Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 08:57 PM EST

PDB ID	:	1ZOI
Title	:	Crystal Structure of a Stereoselective Esterase from Pseudomonas putida IFO12996
Authors	:	Elmi, F.; Lee, H.T.; Huang, J.Y.; Hsieh, Y.C.; Wang, Y.L.; Chen, Y.J.; Shaw, S.Y.; Chen, C.J.
Deposited on	:	2005-05-13
Resolution	:	1.60 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 (i)) were used in the production of this report:

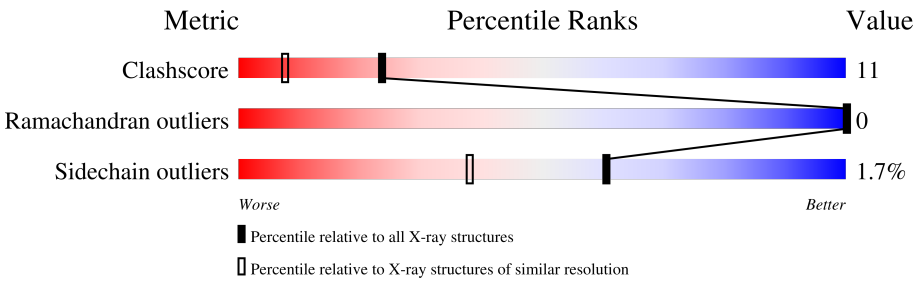
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.60 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))
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	276	81% 18%
1	B	276	79% 19% • •
1	C	276	82% 16% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6694 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 esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	2128	1355	379	388	6	0	0	0
1	B	274	2121	1352	378	385	6	0	0	0
1	C	275	2128	1355	379	388	6	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	LEU	MET	conflict	UNP Q3HWU8
A	112	GLU	ALA	conflict	UNP Q3HWU8
A	133	GLY	ASP	conflict	UNP Q3HWU8
A	175	GLU	ASP	conflict	UNP Q3HWU8
A	216	GLN	THR	conflict	UNP Q3HWU8
A	237	VAL	LEU	conflict	UNP Q3HWU8
A	247	ALA	THR	conflict	UNP Q3HWU8
A	252	LYS	GLN	conflict	UNP Q3HWU8
B	42	LEU	MET	conflict	UNP Q3HWU8
B	112	GLU	ALA	conflict	UNP Q3HWU8
B	133	GLY	ASP	conflict	UNP Q3HWU8
B	175	GLU	ASP	conflict	UNP Q3HWU8
B	216	GLN	THR	conflict	UNP Q3HWU8
B	237	VAL	LEU	conflict	UNP Q3HWU8
B	247	ALA	THR	conflict	UNP Q3HWU8
B	252	LYS	GLN	conflict	UNP Q3HWU8
C	42	LEU	MET	conflict	UNP Q3HWU8
C	112	GLU	ALA	conflict	UNP Q3HWU8
C	133	GLY	ASP	conflict	UNP Q3HWU8
C	175	GLU	ASP	conflict	UNP Q3HWU8
C	216	GLN	THR	conflict	UNP Q3HWU8
C	237	VAL	LEU	conflict	UNP Q3HWU8
C	247	ALA	THR	conflict	UNP Q3HWU8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	252	LYS	GLN	conflict	UNP Q3HWU8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	126	Total O 126 126	0	0
2	B	111	Total O 111 111	0	0
2	C	80	Total O 80 80	0	0

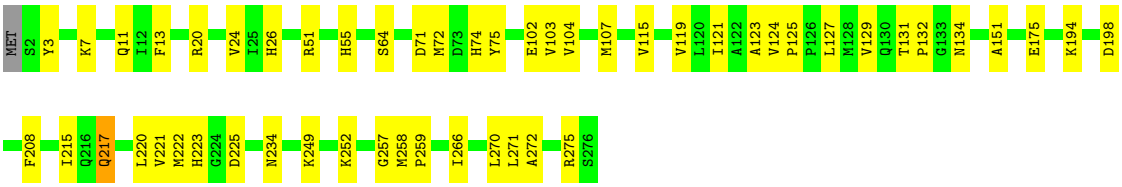
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

