



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 05:31 pm BST

PDB ID : 3UAK
Title : Crystal Structure of De Novo designed cysteine esterase ECH14, Northeast Structural Genomics Consortium Target OR54
Authors : Kuzin, A.; Su, M.; Seetharaman, J.; Sahdev, S.; Xiao, R.; Ciccocanti, C.; Richter, F.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Baker, D.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2011-10-21
Resolution : 3.23 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

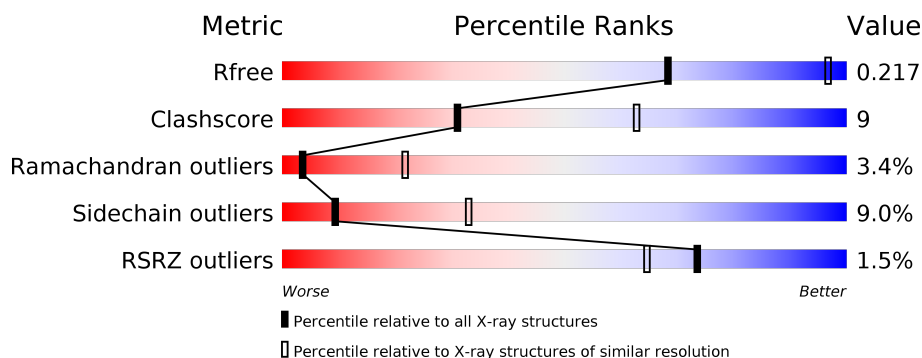
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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 on 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 $\leq 5\%$. 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	406	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 26%, green 68%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 68% 26% • • </div> </div>
1	B	406	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 23%, green 71%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 71% 23% • • </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6144 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.

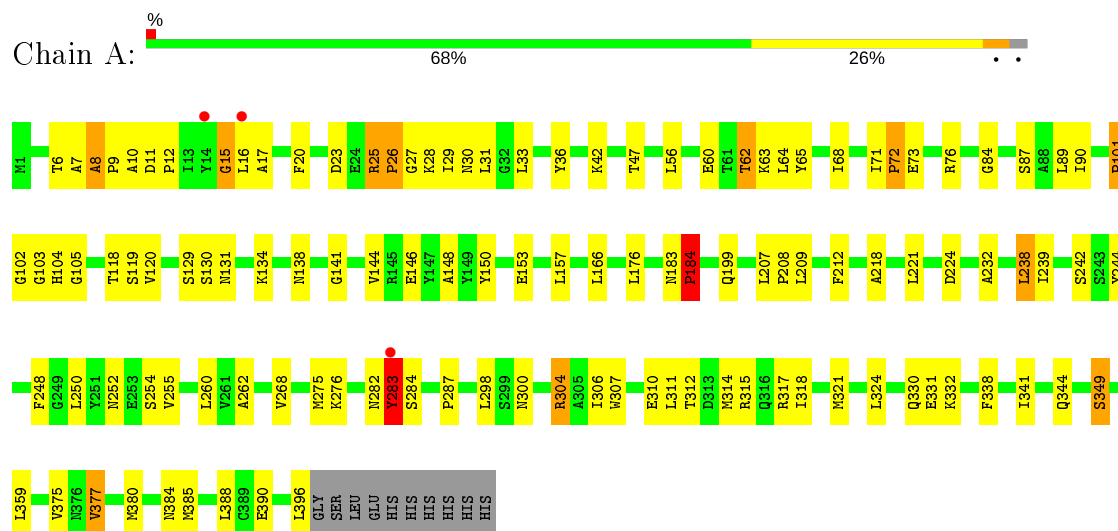
- Molecule 1 is a protein called De Novo designed cysteine esterase ECH14.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	Se	0	0	0
			3072	1944	527	587	6	8			
1	B	396	Total	C	N	O	S	Se	0	0	0
			3072	1944	527	587	6	8			

