Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 11:39 AM EDT

PDB ID	:	4N7R
Title	:	Crystal structure of Arabidopsis glutamyl-tRNA reductase in complex with its binding protein
Authors	:	Zhao, A.; Fang, Y.; Lin, Y.; Gong, W.; Liu, L.
Deposited on	:	2013-10-16
Resolution	:	2.80 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:

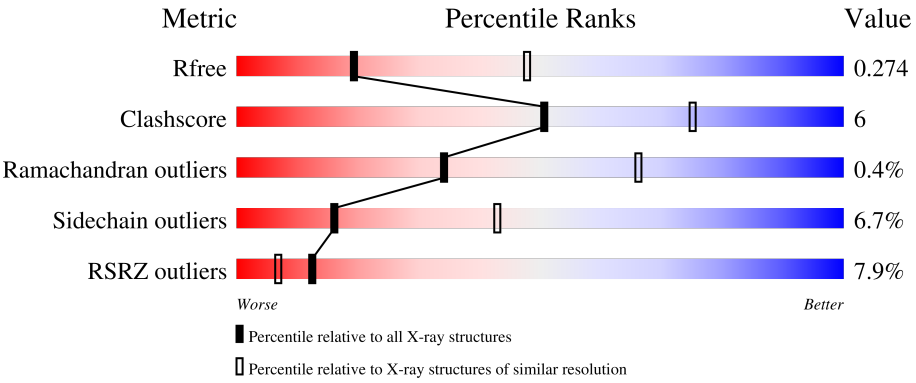
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	472	6% 72% 12% • 14%
1	B	472	13% 68% 12% • 18%
2	C	310	% 62% 18% • 19%
2	D	310	3% 65% 14% • 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9918 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	405	Total	C	N	O	S	5	2	0
			3097	1939	558	576	24			
1	B	385	Total	C	N	O	S	1	0	0
			2844	1779	504	542	19			

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 Genomic DNA, chromosome 3, P1 clone: MXL8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	252	Total	C	N	O	S	0	0	0
			1957	1238	332	374	13			
2	D	251	Total	C	N	O	S	0	0	0
			1975	1249	336	377	13			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	MET	-	expression tag	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

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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	-	expression tag	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

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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 water.

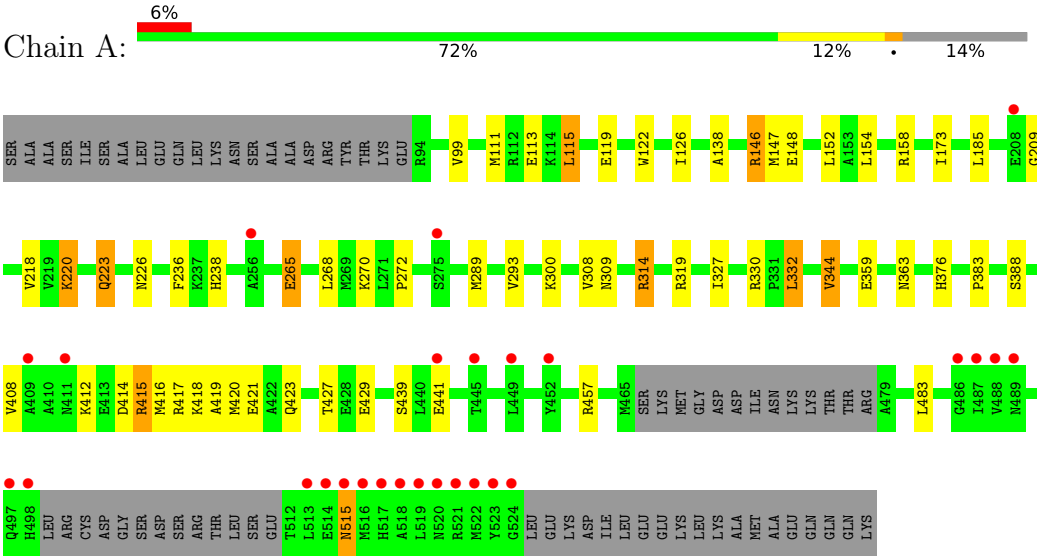
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0
3	C	14	Total O 14 14	0	0
3	D	15	Total O 15 15	0	0

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.

