Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:29 PM JST

PDB ID	:	7XOF
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:

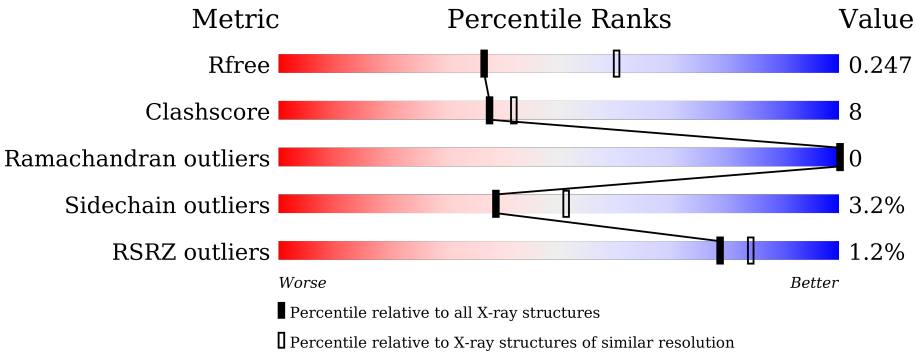
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 <=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	% 70% 18% 12%
1	B	1045	% 70% 17% • 11%

2 Entry composition (i)

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.

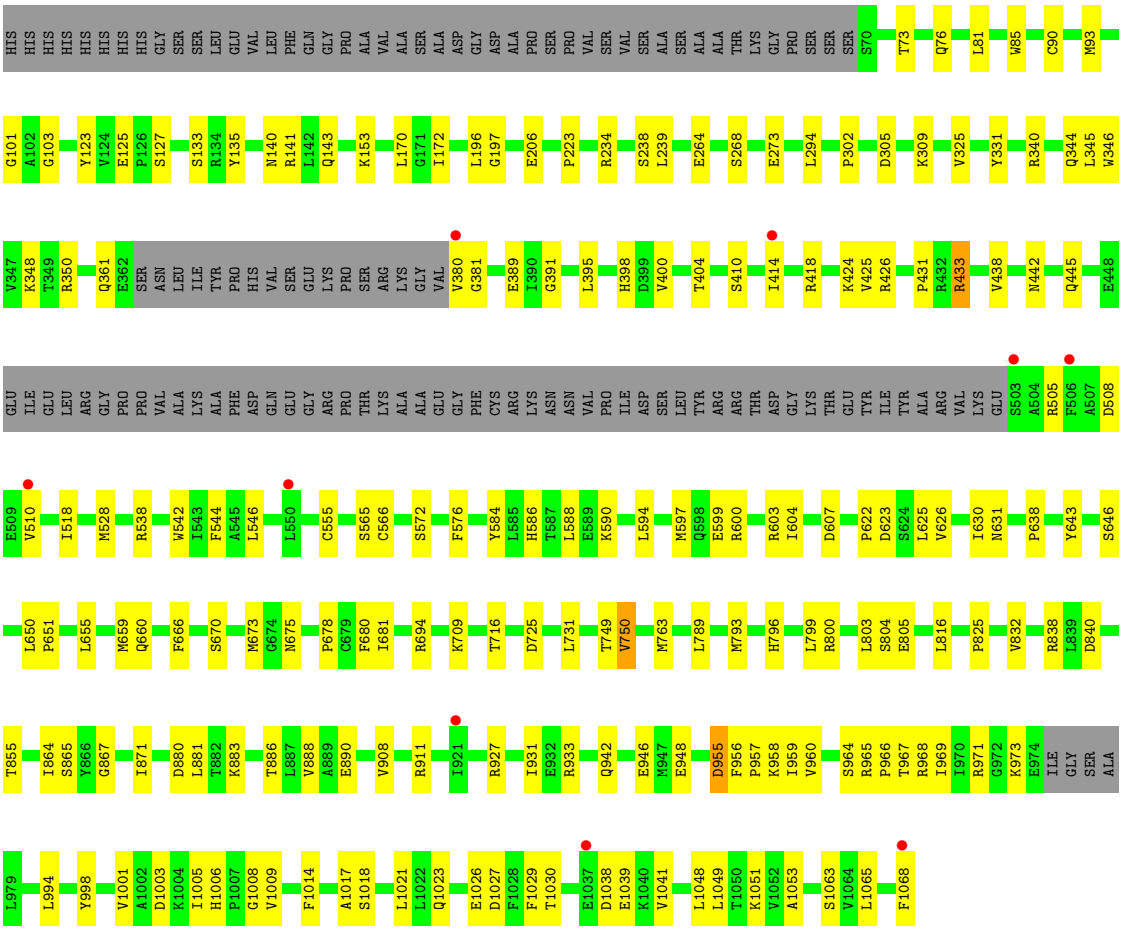
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	128	Total O 128 128	0	0
2	B	90	Total O 90 90	0	0

3 Residue-property plots (i)

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.

