Full wwPDB X-ray Structure Validation Report (i)

Sep 5, 2023 – 08:01 AM EDT

PDB ID	:	3TJN
Title	:	HtrA1 catalytic domain, apo form
Authors	:	Eigenbrot, C.; Ultsch, M.
Deposited on	:	2011-08-24
Resolution	:	3.00 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 (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:

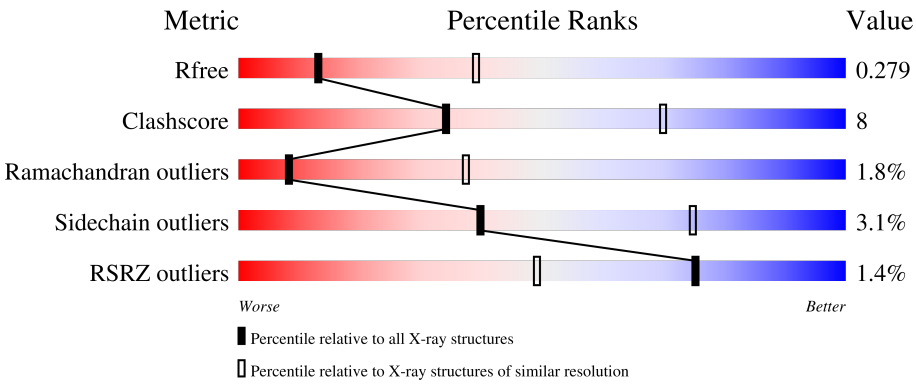
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	A	228	64% 18% • 17%
1	B	228	% 69% 16% • 14%
1	D	228	2% 64% 17% • 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4381 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 HTRA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O				
1	A	190	1458	934	247	277		0	1	0
			Total	C	N	O	S			
1	B	197	1503	960	259	283	1	0	0	0
			Total	C	N	O	S			
1	D	187	1420	909	243	267	1	0	0	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	MET	-	expression tag	UNP Q92743
A	141	GLY	-	expression tag	UNP Q92743
A	142	SER	-	expression tag	UNP Q92743
A	143	SER	-	expression tag	UNP Q92743
A	144	HIS	-	expression tag	UNP Q92743
A	145	HIS	-	expression tag	UNP Q92743
A	146	HIS	-	expression tag	UNP Q92743
A	147	HIS	-	expression tag	UNP Q92743
A	148	HIS	-	expression tag	UNP Q92743
A	149	HIS	-	expression tag	UNP Q92743
A	150	SER	-	expression tag	UNP Q92743
A	151	SER	-	expression tag	UNP Q92743
A	152	GLY	-	expression tag	UNP Q92743
A	153	LEU	-	expression tag	UNP Q92743
A	154	VAL	-	expression tag	UNP Q92743
A	155	PRO	-	expression tag	UNP Q92743
A	156	ARG	-	expression tag	UNP Q92743
A	157	GLY	-	expression tag	UNP Q92743
A	158	SER	-	expression tag	UNP Q92743
A	159	HIS	-	expression tag	UNP Q92743
A	160	MET	-	expression tag	UNP Q92743
B	140	MET	-	expression tag	UNP Q92743
B	141	GLY	-	expression tag	UNP Q92743

Continued on next page...

Continued from previous page...

