



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:08 PM UTC

PDB ID : 7XOF / pdb_00007xof
Title : Crystal structure of Oryza sativa plastid glycyl-tRNA synthetase
Authors : Yu, Z.; Lu, G.; Li, J.
Deposited on : 2022-05-01
Resolution : 2.56 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

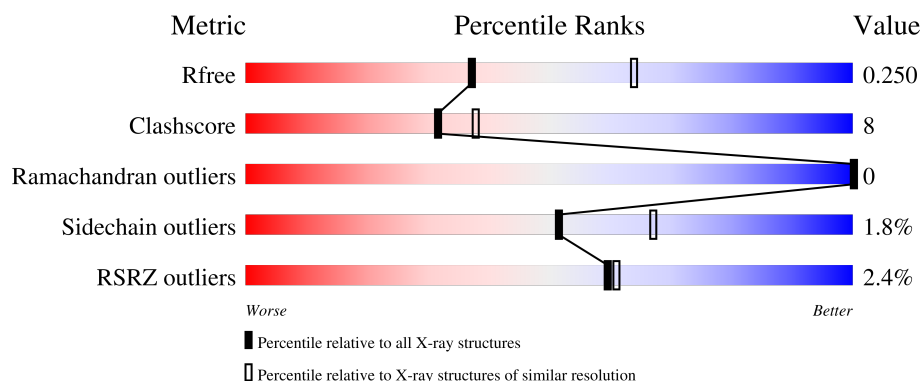
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

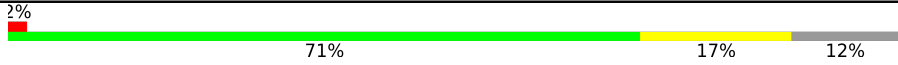
The reported resolution of this entry is 2.56 Å.

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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	1045	
1	B	1045	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14829 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 Glycine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	924	Total	C	N	O	S	0	2	0
			7292	4649	1241	1371	31			
1	B	927	Total	C	N	O	S	0	2	0
			7319	4669	1247	1373	30			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	HIS	-	expression tag	UNP Q0DFB6
A	25	HIS	-	expression tag	UNP Q0DFB6
A	26	HIS	-	expression tag	UNP Q0DFB6
A	27	HIS	-	expression tag	UNP Q0DFB6
A	28	HIS	-	expression tag	UNP Q0DFB6
A	29	HIS	-	expression tag	UNP Q0DFB6
A	30	HIS	-	expression tag	UNP Q0DFB6
A	31	HIS	-	expression tag	UNP Q0DFB6
A	32	GLY	-	expression tag	UNP Q0DFB6
A	33	SER	-	expression tag	UNP Q0DFB6
A	34	SER	-	expression tag	UNP Q0DFB6
A	35	LEU	-	expression tag	UNP Q0DFB6
A	36	GLU	-	expression tag	UNP Q0DFB6
A	37	VAL	-	expression tag	UNP Q0DFB6
A	38	LEU	-	expression tag	UNP Q0DFB6
A	39	PHE	-	expression tag	UNP Q0DFB6
A	40	GLN	-	expression tag	UNP Q0DFB6
A	41	GLY	-	expression tag	UNP Q0DFB6
A	42	PRO	-	expression tag	UNP Q0DFB6
A	481	PRO	LEU	conflict	UNP Q0DFB6
A	967	THR	ALA	conflict	UNP Q0DFB6
A	1040	LYS	ARG	conflict	UNP Q0DFB6
B	24	HIS	-	expression tag	UNP Q0DFB6
B	25	HIS	-	expression tag	UNP Q0DFB6
B	26	HIS	-	expression tag	UNP Q0DFB6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	HIS	-	expression tag	UNP Q0DFB6
B	28	HIS	-	expression tag	UNP Q0DFB6
B	29	HIS	-	expression tag	UNP Q0DFB6
B	30	HIS	-	expression tag	UNP Q0DFB6
B	31	HIS	-	expression tag	UNP Q0DFB6
B	32	GLY	-	expression tag	UNP Q0DFB6
B	33	SER	-	expression tag	UNP Q0DFB6
B	34	SER	-	expression tag	UNP Q0DFB6
B	35	LEU	-	expression tag	UNP Q0DFB6
B	36	GLU	-	expression tag	UNP Q0DFB6
B	37	VAL	-	expression tag	UNP Q0DFB6
B	38	LEU	-	expression tag	UNP Q0DFB6
B	39	PHE	-	expression tag	UNP Q0DFB6
B	40	GLN	-	expression tag	UNP Q0DFB6
B	41	GLY	-	expression tag	UNP Q0DFB6
B	42	PRO	-	expression tag	UNP Q0DFB6
B	481	PRO	LEU	conflict	UNP Q0DFB6
B	967	THR	ALA	conflict	UNP Q0DFB6
B	1040	LYS	ARG	conflict	UNP Q0DFB6

