

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	5CHE
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) 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: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 <=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	А	472	% 7 6%		14%	• 10%
1	В	472	^{3%} 70%		19%	• 10%
2	С	310	2% 66%	14%	·	19%
2	D	310	^{2%} 66%	14%	·	19%
3	Е	159	60%	14%	25	5%
3	F	159	2% 54% 19%	6	26	%



 $\mathbf{2}$

Entry composition (i)

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.

7 7 1		D 11		A /						m
Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
1	۸	497	Total	С	Ν	0	S	0	1	0
T	A	427	3292	2055	591	621	25	0	1	0
1 D	402	Total	С	Ν	0	S	0	0	0	
T	D	420	3243	2029	586	603	25	0	0	0

• Molecule 1 is a protein called Glutamyl-tRNA reductase 1, chloroplastic.

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	72	SER	-	expression tag	UNP P42804
В	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	С	250	Total 1970	C 1246	N 335	O 376	S 13	0	0	0
2	D	250	Total 1992	C 1260	N 339	O 380	S 13	0	1	0

There are 68 discrepancies between the modelled and reference sequences:

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



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Chain	Residue	Modelled	Actual	Comment	Reference
С	18	SER	-	expression tag	UNP Q9LU39
С	19	SER	-	expression tag	UNP Q9LU39
С	20	GLY	-	expression tag	UNP Q9LU39
С	21	LEU	-	expression tag	UNP Q9LU39
С	22	VAL	-	expression tag	UNP Q9LU39
С	23	PRO	-	expression tag	UNP Q9LU39
С	24	ARG	-	expression tag	UNP Q9LU39
С	25	GLY	-	expression tag	UNP Q9LU39
С	26	SER	-	expression tag	UNP Q9LU39
С	27	HIS	-	expression tag	UNP Q9LU39
С	28	MET	-	expression tag	UNP Q9LU39
С	29	ALA	-	expression tag	UNP Q9LU39
С	30	SER	-	expression tag	UNP Q9LU39
С	31	MET	-	expression tag	UNP Q9LU39
С	32	THR	-	expression tag	UNP Q9LU39
С	33	GLY	-	expression tag	UNP Q9LU39
С	34	GLY	-	expression tag	UNP Q9LU39
С	35	GLN	-	expression tag	UNP Q9LU39
С	36	GLN	-	expression tag	UNP Q9LU39
С	37	MET	-	expression tag	UNP Q9LU39
С	38	GLY	-	expression tag	UNP Q9LU39
С	39	ARG	-	expression tag	UNP Q9LU39
С	40	GLY	-	expression tag	UNP Q9LU39
С	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



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		At	oms			ZeroOcc	AltConf	Trace
3	Е	119	Total 951	C 599	N 160	O 190	S 2	0	1	0
3	F	117	Total 917	C 579	N 157	O 179	$\frac{S}{2}$	0	0	0

There are 74 discrepancies between the modelled and reference sequences:

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



Chain	Residue	Modelled	Actual	Comment	Reference
Е	173	LEU	_	expression tag	UNP Q940U6
Е	174	ALA	_	expression tag	UNP Q940U6
Е	175	ALA	_	expression tag	UNP Q940U6
Е	176	GLN	_	expression tag	UNP Q940U6
Е	177	PRO	-	expression tag	UNP Q940U6
Е	178	ALA	-	expression tag	UNP Q940U6
Е	179	MET	-	expression tag	UNP Q940U6
Е	180	ALA	-	expression tag	UNP Q940U6
Е	181	MET	-	expression tag	UNP Q940U6
Е	182	ASP	-	expression tag	UNP Q940U6
Е	183	ILE	-	expression tag	UNP Q940U6
Е	184	GLY	-	expression tag	UNP Q940U6
Е	185	ILE	-	expression tag	UNP Q940U6
Е	186	ASN	-	expression tag	UNP Q940U6
Е	187	SER	-	expression tag	UNP Q940U6
Е	188	ASP	-	expression tag	UNP Q940U6
Е	189	PRO	-	expression tag	UNP Q940U6
Е	190	HIS	-	expression tag	UNP Q940U6
Е	191	HIS	-	expression tag	UNP Q940U6
Е	192	HIS	-	expression tag	UNP Q940U6
Е	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



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	А	2	Total O 2 2	0	0
4	В	2	Total O 2 2	0	0
4	С	2	Total O 2 2	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.



