



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2022 – 06:03 PM JST

PDB ID : 7VGE
Title : Structure of the PDZ deleted variant of HtrA2 protease (S306A)
Authors : Parui, A.L.; Mishra, V.; Bhaumik, P.; Bose, K.
Deposited on : 2021-09-15
Resolution : 4.00 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
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
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)	:	2.28.1

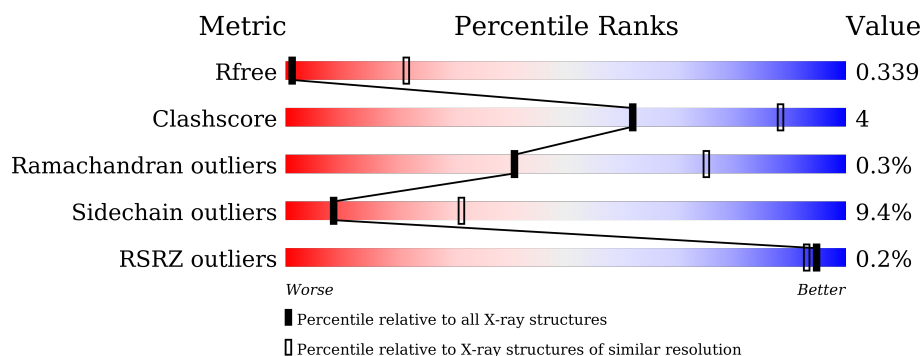
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 $\leq 5\%$. 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	203	<div> <div>69%</div> <div>20%</div> <div>•</div> <div>9%</div> </div>
1	B	203	<div> <div>72%</div> <div>14%</div> <div>•</div> <div>13%</div> </div>
1	C	203	<div> <div>73%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>
2	D	202	<div> <div>73%</div> <div>18%</div> <div>•</div> <div>8%</div> </div>
2	F	202	<div> <div>76%</div> <div>16%</div> <div>7%</div> </div>
3	E	201	<div> <div>78%</div> <div>10%</div> <div>11%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8149 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 Serine protease HTRA2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1382	873	239	268	2			
1	B	176	Total	C	N	O	S	0	0	0
			1307	824	226	255	2			
1	C	179	Total	C	N	O	S	0	0	0
			1332	843	229	258	2			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	306	ALA	SER	engineered mutation	UNP O43464
B	306	ALA	SER	engineered mutation	UNP O43464
C	306	ALA	SER	engineered mutation	UNP O43464

- Molecule 2 is a protein called Serine protease HTRA2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	186	Total	C	N	O	S	0	0	0
			1394	881	244	268	1			
2	F	187	Total	C	N	O	S	0	0	0
			1403	886	246	269	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	306	ALA	SER	engineered mutation	UNP O43464
F	306	ALA	SER	engineered mutation	UNP O43464

- Molecule 3 is a protein called Serine protease HTRA2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	179	Total	C	N	O	S	0	0	0
			1331	838	233	258	2			

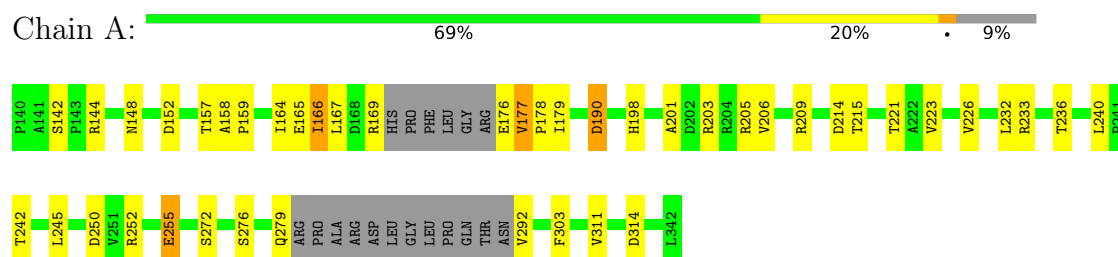
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	306	ALA	SER	engineered mutation	UNP O43464

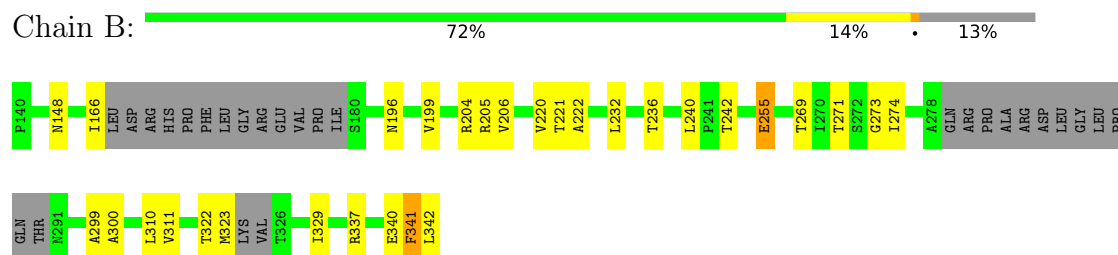
3 Residue-property plots

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.