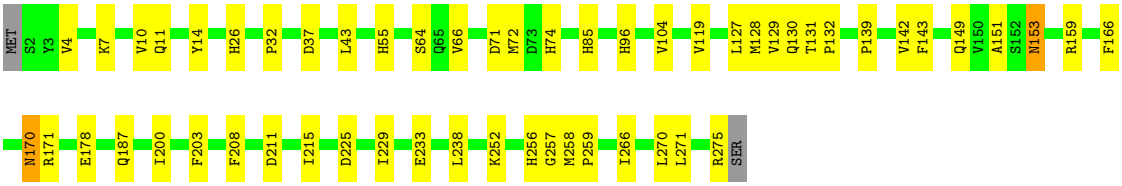
• Molecule 1: esterase

Chain A:



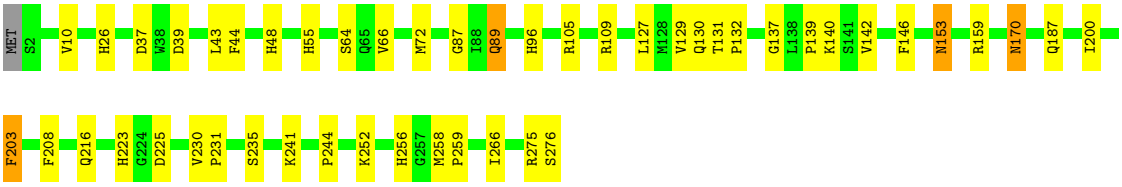
• Molecule 1: esterase

Chain B:



• Molecule 1: esterase

Chain C:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	50.56Å 98.11Å 153.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6694	wwPDB-VP
Average B, all atoms ($Å^2$)	17.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.31	0/2195	0.60	0/2990
1	B	0.31	0/2188	0.60	0/2982
1	C	0.30	0/2195	0.58	0/2990
All	All	0.30	0/6578	0.59	0/8962

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	A	2128	0	2023	49	0
1	B	2121	0	2018	50	0
1	C	2128	0	2023	42	0
2	A	126	0	0	1	0
2	B	111	0	0	2	0
2	C	80	0	0	1	0
All	All	6694	0	6064	139	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 11.

