



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2022 – 12:15 PM JST

PDB ID : 7EGY
Title : Recombinant head-to-tail dimeric E2 protein
Authors : Ru, Q.X.
Deposited on : 2021-03-27
Resolution : 4.20 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	:	2.27
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)	:	2.27

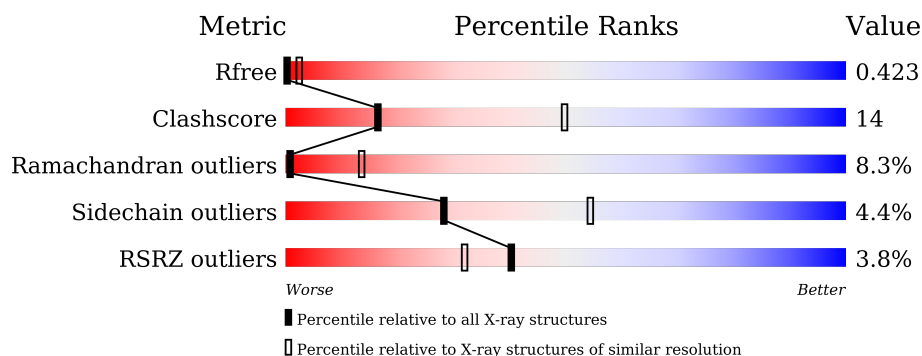
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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	342	<div> <div>2%</div> <div> <div></div> <div>43%</div> <div>26%</div> <div>•</div> <div>30%</div> </div> </div>
1	B	342	<div> <div>3%</div> <div> <div></div> <div>45%</div> <div>22%</div> <div>•</div> <div>30%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3402 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.

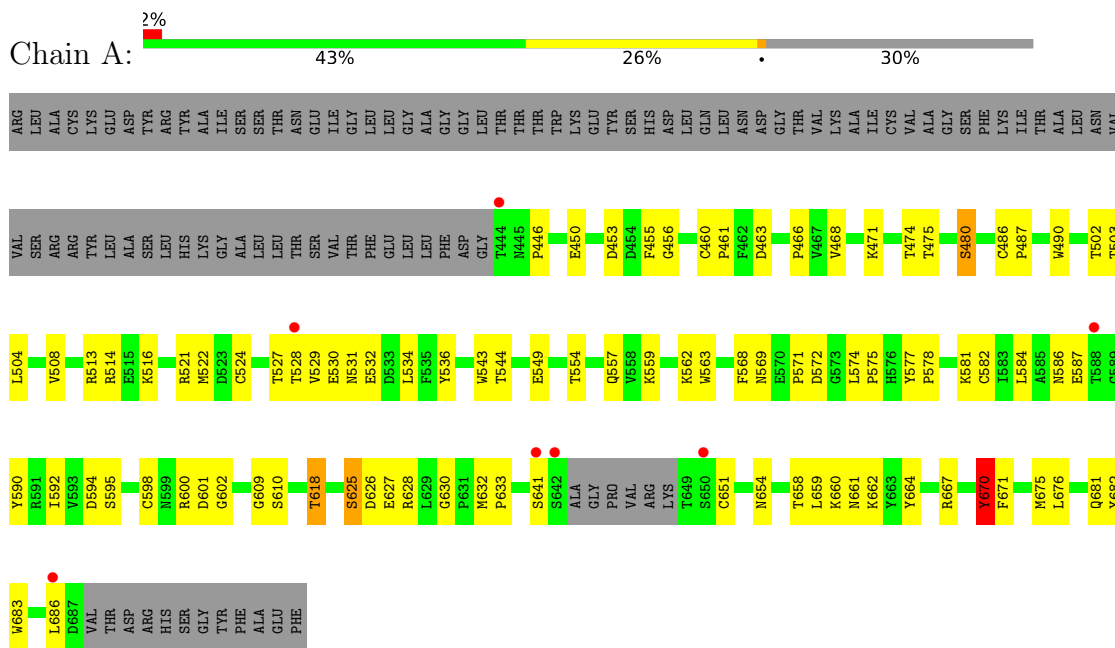
- Molecule 1 is a protein called E2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1701	1082	285	318	16			
1	B	238	Total	C	N	O	S	0	0	0
			1701	1082	285	318	16			