 \bullet Molecule 1: Glutamyl-tRNA reductase 1, chloroplastic



V955 L105 L105 R107 8107 1137 1137 1137 1144 1144 1144 1144 1144	V167 V169 V169 V169 M177 D183 N194	R201 E217 D218 F220 F220 V227	F231 V232 V233 1233 D242 R243	D247 L248 R249 V250 V250 V250 V259 R256 1261
P262 D269 D269 P269 P269 P269 P299 P299 P299 P299 P	SER HIS LYS GLY GLY GLY			
• Molecule 2: Glutamyl-tl	RNA reductase-b	oinding protein	n, chloroplas	tic
Chain D:	66%		14% <mark>•</mark> 1	9%
MET OLY SER SER HIS HIS HIS HIS HIS HIS HIS SER CIY VAL VAL VAL VAL SER SER SER SER SER	HIS MET ALA ALA SER MET GLY GLY GLN GLY GLY	ARG GLY SER CYS CYS SER VAL THR THR THR LLEU	ASP THR PRO ALA ALA ALA SER SER SER	M69 L80 T81 W85 V95
P101 V102 L105 N106 N106 P111 P111 P111 E122 E122 E122 T128 T128 T128 T133	1137 1137 1139 1139 1143 1143 1143 1144 1144	Y167 V168 V169 N174 M177 N194	1203 M216 R221 V227	E235 D242 D247 V269 R260 T261 P262
E270 K271 K271 A284 K289 K289 K289 K289 K289 K289 K289 K299 K29	HIS LLYS GLN GLN GLN			
• Molecule 3: Protein FL	UORESCENT II	N BLUE LIGH	HT, chloropla	astic
Chain E:	60%	14%	25%	
MET LYS TYR TYR LEU LEU PRO PRO PRO PRO LEU LEU LEU LEU LEU LEU LEU LEU LEU PRO PRO PRO PRO PRO PRO PRO	ALLA MET ALLA MET ALSP ALSP CLLY CLLY ALSP SER ASP ASP PRO	HIS HIS HIS HIS HIS TILE VAL E198	1204 1205 8206 8206 1206 1207 1210 1215	N217 Q218 E226 1229 1229 1241 E243 E243
K244 K245 Y260 M269 M269 T73 T284 T284 T284 T284 T284 T284 T284 T284	A312 R313 L314 E315 T316 ASP ASP			
• Molecule 3: Protein FL	UORESCENT II	N BLUE LIGH	HT, chloropla	astic
Chain F:	54%	19%	26%	
MET TYR TYR LEU LEU EEU PRO PRO PRO PRO PRO PRO ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	ALA ALA ALA ALA ALA ASP CLY CLY CLY CLY CLY CLY SSR SSR SSR ASP ASP	HIS HIS HIS HIS HIS TILE VAL CIU PRO	K200 L204 L205 S205 K207 K207 K209 T210	L215 218 7224 7224 728 728 7228 7228
P240 1241 1241 1241 1245 1255 1255 1255 1256 1256 1256 1270 1273	8274 E277 5278 5279 5279 5278 5279 5280 1280 7281 7284 7284 7284	1296 E296 L297 1307 1311 A312 A313	T316 ASP	



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	216.99Å 53.21Å 203.76Å	Depositor
a, b, c, α , β , γ	90.00° 108.36° 90.00°	Depositor
$\mathbf{P}_{\mathrm{oscolution}}(\mathbf{\hat{A}})$	39.27 - 3.20	Depositor
Resolution (A)	48.23 - 3.20	EDS
% Data completeness	87.2 (39.27-3.20)	Depositor
(in resolution range)	87.4 (48.23-3.20)	EDS
R_{merge}	0.13	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	4.00 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
D D.	0.223 , 0.278	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.225 , 0.279	DCC
R_{free} test set	1636 reflections (5.03%)	wwPDB-VP
Wilson B-factor $(Å^2)$	58.7	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29, 5.9	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	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.