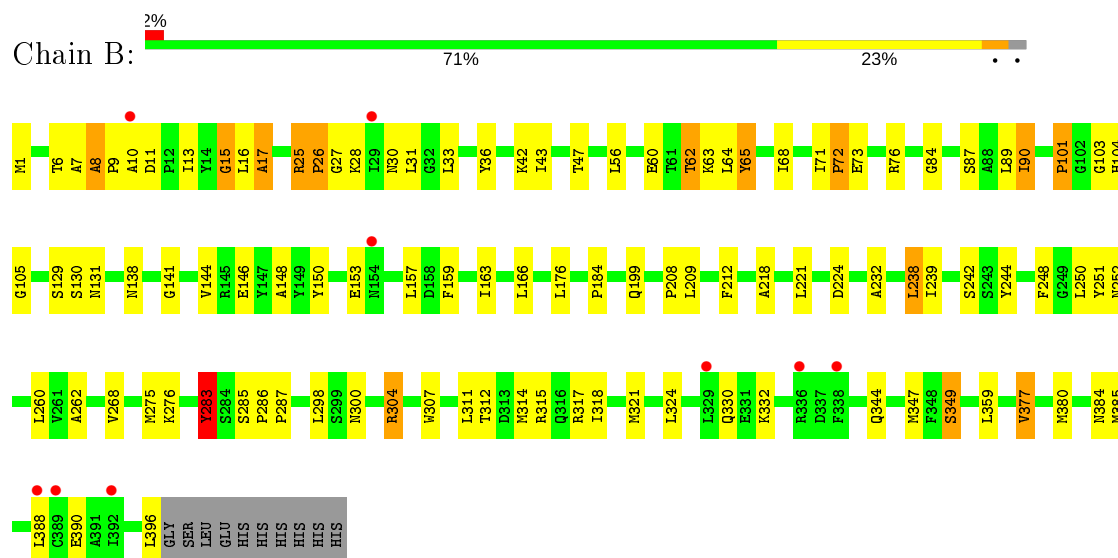
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: De Novo designed cysteine esterase ECH14



- Molecule 1: De Novo designed cysteine esterase ECH14



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.64Å 81.81Å 159.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 3.23 49.56 – 3.23	Depositor EDS
% Data completeness (in resolution range)	96.9 (19.96-3.23) 91.4 (49.56-3.23)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.7.2_869, REFMAC	Depositor
R, R_{free}	0.210 , 0.287 0.207 , 0.217	Depositor DCC
R_{free} test set	722 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6144	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	0.47	0/3126	0.61	0/4224
1	B	0.46	0/3126	0.61	0/4224
All	All	0.47	0/6252	0.61	0/8448