- Molecule 2 is water.

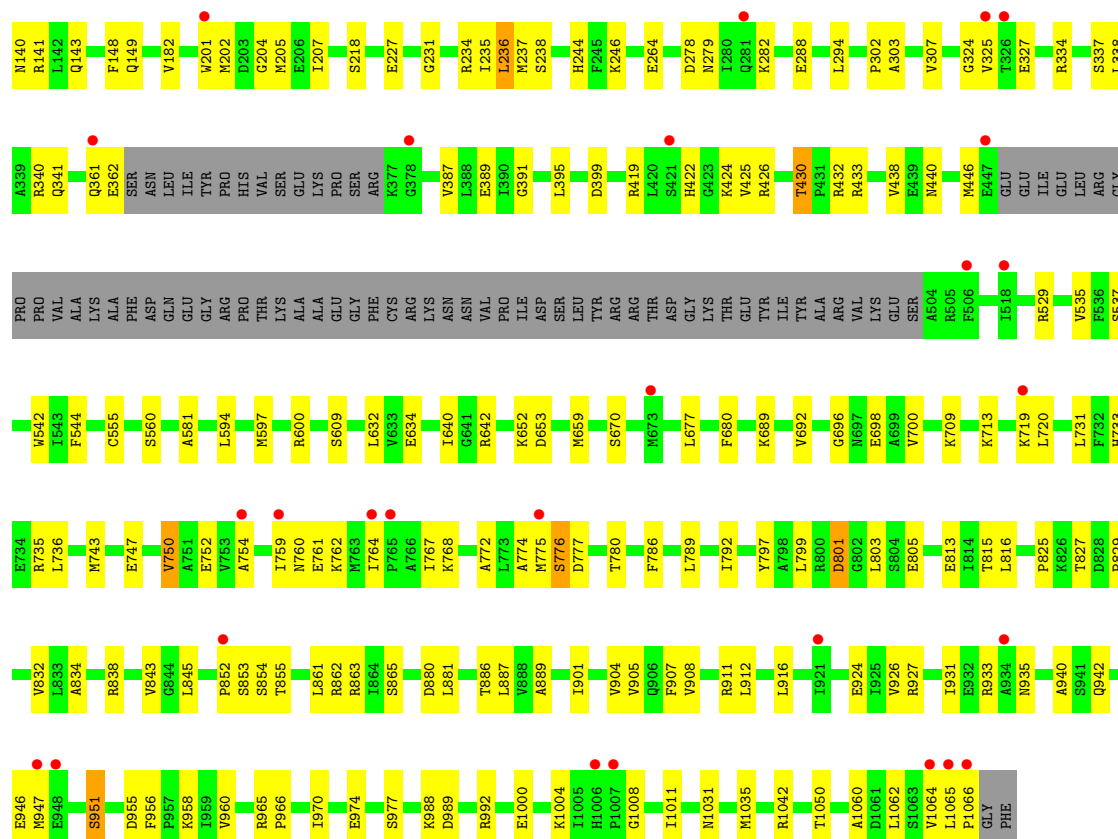
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	128	Total O 128 128	0	0
2	B	90	Total O 90 90	0	0

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

[illegible]

Chain B:

