

Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 01:24 AM JST

PDB ID	:	6IO4
Title	:	Silver-bound Glyceraldehyde-3-phosphate dehydrogenase A
Authors	:	Wang, H.; Sun, H.; Wang, M.
Deposited on	:	2018-10-29
Resolution	:	3.10 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 (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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	329	88%	12%
1	В	329	87%	13% •
1	С	329	.% 89 %	10%
1	D	329	90%	10%
1	Е	329	88%	12%
1	F	329	86%	14%



Mol	Chain	Length	Quality of chain	
1	G	329	90%	10%
1	Н	329	% • 87%	13%
1	Ι	329	88%	12%
1	J	329	84%	16%
1	Κ	329	3% 91%	9%
1	L	329	87%	12%
1	М	329	2% 88%	12%
1	Ν	329	88%	12%
1	О	329	89%	11%
1	Р	329	86%	13%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 38671 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	329	Total	С	Ν	0	S	0	0	0
		020	2405	1519	412	464	10	0	0	0
1	В	320	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	D	525	2428	1532	414	472	10	0	0	0
1	С	320	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
1	U	525	2405	1519	412	464	10	0	0	0
1	Л	320	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0	0
	D	525	2428	1532	414	472	10	0	0	0
1	F	320	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	Ľ	525	2411	1522	415	464	10	0	1 I	0
1	Б	220	Total	С	Ν	0	S	0	0	0
	Г	529	2428	1532	414	472	10	0	0	0
1	С	200	Total	С	Ν	0	S	0	1	0
	G	529	2410	1522	415	463	10			0
1	и	200	Total	С	Ν	0	S	0	0	0
	п	329	2421	1528	413	470	10	0	0	0
1	т	220	Total	С	Ν	0	S	0	1	0
	1	529	2405	1519	414	462	10			
1	т	200	Total	С	Ν	0	S	0	0	0
	1	529	2425	1530	413	472	10	0	0	0
1	V	220	Total	С	Ν	0	S	0	0	0
	Γ	529	2393	1510	411	462	10	0	0	0
1	т	200	Total	С	Ν	0	S	0	0	0
		529	2428	1532	414	472	10	0	0	U
1	м	200	Total	С	Ν	0	S	0	1	0
	IVI	529	2408	1520	414	464	10	0	L	0
1	N	220	Total	С	Ν	0	S	0	0	0
1	IN	529	2424	1529	414	471	10	0	0	0
1	0	220	Total	С	Ν	0	S	0	1	0
		329	2411	1522	415	464	10	U		U
1	р	200	Total	С	Ν	Ο	S	0	0	0
	Г	329	2425	1530	413	472	10	U	U	U

• Molecule 1 is a protein called Glyceraldehyde-3-phosphate dehydrogenase A.



0104

Chain	Residue	Modelled	Actual	Comment	Reference
А	78	GLY	ASP	engineered mutation	UNP P0A9B2
В	78	GLY	ASP	engineered mutation	UNP P0A9B2
С	78	GLY	ASP	engineered mutation	UNP P0A9B2
D	78	GLY	ASP	engineered mutation	UNP P0A9B2
Е	78	GLY	ASP	engineered mutation	UNP P0A9B2
F	78	GLY	ASP	engineered mutation	UNP P0A9B2
G	78	GLY	ASP	engineered mutation	UNP P0A9B2
Н	78	GLY	ASP	engineered mutation	UNP P0A9B2
Ι	78	GLY	ASP	engineered mutation	UNP P0A9B2
J	78	GLY	ASP	engineered mutation	UNP P0A9B2
K	78	GLY	ASP	engineered mutation	UNP P0A9B2
L	78	GLY	ASP	engineered mutation	UNP P0A9B2
М	78	GLY	ASP	engineered mutation	UNP P0A9B2
N	78	GLY	ASP	engineered mutation	UNP P0A9B2
0	78	GLY	ASP	engineered mutation	UNP P0A9B2
Р	78	GLY	ASP	engineered mutation	UNP P0A9B2

There are 16 discrepancies between the modelled and reference sequences:

• Molecule 2 is SILVER ION (three-letter code: AG) (formula: Ag).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Ag 1 1	0	0
2	В	1	Total Ag 1 1	0	0
2	С	1	Total Ag 1 1	0	0
2	D	1	Total Ag 1 1	0	0
2	Е	1	Total Ag 1 1	0	0
2	F	1	Total Ag 1 1	0	0
2	G	1	Total Ag 1 1	0	0
2	Н	1	Total Ag 1 1	0	0
2	Ι	1	Total Ag 1 1	0	0
2	J	1	Total Ag 1 1	0	0
2	К	1	Total Ag 1 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total Ag 1 1	0	0
2	М	1	Total Ag 1 1	0	0
2	Ν	1	Total Ag 1 1	0	0
2	О	1	Total Ag 1 1	0	0
2	Р	1	Total Ag 1 1	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: Glyceraldehyde-3-phosphate dehydrogenase A



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A





• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A





L322 K330

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

Chain E:	88%		12%
11 114 114 114 133 133 133 148 188 198 196 196 196	K131 F135 C149 C149 L154 L154 L171 L171 M172	H176 1156 1156 1194 1194 1194 1198 1198 1198 1200 1203 1203	V217 L225 L225 R231 V232 V233 V237 S238
L242 L242 L271 L271 L271 N277 N311 Y311 Y311			
• Molecule 1: Glyceraldehyde-3-	phosphate dehy	drogenase A	
Chain F:	86%		14%
K11 V3 V3 V3 K13 V15 V15 V15 V15 V15 V15 V15 V15 V15 V15	w84 v87 d88 v89 v89 v89 v89 v89 v89 v89 v89 v89 v	S148 C149 C153 L154 L171 L171 T173 R194 R194	M228 V232 V233 V233 V237 V237 V237 V237 V237
1243 K266 V259 V259 1271 L271 L271 L271 K206 K306 K306 K306 V308 V311 V311 V312	<mark>K330</mark>		
• Molecule 1: Glyceraldehyde-3-	phosphate dehy	drogenase A	
Chain G:	90%		10%
11 1332 1332 1332 1333 1434 1434 1434 14	M172 H176 T179 D186 S200 G227	R231 7232 7233 7233 7237 8238 1243 1243 1243 1243 1243 1243 1243 1243	L271 D277 L300 K306 Y311
<mark></mark>			
• Molecule 1: Glyceraldehyde-3-	phosphate dehy	drogenase A	
Chain H:	070/		1.20/
	0770		13 %
11 R10 R13 F16 F16 F16 E58 E58 C116 B87 V116 K115 V116 V116	6120 P121 F131 F135 F135 F135 F135 S145	S148 C149 C149 E154 E159 G170 C171 T171 R194 R194 S200	V232 V237 V237 V237 1241 1242 T243 V244
R245 K256 V259 V270 L271 C271 C272 C285 C286 C286 C286 C286 C286 C286 C286 C286	1328 8329 K330		
• Molecule 1: Glyceraldehyde-3-	phosphate dehy	drogenase A	
Chain I:	990/		1.20/
Citorin 1.	00 /0		12 /0



