



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2025 – 06:06 PM EST

PDB ID : 9DEL
Title : USP7 in complex with macrocycle MC03
Authors : Ultsch, M.; Tenorio, C.A.; Dueber, E.C.; Harris, S.F.
Deposited on : 2024-08-29
Resolution : 2.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

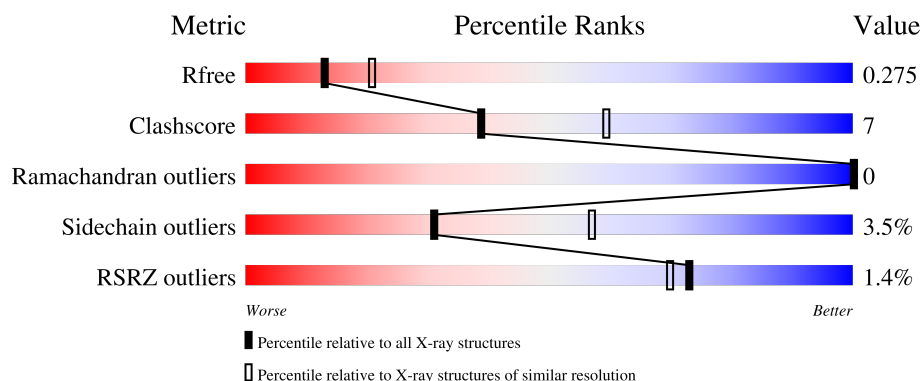
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	368	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>18%</div> <div>• 10%</div> </div> </div>
1	B	368	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 9%</div> </div> </div>
2	C	15	<div> <div></div> <div>73%</div> <div>27%</div> </div>
2	D	15	<div> <div></div> <div>80%</div> <div>20%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5563 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 Ubiquitin carboxyl-terminal hydrolase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2635	1669	439	511	16			
1	B	334	Total	C	N	O	S	0	0	0
			2662	1686	446	514	16			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	MET	-	initiating methionine	UNP Q93009
A	188	GLY	-	expression tag	UNP Q93009
A	189	SER	-	expression tag	UNP Q93009
A	190	SER	-	expression tag	UNP Q93009
A	191	HIS	-	expression tag	UNP Q93009
A	192	HIS	-	expression tag	UNP Q93009
A	193	HIS	-	expression tag	UNP Q93009
A	194	HIS	-	expression tag	UNP Q93009
A	195	HIS	-	expression tag	UNP Q93009
A	196	HIS	-	expression tag	UNP Q93009
A	197	SER	-	expression tag	UNP Q93009
A	198	SER	-	expression tag	UNP Q93009
A	199	GLY	-	expression tag	UNP Q93009
A	200	LEU	-	expression tag	UNP Q93009
A	201	VAL	-	expression tag	UNP Q93009
A	202	PRO	-	expression tag	UNP Q93009
A	203	ARG	-	expression tag	UNP Q93009
A	204	GLY	-	expression tag	UNP Q93009
A	205	SER	-	expression tag	UNP Q93009
A	206	HIS	-	expression tag	UNP Q93009
A	207	MET	-	expression tag	UNP Q93009
B	187	MET	-	initiating methionine	UNP Q93009
B	188	GLY	-	expression tag	UNP Q93009
B	189	SER	-	expression tag	UNP Q93009
B	190	SER	-	expression tag	UNP Q93009

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Chain	Residue	Modelled	Actual	Comment	Reference
B	191	HIS	-	expression tag	UNP Q93009
B	192	HIS	-	expression tag	UNP Q93009
B	193	HIS	-	expression tag	UNP Q93009
B	194	HIS	-	expression tag	UNP Q93009
B	195	HIS	-	expression tag	UNP Q93009
B	196	HIS	-	expression tag	UNP Q93009
B	197	SER	-	expression tag	UNP Q93009
B	198	SER	-	expression tag	UNP Q93009
B	199	GLY	-	expression tag	UNP Q93009
B	200	LEU	-	expression tag	UNP Q93009
B	201	VAL	-	expression tag	UNP Q93009
B	202	PRO	-	expression tag	UNP Q93009
B	203	ARG	-	expression tag	UNP Q93009
B	204	GLY	-	expression tag	UNP Q93009
B	205	SER	-	expression tag	UNP Q93009
B	206	HIS	-	expression tag	UNP Q93009
B	207	MET	-	expression tag	UNP Q93009