Amino Acid	Percentage
HIS	3%
HIS	70%
HIS	70%
HIS	70%
HIS	70%
HIS	70%
HIS	70%
HIS	70%
HIS	70%
GLY	70%
SER	70%
LEU	70%
LEU	70%
VAL	70%
PHE	70%
GLN	70%
GLY	70%
PRO	70%
ALA	70%
VAL	70%
ALA	70%
SER	70%
ALA	70%
ASP	70%
GLY	70%
ASP	70%
ALA	70%
PRO	70%
SER	70%
PRO	70%
VAL	70%
SER	70%
VAL	70%
SER	70%
ALA	70%
ALA	70%
ALA	70%
THR	70%
LYS	70%
GLY	70%
PRO	70%
SER	70%
SER	70%
SER	70%
SER	70%
S70	18%
V71	18%
L72	18%
L81	11%
R112	11%
W119	11%
Y123	11%
R134	11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.13Å 130.94Å 123.39Å 90.00° 101.88° 90.00°	Depositor
Resolution (Å)	65.47 – 2.56 65.47 – 2.56	Depositor EDS
% Data completeness (in resolution range)	92.5 (65.47-2.56) 92.5 (65.47-2.56)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.210 , 0.250 0.210 , 0.250	Depositor DCC
R_{free} test set	3386 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14829	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.25	1/7438 (0.0%)	0.44	0/10086
1	B	0.24	0/7465	0.44	0/10121
All	All	0.25	1/14903 (0.0%)	0.44	0/20207

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	764	ILE	CA-CB	-6.26	1.50	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7292	0	7245	107	0
1	B	7319	0	7312	129	0
2	A	128	0	0	2	0
2	B	90	0	0	3	0
All	All	14829	0	14557	236	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 8.