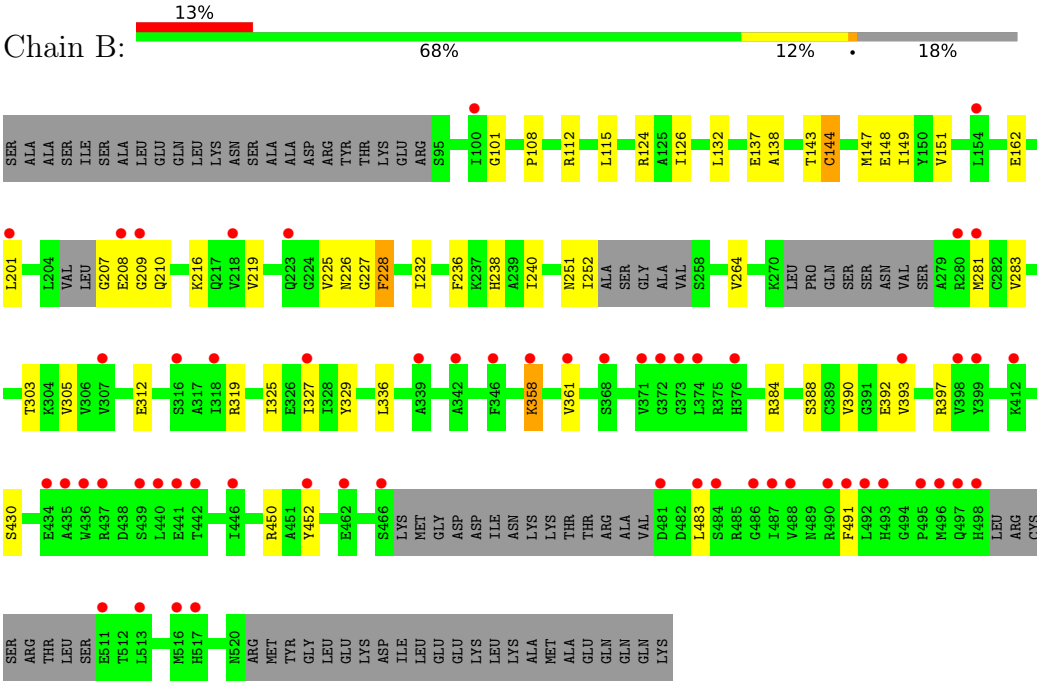
• Molecule 1: Glutamyl-tRNA reductase 1, chloroplastic

Chain A:



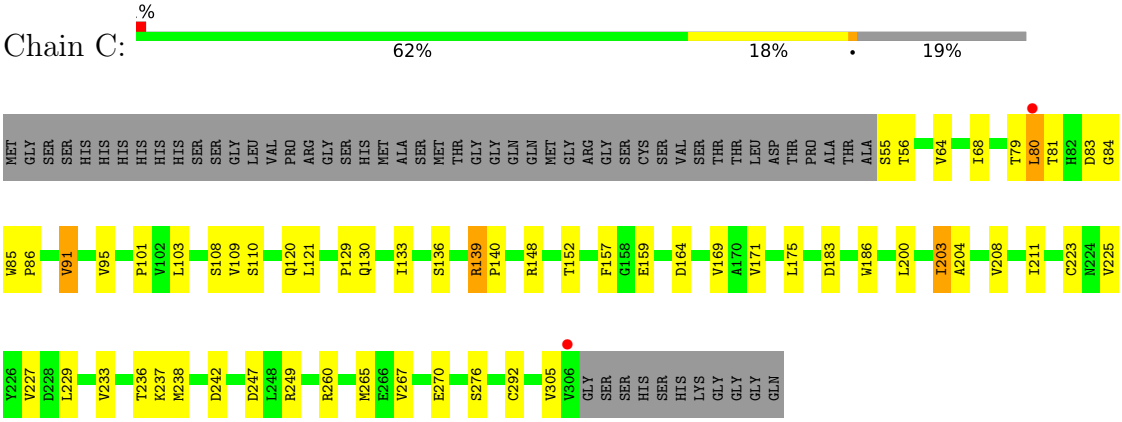
• Molecule 1: Glutamyl-tRNA reductase 1, chloroplastic