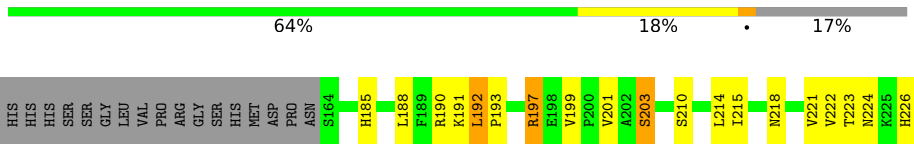
Chain	Residue	Modelled	Actual	Comment	Reference
B	142	SER	-	expression tag	UNP Q92743
B	143	SER	-	expression tag	UNP Q92743
B	144	HIS	-	expression tag	UNP Q92743
B	145	HIS	-	expression tag	UNP Q92743
B	146	HIS	-	expression tag	UNP Q92743
B	147	HIS	-	expression tag	UNP Q92743
B	148	HIS	-	expression tag	UNP Q92743
B	149	HIS	-	expression tag	UNP Q92743
B	150	SER	-	expression tag	UNP Q92743
B	151	SER	-	expression tag	UNP Q92743
B	152	GLY	-	expression tag	UNP Q92743
B	153	LEU	-	expression tag	UNP Q92743
B	154	VAL	-	expression tag	UNP Q92743
B	155	PRO	-	expression tag	UNP Q92743
B	156	ARG	-	expression tag	UNP Q92743
B	157	GLY	-	expression tag	UNP Q92743
B	158	SER	-	expression tag	UNP Q92743
B	159	HIS	-	expression tag	UNP Q92743
B	160	MET	-	expression tag	UNP Q92743
D	140	MET	-	expression tag	UNP Q92743
D	141	GLY	-	expression tag	UNP Q92743
D	142	SER	-	expression tag	UNP Q92743
D	143	SER	-	expression tag	UNP Q92743
D	144	HIS	-	expression tag	UNP Q92743
D	145	HIS	-	expression tag	UNP Q92743
D	146	HIS	-	expression tag	UNP Q92743
D	147	HIS	-	expression tag	UNP Q92743
D	148	HIS	-	expression tag	UNP Q92743
D	149	HIS	-	expression tag	UNP Q92743
D	150	SER	-	expression tag	UNP Q92743
D	151	SER	-	expression tag	UNP Q92743
D	152	GLY	-	expression tag	UNP Q92743
D	153	LEU	-	expression tag	UNP Q92743
D	154	VAL	-	expression tag	UNP Q92743
D	155	PRO	-	expression tag	UNP Q92743
D	156	ARG	-	expression tag	UNP Q92743
D	157	GLY	-	expression tag	UNP Q92743
D	158	SER	-	expression tag	UNP Q92743
D	159	HIS	-	expression tag	UNP Q92743
D	160	MET	-	expression tag	UNP Q92743

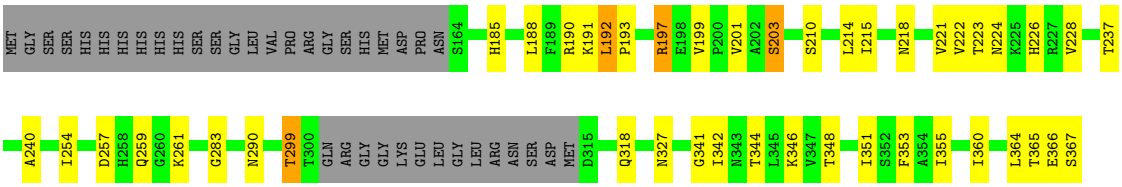
3 Residue-property plots (i)

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: Serine protease HTRA1

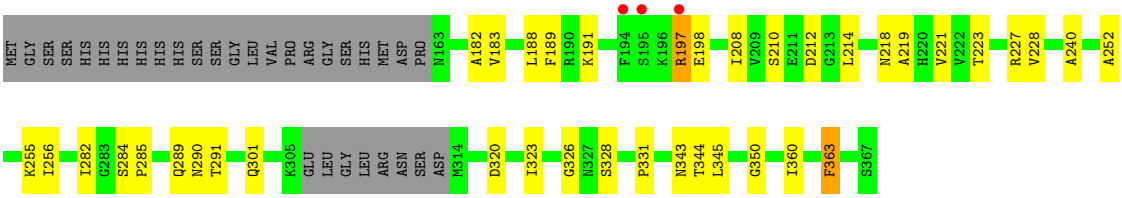
Chain A:





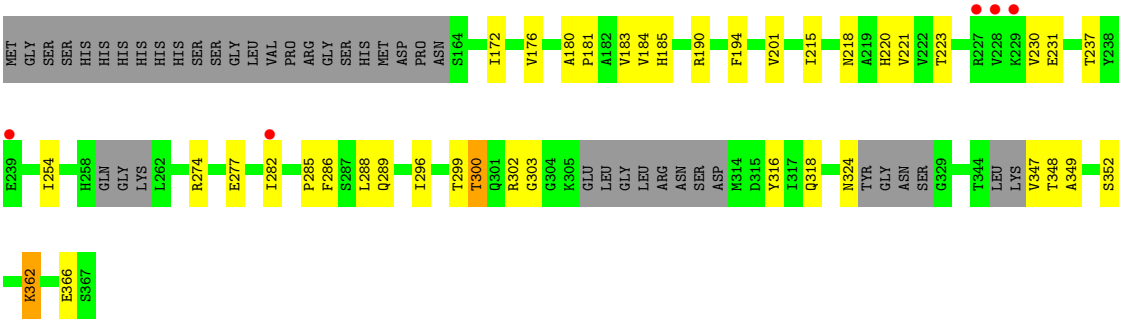
• Molecule 1: Serine protease HTRA1

Chain B:



• Molecule 1: Serine protease HTRA1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	108.50Å 108.50Å 234.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.73 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.00) 99.8 (49.73-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.294 0.234 , 0.279	Depositor DCC
R_{free} test set	799 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å^2)	83.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4381	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.44	0/1481	0.61	0/2006
1	B	0.40	0/1526	0.56	0/2063
1	D	0.39	0/1439	0.54	0/1944
All	All	0.41	0/4446	0.57	0/6013

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	1458	0	1507	26	0
1	B	1503	0	1560	24	0
1	D	1420	0	1465	27	0
All	All	4381	0	4532	75	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 8.