All (236) 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:659:MET:HE2	1:A:680:PHE:HB3	1.59	0.83
1:A:414:ILE:HG12	1:A:518:ILE:HD11	1.66	0.78
1:A:625:LEU:HD22	1:A:660:GLN:HG2	1.64	0.78
1:B:288:GLU:HG3	1:B:338:LEU:HD11	1.63	0.78
1:B:430:THR:HB	1:B:433:ARG:HG2	1.73	0.70
1:A:816:LEU:HB2	1:A:825:PRO:HD3	1.73	0.70
1:B:886:THR:HG22	1:B:901:ILE:HD13	1.73	0.69
1:B:140:ASN:HD22	1:B:237:MET:HE1	1.57	0.69
1:B:927:ARG:O	1:B:931:ILE:HG13	1.93	0.68
1:B:424:LYS:HE2	1:B:426:ARG:HG3	1.75	0.68
1:B:955:ASP:HA	1:B:958:LYS:HE2	1.76	0.68
1:B:659:MET:HE2	1:B:680:PHE:HB3	1.75	0.67
1:B:279:ASN:HA	1:B:282:LYS:HE2	1.77	0.67
1:A:956:PHE:O	1:A:960:VAL:HG23	1.95	0.67
1:A:294:LEU:HD13	1:A:302:PRO:HB2	1.77	0.66
1:A:838:ARG:HG2	1:A:864:ILE:HG23	1.77	0.66
1:B:294:LEU:HD13	1:B:302:PRO:HB2	1.77	0.66
1:B:430:THR:HG22	1:B:432:ARG:H	1.62	0.65
1:A:673:MET:HG3	1:A:675:ASN:H	1.61	0.65
1:B:816:LEU:HB2	1:B:825:PRO:HD3	1.79	0.64
1:B:813:GLU:HA	1:B:816:LEU:HD12	1.78	0.64
1:A:205:MET:HE1	1:A:238:SER:HB3	1.80	0.63
1:B:134:ARG:HG3	1:B:141:ARG:HB3	1.80	0.63
1:B:642:ARG:O	1:B:698:GLU:HG2	1.99	0.63
1:B:743:MET:CE	1:B:775:MET:HB2	2.29	0.63
1:B:863:ARG:NH2	2:B:1102:HOH:O	2.33	0.61
1:A:880:ASP:OD1	1:A:883:LYS:HG3	2.01	0.61
1:A:81:LEU:HG	1:A:170:LEU:HD21	1.81	0.61
1:A:966:PRO:HB3	1:A:1049:LEU:HD22	1.82	0.60
1:B:218:SER:HB2	1:B:340:ARG:HG3	1.82	0.60
1:A:340:ARG:HG2	1:A:344[B]:GLN:NE2	2.16	0.60
1:B:1062:LEU:HD12	1:B:1065:LEU:HD12	1.83	0.60
1:A:964:SER:O	1:A:968:ARG:HG3	2.01	0.60
1:B:324:GLY:N	1:B:327:GLU:OE1	2.30	0.60
1:A:424:LYS:NZ	2:A:1104:HOH:O	2.33	0.60
1:A:345:LEU:HA	1:A:348:LYS:HE2	1.82	0.59
1:B:430:THR:HG23	1:B:634:GLU:HG2	1.84	0.59
1:B:696:GLY:O	1:B:700:VAL:HG23	2.03	0.59
1:A:880:ASP:CG	1:A:883:LYS:HG3	2.27	0.59
1:A:886:THR:O	1:A:890:GLU:HG3	2.03	0.59
1:A:1063:SER:HA	1:A:1068:PHE:CG	2.37	0.59
1:B:907:PHE:O	1:B:911:ARG:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:GLU:O	1:A:1030:THR:HG23	2.02	0.58
1:B:149:GLN:NE2	1:B:227:GLU:OE2	2.35	0.58
1:B:659:MET:CE	1:B:680:PHE:HB3	2.33	0.58
1:B:143:GLN:N	1:B:264:GLU:OE2	2.32	0.57
1:B:743:MET:HE3	1:B:774:ALA:O	2.03	0.57
1:B:288:GLU:OE1	1:B:334:ARG:NH2	2.34	0.57
1:A:626:VAL:O	1:A:630:ILE:HG13	2.04	0.57
1:B:689:LYS:HD3	1:B:692:VAL:HG23	1.86	0.57
1:A:418:ARG:O	1:A:445:GLN:HG2	2.05	0.56
1:A:143:GLN:HG3	1:A:264:GLU:OE2	2.04	0.56
1:A:305:ASP:OD2	1:A:309:LYS:NZ	2.37	0.56
1:B:777:ASP:HA	1:B:780:THR:HG23	1.88	0.56
1:A:965:ARG:HD3	1:A:1029:PHE:CE2	2.40	0.56
1:B:1035:MET:HE3	1:B:1042:ARG:HD3	1.88	0.56
1:B:143:GLN:HG3	1:B:264:GLU:OE2	2.06	0.55
1:B:709:LYS:HE2	1:B:713:LYS:NZ	2.20	0.55
1:B:947:MET:O	1:B:951:SER:OG	2.25	0.55
1:B:709:LYS:HE2	1:B:713:LYS:HZ1	1.72	0.55