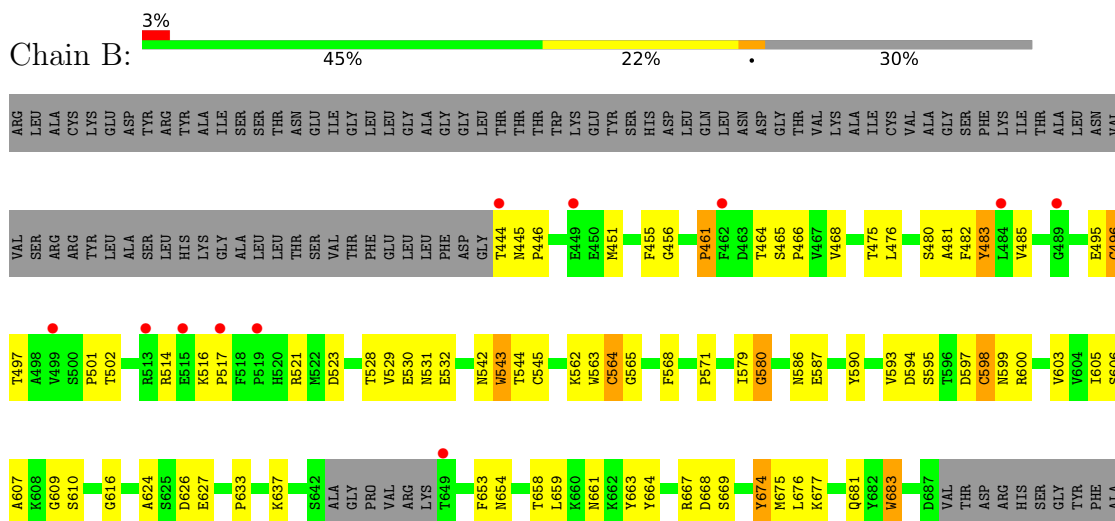
3 Residue-property plots

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: E2 protein



• Molecule 1: E2 protein



GLU
PHE

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	177.17Å 177.17Å 59.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.55 – 4.20 49.20 – 4.20	Depositor EDS
% Data completeness (in resolution range)	87.8 (42.55-4.20) 96.8 (49.20-4.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.381 , 0.444 0.401 , 0.423	Depositor DCC
R_{free} test set	358 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 90.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.042 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.49	EDS
Total number of atoms	3402	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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	0.27	0/1737	0.50	0/2350
1	B	0.27	0/1737	0.51	0/2350
All	All	0.27	0/3474	0.51	0/4700

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	1701	0	1478	48	0
1	B	1701	0	1478	43	0
All	All	3402	0	2956	91	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 14.