- Molecule 2 is a protein called Macrocycle peptide MC03.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	15	Total	C	N	O	S	0	0	0
			126	85	19	21	1			
2	C	15	Total	C	N	O	S	0	0	0
			126	85	19	21	1			

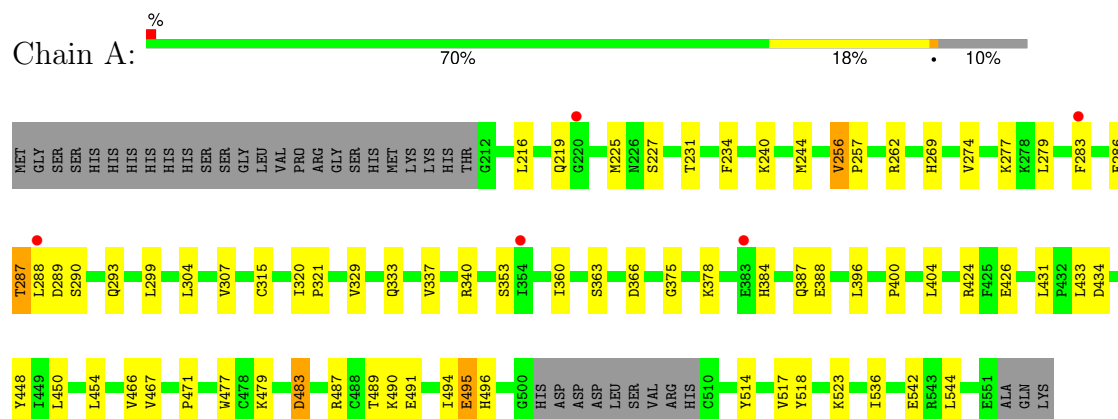
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	10	Total	O	0	0
			10	10		

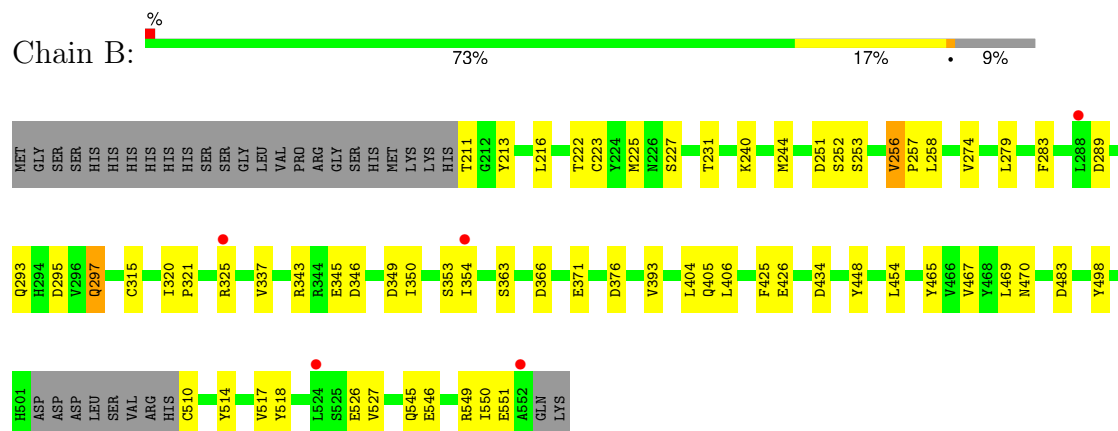
3 Residue-property plots

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.

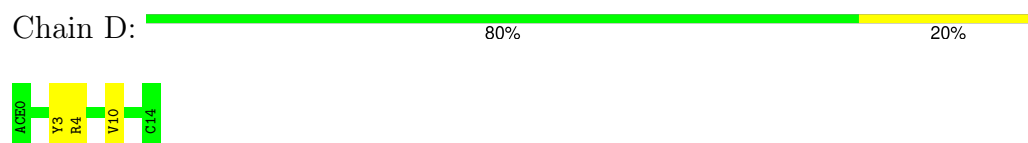
- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 7

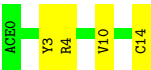


- Molecule 2: Macrocycle peptide MC03



- Molecule 2: Macrocycle peptide MC03





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.91Å 69.42Å 76.41Å 90.00° 91.93° 90.00°	Depositor
Resolution (Å)	42.81 – 2.50 42.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	75.6 (42.81-2.50) 75.6 (42.81-2.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.216 , 0.272 0.219 , 0.275	Depositor DCC
R_{free} test set	1395 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.027 for h,-k,-l 0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5563	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.5806e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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

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	0.25	0/2690	0.46	0/3640
1	B	0.24	0/2719	0.44	0/3679
2	C	0.30	0/130	0.55	0/176
2	D	0.25	0/130	0.49	0/176
All	All	0.25	0/5669	0.45	0/7671

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	2635	0	2519	37	0
1	B	2662	0	2548	35	0
2	C	126	0	104	2	0
2	D	126	0	104	4	0
3	A	4	0	0	0	0
3	B	10	0	0	2	0
All	All	5563	0	5275	73	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 7.