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A

Chain J: 84% 16%

• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A





• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase A







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	87.99Å 110.02Å 139.71Å	Depositor
a, b, c, α , β , γ	87.66° 86.94° 87.26°	Depositor
Bosolution(A)	87.77 - 3.10	Depositor
Resolution (A)	139.41 - 3.10	EDS
% Data completeness	90.2 (87.77-3.10)	Depositor
(in resolution range)	$90.3\ (139.41-3.10)$	EDS
R_{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.46 (at 3.07 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.14_3260:001)	Depositor
B B.	0.175 , 0.240	Depositor
II, II, <i>free</i>	0.174 , 0.239	DCC
R_{free} test set	4138 reflections (4.83%)	wwPDB-VP
Wilson B-factor $(Å^2)$	81.1	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 52.9	EDS
L-test for $twinning^2$	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	38671	wwPDB-VP
Average B, all atoms $(Å^2)$	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.49% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: AG

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	0.24	0/2443	0.43	0/3321
1	В	0.24	0/2466	0.43	0/3348
1	С	0.24	0/2443	0.43	0/3321
1	D	0.24	0/2466	0.42	0/3348
1	Ε	0.24	0/2454	0.43	0/3335
1	F	0.24	0/2466	0.43	0/3348
1	G	0.24	0/2453	0.42	0/3335
1	Н	0.24	0/2459	0.42	0/3340
1	Ι	0.24	0/2448	0.42	0/3329
1	J	0.24	0/2463	0.42	0/3345
1	Κ	0.24	0/2431	0.42	0/3307
1	L	0.24	0/2466	0.43	0/3348
1	М	0.24	0/2451	0.42	0/3332
1	Ν	0.24	0/2462	0.42	0/3345
1	0	0.24	0/2454	0.42	0/3335
1	Р	0.24	0/2463	0.43	0/3345
All	All	0.24	0/39288	0.42	0/53382

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 (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	2405	0	2350	24	0
1	В	2428	0	2382	26	0
1	С	2405	0	2350	22	0
1	D	2428	0	2382	25	0
1	Е	2411	0	2359	24	0
1	F	2428	0	2382	31	0
1	G	2410	0	2359	21	0
1	Н	2421	0	2372	25	0
1	Ι	2405	0	2351	24	0
1	J	2425	0	2376	34	0
1	K	2393	0	2324	19	0
1	L	2428	0	2382	26	0
1	М	2408	0	2353	26	0
1	N	2424	0	2376	27	0
1	0	2411	0	2359	19	0
1	Р	2425	0	2376	29	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Е	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	Н	1	0	0	0	0
2	Ι	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	М	1	0	0	0	0
2	N	1	0	0	1	0
2	0	1	0	0	0	0
2	Р	1	0	0	0	0
All	All	38671	0	37833	335	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 5.

All (335) 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:E:171:LEU:HG	1:F:306:LYS:HE2	1.75	0.69
1:G:176:HIS:HB3	1:G:231[B]:ARG:HD3	1.76	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:M:176:HIS:HB3	1:M:231[B]:ARG:HD3	1.77	0.67
1:A:154:LEU:HD11	1:A:242:LEU:HD13	1.77	0.66
1:P:15:VAL:HG13	1:P:322:LEU:HD11	1.78	0.66
1:F:127:PRO:HG3	1:F:141:GLN:HE21	1.60	0.65
1:M:171:LEU:HG	1:N:306:LYS:HE2	1.78	0.65
1:I:176:HIS:HB3	1:I:231[B]:ARG:HD3	1.80	0.64
1:A:277:ASP:HB3	1:B:194:ARG:HG2	1.78	0.64
1:L:127:PRO:HG3	1:L:141:GLN:HE21	1.64	0.63
1:P:58:GLU:HG2	1:P:65:ILE:HB	1.81	0.63
1:L:200:SER:HA	1:L:233:PRO:HB3	1.82	0.62
1:J:15:VAL:HG13	1:J:322:LEU:HD11	1.82	0.61
1:H:154:LEU:HD11	1:H:242:LEU:HD13	1.83	0.60
1:M:171:LEU:HD23	1:N:243:THR:HG23	1.83	0.60
1:E:306:LYS:HB2	1:F:171:LEU:HD13	1.83	0.60
1:A:176:HIS:HB3	1:A:231:ARG:HD3	1.82	0.60
1:I:277:ASP:HB3	1:J:194:ARG:HG2	1.83	0.60
1:L:10:ARG:HH11	1:L:13:ARG:HH21	1.48	0.60
1:M:277:ASP:HB3	1:N:194:ARG:HG2	1.83	0.59
1:E:171:LEU:HD23	1:F:243:THR:HG23	1.84	0.58
1:C:306:LYS:HB2	1:D:171:LEU:HD13	1.85	0.58
1:D:131:LYS:N	1:D:135:PHE:CE1	2.72	0.58
1:F:121:PRO:HG3	1:F:148:SER:HB3	1.86	0.58
1:D:256:LYS:HD2	1:D:294:ALA:HB1	1.84	0.58
1:K:194:ARG:HG2	1:L:277:ASP:HB3	1.85	0.58
1:J:87:VAL:HG23	1:J:89:VAL:HG23	1.85	0.58
1:K:200:SER:HA	1:K:233:PRO:HB3	1.86	0.58
1:N:106:ARG:NH1	1:N:142:ASP:OD2	2.37	0.58
1:C:176:HIS:HB3	1:C:231:ARG:HD3	1.84	0.57
1:L:87:VAL:HG23	1:L:89:VAL:HG23	1.86	0.57
1:O:277:ASP:HB3	1:P:194:ARG:HG2	1.86	0.57
1:E:306:LYS:HE2	1:F:171:LEU:HB3	1.86	0.57
1:M:200:SER:HA	1:M:233:PRO:HB3	1.87	0.57
1:E:277:ASP:HB3	1:F:194:ARG:HG2	1.87	0.56
1:H:10:ARG:HH11	1:H:13:ARG:HH21	1.53	0.56
1:E:154:LEU:HD11	1:E:242:LEU:HD13	1.86	0.56
1:N:121:PRO:HG3	1:N:148:SER:HB3	1.87	0.56
1:L:15:VAL:HG13	1:L:322:LEU:HD11	1.86	0.56
1:J:106:ARG:NH1	1:J:142:ASP:OD2	2.38	0.56
1:I:120:GLY:O	1:I:145:SER:OG	2.24	0.56
1:I:171:LEU:HD23	1:J:243:THR:HG23	1.86	0.56
1:G:171:LEU:HD23	1:H:243:THR:HG23	1.88	0.55