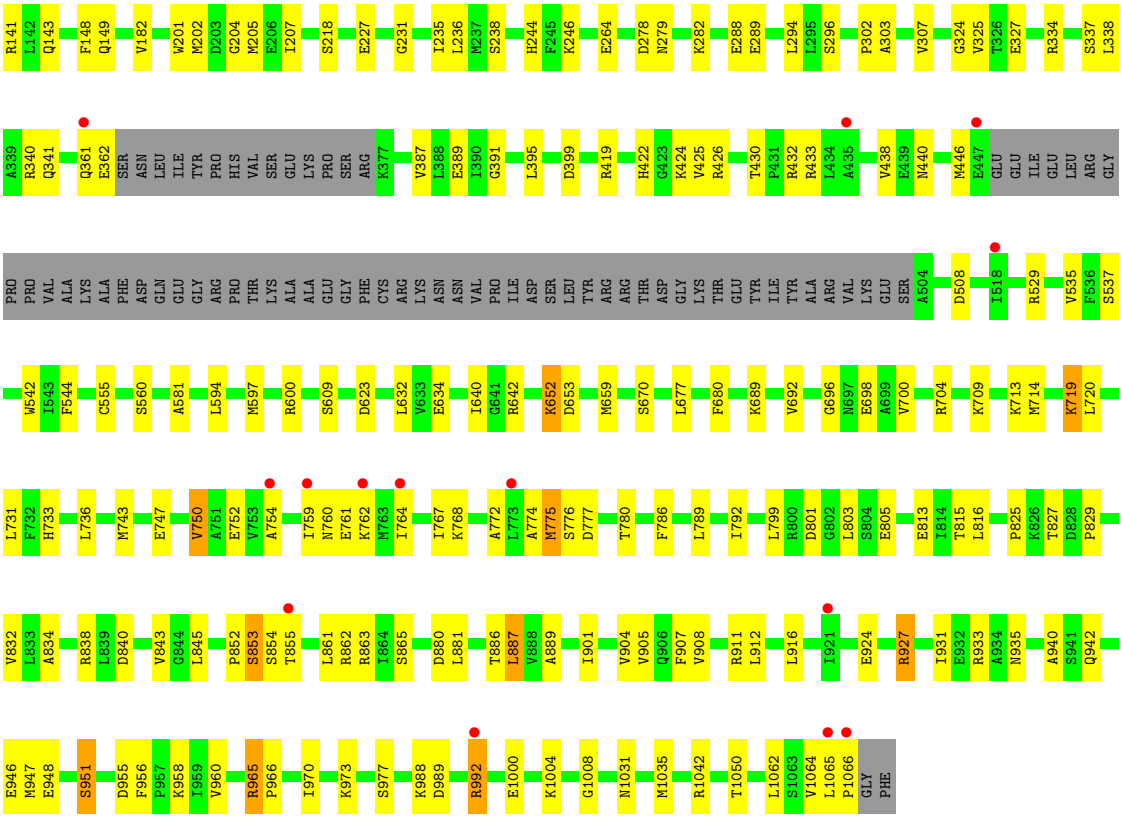
• Molecule 1: Glycine–tRNA ligase

Chain A:



• Molecule 1: Glycine–tRNA ligase

Chain B:


R141 L142 Q143 F148 Q149 V182 W201 M202 D203 G204 M205 E206 I207 S218 E227 G231 I235 L236 M237 S238 H244 F245 K246 E264 D278 N279 K282 E288 E289 L294 L295 S296 P302 A303 V307 G324 V325 T326 E327 R334 S337 L338
A339 R340 Q341 Q361 E362 SER ASN LEU ILE TYR PRO HIS VAL SER GLU LYS PRO SER ARG K377 V387 L388 E389 I390 G391 L395 D399 R419 H422 G423 K424 V425 R426 T430 P431 R432 R433 L434 A435 V438 E439 N440 M446 E447 GLU GLU ILE GLU LEU ARG GLY
PRO PRO VAL ALA LYS ALA PHE ASP GLN GLU GLY ARG PRO THR LYS ALA ALA GLU GLY PHE CYS ARG LYS ASN ASN VAL PRO ILE ASP SER LEU TYR ARG ARG THR ASP GLY LYS THR GLU TYR ILE TYR ALA ARG VAL LYS GLU SER A504 D508 I518 R529 V535 F536 S537
W542 I543 F544 C555 S560 A581 L594 M597 R600 S609 D623 L632 V633 E634 I640 G641 R642 K652 D653 M659 S670 L677 F680 K689 V692 G696 N697 E698 A699 V700 R704 K709 K713 M714 K719 L720
L731 F732 H733 L736 M743 E747 V750 A751 E752 V753 A754 I759 N760 E761 K762 M763 I764 I767 K768 A772 L773 A774 M775 S776 D777 T780 F786 L789 I792 L799 R800 D801 G802 L803 S804 E805 E813 I814 T815 L816 P825 K826 T827 D828 P829
V832 L833 A834 R838 L839 D840 V843 G844 L845 P852 S853 S854 T855 L861 R862 R863 I864 S865 D880 L881 T886 L887 V888 A889 I901 V904 V905 Q906 F907 V908 R911 L912 L916 I921 E924 R927 I931 E932 R933 A934 N935 A940 S941 Q942
E946 M947 E948 S951 D955 F956 P957 K958 I959 V960 R965 P966 I970 K973 S977 K988 D989 R992 E1000 K1004 G1008 N1031 M1035 R1042 T1050 L1062 S1063 V1064 L1065 P1066 GLY PHE