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	3072	0	3020	63	0
1	B	3072	0	3020	57	0
All	All	6144	0	6040	111	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 9.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD11	1:A:388:LEU:HD11	1.53	0.87
1:B:31:LEU:HD11	1:B:388:LEU:HD11	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:PRO:HB3	1:B:287:PRO:HB3	1.61	0.82
1:B:311:LEU:HA	1:B:314:MSE:HE3	1.74	0.69
1:A:208:PRO:HG2	1:A:238:LEU:HB3	1.76	0.67
1:A:311:LEU:HA	1:A:314:MSE:HE3	1.77	0.67
1:B:208:PRO:HG2	1:B:238:LEU:HB3	1.79	0.64
1:A:26:PRO:O	1:A:28:LYS:N	2.31	0.64
1:A:101:PRO:HB2	1:A:105:GLY:HA3	1.79	0.64
1:B:101:PRO:HB2	1:B:105:GLY:HA3	1.82	0.61
1:B:89:LEU:HD11	1:B:232:ALA:HB1	1.83	0.61
1:A:138:ASN:O	1:A:141:GLY:N	2.33	0.60
1:B:317:ARG:NH1	1:B:321:MSE:HE3	2.17	0.59
1:A:344:GLN:HE22	1:A:349:SER:HA	1.68	0.59
1:A:298:LEU:HA	1:A:304:ARG:HG3	1.84	0.59
1:A:332:LYS:HD2	1:A:390:GLU:HG2	1.85	0.58
1:A:324:LEU:HG	1:A:385:MSE:HG2	1.86	0.58
1:A:68:ILE:H	1:A:68:ILE:HD12	1.68	0.57
1:A:120:VAL:HG13	1:B:1:MSE:HE2	1.85	0.57
1:B:15:GLY:O	1:B:17:ALA:N	2.35	0.57
1:B:68:ILE:H	1:B:68:ILE:HD12	1.69	0.57
1:B:298:LEU:HA	1:B:304:ARG:HG3	1.85	0.56
1:B:344:GLN:HE22	1:B:349:SER:HA	1.69	0.56
1:B:26:PRO:O	1:B:28:LYS:N	2.39	0.56
1:A:384:ASN:O	1:A:388:LEU:HB2	2.07	0.55
1:B:324:LEU:HG	1:B:385:MSE:HG2	1.90	0.54
1:A:260:LEU:HD22	1:A:275:MSE:HE3	1.90	0.53
1:A:344:GLN:NE2	1:A:349:SER:HA	2.23	0.53
1:A:84:GLY:O	1:A:87:SER:HB2	2.09	0.53
1:B:138:ASN:O	1:B:141:GLY:N	2.39	0.53
1:A:118:THR:HG21	1:B:1:MSE:HB3	1.90	0.53
1:A:60:GLU:OE2	1:A:63:LYS:NZ	2.42	0.53
1:B:62:THR:HG21	1:B:64:LEU:HD22	1.90	0.53
1:B:311:LEU:HD12	1:B:314:MSE:HE3	1.90	0.52
1:B:318:ILE:HG23	1:B:377:VAL:HG22	1.91	0.52
1:B:332:LYS:HD2	1:B:390:GLU:HG2	1.91	0.52
1:B:344:GLN:NE2	1:B:349:SER:HA	2.25	0.52
1:A:248:PHE:HB3	1:A:250:LEU:HG	1.92	0.51
1:A:262:ALA:HB3	1:A:268:VAL:HB	1.92	0.51
1:B:248:PHE:HB3	1:B:250:LEU:HG	1.92	0.51
1:A:317:ARG:NH1	1:A:321:MSE:HE3	2.26	0.51
1:A:68:ILE:HD13	1:A:276:LYS:HG2	1.93	0.51
1:A:380:MSE:HE3	1:A:385:MSE:HE1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HD11	1:A:232:ALA:HB1	1.92	0.50
1:B:84:GLY:O	1:B:87:SER:HB2	2.11	0.50
1:B:176:LEU:HD12	1:B:209:LEU:HG	1.92	0.50
1:B:60:GLU:OE2	1:B:63:LYS:NZ	2.44	0.50
1:A:71:ILE:HG23	1:A:72:PRO:HD2	1.94	0.49
1:A:15:GLY:O	1:A:17:ALA:N	2.40	0.49
1:A:176:LEU:HD12	1:A:209:LEU:HG	1.95	0.49
1:A:62:THR:HG21	1:A:64:LEU:HD22	1.95	0.48
1:B:68:ILE:HD13	1:B:276:LYS:HG2	1.94	0.48
1:A:283:TYR:HD2	1:B:283:TYR:HD2	1.61	0.48
1:A:218:ALA:HB3	1:A:224:ASP:OD1	2.14	0.48
1:A:244:TYR:O	1:A:248:PHE:HB2	2.14	0.47