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:121:PRO:HG3	1:D:148:SER:HB3	1.88	0.55
1:H:121:PRO:HG3	1:H:148:SER:HB3	1.88	0.55
1:P:22:ARG:HD3	1:P:322:LEU:HD23	1.88	0.55
1:D:131:LYS:HA	1:D:135:PHE:CD1	2.40	0.55
1:C:200:SER:HA	1:C:233:PRO:HB3	1.88	0.55
1:F:15:VAL:HG13	1:F:322:LEU:HD11	1.88	0.55
1:M:306:LYS:HB2	1:N:171:LEU:HD13	1.88	0.55
1:A:306:LYS:HB2	1:B:171:LEU:HD13	1.89	0.55
1:C:277:ASP:HB3	1:D:194:ARG:HG2	1.88	0.55
1:F:87:VAL:HG23	1:F:89:VAL:HG23	1.88	0.54
1:K:232:VAL:HG11	1:L:232:VAL:HG11	1.89	0.54
1:0:176:HIS:HB3	1:O:231[B]:ARG:HD3	1.88	0.54
1:I:306:LYS:HE2	1:J:171:LEU:HB3	1.89	0.54
1:M:306:LYS:HE2	1:N:171:LEU:HB3	1.89	0.54
1:P:10:ARG:HH11	1:P:13:ARG:HH21	1.56	0.54
1:D:106:ARG:NH1	1:D:142:ASP:OD2	2.40	0.54
1:I:128:MET:HG2	1:I:145:SER:HB3	1.89	0.54
1:C:280:SER:HB3	1:D:203:ILE:H	1.73	0.54
1:C:72:ARG:NH2	1:C:83:LYS:O	2.42	0.54
1:I:32:ASP:OD1	1:I:33:LEU:N	2.40	0.54
1:K:176:HIS:HB3	1:K:231:ARG:HD3	1.90	0.54
1:I:200:SER:HA	1:I:233:PRO:HB3	1.90	0.53
1:N:87:VAL:HG23	1:N:89:VAL:HG23	1.91	0.53
1:L:121:PRO:HG3	1:L:148:SER:HB3	1.90	0.53
1:E:200:SER:HA	1:E:233:PRO:HB3	1.91	0.53
1:M:192:ASP:OD2	1:M:231[A]:ARG:NH2	2.33	0.53
1:B:127:PRO:HG3	1:B:141:GLN:HE21	1.74	0.53
1:B:200:SER:HA	1:B:233:PRO:HB3	1.90	0.53
1:N:128:MET:HG2	1:N:145:SER:HB3	1.91	0.53
1:G:171:LEU:HG	1:H:306:LYS:HE2	1.91	0.52
1:F:154:LEU:HD11	1:F:242:LEU:HD13	1.91	0.52
1:H:87:VAL:HG23	1:H:89:VAL:HG23	1.92	0.52
1:P:8:PHE:N	1:P:32:ASP:OD2	2.43	0.52
1:H:259:VAL:HG13	1:H:271:LEU:HD21	1.90	0.52
1:B:87:VAL:HG23	1:B:89:VAL:HG23	1.92	0.52
1:F:259:VAL:HG13	1:F:271:LEU:HD21	1.90	0.52
1:B:121:PRO:HG3	1:B:148:SER:HB3	1.91	0.52
1:H:120:GLY:O	1:H:145:SER:OG	2.27	0.52
1:D:87:VAL:HG23	1:D:89:VAL:HG23	1.92	0.52
1:J:22:ARG:HD3	1:J:322:LEU:HD23	1.92	0.51
1:A:232:VAL:HG11	1:B:232:VAL:HG11	1.92	0.51