Chain B:



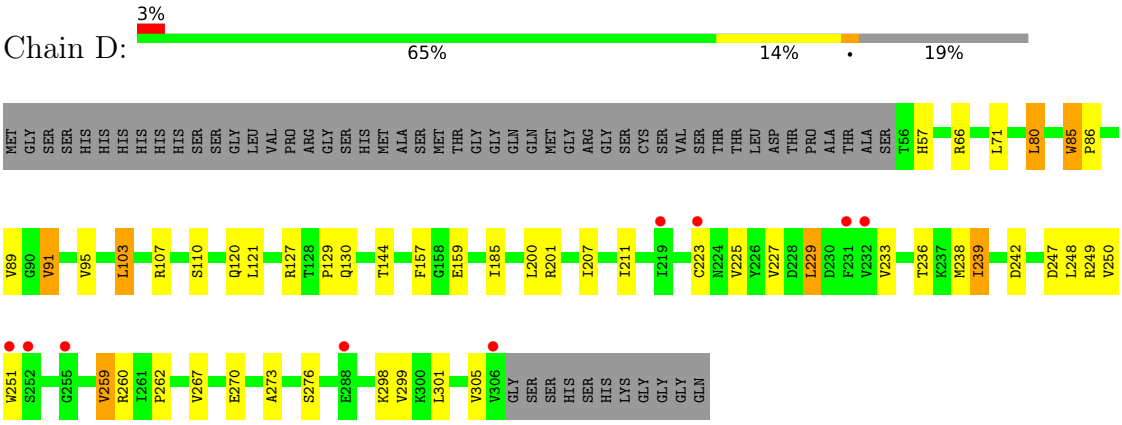
• Molecule 2: Genomic DNA, chromosome 3, P1 clone: MXL8

Chain C:



• Molecule 2: Genomic DNA, chromosome 3, P1 clone: MXL8

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.37Å 84.75Å 359.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 2.80 49.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.56-2.80) 94.2 (49.56-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.71 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.212 , 0.270 0.214 , 0.274	Depositor DCC
R_{free} test set	2189 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9918	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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	0.30	0/3140	0.49	0/4240
1	B	0.23	0/2881	0.41	0/3900
2	C	0.34	0/2000	0.49	0/2718
2	D	0.30	0/2018	0.46	0/2738
All	All	0.29	0/10039	0.46	0/13596

There are no bond length outliers.

There are no bond angle outliers.

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	3097	0	3133	31	0
1	B	2844	0	2763	29	0
2	C	1957	0	1886	31	0
2	D	1975	0	1930	26	0
3	A	16	0	0	1	0
3	C	14	0	0	2	0
3	D	15	0	0	0	0
All	All	9918	0	9712	112	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 6.