All (91) 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:485:VAL:HG11	1:B:543:TRP:HE1	1.44	0.81
1:B:600:ARG:HG3	1:B:633:PRO:HG3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:GLY:O	1:A:625:SER:OG	2.06	0.73
1:A:514:ARG:NE	1:A:516:LYS:O	2.20	0.72
1:B:627:GLU:O	1:B:661:ASN:ND2	2.26	0.69
1:A:563:TRP:HB3	1:A:568:PHE:HE2	1.58	0.67
1:B:455:PHE:O	1:B:521:ARG:NH1	2.27	0.67
1:B:528:THR:OG1	1:B:529:VAL:N	2.29	0.66
1:A:628:ARG:O	1:A:662:LYS:NZ	2.27	0.66
1:A:453:ASP:OD1	1:A:514:ARG:NH2	2.26	0.65
1:B:465:SER:O	1:B:497:THR:OG1	2.14	0.64
1:B:668:ASP:OD1	1:B:669:SER:N	2.31	0.63
1:B:542:ASN:O	1:B:544:THR:N	2.31	0.63
1:A:658:THR:OG1	1:A:659:LEU:N	2.31	0.62
1:A:594:ASP:OD1	1:A:595:SER:N	2.33	0.62
1:B:674:TYR:O	1:B:676:LEU:N	2.34	0.61
1:B:468:VAL:HG21	1:B:475:THR:HG21	1.83	0.61
1:B:542:ASN:C	1:B:544:THR:H	2.08	0.57
1:A:664:TYR:O	1:A:681:GLN:NE2	2.37	0.57
1:A:664:TYR:N	1:A:681:GLN:OE1	2.32	0.56
1:B:597:ASP:O	1:B:599:ASN:N	2.39	0.56
1:A:528:THR:OG1	1:A:529:VAL:N	2.40	0.55
1:B:624:ALA:HB2	1:B:659:LEU:HD23	1.87	0.55
1:A:508:VAL:O	1:A:508:VAL:HG13	2.07	0.55
1:B:654:ASN:O	1:B:683:TRP:N	2.39	0.54
1:B:464:THR:O	1:B:466:PRO:HD3	2.08	0.54
1:B:480:SER:OG	1:B:481:ALA:N	2.40	0.54
1:A:658:THR:OG1	1:A:662:LYS:O	2.21	0.53
1:A:627:GLU:O	1:A:661:ASN:ND2	2.40	0.53
1:A:503:THR:C	1:A:504:LEU:HD22	2.28	0.53
1:B:594:ASP:OD1	1:B:595:SER:N	2.40	0.52
1:A:568:PHE:HD1	1:A:618:THR:HG21	1.74	0.52
1:A:595:SER:O	1:A:595:SER:OG	2.27	0.51
1:B:451:MET:O	1:B:514:ARG:NH2	2.44	0.51
1:A:563:TRP:HB3	1:A:568:PHE:CE2	2.44	0.51
1:B:626:ASP:OD1	1:B:627:GLU:N	2.44	0.51
1:A:468:VAL:HG21	1:A:475:THR:HG21	1.93	0.50
1:A:562:LYS:HB3	1:A:581:LYS:HE2	1.94	0.50
1:B:563:TRP:NE1	1:B:564:CYS:SG	2.84	0.50
1:B:514:ARG:NH1	1:B:517:PRO:O	2.45	0.50
1:B:530:GLU:O	1:B:532:GLU:N	2.45	0.49
1:B:476:LEU:HB2	1:B:483:TYR:O	2.12	0.49
1:A:574:LEU:H	1:A:574:LEU:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:ARG:NH1	1:B:516:LYS:HG3	2.27	0.48
1:B:542:ASN:O	1:B:544:THR:HG23	2.12	0.48
1:B:563:TRP:O	1:B:565:GLY:N	2.47	0.48
1:B:495:GLU:O	1:B:497:THR:N	2.46	0.48
1:B:495:GLU:O	1:B:497:THR:HG23	2.14	0.47
1:A:569:ASN:O	1:A:577:TYR:OH	2.25	0.47
1:A:460:CYS:HB2	1:A:480:SER:O	2.13	0.47
1:B:485:VAL:HG11	1:B:543:TRP:NE1	2.22	0.47
1:A:581:LYS:HE3	1:A:590:TYR:CD1	2.50	0.46
1:A:460:CYS:SG	1:A:466:PRO:HG3	2.56	0.46
1:A:522:MET:O	1:A:524:CYS:N	2.48	0.46
1:B:461:PRO:HD2	1:B:496:CYS:SG	2.56	0.46
1:A:530:GLU:O	1:A:532:GLU:N	2.48	0.46
1:A:529:VAL:HA	1:A:534:LEU:HA	1.96	0.46
1:B:586:ASN:OD1	1:B:587:GLU:N	2.49	0.46
1:A:455:PHE:O	1:A:521:ARG:NH1	2.48	0.46
1:B:658:THR:OG1	1:B:659:LEU:N	2.49	0.46
1:B:562:LYS:HD2	1:B:590:TYR:HE1	1.81	0.45
1:A:632:MET:HG2	1:A:662:LYS:HB3	1.98	0.45
1:B:444:THR:HA	1:B:445:ASN:HA	1.67	0.45
1:A:675:MET:HE3	1:A:682:TYR:HB2	1.98	0.45
1:A:630:GLY:HA3	1:A:662:LYS:HZ2	1.82	0.44
1:A:609:GLY:HA3	1:A:610:SER:HA	1.65	0.44
1:B:667:ARG:HG3	1:B:674:TYR:CE1	2.52	0.44
1:A:670:TYR:CE1	1:A:686:LEU:HB3	2.52	0.44
1:B:664:TYR:N	1:B:681:GLN:OE1	2.38	0.44
1:A:513:ARG:HG2	1:A:514:ARG:N	2.34	0.43
1:B:579:ILE:HG12	1:B:580:GLY:H	1.82	0.43
1:B:599:ASN:HA	1:B:603:VAL:O	2.18	0.43
1:B:609:GLY:HA2	1:B:610:SER:HA	1.55	0.43
1:A:504:LEU:HD22	1:A:504:LEU:N	2.33	0.43
1:A:557:GLN:O	1:A:584:LEU:HD12	2.19	0.42
1:A:575:PRO:HG2	1:A:600:ARG:CZ	2.49	0.42
1:A:586:ASN:OD1	1:A:587:GLU:N	2.51	0.42
1:B:599:ASN:O	1:B:600:ARG:NE	2.47	0.42
1:A:578:PRO:HB2	1:A:582:CYS:SG	2.60	0.42
1:A:641:SER:OG	1:A:654:ASN:OD1	2.36	0.42
1:B:598:CYS:HB3	1:B:605:ILE:HG13	2.02	0.42
1:A:450:GLU:OE2	1:A:513:ARG:HD2	2.20	0.42
1:A:670:TYR:CZ	1:A:686:LEU:O	2.73	0.42
1:B:579:ILE:HG12	1:B:580:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:THR:O	1:A:527:THR:OG1	2.28	0.41
1:A:654:ASN:N	1:A:683:TRP:O	2.30	0.41
1:A:471:LYS:N	1:A:490:TRP:HE1	2.19	0.41
1:A:474:THR:HB	1:A:544:THR:HG21	2.03	0.40
1:A:671:PHE:N	1:A:671:PHE:CD1	2.89	0.40
1:B:606:SER:HB3	1:B:607:ALA:H	1.76	0.40
1:A:536:TYR:N	1:A:549:GLU:O	2.54	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	234/342 (68%)	155 (66%)	58 (25%)	21 (9%)	1	13
1	B	234/342 (68%)	151 (64%)	65 (28%)	18 (8%)	1	15
All	All	468/684 (68%)	306 (65%)	123 (26%)	39 (8%)	1	13