	A + amp 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:15:VAL:HG13	1:B:322:LEU:HD11	1.92	0.51
1:G:179:THR:OG1	1:G:231[B]:ARG:NH1	2.41	0.51
1:M:168:ILE:HD12	1:M:245:ARG:HG2	1.91	0.51
1:H:200:SER:HA	1:H:233:PRO:HB3	1.91	0.51
1:P:32:ASP:OD1	1:P:33:LEU:N	2.43	0.51
1:B:10:ARG:HH11	1:B:13:ARG:HH21	1.59	0.51
1:N:22:ARG:HD3	1:N:322:LEU:HD23	1.93	0.51
1:M:272:GLY:N	1:M:290:SER:O	2.36	0.51
1:L:154:LEU:HD11	1:L:242:LEU:HD13	1.93	0.51
1:A:171:LEU:HG	1:B:306:LYS:HE2	1.91	0.50
1:0:32:ASP:OD1	1:O:33:LEU:N	2.44	0.50
1:A:306:LYS:HE2	1:B:171:LEU:HB3	1.93	0.50
1:M:32:ASP:OD1	1:M:33:LEU:N	2.45	0.50
1:K:171:LEU:HD23	1:L:243:THR:HG23	1.94	0.50
1:N:10:ARG:HH11	1:N:13:ARG:HH21	1.59	0.50
1:A:106:ARG:NH1	1:A:142:ASP:OD2	2.42	0.49
1:N:149:CYS:HG	2:N:401:AG:AG	1.80	0.49
1:K:173:THR:O	1:K:241:ASP:N	2.44	0.49
1:K:277:ASP:HB3	1:L:194:ARG:HG3	1.95	0.49
1:N:154:LEU:HD11	1:N:242:LEU:HD13	1.95	0.49
1:F:173:THR:HB	1:F:241:ASP:HB3	1.94	0.49
1:H:106:ARG:NH1	1:H:142:ASP:OD2	2.45	0.49
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.48	0.49
1:B:106:ARG:NH1	1:B:142:ASP:OD2	2.45	0.49
1:C:115:LYS:HD3	1:C:328:ILE:HD12	1.95	0.49
1:I:245:ARG:HD2	1:J:245:ARG:HD2	1.95	0.49
1:N:259:VAL:HG13	1:N:271:LEU:HD21	1.94	0.49
1:F:10:ARG:HH11	1:F:13:ARG:HH21	1.59	0.49
1:I:171:LEU:HG	1:J:306:LYS:HE2	1.95	0.49
1:G:32:ASP:OD1	1:G:33:LEU:N	2.44	0.49
1:A:171:LEU:HD23	1:B:243:THR:HG23	1.95	0.49
1:O:306:LYS:HB2	1:P:171:LEU:HD13	1.94	0.49
1:P:87:VAL:HG23	1:P:89:VAL:HG23	1.94	0.49
1:M:245:ARG:HD2	1:N:245:ARG:HD2	1.94	0.49
1:H:272:GLY:N	1:H:290:SER:O	2.41	0.48
1:N:256:LYS:HD2	1:N:294:ALA:HB1	1.94	0.48
1:B:22:ARG:HD3	1:B:322:LEU:HD23	1.93	0.48
1:H:115:LYS:NZ	1:H:328:ILE:O	2.45	0.48
1:I:115:LYS:HD3	1:I:328:ILE:HD12	1.96	0.48
1:K:306:LYS:HB2	1:L:171:LEU:HD13	1.96	0.48
1:I:306:LYS:HB2	1:J:171:LEU:HD13	1.96	0.48



A + a 1		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:J:154:LEU:HD11	1:J:242:LEU:HD13	1.95	0.48
1:J:256:LYS:HD2	1:J:294:ALA:HB1	1.94	0.48
1:C:171:LEU:HD23	1:D:243:THR:HG23	1.95	0.48
1:E:176:HIS:HB3	1:E:231[B]:ARG:HD3	1.96	0.48
1:N:15:VAL:HG13	1:N:322:LEU:HD11	1.96	0.48
1:E:232:VAL:HG11	1:F:232:VAL:HG11	1.94	0.48
1:J:106:ARG:HD3	1:J:109:ILE:HD12	1.96	0.48
1:P:259:VAL:HG13	1:P:271:LEU:HD21	1.95	0.48
1:F:58:GLU:HG2	1:F:65:ILE:HB	1.95	0.47
1:J:82:LEU:HD13	1:J:84:TRP:CZ2	2.48	0.47
1:N:127:PRO:HG3	1:N:141:GLN:HE21	1.78	0.47
1:L:106:ARG:NH1	1:L:142:ASP:OD2	2.47	0.47
1:L:256:LYS:HD2	1:L:294:ALA:HB1	1.95	0.47
1:N:200:SER:HA	1:N:233:PRO:HB3	1.95	0.47
1:C:232:VAL:HG11	1:D:232:VAL:HG11	1.96	0.47
1:G:232:VAL:HG11	1:H:232:VAL:HG11	1.96	0.47
1:G:259:VAL:HG13	1:G:271:LEU:HD21	1.96	0.47
1:G:200:SER:HA	1:G:233:PRO:HB3	1.95	0.47
1:B:58:GLU:HG2	1:B:65:ILE:HB	1.95	0.47
1:F:22:ARG:HD3	1:F:322:LEU:HD23	1.96	0.47
1:E:94:GLU:OE2	1:E:96:THR:OG1	2.23	0.47
1:J:94:GLU:OE2	1:J:96:THR:OG1	2.27	0.47
1:P:84:TRP:HB3	1:P:89:VAL:HB	1.97	0.47
1:P:173:THR:HB	1:P:241:ASP:HB3	1.96	0.47
1:B:256:LYS:HD2	1:B:294:ALA:HB1	1.96	0.47
1:D:131:LYS:CA	1:D:135:PHE:CE1	2.98	0.47
1:0:179:THR:OG1	1:O:231[B]:ARG:NH1	2.48	0.47
1:J:121:PRO:HG3	1:J:148:SER:HB3	1.96	0.47
1:P:115:LYS:NZ	1:P:328:ILE:O	2.39	0.47
1:P:200:SER:HA	1:P:233:PRO:HB3	1.96	0.47
1:I:171:LEU:HB2	1:J:304:PHE:CE2	2.50	0.46
1:G:72:ARG:NH2	1:G:83:LYS:O	2.49	0.46
1:G:154:LEU:HD11	1:G:242:LEU:HD13	1.98	0.46
1:M:128:MET:HG2	1:M:145:SER:HB3	1.98	0.46
1:M:170:GLY:HA3	1:M:225:LEU:HD23	1.96	0.46
1:N:58:GLU:HG2	1:N:65:ILE:HB	1.97	0.46
1:G:245:ARG:HD2	1:H:245:ARG:HD2	1.97	0.46
1:I:78:GLY:O	1:I:80:ALA:N	2.43	0.46
1:G:306:LYS:HB2	1:H:171:LEU:HD13	1.98	0.46
1:G:82:LEU:HD13	1:G:84:TRP:CZ2	2.51	0.46
1:K:120:GLY:O	1:K:145:SER:OG	2.29	0.46