All (139) 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:C:10:VAL:HG22	1:C:66:VAL:HG21	1.50	0.91
1:B:139:PRO:O	1:B:142:VAL:HG12	1.69	0.91
1:B:10:VAL:HG22	1:B:66:VAL:HG21	1.54	0.89
1:A:72:MET:HE2	1:A:102:GLU:HA	1.53	0.88
1:A:217:GLN:H	1:A:217:GLN:HE21	1.22	0.88
1:B:127:LEU:HD21	1:B:129:VAL:HG12	1.64	0.79
1:C:225:ASP:OD2	1:C:252:LYS:HA	1.83	0.78
1:A:103:VAL:HG12	1:A:107:MET:HE2	1.65	0.78
1:A:222:MET:HE1	1:A:266:ILE:HG23	1.68	0.76
1:C:127:LEU:HD11	1:C:129:VAL:HG12	1.65	0.76
1:B:4:VAL:HG13	1:B:14:TYR:CE1	2.22	0.74
1:B:166:PHE:HA	1:B:229:ILE:HD11	1.69	0.72
1:A:271:LEU:HG	1:A:275:ARG:NH1	2.04	0.71
1:B:72:MET:HG2	1:B:208:PHE:HE1	1.56	0.70
1:A:222:MET:CE	1:A:266:ILE:HD12	2.21	0.70
1:A:220:LEU:HD12	1:A:222:MET:HG3	1.75	0.69
1:A:121:ILE:HG23	1:A:222:MET:HE2	1.76	0.67
1:A:222:MET:HE3	1:A:266:ILE:HD12	1.77	0.67
1:B:4:VAL:HG12	1:B:85:HIS:CD2	2.30	0.67
1:C:259:PRO:HG2	2:C:329:HOH:O	1.95	0.67
1:C:259:PRO:HA	1:C:266:ILE:HD12	1.76	0.66
1:B:4:VAL:HG13	1:B:14:TYR:HE1	1.60	0.66
1:A:72:MET:CE	1:A:75:TYR:HD2	2.09	0.65
1:B:131:THR:HB	1:B:132:PRO:HD2	1.79	0.65
1:C:130:GLN:HB2	1:C:137:GLY:O	1.97	0.65
1:C:258:MET:HG3	1:C:266:ILE:HD11	1.80	0.63
1:A:271:LEU:HG	1:A:275:ARG:HH11	1.62	0.62
1:A:72:MET:HE3	1:A:75:TYR:HD2	1.63	0.62
1:B:229:ILE:HD12	1:B:256:HIS:CD2	2.35	0.62
1:B:271:LEU:HD21	1:B:275:ARG:NH2	2.15	0.62
1:B:258:MET:N	1:B:259:PRO:HD2	2.15	0.62
1:C:131:THR:HB	1:C:132:PRO:HD2	1.82	0.62
1:B:151:ALA:HA	1:C:43:LEU:HD12	1.82	0.60
1:C:275:ARG:HH11	1:C:275:ARG:HG2	1.67	0.59
1:C:231:PRO:O	1:C:235:SER:HB2	2.03	0.59
1:A:131:THR:HB	1:A:132:PRO:HD2	1.85	0.58
1:B:259:PRO:HA	1:B:266:ILE:HD12	1.86	0.58
1:C:87:GLY:HA2	1:C:89:GLN:HE22	1.68	0.58
1:A:220:LEU:HD13	1:A:221:VAL:N	2.19	0.58
1:A:194:LYS:HE3	1:A:198:ASP:OD2	2.04	0.58
1:B:72:MET:HG2	1:B:208:PHE:CE1	2.37	0.57
1:A:72:MET:HE3	1:A:75:TYR:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:MET:HG2	1:C:208:PHE:CE1	2.41	0.56
1:A:72:MET:HE3	1:A:75:TYR:HB2	1.87	0.56
1:C:275:ARG:O	1:C:276:SER:HB3	2.05	0.55
1:A:72:MET:HE3	1:A:72:MET:HA	1.89	0.55
1:C:72:MET:HG2	1:C:208:PHE:HE1	1.72	0.55
1:A:107:MET:HE3	1:A:215:ILE:HD13	1.89	0.54
1:A:151:ALA:HA	1:B:43:LEU:HD12	1.90	0.54
1:A:127:LEU:C	1:A:127:LEU:HD13	2.27	0.53
1:A:72:MET:HG2	1:A:208:PHE:HE1	1.72	0.53
1:B:11:GLN:HB2	1:B:64:SER:OG	2.08	0.53
1:C:259:PRO:CA	1:C:266:ILE:HD12	2.38	0.53
1:B:170:ASN:HD22	1:B:171:ARG:N	2.06	0.53