1:A:338:PHE:HB3	1:A:341:ILE:HD13	1.97	0.47
1:B:244:TYR:O	1:B:248:PHE:HB2	2.14	0.47
1:B:384:ASN:O	1:B:388:LEU:HB2	2.15	0.47
1:B:72:PRO:HB2	1:B:73:GLU:HG2	1.97	0.47
1:B:380:MSE:HE3	1:B:385:MSE:HE1	1.97	0.47
1:A:72:PRO:HB2	1:A:73:GLU:HG2	1.97	0.46
1:B:159:PHE:CZ	1:B:163:ILE:HD11	2.51	0.46
1:B:25:ARG:HG3	1:B:26:PRO:HD2	1.97	0.46
1:A:250:LEU:HD13	1:A:255:VAL:HG21	1.97	0.45
1:B:71:ILE:HG23	1:B:72:PRO:HD2	1.98	0.45
1:A:252:ASN:HA	1:B:65:TYR:CD2	2.51	0.45
1:A:282:ASN:O	1:A:284:SER:N	2.46	0.45
1:B:30:ASN:HD21	1:B:33:LEU:HD13	1.81	0.45
1:B:129:SER:OG	1:B:130:SER:N	2.50	0.45
1:A:311:LEU:HD12	1:A:314:MSE:HE3	1.99	0.45
1:A:8:ALA:H	1:A:9:PRO:CD	2.30	0.45
1:B:260:LEU:HD22	1:B:275:MSE:HE3	1.99	0.45
1:A:20:PHE:CZ	1:A:30:ASN:HB2	2.53	0.44
1:A:221:LEU:HD21	1:A:307:TRP:CH2	2.53	0.44
1:B:148:ALA:HB1	1:B:150:TYR:CE2	2.53	0.44
1:B:209:LEU:HD13	1:B:239:ILE:HB	2.00	0.44
1:B:262:ALA:HB3	1:B:268:VAL:HB	1.99	0.44
1:A:63:LYS:O	1:B:251:TYR:HB2	2.17	0.44
1:A:260:LEU:HD13	1:A:275:MSE:HE1	2.00	0.43
1:A:36:TYR:CE1	1:A:314:MSE:HG2	2.53	0.43
1:A:64:LEU:C	1:B:252:ASN:HB3	2.39	0.43
1:A:318:ILE:HG23	1:A:377:VAL:HG22	2.01	0.43
1:A:23:ASP:OD1	1:A:25:ARG:HB2	2.19	0.43
1:A:25:ARG:HG3	1:A:26:PRO:HD2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD22	1:B:1:MSE:HG3	2.01	0.43
1:A:283:TYR:HB3	1:B:283:TYR:HB3	2.00	0.43
1:B:312:THR:HG23	1:B:315:ARG:NH1	2.33	0.43
1:A:148:ALA:HB1	1:A:150:TYR:CE2	2.54	0.43
1:B:218:ALA:HB3	1:B:224:ASP:OD1	2.19	0.43
1:B:36:TYR:CE1	1:B:314:MSE:HG2	2.53	0.42
1:A:134:LYS:HB2	1:A:134:LYS:HE2	1.72	0.42
1:A:183:ASN:HA	1:A:184:PRO:HA	1.80	0.42
1:B:11:ASP:O	1:B:13:ILE:N	2.47	0.42
1:B:221:LEU:HD21	1:B:307:TRP:CH2	2.54	0.42
1:A:30:ASN:HD21	1:A:33:LEU:HD13	1.84	0.42
1:B:8:ALA:H	1:B:9:PRO:CD	2.32	0.42
1:A:102:GLY:H	1:A:254:SER:HB3	1.85	0.42
1:A:11:ASP:HA	1:A:12:PRO:HD2	1.98	0.41
1:A:129:SER:OG	1:A:130:SER:N	2.53	0.41
1:A:29:ILE:HG21	1:A:388:LEU:HD13	2.02	0.41
1:B:36:TYR:O	1:B:43:ILE:HG23	2.21	0.41
1:A:209:LEU:HD13	1:A:239:ILE:HB	2.02	0.41
1:B:260:LEU:HD13	1:B:275:MSE:HE1	2.02	0.41
1:B:87:SER:HB3	1:B:90:ILE:HG13	2.02	0.41
1:A:306:ILE:O	1:A:310:GLU:HG3	2.21	0.41
1:B:317:ARG:HH11	1:B:321:MSE:HE3	1.84	0.41
1:B:285:SER:HA	1:B:286:PRO:HD3	1.93	0.40
1:A:29:ILE:HG12	1:A:384:ASN:HB2	2.04	0.40
1:A:312:THR:HG23	1:A:315:ARG:NH1	2.36	0.40
1:A:8:ALA:H	1:A:9:PRO:HD2	1.87	0.40
1:B:347:MSE:HB3	1:B:347:MSE:HE3	1.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	394/406 (97%)	357 (91%)	24 (6%)	13 (3%)	4	22
1	B	394/406 (97%)	355 (90%)	25 (6%)	14 (4%)	3	20
All	All	788/812 (97%)	712 (90%)	49 (6%)	27 (3%)	3	22