All (112) 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)
2:D:120:GLN:HG2	2:D:130:GLN:HG2	1.70	0.74
2:D:227:VAL:HG12	2:D:299:VAL:HB	1.69	0.72
2:C:120:GLN:HG2	2:C:130:GLN:HG2	1.74	0.70
2:C:83:ASP:O	2:C:85:TRP:N	2.24	0.70
2:C:211:ILE:HD12	2:C:238:MET:HE1	1.75	0.68
2:D:57:HIS:HB3	2:D:262:PRO:HB3	1.75	0.66
1:A:416:MET:O	1:A:420:MET:N	2.28	0.65
1:A:158:ARG:NH1	3:A:615:HOH:O	2.30	0.65
2:C:55:SER:N	2:C:56:THR:HA	2.12	0.64
2:D:242:ASP:OD1	2:D:260:ARG:NH2	2.29	0.64
1:B:207:GLY:HA2	1:B:210:GLN:HB3	1.80	0.64
2:D:236:THR:HG22	2:D:250:VAL:HA	1.80	0.64
2:C:183:ASP:O	2:D:107:ARG:NH2	2.32	0.62
1:B:137:GLU:HB2	1:B:232:ILE:HD13	1.85	0.59
1:A:210:GLN:O	1:A:214:GLN:N	2.34	0.59
1:B:303:THR:HA	1:B:325:ILE:HG13	1.85	0.58
2:C:242:ASP:OD1	2:C:260:ARG:NH2	2.34	0.57
1:B:264:VAL:HG21	1:B:296:HIS:HB3	1.86	0.57
1:B:225:VAL:HG12	1:B:227:GLY:H	1.70	0.56
2:D:248:LEU:HB2	2:D:259:VAL:HG23	1.88	0.55
1:A:265:GLU:OE1	1:A:300:LYS:NZ	2.34	0.54
1:A:483:LEU:HD23	1:B:483:LEU:HD23	1.89	0.54
2:C:139:ARG:HG3	2:C:140:PRO:HD2	1.89	0.54
2:D:71:LEU:HD11	2:D:201:ARG:HB2	1.89	0.54
1:B:251:ASN:N	1:B:252:ILE:HA	2.22	0.54
1:A:115:LEU:HB3	1:A:147:MET:HG2	1.89	0.54
2:C:101:PRO:HG2	2:C:169:VAL:HB	1.90	0.53
1:A:344:VAL:HB	1:A:376:HIS:HB2	1.91	0.53
2:C:249:ARG:NH1	2:C:305:VAL:HG11	2.23	0.53
2:C:133:ILE:HG23	2:C:171:VAL:HG13	1.92	0.52
1:B:281:MET:HB2	1:B:305:VAL:HG12	1.92	0.52
1:A:414:ASP:HA	1:A:417:ARG:HB3	1.91	0.52
2:C:242:ASP:CG	2:C:260:ARG:HH22	2.13	0.51
2:D:223:CYS:SG	2:D:236:THR:HG21	2.50	0.51
1:B:228:PHE:HE1	1:B:232:ILE:HG22	1.75	0.51
1:B:132:LEU:HD13	1:B:162:GLU:HB3	1.91	0.51
2:D:249:ARG:NH1	2:D:305:VAL:HG21	2.26	0.51
1:A:405:LYS:O	1:A:408:VAL:HG23	2.10	0.51
1:A:146[A]:ARG:HG2	1:A:148:GLU:HG3	1.92	0.51
2:C:56:THR:N	3:C:411:HOH:O	2.38	0.50
1:A:220:LYS:O	1:A:223:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HG23	1:A:138:ALA:HB3	1.94	0.50
1:A:412:LYS:O	1:A:415:ARG:NH1	2.40	0.50
2:C:91:VAL:HG11	2:C:103:LEU:HD22	1.92	0.49
1:B:126:ILE:HG23	1:B:138:ALA:HB3	1.94	0.49
1:A:119:GLU:HA	1:A:122:TRP:CE2	2.48	0.48
1:B:115:LEU:HD13	1:B:171:SER:HB3	1.96	0.48
2:D:267:VAL:HG11	2:D:273:ALA:HB2	1.95	0.48
2:D:121:LEU:O	2:D:129:PRO:HD2	2.14	0.47
1:A:416:MET:HA	1:A:419:ALA:HB3	1.95	0.47
2:C:208:VAL:HA	2:C:238:MET:HE2	1.96	0.47
2:D:85:TRP:CD1	2:D:86:PRO:HD2	2.50	0.47
2:C:108:SER:O	2:C:110:SER:N	2.40	0.46
1:B:358:LYS:HE3	1:B:392:GLU:HB2	1.95	0.46
1:B:312:GLU:HG2	1:B:329:TYR:CZ	2.50	0.46
1:B:208:GLU:HA	1:B:209:GLY:HA2	1.58	0.45
2:C:86:PRO:HD3	2:D:80:LEU:HD22	1.97	0.45
1:A:119:GLU:HA	1:A:122:TRP:CD2	2.52	0.45
1:A:309:ASN:HD21	1:A:314:ARG:NH1	2.14	0.45
2:C:204:ALA:O	2:C:208:VAL:HG23	2.17	0.45