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.04 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.210 , 0.250 0.208 , 0.247	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)	0.34 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.31	0/7438	0.54	0/10086
1	B	0.31	1/7465 (0.0%)	0.54	1/10121 (0.0%)
All	All	0.31	1/14903 (0.0%)	0.54	1/20207 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	719	LYS	CD-CE	5.12	1.64	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	775	MET	CG-SD-CE	5.68	109.29	100.20

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	7292	0	7245	104	0
1	B	7319	0	7312	120	0
2	A	128	0	0	2	0
2	B	90	0	0	2	0
All	All	14829	0	14557	224	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 (224) 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: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: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: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: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:659:MET:HE2	1:B:680:PHE:HB3	1.82	0.62
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:PHE:O	1:B:911:ARG:HG2	2.02	0.59
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: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:A:643:TYR:CE1	1:A:659:MET:HE1	2.40	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: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:A:880:ASP:CG	1:A:883:LYS:HG3	2.27	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: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: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: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: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:391:GLY:HA3	1:A:542:TRP:CE2	2.48	0.49
1:A:659:MET:CE	1:A:680:PHE:HB3	2.42	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: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
1:B:924:GLU:HB3	1:B:1064:VAL:HG12	1.95	0.47
1:B:743:MET:HE3	1:B:774:ALA:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:TYR:CZ	1:A:588:LEU:HD11	2.50	0.47
1:B:743:MET:HE3	1:B:775:MET:HB2	1.95	0.46
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: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:B:399:ASP:OD2	1:B:537:SER:OG	2.22	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:A:431:PRO:HG3	1:A:631:ASN:O	2.18	0.43
1:B:325:VAL:CG1	1:B:731:LEU:HB2	2.49	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LEU:HD12	1:A:528:MET:HB3	1.99	0.43
1:A:659:MET:HE3	1:A:680:PHE:HB3	2.01	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: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:597:MET:HB2	1:A:597:MET:HE2	1.76	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 (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	918/1045 (88%)	897 (98%)	21 (2%)	0	100	100
1	B	923/1045 (88%)	901 (98%)	22 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1841/2090 (88%)	1798 (98%)	43 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	790/898 (88%)	765 (97%)	25 (3%)	39 51
1	B	795/898 (88%)	768 (97%)	27 (3%)	37 49
All	All	1585/1796 (88%)	1533 (97%)	52 (3%)	39 50

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	141	ARG
1	A	238	SER
1	A	331	TYR
1	A	426	ARG
1	A	433	ARG
1	A	442	ASN
1	A	508	ASP
1	A	555	CYS
1	A	572	SER
1	A	603	ARG
1	A	623	ASP
1	A	646	SER
1	A	694	ARG
1	A	725	ASP
1	A	749	THR
1	A	750	VAL
1	A	763	MET
1	A	803	LEU
1	A	804	SER

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Mol	Chain	Res	Type
1	A	855	THR
1	A	948	GLU
1	A	955	ASP
1	A	1003	ASP
1	A	1039	GLU
1	B	238	SER
1	B	289	GLU
1	B	296	SER
1	B	508[A]	ASP
1	B	508[B]	ASP
1	B	560	SER
1	B	609	SER
1	B	623	ASP
1	B	640	ILE
1	B	652	LYS
1	B	704	ARG
1	B	714	MET
1	B	750	VAL
1	B	801	ASP
1	B	815	THR
1	B	840	ASP
1	B	853	SER
1	B	855	THR
1	B	881	LEU
1	B	887	LEU
1	B	927	ARG
1	B	948	GLU
1	B	951	SER
1	B	965	ARG
1	B	973	LYS
1	B	977	SER
1	B	992	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	82	GLN
1	A	398	HIS
1	A	1023	GLN
1	B	140	ASN
1	B	177	HIS

5.3.3 RNA

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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%)	0.20	9 (0%) 82 87	34, 50, 74, 92	0
1	B	927/1045 (88%)	0.18	14 (1%) 73 80	34, 54, 75, 92	0
All	All	1851/2090 (88%)	0.19	23 (1%) 79 84	34, 52, 75, 92	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	SER	5.0
1	A	1068	PHE	3.9
1	B	518	ILE	3.4
1	B	764	ILE	3.1
1	A	1037	GLU	3.0
1	A	921	ILE	3.0
1	A	380	VAL	2.8
1	B	992	ARG	2.7
1	B	759	ILE	2.7
1	A	550	LEU	2.5
1	B	921	ILE	2.5
1	B	855	THR	2.4
1	A	510	VAL	2.3
1	A	506	PHE	2.3
1	B	754	ALA	2.3
1	B	762	LYS	2.2
1	B	1066	PRO	2.2
1	B	773	LEU	2.2
1	B	435	ALA	2.1
1	A	414	ILE	2.1
1	B	1065	LEU	2.0
1	B	361	GLN	2.0
1	B	447	GLU	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 monosaccharides 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.