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:H:58:GLU:HG2	1:H:65:ILE:HB	1.98	0.46
1:I:135:PHE:O	1:I:327:HIS:NE2	2.48	0.46
1:O:200:SER:HA	1:O:233:PRO:HB3	1.97	0.46
1:P:84:TRP:CE3	1:P:89:VAL:HG21	2.51	0.46
1:J:131:LYS:HG2	1:J:270:VAL:HG21	1.98	0.46
1:A:200:SER:HA	1:A:233:PRO:HB3	1.98	0.46
1:E:198:GLY:O	1:E:202:ASN:ND2	2.41	0.46
1:I:72:ARG:NH1	1:I:82:LEU:O	2.49	0.46
1:M:171:LEU:HB2	1:N:304:PHE:CE2	2.51	0.46
1:D:131:LYS:HB2	1:D:135:PHE:CZ	2.51	0.45
1:M:171:LEU:HD12	1:M:171:LEU:HA	1.82	0.45
1:P:168:ILE:HD11	1:P:247:GLU:HA	1.99	0.45
1:C:10:ARG:HH11	1:C:13:ARG:NH2	2.15	0.45
1:F:153:CYS:HA	1:F:290:SER:HB2	1.99	0.45
1:I:232:VAL:HG11	1:J:232:VAL:HG11	1.98	0.45
1:A:32:ASP:OD1	1:A:33:LEU:N	2.48	0.45
1:D:58:GLU:HG2	1:D:65:ILE:HB	1.98	0.45
1:C:203:ILE:H	1:D:280:SER:HB3	1.82	0.45
1:I:154:LEU:HD11	1:I:242:LEU:HD13	1.97	0.45
1:A:79:PRO:HB2	1:A:107:LYS:HB2	1.98	0.45
1:C:82:LEU:HD13	1:C:84:TRP:CZ2	2.52	0.45
1:G:243:THR:HG23	1:H:171:LEU:HD12	1.99	0.45
1:J:85:ASP:OD1	1:J:85:ASP:N	2.50	0.45
1:O:243:THR:HG23	1:P:171:LEU:HD12	1.99	0.45
1:D:15:VAL:HG13	1:D:322:LEU:HD11	1.99	0.44
1:E:203:ILE:H	1:F:280:SER:HB3	1.82	0.44
1:K:136:ASP:N	1:K:136:ASP:OD1	2.50	0.44
1:K:239:VAL:HB	1:K:310:TRP:CE3	2.52	0.44
1:B:154:LEU:HD11	1:B:242:LEU:HD13	1.99	0.44
1:E:238:SER:HB2	1:E:311:TYR:CZ	2.52	0.44
1:F:3:VAL:HB	1:F:27:ILE:HD13	1.99	0.44
1:H:15:VAL:HG13	1:H:322:LEU:HD11	1.98	0.44
1:J:58:GLU:HG2	1:J:65:ILE:HB	1.99	0.44
1:K:171:LEU:HB2	1:L:304:PHE:CE2	2.52	0.44
1:F:82:LEU:HD13	1:F:84:TRP:CZ2	2.53	0.44
1:P:121:PRO:HG3	1:P:148:SER:HB3	1.98	0.44
1:B:38:ASP:HA	1:B:59:VAL:HG21	1.99	0.44
1:P:85:ASP:OD1	1:P:85:ASP:N	2.51	0.44
1:F:24:ASP:OD1	1:F:24:ASP:N	2.49	0.44
1:G:171:LEU:HB2	1:H:304:PHE:CE2	2.53	0.44
1:J:10:ARG:HH11	1:J:13:ARG:HH21	1.66	0.44