1:A:270:LYS:HG2	1:A:399:TYR:OH	2.17	0.44
2:D:229:LEU:HD23	2:D:233:VAL:HG21	1.98	0.44
1:A:218:VAL:HG11	1:A:236:PHE:CE1	2.53	0.44
2:D:157:PHE:O	2:D:159:GLU:HG3	2.16	0.44
1:A:308:VAL:HG12	1:A:332:LEU:HD12	1.99	0.44
1:B:143:THR:HG22	1:B:144:CYS:H	1.83	0.44
2:C:247:ASP:OD1	2:C:260:ARG:HD3	2.17	0.44
2:D:91:VAL:HG11	2:D:103:LEU:HD13	1.98	0.44
2:D:211:ILE:HD12	2:D:238:MET:HE1	2.00	0.44
1:B:291:LYS:HE2	1:B:295:LYS:HE3	2.00	0.44
1:B:101:GLY:HA3	1:B:148:GLU:HG2	1.99	0.43
1:A:289:MET:O	1:A:293:VAL:HG23	2.17	0.43
1:B:236:PHE:O	1:B:240:ILE:HG13	2.18	0.43
2:C:86:PRO:HB3	2:D:80:LEU:HD13	1.99	0.43
2:C:249:ARG:HH11	2:C:305:VAL:HG11	1.83	0.43
1:B:216:LYS:HA	1:B:219:VAL:HG22	2.01	0.43
1:B:108:PRO:O	1:B:112:ARG:HG3	2.19	0.42
1:B:361:VAL:HG11	1:B:390:VAL:HG13	2.00	0.42
2:D:239:ILE:HG12	2:D:247:ASP:O	2.19	0.42
1:A:115:LEU:HD13	1:A:115:LEU:HA	1.84	0.42
2:D:247:ASP:OD1	2:D:260:ARG:HD3	2.18	0.42
1:A:515:ASN:OD1	1:A:515:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ILE:O	1:B:430:SER:OG	2.29	0.42
1:B:319:ARG:HA	1:B:327:ILE:HD13	2.00	0.42
2:C:148:ARG:O	2:C:152:THR:HG23	2.20	0.42
1:B:384:ARG:NH1	1:B:388:SER:HB2	2.35	0.42
2:C:223:CYS:HB3	2:C:233:VAL:HG21	2.01	0.42
1:B:390:VAL:O	1:B:393:VAL:HG22	2.20	0.42
1:A:111:MET:HG3	1:A:173:ILE:HD13	2.01	0.42
2:D:200:LEU:HD11	2:D:267:VAL:HG12	2.02	0.42
2:C:175:LEU:HB2	2:C:186:TRP:CZ3	2.55	0.41
1:A:308:VAL:HA	1:A:330:ARG:O	2.20	0.41
1:A:418:LYS:HA	1:A:421:GLU:HB2	2.02	0.41
2:C:203:ILE:HD12	2:C:270:GLU:HB2	2.02	0.41
1:B:216:LYS:HG2	1:B:240:ILE:HD13	2.01	0.41
2:D:249:ARG:HH11	2:D:305:VAL:HG21	1.86	0.41
2:C:237:LYS:HE2	2:C:237:LYS:HB3	1.95	0.41
1:A:113:GLU:HB2	1:A:383:PRO:HA	2.03	0.41
1:A:209:GLY:O	1:A:211:ILE:N	2.54	0.41
1:A:319:ARG:HA	1:A:327:ILE:HD12	2.01	0.41
2:C:85:TRP:CD1	2:C:86:PRO:HD2	2.56	0.41
2:C:121:LEU:O	2:C:129:PRO:HD2	2.21	0.41
1:B:149:ILE:HG22	1:B:151:VAL:HG13	2.03	0.41
1:A:99:VAL:CG1	1:A:185:LEU:HB2	2.51	0.40
1:B:228:PHE:CE1	1:B:232:ILE:HG22	2.55	0.40
2:D:249:ARG:HD2	2:D:251:TRP:CH2	2.56	0.40
1:A:423:GLN:O	1:A:427:THR:HG23	2.22	0.40
2:C:64:VAL:O	2:C:68:ILE:HG13	2.22	0.40
2:C:80:LEU:HD21	2:D:80:LEU:HD21	2.03	0.40
2:C:139:ARG:NH2	3:C:405:HOH:O	2.54	0.40
2:C:157:PHE:O	2:C:159:GLU:HG3	2.22	0.40
2:D:207:ILE:HD11	2:D:270:GLU:HG3	2.03	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	401/472 (85%)	379 (94%)	20 (5%)	2 (0%)	29	61
1	B	373/472 (79%)	352 (94%)	21 (6%)	0	100	100
2	C	250/310 (81%)	241 (96%)	7 (3%)	2 (1%)	19	49
2	D	249/310 (80%)	239 (96%)	9 (4%)	1 (0%)	34	66
All	All	1273/1564 (81%)	1211 (95%)	57 (4%)	5 (0%)	34	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
2	C	84	GLY
1	A	272	PRO
2	C	109	VAL
2	D	110	SER

