.75	0.51
2:D:57:HIS:CG	2:D:262:PRO:HB3	2.46	0.51
1:B:185:LEU:HD11	2:D:271:LYS:HG3	1.92	0.51
3:E:207:LYS:NZ	3:E:226:GLU:OE1	2.43	0.51
1:A:500:ARG:HG2	3:E:308:ASP:OD1	2.10	0.50
1:B:446:ILE:HG23	1:B:496:MET:SD	2.50	0.50
2:D:122:GLU:HA	2:D:128:THR:HG22	1.94	0.50
2:D:247:ASP:OD2	2:D:260:ARG:NH1	2.43	0.50
2:C:85:TRP:CD1	2:C:86:PRO:HD2	2.46	0.50
1:B:252:ILE:CG2	1:B:418:LYS:HB3	2.36	0.50
2:C:231:PHE:HB3	2:C:254:ARG:HE	1.77	0.50
1:B:358:LYS:HE2	1:B:389:CYS:SG	2.51	0.49
2:C:259:VAL:HG12	2:C:302:LEU:HD22	1.94	0.49
2:D:80:LEU:HD12	2:D:112:ASP:OD2	2.13	0.49
2:C:231:PHE:CD1	2:C:254:ARG:HD2	2.47	0.49
3:E:241:THR:HG22	3:E:245:LYS:HE3	1.95	0.49
1:B:361:VAL:HG13	1:B:364:LEU:HD12	1.94	0.48
2:D:102:VAL:HG21	2:D:149:LEU:HD22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ILE:HA	1:A:418:LYS:HD3	1.96	0.48
2:C:137:ILE:HG12	2:C:169:VAL:HG22	1.96	0.48
1:B:105:HIS:HA	1:B:405:LYS:HZ1	1.78	0.48
2:D:105:LEU:HB2	2:D:167:TYR:CE2	2.49	0.48
2:C:233:VAL:HG13	2:C:250:VAL:HG13	1.95	0.48
1:B:413:GLU:HG3	1:B:414:ASP:H	1.79	0.48
3:F:269:MET:O	3:F:273:ILE:HG13	2.13	0.47
1:A:315:VAL:HG21	1:A:329:TYR:HD1	1.79	0.47
2:C:130:GLN:HG3	2:C:177:MET:HG3	1.97	0.47
3:E:315:GLU:N	3:E:316:THR:HA	2.28	0.47
1:B:409:ALA:HB2	1:B:415:ARG:NH2	2.30	0.47
3:F:251:GLY:O	3:F:255:GLN:HG3	2.15	0.47
3:E:206:SER:O	3:E:210:THR:OG1	2.26	0.47
3:F:284:THR:OG1	3:F:313:ARG:NE	2.40	0.46
2:C:143:ASP:OD1	2:C:145:VAL:HG22	2.15	0.46
1:A:272:PRO:C	1:A:274:SER:H	2.24	0.46
1:A:134:HIS:HA	1:A:154:LEU:HD23	1.97	0.46
1:B:124:ARG:HB2	1:B:124:ARG:HH11	1.80	0.46
1:B:361:VAL:HA	1:B:364:LEU:HG	1.96	0.46
1:A:115:LEU:HG	1:A:147:MET:HE2	1.97	0.46
1:B:132:LEU:HD13	1:B:162:GLU:HB3	1.97	0.46
3:F:224:TYR:CE2	3:F:228:LYS:HD2	2.50	0.46
1:B:285:GLY:HA3	1:B:348:SER:O	2.16	0.46
1:B:289:MET:O	1:B:293:VAL:HG23	2.16	0.46
1:A:374:LEU:HD13	1:A:397:ARG:HE	1.80	0.45
1:B:408:VAL:HG12	1:B:409:ALA:N	2.31	0.45
1:A:332:LEU:H	1:A:332:LEU:HD22	1.81	0.45
1:B:382:VAL:CA	1:B:383:PRO:C	2.89	0.45
1:A:208:GLU:HG3	1:A:292:LEU:HD21	1.98	0.45
1:B:472:ILE:HA	1:B:473:ASN:HA	1.79	0.45
3:F:206:SER:O	3:F:210:THR:OG1	2.20	0.45
1:A:347:THR:OG1	1:A:385:ASN:HB2	2.17	0.45
3:F:307:TYR:O	3:F:311:ILE:HG12	2.17	0.45
2:C:289:LYS:HB3	2:C:291:TYR:CE2	2.51	0.45
2:D:221:ARG:HG2	2:D:284:ALA:HB1	1.99	0.45
3:E:269:MET:O	3:E:273:ILE:HG13	2.17	0.45
1:A:227:GLY:O	1:A:228:PHE:C	2.54	0.44
1:A:219:VAL:O	1:A:223:GLN:HG2	2.17	0.44
1:A:225:VAL:HG12	1:A:227:GLY:H	1.82	0.44
1:A:329:TYR:O	1:A:330:ARG:HD2	2.18	0.44
1:B:284:ILE:HG13	1:B:308:VAL:HB	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:56:THR:HG22	2:C:57:HIS:H	1.82	0.44