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:16:PHE:CE2	1:B:44:LEU:HD11	2.52	0.44
1:J:120:GLY:O	1:J:145:SER:OG	2.32	0.44
1:O:259:VAL:HG13	1:O:271:LEU:HD21	2.00	0.44
1:E:259:VAL:HG13	1:E:271:LEU:HD21	2.00	0.44
1:F:238:SER:HB2	1:F:311:TYR:CZ	2.52	0.44
1:J:238:SER:HB2	1:J:311:TYR:CZ	2.53	0.44
1:L:8:PHE:N	1:L:32:ASP:OD2	2.48	0.44
1:O:194:ARG:HG2	1:P:277:ASP:HB3	1.99	0.44
1:C:306:LYS:HE2	1:D:171:LEU:HB3	1.99	0.43
1:O:153:CYS:HA	1:O:290:SER:HB2	2.00	0.43
1:L:17:ARG:NH2	1:L:51:GLY:O	2.49	0.43
1:0:173:THR:0	1:O:241:ASP:N	2.51	0.43
1:F:22:ARG:NH1	1:F:323:ASP:OD1	2.50	0.43
1:A:194:ARG:NH1	1:B:278:VAL:O	2.50	0.43
1:F:68:GLY:HA3	1:J:265:GLY:HA2	1.99	0.43
1:F:84:TRP:HB3	1:F:89:VAL:HB	2.01	0.43
1:G:120:GLY:O	1:G:145:SER:OG	2.32	0.43
1:H:256:LYS:HD2	1:H:294:ALA:HB1	2.00	0.43
1:K:300:LEU:HD23	1:L:226:THR:HG22	2.01	0.43
1:M:15:VAL:HG13	1:M:322:LEU:HD21	2.01	0.43
1:M:25:ILE:HG21	1:M:322:LEU:HD12	2.00	0.43
1:M:259:VAL:HG13	1:M:271:LEU:HD21	1.99	0.43
1:E:130:VAL:HG23	1:E:217:VAL:HG11	2.00	0.43
1:F:23:SER:HB2	1:J:327:HIS:ND1	2.34	0.43
1:E:204:ILE:HB	1:E:231[B]:ARG:HB2	2.01	0.43
1:J:38:ASP:HA	1:J:59:VAL:HG21	2.00	0.43
1:C:242:LEU:HG	1:C:244:VAL:HG13	2.01	0.43
1:D:3:VAL:HB	1:D:27:ILE:HD13	2.01	0.43
1:I:239:VAL:HB	1:I:310:TRP:CE3	2.54	0.43
1:A:228:MET:HE3	1:A:228:MET:HB2	1.97	0.43
1:A:238:SER:HB2	1:A:311:TYR:CZ	2.54	0.43
1:C:243:THR:HG23	1:D:171:LEU:HD12	2.00	0.43
1:J:198:GLY:O	1:J:202:ASN:ND2	2.44	0.43
1:K:171:LEU:HG	1:L:306:LYS:HE2	2.00	0.43
1:O:232:VAL:HG11	1:P:232:VAL:HG11	2.01	0.43
1:G:238:SER:HB2	1:G:311:TYR:CZ	2.54	0.43
1:K:238:SER:HB2	1:K:311:TYR:CZ	2.54	0.43
1:0:115:LYS:HD3	1:O:328:ILE:HD12	1.99	0.43
1:E:82:LEU:HD13	1:E:84:TRP:CZ2	2.54	0.42
1:G:277:ASP:HB3	1:H:194:ARG:HG2	2.00	0.42
1:J:128:MET:HG2	1:J:145:SER:HB3	2.00	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:P:129:PHE:HD2	1:P:144:VAL:HG13	1.84	0.42
1:C:32:ASP:OD1	1:C:33:LEU:N	2.47	0.42
1:C:259:VAL:HG13	1:C:271:LEU:HD21	2.01	0.42
1:D:85:ASP:OD1	1:D:85:ASP:N	2.51	0.42
1:E:194:ARG:HG3	1:F:277:ASP:HB3	2.00	0.42
1:N:286:GLU:HG3	1:N:288:CYS:H	1.84	0.42
1:E:170:GLY:HA3	1:E:225:LEU:HD23	2.01	0.42
1:H:16:PHE:CE2	1:H:44:LEU:HD11	2.54	0.42
1:L:153:CYS:HA	1:L:290:SER:HB2	2.01	0.42
1:C:171:LEU:HD12	1:C:171:LEU:HA	1.82	0.42
1:L:85:ASP:OD1	1:L:85:ASP:N	2.51	0.42
1:N:16:PHE:CE2	1:N:44:LEU:HD11	2.54	0.42
1:P:84:TRP:HE3	1:P:89:VAL:HG21	1.84	0.42
1:D:170:GLY:HA3	1:D:244:VAL:HG12	2.00	0.42
1:P:154:LEU:HD11	1:P:242:LEU:HD13	2.01	0.42
1:D:259:VAL:HG13	1:D:271:LEU:HD21	2.01	0.42
1:F:84:TRP:CE3	1:F:89:VAL:HG21	2.54	0.42
1:I:238:SER:HB2	1:I:311:TYR:CZ	2.55	0.42
1:L:157:LEU:HD22	1:L:309:SER:HB2	2.02	0.42
1:M:238:SER:HB2	1:M:311:TYR:CZ	2.55	0.42
1:O:238:SER:HB2	1:0:311:TYR:CZ	2.55	0.42
1:A:45:LYS:HD2	1:A:46:TYR:CE2	2.55	0.42
1:D:16:PHE:CE2	1:D:44:LEU:HD11	2.55	0.42
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.54	0.42
1:C:172:MET:HG3	1:C:227:GLY:HA3	2.01	0.42
1:K:154:LEU:HD11	1:K:242:LEU:HD13	2.01	0.42
1:F:256:LYS:HD2	1:F:294:ALA:HB1	2.02	0.42
1:M:232:VAL:HG11	1:N:232:VAL:HG11	2.01	0.42
1:A:87:VAL:HG13	1:A:89:VAL:HG23	2.02	0.41
1:A:136:ASP:OD1	1:A:136:ASP:N	2.53	0.41
1:B:3:VAL:HB	1:B:27:ILE:HD13	2.02	0.41
1:E:62:GLY:O	1:E:63:HIS:ND1	2.53	0.41
1:P:106:ARG:NH1	1:P:142:ASP:OD2	2.53	0.41
1:C:154:LEU:HD11	1:C:242:LEU:HD13	2.01	0.41
1:E:171:LEU:HD12	1:E:171:LEU:HA	1.82	0.41
1:P:127:PRO:HG3	1:P:141:GLN:HE21	1.85	0.41
1:B:160:VAL:O	1:B:164:ASN:ND2	2.38	0.41
1:C:300:LEU:HD23	1:D:226:THR:HG22	2.02	0.41
1:E:10:ARG:O	1:E:14:ILE:HG12	2.20	0.41
1:O:239:VAL:HB	1:O:310:TRP:CE3	2.56	0.41
1:A:72:ARG:HD3	1:A:74:THR:HG23	2.01	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:171:LEU:HB2	1:B:304:PHE:CE2	2.55	0.41
1:F:84:TRP:HE3	1:F:89:VAL:HG21	1.85	0.41
1:G:172:MET:HG3	1:G:227:GLY:HA3	2.02	0.41
1:H:286:GLU:HG3	1:H:288:CYS:H	1.86	0.41
1:I:10:ARG:O	1:I:14:ILE:HG12	2.20	0.41
1:I:194:ARG:HG3	1:J:277:ASP:HB3	2.03	0.41
1:P:82:LEU:HD13	1:P:84:TRP:CZ2	2.55	0.41
1:E:32:ASP:OD1	1:E:33:LEU:N	2.47	0.41
1:J:200:SER:HA	1:J:233:PRO:HB3	2.02	0.41
1:K:82:LEU:HD13	1:K:84:TRP:CZ2	2.56	0.41
1:A:115:LYS:HD3	1:A:328:ILE:HD12	2.03	0.41
1:D:131:LYS:HA	1:D:135:PHE:CE1	2.56	0.41
1:J:10:ARG:HD2	1:J:10:ARG:HA	1.88	0.41
1:M:78:GLY:HA2	1:M:79:PRO:HD3	1.95	0.41
1:M:239:VAL:HB	1:M:310:TRP:CE3	2.56	0.41
1:A:25:ILE:HD12	1:A:322:LEU:HB3	2.02	0.41
1:L:136:ASP:OD1	1:L:136:ASP:N	2.53	0.41
1:N:238:SER:HB2	1:N:311:TYR:CZ	2.56	0.41
1:B:149:CYS:HB3	1:B:317:TYR:HB2	2.03	0.41
1:G:300:LEU:HD13	1:H:169:GLU:HB2	2.02	0.41
1:K:3:VAL:HB	1:K:27:ILE:HD13	2.03	0.41
1:M:243:THR:HG23	1:N:171:LEU:HD12	2.02	0.41
1:B:238:SER:HB2	1:B:311:TYR:CZ	2.56	0.41
1:L:82:LEU:HD13	1:L:84:TRP:CZ2	2.56	0.41
1:0:192:ASP:OD2	1:O:231[A]:ARG:NH2	2.50	0.41
1:E:131:LYS:HD2	1:E:135:PHE:CE2	2.55	0.40
1:F:200:SER:HA	1:F:233:PRO:HB3	2.01	0.40
1:H:131:LYS:HG2	1:H:270:VAL:HG21	2.03	0.40
1:I:172:MET:HG3	1:I:227:GLY:HA3	2.03	0.40
1:A:173:THR:O	1:A:241:ASP:N	2.54	0.40
1:J:8:PHE:N	1:J:32:ASP:OD2	2.49	0.40
1:K:172:MET:HG2	1:K:211:ALA:HB2	2.02	0.40
1:L:16:PHE:CE2	1:L:44:LEU:HD11	2.56	0.40
1:M:154:LEU:HD11	1:M:242:LEU:HD13	2.02	0.40
1:O:275:GLU:HG2	1:O:294:ALA:HB3	2.03	0.40
1:G:87:VAL:HG13	1:G:89:VAL:HG23	2.03	0.40
1:C:136:ASP:OD1	1:C:136:ASP:N	2.54	0.40
1:I:84:TRP:HB3	1:I:89:VAL:HB	2.04	0.40
1:J:16:PHE:CE2	1:J:44:LEU:HD11	2.57	0.40
1:L:10:ARG:HA	1:L:10:ARG:HD2	1.86	0.40
1:O:94:GLU:OE2	1:O:96:THR:OG1	2.27	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:16:PHE:CE2	1:P:44:LEU:HD11	2.57	0.40
1:P:155:ALA:HB3	1:P:156:PRO:HD3	2.02	0.40
1:B:283:PHE:CE1	1:B:291:VAL:HG11	2.57	0.40
1:M:94:GLU:OE2	1:M:96:THR:OG1	2.27	0.40
1:N:136:ASP:OD1	1:N:136:ASP:N	2.55	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	Perce	ntiles
1	А	327/329~(99%)	305~(93%)	20~(6%)	2(1%)	25	59
1	В	327/329~(99%)	304 (93%)	22 (7%)	1 (0%)	41	73
1	С	327/329~(99%)	307~(94%)	18 (6%)	2 (1%)	25	59
1	D	327/329~(99%)	305~(93%)	21 (6%)	1 (0%)	41	73
1	Е	328/329~(100%)	309 (94%)	17 (5%)	2 (1%)	25	59
1	F	327/329~(99%)	303~(93%)	23~(7%)	1 (0%)	41	73
1	G	328/329~(100%)	310 (94%)	16 (5%)	2 (1%)	25	59
1	Н	327/329~(99%)	309 (94%)	17 (5%)	1 (0%)	41	73
1	Ι	328/329~(100%)	304 (93%)	22 (7%)	2 (1%)	25	59
1	J	327/329~(99%)	306 (94%)	20 (6%)	1 (0%)	41	73
1	K	327/329~(99%)	308 (94%)	17 (5%)	2 (1%)	25	59
1	L	327/329~(99%)	306 (94%)	20 (6%)	1 (0%)	41	73
1	М	328/329~(100%)	308 (94%)	18 (6%)	2 (1%)	25	59
1	Ν	327/329~(99%)	306 (94%)	20 (6%)	1 (0%)	41	73
1	Ο	328/329~(100%)	311 (95%)	14 (4%)	3 (1%)	17	52
1	Р	327/329~(99%)	308 (94%)	18 (6%)	1 (0%)	41	73