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	332/400 (83%)	309 (93%)	23 (7%)	15	41
1	B	291/400 (73%)	277 (95%)	14 (5%)	25	58
2	C	214/269 (80%)	196 (92%)	18 (8%)	11	31
2	D	220/269 (82%)	203 (92%)	17 (8%)	13	35
All	All	1057/1338 (79%)	985 (93%)	72 (7%)	16	42

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	146[A]	ARG
1	A	146[B]	ARG

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Mol	Chain	Res	Type
1	A	152	LEU
1	A	154	LEU
1	A	220	LYS
1	A	223	GLN
1	A	226	ASN
1	A	238	HIS
1	A	265	GLU
1	A	268	LEU
1	A	314	ARG
1	A	332	LEU
1	A	344	VAL
1	A	359	GLU
1	A	363	ASN
1	A	388	SER
1	A	415	ARG
1	A	429	GLU
1	A	439	SER
1	A	441	GLU
1	A	457	ARG
1	A	515	ASN
2	C	79	THR
2	C	80	LEU
2	C	81	THR
2	C	91	VAL
2	C	95	VAL
2	C	136	SER
2	C	139	ARG
2	C	164	ASP
2	C	200	LEU
2	C	203	ILE
2	C	225	VAL
2	C	227	VAL
2	C	229	LEU
2	C	236	THR
2	C	265	MET
2	C	267	VAL
2	C	276	SER
2	C	292	CYS
1	B	124	ARG
1	B	144	CYS
1	B	147	MET
1	B	201	LEU

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Mol	Chain	Res	Type
1	B	226	ASN
1	B	228	PHE
1	B	238	HIS
1	B	283	VAL
1	B	336	LEU
1	B	358	LYS
1	B	397	ARG
1	B	450	ARG
1	B	452	TYR
1	B	491	PHE
2	D	66	ARG
2	D	80	LEU
2	D	85	TRP
2	D	89	VAL
2	D	91	VAL
2	D	95	VAL
2	D	103	LEU
2	D	127	ARG
2	D	144	THR
2	D	185	ILE
2	D	225	VAL
2	D	229	LEU
2	D	239	ILE
2	D	259	VAL
2	D	276	SER
2	D	298	LYS
2	D	301	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