All (75) 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:284:SER:HB3	1:B:289:GLN:HA	1.34	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:THR:HG23	1:D:300:THR:N	1.89	0.86
1:A:259:GLN:HG3	1:B:301:GLN:HE21	1.50	0.76
1:D:299:THR:CG2	1:D:318:GLN:H	1.99	0.75
1:A:218:ASN:HB2	1:A:221:VAL:HG23	1.71	0.73
1:D:362:LYS:O	1:D:366:GLU:HG2	1.92	0.69
1:A:228:VAL:HG23	1:A:240:ALA:HB3	1.74	0.68
1:A:344:THR:HG22	1:A:346:LYS:H	1.59	0.68
1:D:190:ARG:HB2	1:D:201:VAL:HG21	1.75	0.67
1:B:284:SER:HB3	1:B:289:GLN:CA	2.21	0.67
1:A:283:GLY:O	1:A:290:ASN:HB2	1.96	0.64
1:D:299:THR:HG21	1:D:318:GLN:H	1.61	0.64
1:A:299:THR:HG22	1:A:318:GLN:HB2	1.80	0.63
1:D:231:GLU:HG2	1:D:237:THR:HG22	1.80	0.62
1:D:299:THR:HG23	1:D:300:THR:H	1.62	0.61
1:D:299:THR:HG22	1:D:318:GLN:H	1.65	0.60
1:B:255:LYS:HG3	1:B:256:ILE:N	2.15	0.60
1:A:191:LYS:O	1:A:192:LEU:HB2	2.01	0.60
1:A:364:LEU:HD13	1:D:194:PHE:HZ	1.68	0.58
1:A:283:GLY:HA3	1:A:327:ASN:HA	1.84	0.58
1:B:182:ALA:HA	1:B:208:ILE:HD12	1.86	0.58
1:D:285:PRO:HB3	1:D:324:ASN:HB2	1.86	0.57
1:A:348:THR:HG22	1:A:353:PHE:HE2	1.70	0.56
1:D:302:ARG:O	1:D:316:TYR:N	2.30	0.56
1:B:219:ALA:HA	1:B:252:ALA:HB2	1.90	0.54
1:A:210:SER:OG	1:A:214:LEU:HB2	2.07	0.54
1:B:228:VAL:HG23	1:B:240:ALA:HB3	1.92	0.52
1:A:348:THR:HG22	1:A:353:PHE:CE2	2.44	0.52
1:D:215:ILE:HB	1:D:254:ILE:HG13	1.91	0.52
1:D:286:PHE:C	1:D:288:LEU:H	2.12	0.52
1:B:289:GLN:O	1:B:290:ASN:HB2	2.09	0.52
1:D:183:VAL:HG11	1:D:282:ILE:HG22	1.92	0.51
1:A:344:THR:CG2	1:A:346:LYS:H	2.23	0.51
1:B:212:ASP:HB3	1:B:255:LYS:HZ1	1.74	0.51
1:B:188:LEU:HD11	1:B:221:VAL:O	2.10	0.51
1:A:344:THR:HB	1:A:353:PHE:O	2.11	0.50
1:A:342:ILE:HG13	1:A:360:ILE:HD11	1.92	0.50
1:D:185:HIS:HB3	1:D:231:GLU:HB2	1.94	0.50
1:B:328:SER:HA	1:B:343:ASN:O	2.13	0.49
1:A:190:ARG:HB2	1:A:201:VAL:HG21	1.94	0.49
1:B:285:PRO:HD2	1:B:291:THR:HB	1.95	0.48
1:A:341:GLY:HA2	1:A:355:ILE:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:HA	1:B:198:GLU:HG2	1.96	0.47
1:D:180:ALA:HB3	1:D:181:PRO:HD3	1.95	0.47
1:A:222:VAL:HG23	1:A:223:THR:H	1.79	0.47
1:B:189:PHE:HB2	1:B:227:ARG:HB3	1.96	0.47
1:A:191:LYS:HB2	1:A:226:HIS:NE2	2.30	0.47
1:D:218:ASN:HB2	1:D:221:VAL:HG23	1.98	0.46
1:D:299:THR:HB	1:D:318:GLN:HB3	1.98	0.46
1:B:218:ASN:HD21	1:B:344:THR:HA	1.82	0.45
1:D:299:THR:CG2	1:D:300:THR:H	2.20	0.44
1:A:365:THR:C	1:A:367:SER:H	2.21	0.44
1:A:185:HIS:HE1	1:A:203:SER:OG	2.01	0.44
1:D:172:ILE:O	1:D:176:VAL:HG23	2.18	0.44
1:B:188:LEU:HD23	1:B:228:VAL:HG12	2.00	0.44