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5237/5264~(100%)	4909 (94%)	303~(6%)	25~(0%)	29 64

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	186	ASP
1	G	186	ASP
1	М	186	ASP
1	А	186	ASP
1	Е	186	ASP
1	F	237	VAL
1	Н	237	VAL
1	Ι	186	ASP
1	Ι	237	VAL
1	Κ	186	ASP
1	В	237	VAL
1	С	237	VAL
1	Е	237	VAL
1	G	237	VAL
1	Κ	237	VAL
1	L	237	VAL
1	Ν	237	VAL
1	0	237	VAL
1	Р	237	VAL
1	A	237	VAL
1	D	237	VAL
1	J	237	VAL
1	М	237	VAL
1	0	186	ASP
1	0	166	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	239/263~(91%)	237~(99%)	2(1%)	81 92



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	В	246/263~(94%)	243~(99%)	3~(1%)	71	88
1	\mathbf{C}	239/263~(91%)	235~(98%)	4(2%)	60	83
1	D	246/263~(94%)	245~(100%)	1 (0%)	91	96
1	Ε	240/263~(91%)	237~(99%)	3~(1%)	69	87
1	F	246/263~(94%)	244 (99%)	2(1%)	81	92
1	G	240/263~(91%)	238~(99%)	2(1%)	81	92
1	Η	245/263~(93%)	243~(99%)	2(1%)	81	92
1	Ι	239/263~(91%)	236~(99%)	3~(1%)	69	87
1	J	246/263~(94%)	245 (100%)	1 (0%)	91	96
1	Κ	236/263~(90%)	234 (99%)	2(1%)	81	92
1	L	246/263~(94%)	244 (99%)	2(1%)	81	92
1	М	240/263~(91%)	238~(99%)	2(1%)	81	92
1	Ν	246/263~(94%)	246 (100%)	0	100	100
1	О	240/263~(91%)	238~(99%)	2 (1%)	81	92
1	Р	246/263~(94%)	244 (99%)	2 (1%)	81	92
All	All	3880/4208~(92%)	3847~(99%)	33 (1%)	78	91