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ALA
1	A	27	GLY
1	B	10	ALA
1	B	27	GLY
1	A	8	ALA
1	A	103	GLY
1	A	283	TYR
1	B	8	ALA
1	B	26	PRO
1	B	103	GLY
1	A	7	ALA
1	A	26	PRO
1	A	72	PRO
1	B	7	ALA
1	B	16	LEU
1	B	72	PRO
1	A	15	GLY
1	A	16	LEU
1	A	131	ASN
1	B	15	GLY
1	B	101	PRO
1	A	101	PRO
1	B	17	ALA
1	B	131	ASN
1	B	283	TYR
1	A	184	PRO
1	B	184	PRO

5.3.2 Protein sidechains ⓘ

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	322/323 (100%)	291 (90%)	31 (10%)	8	30
1	B	322/323 (100%)	295 (92%)	27 (8%)	11	37
All	All	644/646 (100%)	586 (91%)	58 (9%)	9	33

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	25	ARG
1	A	42	LYS
1	A	47	THR
1	A	56	LEU
1	A	62	THR
1	A	65	TYR
1	A	76	ARG
1	A	90	ILE
1	A	104	HIS
1	A	119	SER
1	A	144	VAL
1	A	146	GLU
1	A	153	GLU
1	A	157	LEU
1	A	166	LEU
1	A	184	PRO
1	A	199	GLN
1	A	212	PHE
1	A	238	LEU
1	A	242	SER
1	A	283	TYR
1	A	300	ASN
1	A	304	ARG
1	A	330	GLN
1	A	331	GLU
1	A	349	SER
1	A	359	LEU
1	A	375	VAL
1	A	377	VAL
1	A	396	LEU
1	B	6	THR
1	B	25	ARG
1	B	42	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	47	THR
1	B	56	LEU
1	B	62	THR
1	B	65	TYR
1	B	76	ARG
1	B	90	ILE
1	B	104	HIS
1	B	144	VAL
1	B	146	GLU
1	B	153	GLU
1	B	157	LEU
1	B	166	LEU
1	B	199	GLN
1	B	212	PHE
1	B	238	LEU
1	B	242	SER
1	B	283	TYR
1	B	300	ASN
1	B	304	ARG
1	B	330	GLN
1	B	349	SER
1	B	359	LEU
1	B	377	VAL
1	B	396	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	GLN
1	B	344	GLN

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 carbohydrates 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, 95th 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	388/406 (95%)	-0.19	3 (0%) 86 80	29, 62, 125, 241	0
1	B	388/406 (95%)	0.02	9 (2%) 60 50	23, 70, 141, 293	0
All	All	776/812 (95%)	-0.09	12 (1%) 73 64	23, 66, 134, 293	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	ALA	4.5
1	B	329	LEU	3.3
1	B	388	LEU	3.3
1	B	389	CYS	3.2
1	B	154	ASN	2.8
1	A	16	LEU	2.4
1	B	392	ILE	2.4
1	A	14	TYR	2.3
1	B	336	ARG	2.2
1	B	29	ILE	2.1
1	A	283	TYR	2.0
1	B	338	PHE	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 carbohydrates 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.