All (73) 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:384:HIS:O	1:A:387:GLN:NE2	2.25	0.69
1:B:371:GLU:OE2	2:D:4:ARG:NH1	2.26	0.69
1:A:448:TYR:HB3	1:A:518:TYR:HB3	1.84	0.60
1:A:329:VAL:HG23	1:A:396:LEU:HD11	1.82	0.60
1:A:353:SER:O	1:A:363:SER:OG	2.18	0.59
1:A:477:TRP:CD1	1:A:490:LYS:HG2	2.37	0.59
1:B:353:SER:O	1:B:363:SER:OG	2.20	0.58
1:A:256:VAL:HG13	1:A:257:PRO:HD3	1.88	0.56
1:A:378:LYS:HD3	1:A:388:GLU:HG3	1.87	0.56
1:A:287:THR:HG23	1:A:290:SER:HB3	1.87	0.55
1:B:289:ASP:O	1:B:293:GLN:HG2	2.06	0.55
1:A:489:THR:HG22	1:A:491:GLU:H	1.72	0.54
1:B:448:TYR:HB3	1:B:518:TYR:HB3	1.89	0.54
1:B:510:CYS:N	3:B:602:HOH:O	2.41	0.53
1:B:546:GLU:O	1:B:550:ILE:HG12	2.09	0.53
1:B:470:ASN:ND2	3:B:603:HOH:O	2.42	0.52
1:B:223:CYS:HB3	1:B:465:TYR:CE1	2.45	0.52
1:A:466:VAL:HG11	1:A:479:LYS:HE3	1.90	0.52
1:B:222:THR:HB	1:B:225:MET:HB3	1.92	0.51
1:A:269:HIS:HE1	1:A:536:ILE:HD12	1.75	0.51
1:A:216:LEU:HD23	1:A:274:VAL:HB	1.93	0.51
1:A:483:ASP:N	1:A:483:ASP:OD1	2.41	0.51
1:A:219:GLN:NE2	1:A:277:LYS:HG3	2.26	0.50
1:A:450:LEU:HD23	1:A:494:ILE:HD12	1.94	0.50
1:A:225:MET:HG3	1:A:299:LEU:HD21	1.94	0.49
1:A:289:ASP:O	1:A:293:GLN:HG2	2.12	0.49
2:C:3:TYR:CE2	2:C:4:ARG:HG2	2.47	0.49
1:B:325:ARG:NH2	1:B:346:ASP:OD2	2.43	0.49
1:B:366:ASP:O	2:D:4:ARG:NH2	2.43	0.49
1:B:256:VAL:HG13	1:B:257:PRO:HD3	1.94	0.49
1:B:211:THR:HG23	1:B:213:TYR:H	1.78	0.48
1:B:279:LEU:HG	1:B:283:PHE:HE2	1.77	0.48
1:B:354:ILE:HG13	1:B:425:PHE:CG	2.49	0.48
2:D:3:TYR:CE2	2:D:4:ARG:HG2	2.50	0.47
1:B:231:THR:HG21	1:B:517:VAL:HG21	1.97	0.46
1:A:240:LYS:O	1:A:244:MET:HG2	2.15	0.46
1:B:216:LEU:HD23	1:B:274:VAL:HB	1.97	0.46
1:B:343:ARG:NH2	1:B:345:GLU:OE2	2.49	0.46
1:B:454:LEU:HB3	1:B:514:TYR:CZ	2.51	0.46
1:A:400:PRO:HB3	1:A:523:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LYS:O	1:B:244:MET:HG2	2.16	0.46
1:B:354:ILE:HD11	1:B:406:LEU:HD22	1.99	0.45
1:A:454:LEU:HB3	1:A:514:TYR:CZ	2.52	0.45
1:B:289:ASP:OD1	1:B:289:ASP:N	2.48	0.45
1:A:227:SER:HB3	1:A:467:VAL:HB	1.98	0.45
1:A:279:LEU:HG	1:A:283:PHE:HE2	1.81	0.45
1:A:477:TRP:HD1	1:A:490:LYS:HG2	1.79	0.45
1:B:252:SER:HA	1:B:258:LEU:HD23	1.98	0.44
1:A:262:ARG:HG3	1:A:544:LEU:HD22	1.98	0.44
1:A:375:GLY:O	1:A:378:LYS:NZ	2.46	0.44
1:A:366:ASP:O	2:C:4:ARG:NH2	2.45	0.43
1:B:426:GLU:HG3	1:B:498:TYR:CE2	2.53	0.43
1:B:251:ASP:OD2	1:B:253:SER:OG	2.31	0.43
1:A:333:GLN:HB2	1:A:340:ARG:HH11	1.84	0.43
1:A:431:LEU:HG	1:A:433:LEU:HG	1.99	0.43
1:A:315:CYS:HB3	1:B:315:CYS:O	2.19	0.43
1:A:320:ILE:HB	1:A:321:PRO:HD3	2.00	0.42
1:A:495:GLU:H	1:A:495:GLU:HG2	1.54	0.42
1:A:234:PHE:CD1	1:A:471:PRO:HB3	2.54	0.42
1:B:297:GLN:HG2	1:B:405:GLN:HG2	2.01	0.42
1:A:424:ARG:NH1	1:A:426:GLU:OE2	2.52	0.42
1:B:545:GLN:O	1:B:549:ARG:HG3	2.18	0.42
1:B:376:ASP:OD1	1:B:376:ASP:N	2.52	0.42
1:A:360:ILE:HD11	1:A:404:LEU:HD13	2.02	0.42
1:A:337:VAL:HG21	1:A:384:HIS:HB3	2.02	0.41
1:B:295:ASP:OD2	2:D:10:VAL:HG13	2.20	0.41
1:B:320:ILE:HB	1:B:321:PRO:HD3	2.03	0.41
1:B:350:ILE:HB	1:B:404:LEU:HD23	2.02	0.41
1:B:227:SER:HB3	1:B:467:VAL:HB	2.03	0.41
1:A:304:LEU:HA	1:A:307:VAL:HG22	2.03	0.41
1:A:231:THR:HG21	1:A:517:VAL:HG21	2.03	0.40
1:B:526:GLU:HG3	1:B:527:VAL:N	2.36	0.40
1:B:321:PRO:O	1:B:325:ARG:HB3	2.21	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	327/368 (89%)	319 (98%)	8 (2%)	0	100	100
1	B	330/368 (90%)	320 (97%)	10 (3%)	0	100	100
2	C	13/15 (87%)	10 (77%)	3 (23%)	0	100	100
2	D	13/15 (87%)	12 (92%)	1 (8%)	0	100	100
All	All	683/766 (89%)	661 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	287/332 (86%)	277 (96%)	10 (4%)	31	57
1	B	290/332 (87%)	281 (97%)	9 (3%)	35	62
2	C	11/11 (100%)	9 (82%)	2 (18%)	1	2
2	D	11/11 (100%)	11 (100%)	0	100	100
All	All	599/686 (87%)	578 (96%)	21 (4%)	31	57