1:A:258:MET:N	1:A:259:PRO:HD2	2.23	0.52
1:B:127:LEU:HD23	1:B:128:MET:N	2.25	0.52
1:A:72:MET:HG2	1:A:208:PHE:CE1	2.45	0.52
1:A:220:LEU:CD1	1:A:222:MET:HG3	2.40	0.52
1:B:238:LEU:HD12	1:B:238:LEU:N	2.26	0.51
1:B:257:GLY:C	1:B:259:PRO:HD2	2.31	0.51
1:A:115:VAL:O	1:A:217:GLN:HG2	2.10	0.51
1:C:87:GLY:CA	1:C:89:GLN:HE22	2.24	0.51
1:A:72:MET:CE	1:A:102:GLU:HA	2.35	0.51
1:B:225:ASP:OD2	1:B:252:LYS:HA	2.11	0.51
1:C:140:LYS:NZ	1:C:140:LYS:HB3	2.26	0.51
1:A:222:MET:HE1	1:A:266:ILE:HD12	1.92	0.50
1:C:89:GLN:H	1:C:89:GLN:CD	2.13	0.50
1:C:203:PHE:C	1:C:203:PHE:CD1	2.85	0.50
1:B:142:VAL:HG13	1:B:143:PHE:N	2.26	0.50
1:C:37:ASP:HB2	1:C:187:GLN:HE22	1.76	0.49
1:A:26:HIS:HE1	1:A:55:HIS:ND1	2.11	0.49
1:A:11:GLN:HB2	1:A:64:SER:OG	2.13	0.48
1:A:127:LEU:CD1	1:A:129:VAL:O	2.61	0.48
1:B:104:VAL:HG12	1:B:211:ASP:CB	2.43	0.48
1:A:217:GLN:HE21	1:A:217:GLN:N	2.03	0.48
1:B:71:ASP:OD1	1:B:74:HIS:HD2	1.96	0.48
1:C:170:ASN:HD22	1:C:170:ASN:N	2.11	0.48
1:C:216:GLN:NE2	1:C:244:PRO:HG3	2.28	0.48
1:C:275:ARG:HG2	1:C:275:ARG:NH1	2.28	0.48
1:B:166:PHE:CD2	1:B:229:ILE:CD1	2.97	0.47
1:B:149:GLN:NE2	1:B:153:ASN:HD21	2.12	0.47
1:B:170:ASN:HD22	1:B:170:ASN:N	2.11	0.47
1:C:153:ASN:N	1:C:153:ASN:HD22	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASN:HD22	1:B:153:ASN:N	2.12	0.47
1:C:26:HIS:HE1	1:C:55:HIS:ND1	2.13	0.47
1:C:258:MET:N	1:C:259:PRO:HD2	2.30	0.46
1:B:233:GLU:O	1:B:238:LEU:CD1	2.64	0.46
1:A:71:ASP:OD1	1:A:74:HIS:HD2	1.99	0.46
1:C:105:ARG:O	1:C:109:ARG:HG2	2.15	0.46
1:A:225:ASP:OD2	1:A:252:LYS:HA	2.16	0.46
1:B:104:VAL:HG12	1:B:211:ASP:HB3	1.97	0.46
2:B:321:HOH:O	1:C:39:ASP:HB3	2.15	0.46
1:A:220:LEU:HD13	1:A:220:LEU:C	2.36	0.45
1:B:127:LEU:HD22	1:B:129:VAL:O	2.16	0.45
1:A:7:LYS:HG3	2:A:387:HOH:O	2.16	0.45
1:C:223:HIS:HE1	1:C:230:VAL:O	1.99	0.45
1:C:241:LYS:HD3	1:C:241:LYS:O	2.16	0.45
1:B:26:HIS:HE1	1:B:55:HIS:ND1	2.14	0.45
1:C:142:VAL:HG12	1:C:146:PHE:CE2	2.52	0.45
1:B:259:PRO:CA	1:B:266:ILE:HD12	2.47	0.44
1:C:96:HIS:HE1	1:C:256:HIS:O	2.00	0.44
1:B:200:ILE:HA	1:B:203:PHE:CE2	2.52	0.44
1:B:258:MET:N	1:B:259:PRO:CD	2.81	0.44
1:A:134:ASN:HD21	1:A:234:ASN:HD21	1.64	0.44
1:C:258:MET:CG	1:C:266:ILE:HD11	2.47	0.44
1:C:170:ASN:HD22	1:C:170:ASN:H	1.66	0.44
1:A:72:MET:HE2	1:A:102:GLU:CA	2.37	0.43
1:B:119:VAL:HG11	1:B:270:LEU:CD2	2.48	0.43
1:B:127:LEU:HD23	1:B:127:LEU:C	2.39	0.43
1:C:44:PHE:O	1:C:48:HIS:HD2	2.00	0.43
1:B:127:LEU:HD21	1:B:129:VAL:CG1	2.41	0.43