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.



¹Intensities estimated from amplitudes.

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	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.32	0/3338	0.52	3/4501~(0.1%)
1	В	0.33	0/3283	0.57	6/4423~(0.1%)
2	С	0.29	0/2013	0.45	0/2731
2	D	0.31	0/2034	0.46	1/2755~(0.0%)
3	Е	0.30	0/967	0.47	0/1294
3	F	0.26	0/929	0.44	0/1243
All	All	0.31	0/12564	0.50	10/16947~(0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	187	ASN	CB-CA-C	9.99	130.39	110.40
1	А	502	ASP	N-CA-C	-8.89	86.98	111.00
1	В	188	LYS	N-CA-CB	-8.62	95.08	110.60
1	А	186	TYR	N-CA-C	7.29	130.67	111.00
1	В	186	TYR	CB-CA-C	-5.86	98.67	110.40

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	А	3292	0	3363	37	0
1	В	3243	0	3309	54	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	С	1970	0	1928	27	0
2	D	1992	0	1955	24	0
3	Е	951	0	959	16	0
3	F	917	0	926	18	0
4	А	2	0	0	1	0
4	В	2	0	0	0	0
4	С	2	0	0	1	0
All	All	12371	0	12440	166	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.

The worst 5 of 166 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
3:F:215:LEU:O	3:F:256:ARG:NH1	2.21	0.73

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	Perce	ntiles
1	А	422/472~(89%)	406 (96%)	14 (3%)	2 (0%)	29	67
1	В	411/472 (87%)	392 (95%)	16 (4%)	3 (1%)	22	61
2	С	248/310~(80%)	241 (97%)	7 (3%)	0	100	100
2	D	247/310~(80%)	241 (98%)	6 (2%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
3	Е	118/159~(74%)	115 (98%)	3(2%)	0	100	100
3	F	115/159~(72%)	114 (99%)	1 (1%)	0	100	100
All	All	1561/1882 (83%)	1509 (97%)	47 (3%)	5 (0%)	41	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	505	ASP
1	А	506	SER
1	В	203	SER
1	А	187	ASN
1	В	255	GLY

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	А	363/400~(91%)	356~(98%)	7(2%)	57 81
1	В	352/400~(88%)	339~(96%)	13~(4%)	34 68
2	С	220/269~(82%)	214 (97%)	6 (3%)	44 75
2	D	224/269~(83%)	217~(97%)	7 (3%)	40 72
3	Е	99/129~(77%)	98~(99%)	1 (1%)	76 90
3	F	93/129~(72%)	92~(99%)	1 (1%)	73 88
All	All	1351/1596~(85%)	1316 (97%)	35 (3%)	46 76

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	109	VAL
2	D	114	ARG
2	D	259	VAL
1	В	260	SER
1	В	257	VAL



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	385	ASN
2	D	120	GLN
2	D	134	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 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 (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, 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	А	427/472~(90%)	-0.12	3 (0%) 87 81	2, 12, 45, 90	0
1	В	423/472~(89%)	0.18	14 (3%) 46 30	5, 25, 63, 85	0
2	С	250/310~(80%)	0.15	5 (2%) 65 51	4, 21, 59, 83	0
2	D	250/310~(80%)	0.06	5 (2%) 65 51	6, 24, 65, 87	0
3	Е	119/159~(74%)	-0.04	2 (1%) 70 57	6, 22, 47, 58	0
3	F	117/159~(73%)	0.15	3 (2%) 56 40	17, 48, 71, 83	0
All	All	1586/1882~(84%)	0.06	32 (2%) 65 51	2, 21, 64, 90	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	218	GLN	4.2
1	А	476	THR	4.0
2	D	194	ASN	3.4
1	А	414	ASP	3.4
3	Е	218	GLN	3.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no 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.