3:F:274:SER:HB3	3:F:279:GLU:O	2.18	0.44
1:B:409:ALA:HB2	1:B:415:ARG:HH22	1.83	0.44
2:D:110:SER:HB2	2:D:111:PRO:HD2	1.99	0.44
1:A:217:GLN:O	1:A:221:VAL:HG23	2.18	0.44
1:B:187:ASN:O	1:B:190:ALA:HB3	2.18	0.44
2:D:109:VAL:HG13	2:D:167:TYR:CE1	2.49	0.44
3:F:241:THR:HG22	3:F:245:LYS:HE3	2.00	0.44
1:A:212:LEU:HD11	1:A:240:ILE:HG23	2.00	0.43
1:A:473:ASN:HB2	1:A:477:THR:OG1	2.18	0.43
1:A:111:MET:HG3	1:A:173:ILE:HD13	2.00	0.43
1:B:104:ILE:HA	1:B:112:ARG:NH1	2.34	0.43
1:A:516:MET:HE3	1:A:517:HIS:CE1	2.53	0.43
3:E:204:LEU:HD21	3:E:242:GLU:HB3	2.00	0.43
1:A:132:LEU:HD13	1:A:162:GLU:HB3	2.01	0.43
1:A:119:GLU:HA	1:A:122:TRP:CD2	2.54	0.43
2:D:242:ASP:CG	2:D:260:ARG:HH22	2.23	0.43
1:B:346:PHE:HD1	1:B:378:VAL:HB	1.83	0.43
1:A:355:LEU:N	1:A:385:ASN:O	2.38	0.43
1:A:505:ASP:O	1:A:507:ARG:N	2.52	0.43
2:D:221:ARG:HD3	2:D:284:ALA:C	2.44	0.43
2:C:63:GLU:OE1	2:C:243:ARG:NH2	2.36	0.42
2:C:217:GLU:OE1	4:C:401:HOH:O	2.21	0.42
2:C:197:PRO:HB2	2:C:201:ARG:NH1	2.35	0.42
2:D:289:LYS:HB3	2:D:291:TYR:CE2	2.54	0.42
3:F:240:PRO:HB3	3:F:277:GLU:HG3	2.01	0.42
2:C:105:LEU:HG	2:C:107:ARG:H	1.83	0.42
2:D:134:GLN:HE22	2:D:173:ARG:HH21	1.66	0.42
3:F:283:ILE:HB	3:F:313:ARG:NH2	2.35	0.42
1:A:272:PRO:C	1:A:274:SER:N	2.77	0.42
1:B:293:VAL:O	1:B:297:LEU:HB2	2.19	0.42
1:B:105:HIS:HA	1:B:405:LYS:NZ	2.35	0.42
1:B:447:LYS:HD3	3:F:295:THR:HB	2.00	0.42
2:D:133:ILE:HG12	2:D:174:VAL:HG22	2.00	0.42
2:D:142:ASP:OD2	2:D:144:THR:OG1	2.26	0.42
1:B:207:GLY:O	1:B:210:GLN:HG3	2.20	0.42
1:A:361:VAL:HA	1:A:364:LEU:HG	2.01	0.41
1:A:188:LYS:HG2	1:A:434:GLU:CD	2.45	0.41
1:B:271:LEU:HA	1:B:272:PRO:HD2	1.77	0.41
2:C:57:HIS:HB3	2:C:262:PRO:HB3	2.01	0.41
1:B:346:PHE:CD1	1:B:378:VAL:HB	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:SER:OG	1:A:173:ILE:O	2.30	0.41
1:A:275:SER:HB3	1:A:278:SER:CB	2.50	0.41
1:B:119:GLU:HA	1:B:122:TRP:CE2	2.56	0.41
3:E:241:THR:HA	3:E:244:LYS:HE2	2.02	0.41
1:B:206:LEU:HB3	1:B:210:GLN:HB2	2.02	0.41
2:C:247:ASP:OD1	2:C:260:ARG:HD3	2.20	0.41
1:B:168:SER:OG	1:B:173:ILE:O	2.34	0.41
1:B:500:ARG:HD2	1:B:500:ARG:HA	1.97	0.40
1:A:272:PRO:O	1:A:274:SER:N	2.54	0.40
1:A:291:LYS:CE	1:A:314:ARG:HH22	2.33	0.40
1:B:461:LEU:O	1:B:465:MET:HG2	2.22	0.40
2:C:137:ILE:HG23	2:C:167:TYR:HB3	2.03	0.40
2:D:227:VAL:HG11	2:D:259:VAL:HG11	2.02	0.40
1:B:357:LEU:HD23	1:B:360:HIS:CE1	2.55	0.40
2:C:242:ASP:OD1	2:C:260:ARG:NH2	2.38	0.40
1:B:134:HIS:HA	1:B:154:LEU:HD23	2.02	0.40
2:C:219:ILE:HD13	2:C:219:ILE:HA	1.96	0.40
2:D:113:LYS:O	2:D:137:ILE:HG22	2.21	0.40
3:E:284:THR:HG22	3:E:313:ARG:NE	2.33	0.40