1:A:600:ARG:O	1:A:604:ILE:HG13	2.06	0.55
1:B:956:PHE:O	1:B:960:VAL:HG23	2.07	0.55
1:A:340:ARG:HE	1:A:344[B]:GLN:HE22	1.52	0.54
1:A:389:GLU:HB3	1:A:544:PHE:HB3	1.89	0.54
1:A:964:SER:HA	1:A:1068:PHE:CZ	2.42	0.54
1:B:933:ARG:NH2	1:B:1008:GLY:H	2.05	0.54
1:A:433:ARG:NH2	1:A:566:CYS:O	2.40	0.54
1:A:346:TRP:CZ2	1:A:350:ARG:HD3	2.43	0.54
1:A:750:VAL:HG22	1:A:832:VAL:HG12	1.88	0.54
1:B:852:PRO:HG3	1:B:861:LEU:HB2	1.89	0.54
1:B:760:ASN:OD1	1:B:762:LYS:HG2	2.08	0.54
1:B:865:SER:OG	1:B:911:ARG:HG3	2.08	0.54
1:A:867:GLY:O	1:A:871:ILE:HG13	2.07	0.54
1:A:968:ARG:HA	1:A:971:ARG:HG2	1.90	0.53
1:B:843:VAL:HG11	1:B:889:ALA:HA	1.89	0.53
1:A:1005:ILE:CD1	1:A:1014:PHE:HA	2.39	0.53
1:A:325:VAL:HG22	1:A:731:LEU:HB2	1.91	0.53
1:A:401:ILE:CD1	1:A:597:MET:HE1	2.39	0.53
1:B:970:ILE:HD13	1:B:1050:THR:HA	1.91	0.53
1:B:278:ASP:O	1:B:282:LYS:HG3	2.09	0.53
1:B:845:LEU:HD12	1:B:861:LEU:HD21	1.90	0.53
1:A:956:PHE:HB3	1:A:957:PRO:HD3	1.90	0.53
1:B:325:VAL:HG12	1:B:731:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:ASP:O	1:A:959:ILE:HD12	2.10	0.52
1:B:947:MET:HE1	1:B:1060:ALA:CB	2.38	0.52
1:A:651:PRO:HB3	1:A:796:HIS:CE1	2.45	0.52
1:B:761:GLU:O	1:B:761:GLU:HG2	2.10	0.52
1:B:750:VAL:HG22	1:B:832:VAL:HG12	1.91	0.52
1:B:399:ASP:OD2	1:B:537:SER:OG	2.22	0.51
1:A:361:GLN:NE2	2:A:1116:HOH:O	2.44	0.51
1:B:419:ARG:HB3	1:B:446:MET:H	1.76	0.51
1:A:650:LEU:HD21	1:A:709:LYS:HA	1.93	0.50
1:B:1004:LYS:NZ	2:B:1104:HOH:O	2.43	0.50
1:A:942:GLN:O	1:A:946:GLU:HG2	2.10	0.50
1:A:622:PRO:O	1:A:626:VAL:HG23	2.12	0.50
1:A:947:MET:HE2	1:A:1065:LEU:HD11	1.94	0.50
1:A:391:GLY:HA3	1:A:542:TRP:CE2	2.48	0.49
1:A:1018:SER:HA	1:A:1021:LEU:HD12	1.93	0.49
1:B:752:GLU:HB3	1:B:887:LEU:HD11	1.93	0.49
1:A:933:ARG:HH21	1:A:1008:GLY:H	1.59	0.49
1:A:1001:VAL:HG13	1:A:1017:ALA:HB1	1.94	0.49
1:B:912:LEU:O	1:B:916:LEU:HG	2.12	0.49
1:A:607:ASP:HB2	1:A:638:PRO:HG2	1.95	0.49
1:B:422:HIS:HA	1:B:440:ASN:O	2.12	0.49
1:A:789:LEU:HB3	1:A:793:MET:HG2	1.95	0.49
1:A:143:GLN:N	1:A:264:GLU:OE2	2.46	0.48
1:A:799:LEU:HD21	1:A:805:GLU:HG3	1.95	0.48
1:B:933:ARG:HH21	1:B:1008:GLY:H	1.62	0.48
1:B:1062:LEU:HD22	1:B:1062:LEU:H	1.79	0.48
1:B:754:ALA:HB1	1:B:759:ILE:HD11	1.94	0.48
1:B:670:SER:HB2	1:B:677:LEU:HD21	1.95	0.48
1:A:398:HIS:CD2	1:A:398:HIS:H	2.31	0.48
1:B:207:ILE:HB	1:B:235:ILE:HG12	1.95	0.48
1:B:244:HIS:ND1	1:B:246:LYS:HG2	2.28	0.48
1:B:555:CYS:SG	2:B:1186:HOH:O	2.61	0.48
1:B:425:VAL:HG22	1:B:438:VAL:HG13	1.94	0.48
1:B:764:ILE:HA	1:B:767:ILE:HD12	1.95	0.48
1:A:650:LEU:HB2	1:A:655:LEU:HD21	1.96	0.48
1:B:71:VAL:HG12	1:B:72:LEU:H	1.79	0.48
1:A:410:SER:HB2	1:A:518:ILE:HG23	1.96	0.47
1:B:140:ASN:ND2	1:B:237:MET:HE1	2.26	0.47
1:B:813:GLU:OE1	1:B:827:THR:HB	2.13	0.47