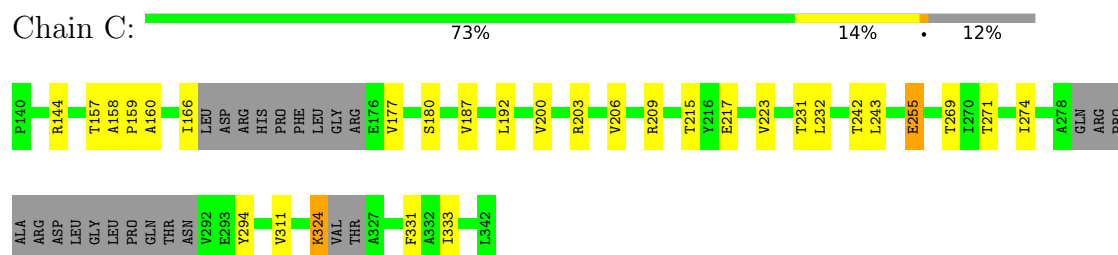
• Molecule 1: Serine protease HTRA2, mitochondrial



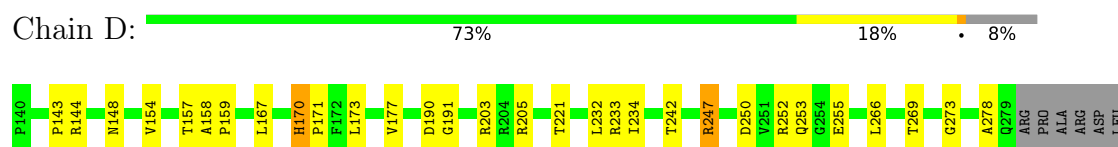
• Molecule 1: Serine protease HTRA2, mitochondrial



• Molecule 1: Serine protease HTRA2, mitochondrial



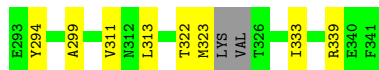
• Molecule 2: Serine protease HTRA2, mitochondrial





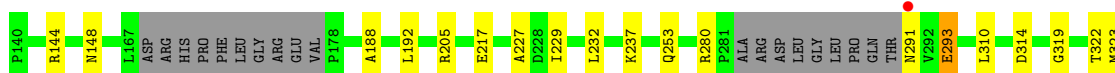
- Molecule 2: Serine protease HTRA2, mitochondrial

Chain F: 76% 16% 7%



- Molecule 3: Serine protease HTRA2, mitochondrial

Chain E: 78% 10% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.88Å 82.88Å 395.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.53 – 4.00 39.53 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.9 (39.53-4.00) 95.1 (39.53-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.265 , 0.336 0.264 , 0.339	Depositor DCC
R_{free} test set	595 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	107.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8149	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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

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	0.72	0/1402	0.88	0/1911
1	B	0.70	0/1325	0.87	0/1805
1	C	0.73	0/1351	0.83	0/1840
2	D	0.72	0/1417	0.84	0/1932
2	F	0.70	0/1426	0.87	0/1944
3	E	0.72	0/1350	0.83	0/1839
All	All	0.72	0/8271	0.85	0/11271

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	340	GLU	Peptide

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	1382	0	1399	13	0
1	B	1307	0	1313	12	1
1	C	1332	0	1346	13	1
2	D	1394	0	1400	21	0
2	F	1403	0	1408	15	1
3	E	1331	0	1344	12	1
All	All	8149	0	8210	72	2

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 4.