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	422/472 (89%)	406 (96%)	14 (3%)	2 (0%)	24	59
1	B	411/472 (87%)	392 (95%)	16 (4%)	3 (1%)	18	52
2	C	248/310 (80%)	241 (97%)	7 (3%)	0	100	100
2	D	247/310 (80%)	241 (98%)	6 (2%)	0	100	100
3	E	118/159 (74%)	115 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	115/159 (72%)	114 (99%)	1 (1%)	0	100	100
All	All	1561/1882 (83%)	1509 (97%)	47 (3%)	5 (0%)	36	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	505	ASP
1	A	506	SER
1	B	203	SER
1	A	187	ASN
1	B	255	GLY

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	363/400 (91%)	352 (97%)	11 (3%)	36	66
1	B	352/400 (88%)	339 (96%)	13 (4%)	30	63
2	C	220/269 (82%)	215 (98%)	5 (2%)	44	70
2	D	224/269 (83%)	214 (96%)	10 (4%)	24	58
3	E	99/129 (77%)	98 (99%)	1 (1%)	68	80
3	F	93/129 (72%)	92 (99%)	1 (1%)	65	79
All	All	1351/1596 (85%)	1310 (97%)	41 (3%)	36	66

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	VAL
1	A	110	GLU
1	A	152	LEU
1	A	250	THR
1	A	278	SER
1	A	344	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	347	THR
1	A	390	VAL
1	A	400	ASN
1	A	407	VAL
1	A	500	ARG
1	B	110	GLU
1	B	152	LEU
1	B	205	VAL
1	B	206	LEU
1	B	252	ILE
1	B	257	VAL
1	B	260	SER
1	B	344	VAL
1	B	359	GLU
1	B	389	CYS
1	B	416	MET
1	B	417	ARG
1	B	501	CYS
2	C	56	THR
2	C	87	LEU
2	C	161	VAL
2	C	177	MET
2	C	220	PHE
2	D	81	THR
2	D	85	TRP
2	D	109	VAL
2	D	113	LYS
2	D	137	ILE
2	D	161	VAL
2	D	177	MET
2	D	203	ILE
2	D	216	MET
2	D	259	VAL
3	E	217	ASN
3	F	208	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	231	ASN
1	A	493	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	517	HIS
1	B	210	GLN
1	B	376	HIS
1	B	385	ASN
1	B	432	GLN
2	C	57	HIS
2	C	215	ASN
2	D	120	GLN
2	D	215	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](#)

There are no ligands in this entry.

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	427/472 (90%)	-0.30	3 (0%) 84 69	2, 12, 45, 90	1 (0%)
1	B	423/472 (89%)	-0.10	6 (1%) 73 54	5, 25, 63, 85	0
2	C	250/310 (80%)	-0.19	2 (0%) 82 67	4, 21, 59, 83	0
2	D	250/310 (80%)	-0.20	1 (0%) 88 79	5, 24, 65, 87	1 (0%)
3	E	119/159 (74%)	-0.14	0 100 100	6, 22, 47, 58	1 (0%)
3	F	117/159 (73%)	0.11	0 100 100	17, 48, 71, 83	0
All	All	1586/1882 (84%)	-0.17	12 (0%) 82 67	2, 21, 64, 90	3 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	108	SER	4.0
2	D	307	GLY	3.3
1	A	502	ASP	3.0
1	A	476	THR	2.9
2	C	142	ASP	2.8
1	B	506	SER	2.5
1	B	224	GLY	2.4
1	B	472	ILE	2.2
1	B	351	SER	2.2
1	B	481	ASP	2.1
1	B	409	ALA	2.1
1	A	414	ASP	2.1

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.