1:B:183:VAL:HG11	1:B:282:ILE:HG12	2.00	0.43
1:D:274:ARG:HB2	1:D:277:GLU:HG3	1.99	0.43
1:B:282:ILE:HG23	1:B:331:PRO:HG2	2.00	0.43
1:B:212:ASP:HB3	1:B:255:LYS:NZ	2.32	0.43
1:B:360:ILE:O	1:B:363:PHE:HB2	2.19	0.43
1:B:218:ASN:HD22	1:B:328:SER:HB2	1.84	0.43
1:D:184:VAL:HB	1:D:230:VAL:HG13	2.01	0.43
1:A:215:ILE:HB	1:A:254:ILE:HG13	2.00	0.42
1:D:286:PHE:C	1:D:288:LEU:N	2.72	0.42
1:D:289:GLN:NE2	1:D:289:GLN:HA	2.35	0.42
1:B:210:SER:OG	1:B:214:LEU:HB3	2.20	0.42
1:A:348:THR:O	1:A:351:ILE:HG13	2.20	0.41
1:A:192:LEU:HD12	1:A:197:ARG:HB2	2.03	0.41
1:A:190:ARG:HA	1:A:226:HIS:HB2	2.03	0.41
1:D:277:GLU:O	1:D:296:ILE:HA	2.20	0.41
1:A:191:LYS:HB2	1:A:226:HIS:CD2	2.56	0.40
1:B:285:PRO:HA	1:B:326:GLY:HA3	2.03	0.40
1:D:286:PHE:HB2	1:D:288:LEU:HG	2.03	0.40
1:B:320:ASP:HA	1:B:350:GLY:O	2.21	0.40
1:D:220:HIS:HA	1:D:223:THR:HG22	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	186/228 (82%)	175 (94%)	6 (3%)	5 (3%)	5 26
1	B	193/228 (85%)	182 (94%)	10 (5%)	1 (0%)	29 68
1	D	177/228 (78%)	160 (90%)	13 (7%)	4 (2%)	6 30
All	All	556/684 (81%)	517 (93%)	29 (5%)	10 (2%)	8 37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	ARG
1	A	366	GLU
1	A	193	PRO
1	A	197	ARG
1	A	224	ASN
1	D	300	THR
1	A	192	LEU
1	D	349	ALA
1	D	362	LYS
1	D	303	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	A	163/194 (84%)	156 (96%)	7 (4%)	29 66
1	B	167/194 (86%)	162 (97%)	5 (3%)	41 75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	157/194 (81%)	154 (98%)	3 (2%)	57 84
All	All	487/582 (84%)	472 (97%)	15 (3%)	40 75

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LEU
1	A	199	VAL
1	A	203	SER
1	A	237	THR
1	A	257	ASP
1	A	261	LYS
1	A	299	THR
1	B	197	ARG
1	B	223	THR
1	B	323	ILE
1	B	345	LEU
1	B	363	PHE
1	D	347	VAL
1	D	348	THR
1	D	352	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	259	GLN
1	B	218	ASN
1	B	301	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, 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	190/228 (83%)	-0.24	0	100	100	37, 60, 94, 126	0
1	B	197/228 (86%)	-0.17	3 (1%)	73	46	52, 82, 129, 164	1 (0%)
1	D	187/228 (82%)	0.27	5 (2%)	54	26	73, 110, 143, 156	0
All	All	574/684 (83%)	-0.05	8 (1%)	75	49	37, 87, 133, 164	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	228	VAL	2.9
1	D	229	LYS	2.7
1	D	227	ARG	2.6
1	B	194	PHE	2.5
1	B	197	ARG	2.3
1	D	282	ILE	2.2
1	B	195	SER	2.2
1	D	239	GLU	2.1

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.