1:A:716:THR:HB	1:A:800:ARG:CZ	2.44	0.47
1:A:881:LEU:HD21	1:A:908:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:924:GLU:HB3	1:B:1064:VAL:HG12	1.95	0.47
1:B:752:GLU:HB2	1:B:887:LEU:HD21	1.96	0.47
1:B:989:ASP:O	1:B:992:ARG:HG3	2.15	0.47
1:A:584:TYR:CZ	1:A:588:LEU:HD11	2.50	0.47
1:B:123:TYR:CZ	1:B:149:GLN:HG2	2.50	0.46
1:B:653:ASP:HB3	1:B:792:ILE:HD13	1.97	0.46
1:A:206:GLU:HB2	1:A:234:ARG:HH12	1.80	0.46
1:A:395:LEU:HD23	1:A:538:ARG:HB2	1.97	0.46
1:B:904:VAL:O	1:B:908:VAL:HG23	2.15	0.46
1:B:956:PHE:CZ	1:B:1065:LEU:HD13	2.51	0.46
1:A:346:TRP:O	1:A:350:ARG:HG2	2.15	0.46
1:B:853:SER:OG	1:B:854:SER:N	2.47	0.46
1:B:395:LEU:HD22	1:B:537:SER:HB3	1.97	0.46
1:B:389:GLU:HB3	1:B:544:PHE:HB3	1.98	0.46
1:B:709:LYS:HG2	1:B:713:LYS:HZ2	1.80	0.46
1:A:1006:HIS:O	1:A:1009:VAL:HG13	2.16	0.45
1:B:942:GLN:O	1:B:946:GLU:HG3	2.16	0.45
1:A:716:THR:HB	1:A:800:ARG:NH2	2.31	0.45
1:B:205:MET:HE2	1:B:234:ARG:HG2	1.99	0.45
1:B:430:THR:CG2	1:B:634:GLU:HG2	2.44	0.45
1:A:840:ASP:HA	1:A:888:VAL:HG11	1.98	0.45
1:A:967:THR:OG1	1:A:1053:ALA:HB1	2.17	0.45
1:B:337:SER:O	1:B:341:GLN:HG3	2.16	0.45
1:B:733:HIS:HB3	1:B:736:LEU:HB2	1.98	0.45
1:A:135:TYR:OH	1:A:273:GLU:OE2	2.24	0.45
1:B:391:GLY:HA3	1:B:542:TRP:CE2	2.51	0.45
1:A:659:MET:HE2	1:A:680:PHE:CB	2.38	0.45
1:B:880:ASP:OD1	1:B:935:ASN:ND2	2.38	0.45
1:B:202:MET:HB2	1:B:207:ILE:HD13	1.99	0.45
1:B:432:ARG:HD3	1:B:634:GLU:OE1	2.17	0.45
1:A:994:LEU:HD23	1:A:1048:LEU:HD21	2.00	0.44
1:B:965:ARG:HB3	1:B:966:PRO:HD3	1.99	0.44
1:A:927:ARG:O	1:A:931:ILE:HG13	2.17	0.44
1:A:85:TRP:O	1:A:90:CYS:HB2	2.16	0.44
1:B:863:ARG:HD3	1:B:863:ARG:HA	1.72	0.44
1:B:834:ALA:O	1:B:838:ARG:HG3	2.17	0.44
1:B:1035:MET:HA	1:B:1042:ARG:HG3	1.98	0.44
1:B:947:MET:HE2	1:B:1011:ILE:HD12	2.00	0.44
1:A:431:PRO:HG3	1:A:631:ASN:O	2.18	0.43
1:A:880:ASP:CG	1:A:935:ASN:HD21	2.26	0.43
1:B:325:VAL:CG1	1:B:731:LEU:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:MET:HG2	1:B:600:ARG:NH2	2.33	0.43
1:B:720:LEU:HD11	1:B:776:SER:HB2	2.00	0.43
1:B:752:GLU:CB	1:B:887:LEU:HD11	2.48	0.43
1:B:764:ILE:O	1:B:768:LYS:HG3	2.19	0.43
1:A:956:PHE:HZ	1:A:1065:LEU:HD13	1.83	0.43
1:A:196:LEU:HD12	1:A:528:MET:HB3	1.99	0.43
1:A:93:MET:HB2	1:A:123:TYR:HB3	2.01	0.43
1:A:414:ILE:O	1:A:418:ARG:HB2	2.19	0.43
1:B:1065:LEU:CD2	1:B:1066:PRO:HD2	2.49	0.43
1:A:153:LYS:HE2	1:A:223:PRO:HD2	2.00	0.43
1:A:172:ILE:HG12	1:A:239:LEU:HD21	2.00	0.43
1:A:565:SER:HB3	1:A:576:PHE:CZ	2.54	0.43
1:A:586:HIS:NE2	1:A:590:LYS:HD2	2.34	0.42
1:A:969:ILE:O	1:A:973:LYS:HD3	2.19	0.42
1:B:182:VAL:HG22	1:B:632:LEU:HD22	2.01	0.42
1:B:361:GLN:O	1:B:362:GLU:HB3	2.19	0.42
1:B:387:VAL:HG23	1:B:581:ALA:HB1	2.01	0.42
1:A:391:GLY:HA3	1:A:542:TRP:CD2	2.54	0.42