1:A:272:ALA:HA	1:A:275:ARG:NH1	2.33	0.43
1:C:10:VAL:HG13	1:C:64:SER:OG	2.19	0.43
1:B:166:PHE:CA	1:B:229:ILE:HD11	2.44	0.42
1:C:170:ASN:H	1:C:170:ASN:ND2	2.17	0.42
1:C:200:ILE:HA	1:C:203:PHE:CE2	2.54	0.42
1:B:211:ASP:O	1:B:215:ILE:HG12	2.18	0.42
1:B:96:HIS:HE1	1:B:256:HIS:O	2.02	0.42
1:B:159:ARG:NH2	1:B:178:GLU:OE2	2.53	0.42
1:C:87:GLY:C	1:C:89:GLN:NE2	2.73	0.42
1:A:220:LEU:HD11	1:A:249:LYS:HB2	2.02	0.42
1:B:37:ASP:HB2	1:B:187:GLN:HE22	1.85	0.42
1:B:7:LYS:HG2	2:B:375:HOH:O	2.19	0.42
1:A:104:VAL:HA	1:A:107:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:TYR:CE1	1:A:13:PHE:HB2	2.55	0.42
1:C:129:VAL:HG22	1:C:130:GLN:N	2.35	0.42
1:B:149:GLN:CD	1:B:153:ASN:HD21	2.23	0.41
1:B:203:PHE:C	1:B:203:PHE:CD1	2.93	0.41
1:A:24:VAL:HG22	1:A:51:ARG:HD3	2.01	0.41
1:A:124:VAL:N	1:A:125:PRO:CD	2.84	0.41
1:A:127:LEU:HD12	1:A:134:ASN:HD22	1.85	0.41
1:B:129:VAL:HG22	1:B:130:GLN:N	2.36	0.41
1:A:257:GLY:C	1:A:259:PRO:HD2	2.41	0.41
1:A:123:ALA:HB1	1:A:125:PRO:HD2	2.03	0.40
1:A:175:GLU:OE2	1:A:175:GLU:N	2.40	0.40
1:B:258:MET:HB2	1:B:266:ILE:HD11	2.03	0.40
1:A:119:VAL:HG11	1:A:270:LEU:CD2	2.52	0.40
1:B:258:MET:C	1:B:266:ILE:HD12	2.42	0.40
1:C:139:PRO:HG2	1:C:142:VAL:HG23	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	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
1	B	272/276 (99%)	262 (96%)	10 (4%)	0	100	100
1	C	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
All	All	818/828 (99%)	789 (96%)	29 (4%)	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	216/217 (100%)	213 (99%)	3 (1%)	67	47
1	B	215/217 (99%)	212 (99%)	3 (1%)	67	47
1	C	216/217 (100%)	211 (98%)	5 (2%)	50	25
All	All	647/651 (99%)	636 (98%)	11 (2%)	60	38

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	217	GLN
1	A	223	HIS
1	B	32	PRO
1	B	153	ASN
1	B	170	ASN
1	C	89	GLN
1	C	153	ASN
1	C	159	ARG
1	C	170	ASN
1	C	203	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	74	HIS
1	A	134	ASN
1	A	216	GLN
1	A	217	GLN
1	B	11	GLN
1	B	26	HIS
1	B	48	HIS
1	B	74	HIS
1	B	85	HIS

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Mol	Chain	Res	Type
1	B	96	HIS
1	B	130	GLN
1	B	149	GLN
1	B	153	ASN
1	B	170	ASN
1	B	187	GLN
1	B	216	GLN
1	B	223	HIS
1	B	228	GLN
1	C	11	GLN
1	C	26	HIS
1	C	48	HIS
1	C	74	HIS
1	C	89	GLN
1	C	96	HIS
1	C	153	ASN
1	C	170	ASN
1	C	187	GLN
1	C	216	GLN
1	C	223	HIS
1	C	228	GLN
1	C	245	ASN

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.