All (72) 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:253:GLN:HB3	2:D:278:ALA:HB2	1.57	0.87
3:E:148:ASN:HD21	2:F:255:GLU:HG3	1.50	0.76
2:D:157:THR:HG21	2:D:311:VAL:HG11	1.70	0.74
2:F:168:ASP:HB3	2:F:203:ARG:HH21	1.54	0.73
2:D:170:HIS:HB3	2:D:171:PRO:HD3	1.75	0.66
3:E:148:ASN:ND2	2:F:255:GLU:HG3	2.11	0.65
2:D:247:ARG:HG3	2:D:250:ASP:HB2	1.79	0.64
3:E:227:ALA:HB3	3:E:229:ILE:HG12	1.81	0.63
2:F:245:LEU:HD13	2:F:339:ARG:HG2	1.81	0.62
1:A:255:GLU:OE2	1:C:144:ARG:NE	2.33	0.62
2:F:157:THR:HG21	2:F:311:VAL:HG11	1.82	0.62
2:F:218:ALA:HB2	2:F:234:ILE:HG22	1.85	0.57
2:D:255:GLU:CD	2:F:144:ARG:HE	2.08	0.56
2:D:170:HIS:CB	2:D:171:PRO:HD3	2.36	0.56
1:A:177:VAL:HG22	1:A:178:PRO:HD2	1.89	0.54
2:D:273:GLY:HA3	2:D:299:ALA:HB2	1.89	0.54
3:E:319:GLY:HA2	3:E:333:ILE:O	2.08	0.54
1:A:314:ASP:OD1	1:C:144:ARG:HB3	2.07	0.54
1:A:252:ARG:O	1:A:255:GLU:HB2	2.08	0.53
1:C:324:LYS:HD3	1:C:324:LYS:H	1.74	0.53
1:B:255:GLU:O	1:B:274:ILE:HA	2.08	0.52
1:A:190:ASP:HB2	1:A:233:ARG:HH22	1.75	0.52
1:A:157:THR:HG21	1:A:311:VAL:HG11	1.92	0.51
2:D:301:ILE:HD12	2:D:330:SER:HB3	1.93	0.51
1:B:273:GLY:HA3	1:B:299:ALA:HB2	1.94	0.49
1:B:196:ASN:HD21	1:B:322:THR:HA	1.76	0.49
3:E:144:ARG:NE	2:F:255:GLU:OE2	2.46	0.48
1:C:158:ALA:HB3	1:C:159:PRO:HD3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:GLY:HA3	2:D:234:ILE:O	2.13	0.48
3:E:188:ALA:HB3	3:E:192:LEU:HB3	1.95	0.48
2:D:170:HIS:HB3	2:D:171:PRO:CD	2.44	0.47
2:D:335:SER:O	2:D:338:LEU:HB3	2.14	0.47
1:C:209:ARG:CZ	2:D:177:VAL:HG11	2.43	0.47
1:B:222:ALA:HB2	1:B:341:PHE:CZ	2.49	0.47
1:C:294:TYR:HB3	1:C:331:PHE:HB3	1.96	0.47
2:D:154:VAL:HG11	3:E:253:GLN:HE21	1.79	0.46
2:F:191:GLY:O	2:F:233:ARG:HA	2.15	0.46
1:B:166:ILE:HG23	1:B:206:VAL:HG12	1.98	0.46
1:C:157:THR:HG21	1:C:311:VAL:HG11	1.97	0.46
1:B:271:THR:HG21	1:B:300:ALA:HB3	1.98	0.46
2:D:143:PRO:HD2	3:E:314:ASP:OD1	2.16	0.45
1:C:209:ARG:HG3	1:C:215:THR:HG22	1.98	0.45
2:D:266:LEU:HB2	2:D:303:PHE:CD2	2.52	0.45
1:A:250:ASP:O	1:C:144:ARG:NH2	2.50	0.44
1:C:160:ALA:HB3	1:C:243:LEU:HG	2.00	0.44
1:C:166:ILE:HB	1:C:180:SER:HB2	2.00	0.43
2:D:247:ARG:HG3	2:D:250:ASP:CB	2.47	0.43
2:F:153:VAL:HG21	2:F:313:LEU:HA	1.98	0.43
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.93	0.43
2:F:273:GLY:HA3	2:F:299:ALA:HB2	2.01	0.43
1:A:144:ARG:NH2	1:B:255:GLU:OE2	2.52	0.42
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.92	0.42
1:B:236:THR:HG21	1:B:240:LEU:HD21	2.01	0.42
1:A:158:ALA:HB3	1:A:159:PRO:HD3	2.01	0.42
2:D:205:ARG:HD3	2:D:205:ARG:HA	1.91	0.42
1:C:255:GLU:O	1:C:274:ILE:HA	2.20	0.41
3:E:310:LEU:HD12	3:E:310:LEU:HA	1.90	0.41
1:A:166:ILE:O	2:F:178:PRO:HD3	2.20	0.41
1:C:192:LEU:HD11	1:C:231:THR:HB	2.03	0.41
2:F:294:TYR:CE1	2:F:333:ILE:HD13	2.56	0.41
1:B:196:ASN:HB2	1:B:199:VAL:HG23	2.03	0.41
1:B:204:ARG:HG3	1:B:220:VAL:HB	2.03	0.41
3:E:293:GLU:O	3:E:334:PRO:HD3	2.21	0.41
1:A:198:HIS:O	1:A:201:ALA:HB2	2.21	0.40
1:B:337:ARG:HD2	1:B:337:ARG:HA	1.95	0.40
2:D:190:ASP:HB3	2:D:233:ARG:HH22	1.85	0.40
2:D:319:GLY:HA2	2:D:333:ILE:O	2.21	0.40
3:E:232:LEU:N	3:E:232:LEU:HD23	2.37	0.40
2:D:158:ALA:HB3	2:D:159:PRO:HD3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD22	2:F:177:VAL:N	2.36	0.40
2:D:154:VAL:CG1	3:E:253:GLN:HE21	2.34	0.40
2:F:189:ALA:C	2:F:191:GLY:H	2.24	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:GLU:OE2	2:F:235:GLN:OE1[1_655]	1.78	0.42
1:B:342:LEU:CD2	3:E:339:ARG:O[6_435]	2.10	0.10