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	VAL
1	A	286	GLU

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Mol	Chain	Res	Type
1	A	287	THR
1	A	288	LEU
1	A	434	ASP
1	A	483	ASP
1	A	487	ARG
1	A	495	GLU
1	A	496	HIS
1	A	542	GLU
1	B	256	VAL
1	B	297	GLN
1	B	337	VAL
1	B	349	ASP
1	B	393	VAL
1	B	434	ASP
1	B	469	LEU
1	B	483	ASP
1	B	551	GLU
2	C	10	VAL
2	C	14	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	293	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 ⓘ

There are no oligosaccharides 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	331/368 (89%)	0.15	5 (1%) 71 68	59, 86, 138, 179	0
1	B	334/368 (90%)	0.08	5 (1%) 71 68	53, 79, 134, 178	0
2	C	14/15 (93%)	0.28	0 100 100	78, 96, 108, 109	0
2	D	14/15 (93%)	0.17	0 100 100	69, 80, 90, 92	0
All	All	693/766 (90%)	0.12	10 (1%) 73 70	53, 84, 137, 179	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	552	ALA	3.3
1	A	220	GLY	2.7
1	B	524	LEU	2.7
1	B	288	LEU	2.6
1	B	354	ILE	2.6
1	A	383	GLU	2.3
1	A	283	PHE	2.2
1	A	354	ILE	2.2
1	B	325	ARG	2.1
1	A	288	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.