1:A:865:SER:OG	1:A:911:ARG:HG3	2.19	0.42
1:B:1000:GLU:OE2	1:B:1004:LYS:HE3	2.19	0.42
1:B:652:LYS:HG3	1:B:653:ASP:N	2.34	0.42
1:B:797:TYR:O	1:B:801:ASP:CG	2.62	0.42
1:A:400:VAL:O	1:A:404:THR:HG23	2.20	0.42
1:B:303:ALA:O	1:B:307:VAL:HG23	2.20	0.42
1:B:719:LYS:HD3	1:B:719:LYS:HA	1.62	0.42
1:A:505:ARG:NH2	1:A:510:VAL:HG12	2.34	0.42
1:A:998:TYR:CZ	1:A:1051:LYS:HB3	2.55	0.42
1:A:1023:GLN:NE2	1:A:1027:ASP:OD1	2.51	0.42
1:A:425:VAL:HG22	1:A:438:VAL:HG13	2.02	0.42
1:A:1065:LEU:HD23	1:A:1065:LEU:HA	1.83	0.42
1:B:767:ILE:HG12	1:B:829:PRO:HB3	2.02	0.42
1:B:1000:GLU:O	1:B:1004:LYS:HG3	2.20	0.42
1:A:197:GLY:O	1:A:538:ARG:NH2	2.50	0.42
1:A:956:PHE:CZ	1:A:1065:LEU:HD13	2.55	0.42
1:A:92:VAL:C	1:A:93:MET:HE2	2.44	0.42
1:A:670:SER:HB3	1:A:673:MET:HG2	2.02	0.42
1:B:81:LEU:HB3	1:B:148:PHE:CE2	2.54	0.42
1:B:204:GLY:O	1:B:700:VAL:HG11	2.19	0.42
1:A:789:LEU:HD23	1:A:789:LEU:HA	1.92	0.42
1:A:73:THR:OG1	1:A:76:GLN:HG3	2.19	0.42
1:B:236:LEU:HD13	1:B:236:LEU:HA	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:GLU:HA	1:B:764:ILE:CD1	2.50	0.42
1:B:786:PHE:HB2	1:B:789:LEU:HD12	2.01	0.42
1:B:947:MET:HE1	1:B:1060:ALA:HB2	2.02	0.42
1:A:643:TYR:CZ	1:A:678:PRO:HA	2.55	0.41
1:A:103:GLY:HA2	1:A:125:GLU:HG2	2.03	0.41
1:A:666:PHE:HB2	1:A:681:ILE:HB	2.03	0.41
1:B:361:GLN:OE1	1:B:362:GLU:N	2.53	0.41
1:B:761:GLU:HA	1:B:764:ILE:HD13	2.01	0.41
1:B:112:ARG:HG3	1:B:119:TRP:CZ2	2.55	0.41
1:B:901:ILE:O	1:B:905:VAL:HG23	2.20	0.41
1:A:101:GLY:O	1:A:127:SER:HB3	2.21	0.41
1:B:747:GLU:OE2	1:B:772:ALA:HA	2.20	0.41
1:A:955:ASP:HA	1:A:958:LYS:HE3	2.03	0.41
1:A:133:SER:HB3	1:A:268:SER:HA	2.02	0.41
1:A:594:LEU:HD22	1:A:599:GLU:HG2	2.02	0.41
1:B:760:ASN:C	1:B:762:LYS:H	2.27	0.41
1:B:799:LEU:HD21	1:B:805:GLU:HA	2.03	0.41
1:A:380:VAL:HB	1:A:381:GLY:H	1.61	0.41
1:B:231:GLY:O	1:B:235:ILE:HG13	2.21	0.41
1:A:1038:ASP:HB3	1:A:1041:VAL:HB	2.03	0.41
1:B:529:ARG:HG3	1:B:535:VAL:HG12	2.03	0.41
1:B:594:LEU:O	1:B:600:ARG:HD3	2.21	0.41
1:B:803:LEU:HD23	1:B:803:LEU:HA	1.97	0.41
1:B:933:ARG:O	1:B:940[A]:ALA:HB2	2.21	0.41
1:B:933:ARG:O	1:B:940[B]:ALA:HB2	2.21	0.41
1:A:546:LEU:HD12	1:A:546:LEU:HA	1.92	0.40
1:B:862:ARG:HG2	1:B:911:ARG:NE	2.36	0.40
1:A:1001:VAL:HG11	1:A:1021:LEU:HD11	2.02	0.40
1:B:201:TRP:HA	1:B:205:MET:O	2.21	0.40
1:B:988:LYS:HE3	1:B:1031:ASN:O	2.21	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	918/1045 (88%)	897 (98%)	21 (2%)	0	100	100
1	B	923/1045 (88%)	901 (98%)	22 (2%)	0	100	100
All	All	1841/2090 (88%)	1798 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	790/898 (88%)	778 (98%)	12 (2%)	57	71
1	B	795/898 (88%)	778 (98%)	17 (2%)	47	63
All	All	1585/1796 (88%)	1556 (98%)	29 (2%)	51	67