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	149	CYS
1	А	172	MET
1	В	135	PHE
1	В	141	GLN
1	В	149	CYS
1	С	8	PHE
1	С	39	TYR
1	С	149	CYS
1	С	172	MET
1	D	149	CYS
1	Е	39	TYR
1	Е	149	CYS
1	Е	172	MET
1	F	149	CYS
1	F	228	MET
1	G	149	CYS
1	G	172	MET



Mol	Chain	Res	Type
1	Н	135	PHE
1	Н	149	CYS
1	Ι	39	TYR
1	Ι	149	CYS
1	Ι	172	MET
1	J	149	CYS
1	Κ	8	PHE
1	Κ	172	MET
1	L	141	GLN
1	L	149	CYS
1	М	149	CYS
1	М	172	MET
1	0	135	PHE
1	0	172	MET
1	Р	141	GLN
1	Р	149	CYS

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

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)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\langle RSRZ \rangle$	$\# RSRZ {>}2$	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	329/329~(100%)	-0.08	0 100 100	51, 85, 115, 149	0
1	В	329/329~(100%)	-0.19	0 100 100	49, 73, 106, 133	0
1	С	329/329~(100%)	-0.08	3 (0%) 84 69	51, 85, 123, 140	0
1	D	329/329~(100%)	-0.10	0 100 100	46, 75, 111, 150	0
1	E	329/329~(100%)	-0.01	1 (0%) 94 88	65, 90, 127, 165	0
1	F	329/329~(100%)	-0.01	2 (0%) 89 78	57, 87, 118, 141	0
1	G	329/329~(100%)	-0.05	0 100 100	52, 89, 125, 157	0
1	Н	329/329~(100%)	0.03	3 (0%) 84 69	53, 103, 135, 167	0
1	Ι	329/329~(100%)	0.17	9 (2%) 54 31	60, 120, 155, 187	0
1	J	329/329~(100%)	0.02	0 100 100	56, 89, 129, 153	0
1	K	329/329~(100%)	0.28	10 (3%) 50 27	71, 120, 158, 174	0
1	L	329/329~(100%)	-0.03	1 (0%) 94 88	57, 84, 120, 167	0
1	М	329/329~(100%)	0.21	8 (2%) 59 37	66, 121, 155, 198	0
1	N	329/329~(100%)	0.29	15 (4%) 32 16	69, 123, 162, 197	0
1	Ο	329/329~(100%)	-0.11	0 100 100	56, 81, 120, 161	0
1	Р	329/329~(100%)	-0.12	0 100 100	53, 71, 95, 146	0
All	All	5264/5264 (100%)	0.01	52 (0%) 82 67	46, 90, 143, 198	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Ι	241	ASP	5.8
1	Ν	93	ALA	3.9
1	Ν	144	VAL	3.8
1	N	241	ASP	3.6
1	Κ	62	GLY	3.6



6IO4

Mol	Chain	Res	Type	RSRZ
1	K	118	MET	3.4
1	K	8	PHE	3.2
1	Κ	5	ILE	3.2
1	Ν	167	ILE	3.1
1	Ι	173	THR	2.9
1	М	241	ASP	2.9
1	Ι	167	ILE	2.9
1	Ι	246	LEU	2.9
1	Ι	82	LEU	2.8
1	М	169	GLU	2.8
1	Κ	223	GLY	2.7
1	Ν	171	LEU	2.7
1	Ν	198	GLY	2.7
1	N	172	MET	2.6
1	Ι	158	ALA	2.5
1	М	300	LEU	2.5
1	Κ	143	ILE	2.5
1	Κ	178	THR	2.5
1	L	178	THR	2.5
1	Ν	174	THR	2.5
1	N	118	MET	2.4
1	М	279	VAL	2.4
1	Н	241	ASP	2.4
1	Κ	30	ILE	2.4
1	Н	117	VAL	2.3
1	Ν	231	ARG	2.3
1	Е	93	ALA	2.3
1	Κ	234	THR	2.3
1	Ι	169	GLU	2.3
1	Н	173	THR	2.3
1	Κ	240	VAL	2.2
1	Ν	246	LEU	2.2
1	М	234	THR	2.2
1	Ι	90	ASP	2.2
1	М	117	VAL	2.2
1	М	93	ALA	2.2
1	C	241	ASP	2.2
1	F	241	ASP	2.2
1	Ι	5	ILE	2.1
1	М	167	ILE	2.1
1	C	3	VAL	2.1
1	Ν	8	PHE	2.1



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	Ν	146	ASN	2.1
1	Ν	117	VAL	2.0
1	N	157	LEU	2.0
1	F	308	VAL	2.0
1	С	4	GLY	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	AG	Р	401	1/1	0.84	0.43	175,175,175,175	1
2	AG	Ν	401	1/1	0.90	0.19	98,98,98,98	1
2	AG	K	401	1/1	0.93	0.20	101,101,101,101	1
2	AG	Ι	401	1/1	0.95	0.14	92,92,92,92	1
2	AG	А	401	1/1	0.96	0.27	112,112,112,112	1
2	AG	В	401	1/1	0.96	0.36	154,154,154,154	1
2	AG	L	401	1/1	0.96	0.32	144,144,144,144	0
2	AG	М	401	1/1	0.96	0.15	82,82,82,82	1
2	AG	F	401	1/1	0.96	0.23	112,112,112,112	1
2	AG	G	401	1/1	0.96	0.28	129,129,129,129	1
2	AG	J	401	1/1	0.97	0.28	113,113,113,113	1
2	AG	Е	401	1/1	0.97	0.19	96,96,96,96	1
2	AG	D	401	1/1	0.97	0.27	112,112,112,112	1
2	AG	0	401	1/1	0.98	0.15	76,76,76,76	1
2	AG	Н	401	1/1	0.98	0.11	82,82,82,82	1
2	AG	С	401	1/1	0.99	0.18	79,79,79,79	1



6.5 Other polymers (i)

There are no such residues in this entry.