There are no monosaccharides 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, 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	405/472 (85%)	0.31	30 (7%) 14 8	15, 36, 125, 133	7 (1%)
1	B	385/472 (81%)	0.72	61 (15%) 2 1	57, 97, 139, 155	4 (1%)
2	C	252/310 (81%)	-0.05	2 (0%) 86 81	14, 31, 69, 80	0
2	D	251/310 (80%)	0.20	9 (3%) 42 32	17, 48, 99, 116	0
All	All	1293/1564 (82%)	0.34	102 (7%) 12 7	14, 55, 130, 155	11 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	495	PRO	7.9
1	A	496	MET	7.3
1	A	523	TYR	6.2
1	B	491	PHE	6.2
1	B	496	MET	5.6
1	B	483	LEU	5.5
1	A	489	ASN	5.1
1	B	281	MET	5.0
1	A	492	LEU	5.0
1	A	517	HIS	5.0
1	B	484	SER	4.8
1	B	201	LEU	4.8
1	B	435	ALA	4.5
1	A	488	VAL	4.5
1	A	524	GLY	4.2
1	A	515	ASN	4.2
1	B	498	HIS	4.0
1	A	497	GLN	4.0
1	B	376	HIS	3.9
1	A	449	LEU	3.9
1	B	426	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	223	CYS	3.8
1	B	516	MET	3.8
1	B	318	ILE	3.7
1	A	521	ARG	3.7
1	B	511	GLU	3.7
1	B	513	LEU	3.7
1	B	517	HIS	3.6
1	B	487	ILE	3.6
1	B	307	VAL	3.6
1	B	327	ILE	3.6
1	B	441	GLU	3.6
1	A	522	MET	3.5
1	B	452	TYR	3.5
1	B	495	PRO	3.5
2	C	306	VAL	3.3
1	B	373	GLY	3.2
1	B	442	THR	3.2
1	A	498	HIS	3.1
1	B	492	LEU	3.1
1	B	374	LEU	3.1
1	A	519	LEU	3.0
1	B	493	HIS	3.0
1	B	488	VAL	3.0
1	A	518	ALA	2.9
1	B	371	VAL	2.9
1	A	275	SER	2.9
1	A	452	TYR	2.9
1	B	154	LEU	2.8
1	B	490	ARG	2.8
1	B	497	GLN	2.8
1	B	439	SER	2.8
1	B	440	LEU	2.8
2	D	231	PHE	2.7
1	B	198	SER	2.7
1	B	346	PHE	2.7
1	A	409	ALA	2.7
1	B	462	GLU	2.7
2	D	255	GLY	2.6
1	B	100	ILE	2.6
1	A	411	ASN	2.6
1	B	342	ALA	2.6
1	B	316	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	256	ALA	2.5
1	A	516	MET	2.5
1	A	520	ASN	2.5
1	A	441	GLU	2.5
1	B	209	GLY	2.5
1	B	399	TYR	2.5
1	B	486	GLY	2.4
1	B	436	TRP	2.4
1	A	487	ILE	2.4
1	A	514	GLU	2.3
1	B	481	ASP	2.3
1	B	358	LYS	2.3
2	D	252	SER	2.3
1	B	420	MET	2.3
2	C	80	LEU	2.3
1	B	398	VAL	2.2
1	B	368	SER	2.2
1	B	437	ARG	2.2
1	B	393	VAL	2.2
2	D	251	TRP	2.2
1	A	208	GLU	2.2
1	B	208	GLU	2.2
1	A	486	GLY	2.2
1	B	466	SER	2.2
2	D	232	VAL	2.2
1	A	513	LEU	2.1
1	B	223	GLN	2.1
1	B	412	LYS	2.1
2	D	288	GLU	2.1
1	B	361	VAL	2.1
1	B	339	ALA	2.1
1	B	446	ILE	2.1
2	D	306	VAL	2.1
1	B	434	GLU	2.1
2	D	219	ILE	2.0
1	B	372	GLY	2.0
1	A	445	THR	2.0
1	B	218	VAL	2.0
1	B	280	ARG	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.