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	SER
1	A	433	ARG
1	A	534	ILE
1	A	572	SER
1	A	623	ASP
1	A	646	SER
1	A	713	LYS
1	A	749	THR
1	A	750	VAL
1	A	782	ILE
1	A	827	THR
1	A	855	THR
1	B	236	LEU
1	B	238	SER
1	B	430	THR

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Mol	Chain	Res	Type
1	B	560	SER
1	B	609	SER
1	B	640	ILE
1	B	735	ARG
1	B	750	VAL
1	B	776	SER
1	B	801	ASP
1	B	815	THR
1	B	855	THR
1	B	881	LEU
1	B	926	VAL
1	B	951	SER
1	B	974	GLU
1	B	977	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	165	HIS
1	A	341	GLN
1	A	398	HIS
1	A	413	GLN
1	A	564	GLN
1	A	663	GLN
1	A	781	ASN
1	A	806	GLN
1	A	856	ASN
1	A	870	GLN
1	A	878	ASN
1	A	1023	GLN
1	B	120	ASN
1	B	140	ASN
1	B	165	HIS
1	B	177	HIS
1	B	341	GLN
1	B	781	ASN
1	B	892	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

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	924/1045 (88%)	0.28	17 (1%) 67 69	26, 50, 74, 92	2 (0%)
1	B	927/1045 (88%)	0.41	27 (2%) 53 55	31, 54, 75, 92	2 (0%)
All	All	1851/2090 (88%)	0.35	44 (2%) 59 61	26, 52, 75, 92	4 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	VAL	4.5
1	A	980	GLU	4.4
1	B	1066	PRO	3.8
1	B	326	THR	3.6
1	A	1068	PHE	3.5
1	A	979	LEU	3.3
1	B	764	ILE	3.3
1	A	961	GLU	3.2
1	B	378	GLY	3.1
1	B	947	MET	3.1
1	B	934	ALA	3.0
1	A	506	PHE	3.0
1	B	673	MET	2.9
1	A	944	ALA	2.9
1	B	759	ILE	2.9
1	B	1065	LEU	2.8
1	A	503	SER	2.7
1	A	924	GLU	2.7
1	A	414	ILE	2.6
1	B	1007	PRO	2.5
1	B	775	MET	2.5
1	B	506	PHE	2.4
1	B	447	GLU	2.4
1	B	421	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	852	PRO	2.3
1	A	1066	PRO	2.3
1	B	325	VAL	2.3
1	B	948	GLU	2.3
1	B	281	GLN	2.3
1	A	894	ILE	2.3
1	A	637	MET	2.3
1	B	1006	HIS	2.2
1	A	1030	THR	2.2
1	B	1064	VAL	2.1
1	B	754	ALA	2.1
1	B	852	PRO	2.1
1	A	974	GLU	2.1
1	B	765	PRO	2.1
1	B	201	TRP	2.1
1	B	921	ILE	2.1
1	B	361	GLN	2.0
1	A	362	GLU	2.0
1	B	518	ILE	2.0
1	B	719	LYS	2.0

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.