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	PRO
1	A	461	PRO
1	B	446	PRO
1	B	461	PRO
1	B	543	TRP
1	B	564	CYS
1	A	531	ASN
1	B	496	CYS
1	B	523	ASP
1	B	531	ASN
1	B	580	GLY

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Mol	Chain	Res	Type
1	B	593	VAL
1	B	598	CYS
1	B	674	TYR
1	B	675	MET
1	A	487	PRO
1	A	502	THR
1	A	559	LYS
1	A	660	LYS
1	B	483	TYR
1	B	637	LYS
1	A	463	ASP
1	A	543	TRP
1	A	554	THR
1	A	572	ASP
1	A	651	CYS
1	B	545	CYS
1	A	618	THR
1	A	625	SER
1	A	670	TYR
1	A	592	ILE
1	A	598	CYS
1	A	601	ASP
1	B	456	GLY
1	B	502	THR
1	B	616	GLY
1	A	456	GLY
1	A	633	PRO
1	A	486	CYS

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	158/295 (54%)	152 (96%)	6 (4%)	33	58
1	B	159/295 (54%)	151 (95%)	8 (5%)	24	51
All	All	317/590 (54%)	303 (96%)	14 (4%)	28	54

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	480	SER
1	A	571	PRO
1	A	626	ASP
1	A	667	ARG
1	A	670	TYR
1	A	676	LEU
1	B	482	PHE
1	B	501	PRO
1	B	568	PHE
1	B	571	PRO
1	B	653	PHE
1	B	663	TYR
1	B	677	LYS
1	B	683	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	238/342 (69%)	0.11	7 (2%) 51 41	29, 62, 95, 133	0
1	B	238/342 (69%)	0.23	11 (4%) 32 27	31, 70, 106, 147	0
All	All	476/684 (69%)	0.17	18 (3%) 40 32	29, 66, 102, 147	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	649	THR	3.4
1	B	519	PRO	3.3
1	B	515	GLU	3.2
1	B	444	THR	3.2
1	A	650	SER	2.8
1	A	642	SER	2.7
1	A	528	THR	2.7
1	B	499	VAL	2.6
1	A	686	LEU	2.4
1	B	513	ARG	2.3
1	B	449	GLU	2.3
1	B	462	PHE	2.3
1	B	517	PRO	2.1
1	A	641	SER	2.1
1	A	444	THR	2.0
1	B	484	LEU	2.0
1	A	588	THR	2.0
1	B	489	GLY	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.