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	179/203 (88%)	163 (91%)	15 (8%)	1 (1%)	25	63
1	B	168/203 (83%)	157 (94%)	11 (6%)	0	100	100
1	C	171/203 (84%)	166 (97%)	5 (3%)	0	100	100
2	D	180/202 (89%)	168 (93%)	11 (6%)	1 (1%)	25	63
2	F	179/202 (89%)	162 (90%)	16 (9%)	1 (1%)	25	63
3	E	171/201 (85%)	159 (93%)	12 (7%)	0	100	100
All	All	1048/1214 (86%)	975 (93%)	70 (7%)	3 (0%)	41	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	170	HIS
2	F	190	ASP
1	A	142	SER

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	150/165 (91%)	121 (81%)	29 (19%)	1	9
1	B	141/165 (86%)	130 (92%)	11 (8%)	12	39
1	C	144/165 (87%)	131 (91%)	13 (9%)	9	34
2	D	150/164 (92%)	139 (93%)	11 (7%)	14	42
2	F	152/164 (93%)	141 (93%)	11 (7%)	14	42
3	E	144/163 (88%)	136 (94%)	8 (6%)	21	49
All	All	881/986 (89%)	798 (91%)	83 (9%)	8	31

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	152	ASP
1	A	164	ILE
1	A	165	GLU
1	A	166	ILE
1	A	169	ARG
1	A	176	GLU
1	A	177	VAL
1	A	179	ILE
1	A	190	ASP
1	A	203	ARG
1	A	205	ARG
1	A	206	VAL
1	A	209	ARG
1	A	214	ASP
1	A	215	THR
1	A	221	THR
1	A	223	VAL
1	A	226	VAL
1	A	232	LEU
1	A	236	THR
1	A	242	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	245	LEU
1	A	255	GLU
1	A	272	SER
1	A	276	SER
1	A	279	GLN
1	A	292	VAL
1	A	303	PHE
1	B	148	ASN
1	B	205	ARG
1	B	221	THR
1	B	232	LEU
1	B	242	THR
1	B	255	GLU
1	B	269	THR
1	B	311	VAL
1	B	323	MET
1	B	329	ILE
1	B	341	PHE
1	C	177	VAL
1	C	187	VAL
1	C	200	VAL
1	C	203	ARG
1	C	206	VAL
1	C	223	VAL
1	C	232	LEU
1	C	242	THR
1	C	255	GLU
1	C	269	THR
1	C	271	THR
1	C	324	LYS
1	C	333	ILE
2	D	144	ARG
2	D	148	ASN
2	D	167	LEU
2	D	173	LEU
2	D	203	ARG
2	D	221	THR
2	D	232	LEU
2	D	242	THR
2	D	247	ARG
2	D	252	ARG
2	D	269	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	205	ARG
3	E	217	GLU
3	E	237	LYS
3	E	280	ARG
3	E	291	ASN
3	E	293	GLU
3	E	322	THR
3	E	323	MET
2	F	167	LEU
2	F	177	VAL
2	F	200	VAL
2	F	202	ASP
2	F	232	LEU
2	F	242	THR
2	F	267	GLN
2	F	268	ASN
2	F	292	VAL
2	F	322	THR
2	F	323	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	146	GLN
1	B	196	ASN
3	E	253	GLN
3	E	291	ASN
2	F	196	ASN
2	F	279	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 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, 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	185/203 (91%)	-0.36	0	100 100	80, 104, 133, 140	0
1	B	176/203 (86%)	-0.38	0	100 100	81, 115, 145, 172	0
1	C	179/203 (88%)	-0.42	0	100 100	86, 116, 144, 155	0
2	D	186/202 (92%)	-0.29	0	100 100	91, 114, 154, 176	0
2	F	187/202 (92%)	-0.24	1 (0%)	91 85	81, 112, 149, 175	0
3	E	179/201 (89%)	-0.30	1 (0%)	89 84	96, 120, 144, 162	0
All	All	1092/1214 (89%)	-0.33	2 (0%)	95 93	80, 113, 146, 176	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	279	GLN	2.7
3	E	291	ASN	2.5

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.