



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 10:09 PM UTC

PDB ID : 8COI / pdb_00008coi
Title : Human adenovirus-derived synthetic ADDobody binder
Authors : Buzas, D.; Toelzer, C.; Gupta, K.; Berger-Schaffitzel, C.; Berger, I.
Deposited on : 2023-02-28
Resolution : 3.17 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

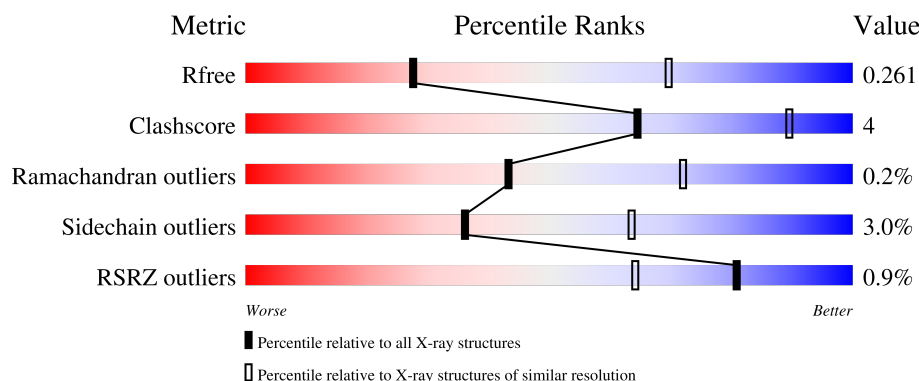
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

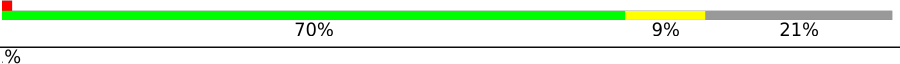
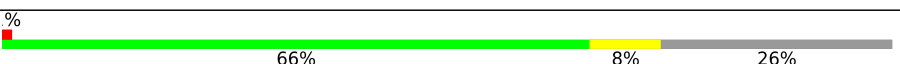
The reported resolution of this entry is 3.17 Å.

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}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	310	 70% 9% 21%
1	B	310	 70% 9% 21%
1	C	310	 70% 10% 20%
1	D	310	 70% 8% 21%
1	E	310	 66% 8% 26%

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Mol	Chain	Length	Quality of chain
1	F	310	
1	G	310	
1	H	310	
1	I	310	
1	J	310	
1	K	310	
1	L	310	
1	M	310	
1	N	310	
1	O	310	
1	P	310	
1	Q	310	
1	R	310	
1	S	310	
1	T	310	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 37335 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 ADDobody.

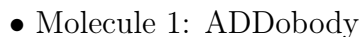
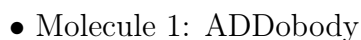
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1927	1235	325	360	7			
1	B	246	Total	C	N	O	S	0	0	0
			1956	1252	326	371	7			
1	C	249	Total	C	N	O	S	0	0	0
			1935	1236	328	364	7			
1	D	244	Total	C	N	O	S	0	0	0
			1938	1237	327	367	7			
1	E	228	Total	C	N	O	S	0	0	0
			1818	1167	301	343	7			
1	F	240	Total	C	N	O	S	0	0	0
			1941	1245	325	363	8			
1	G	243	Total	C	N	O	S	0	0	0
			1920	1227	325	361	7			
1	H	243	Total	C	N	O	S	0	0	0
			1931	1238	324	362	7			
1	I	249	Total	C	N	O	S	0	0	0
			1964	1258	326	373	7			
1	J	243	Total	C	N	O	S	0	0	0
			1917	1232	319	359	7			
1	K	250	Total	C	N	O	S	0	0	0
			1985	1271	332	375	7			
1	L	244	Total	C	N	O	S	0	0	0
			1928	1234	322	366	6			
1	M	237	Total	C	N	O	S	0	0	0
			1882	1203	314	358	7			
1	N	232	Total	C	N	O	S	0	0	0
			1838	1175	307	349	7			
1	O	229	Total	C	N	O	S	0	0	0
			1788	1140	304	338	6			
1	P	243	Total	C	N	O	S	0	0	0
			1855	1184	310	355	6			

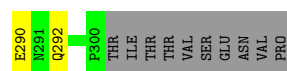
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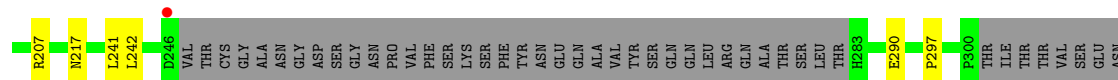
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	232	Total	C	N	O	S	0	0	0
			1796	1148	296	345	7			
1	R	227	Total	C	N	O	S	0	0	0
			1774	1142	291	334	7			
1	S	230	Total	C	N	O	S	0	0	0
			1645	1050	274	318	3			
1	T	212	Total	C	N	O	S	0	0	0
			1597	1019	267	306	5			

- Molecule 1: ADDobody

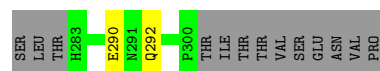
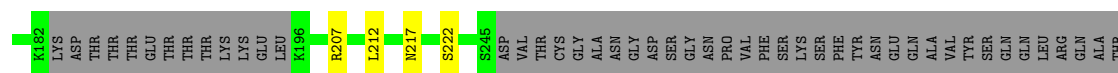




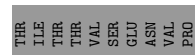
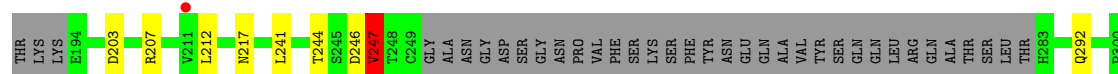
• Molecule 1: ADDobody



• Molecule 1: ADDobody

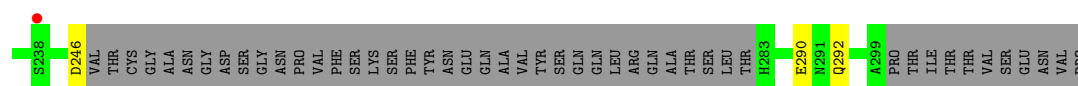


• Molecule 1: ADDobody

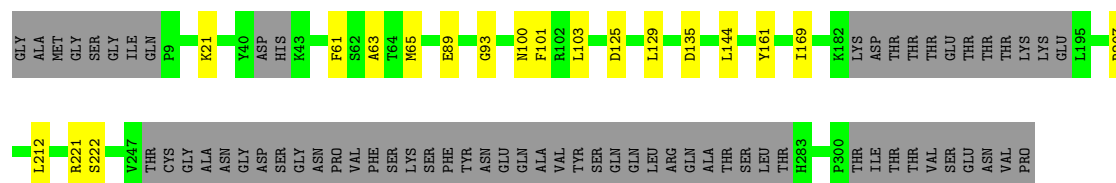


• Molecule 1: ADDobody

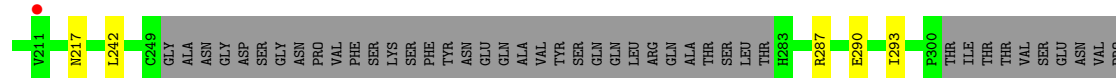




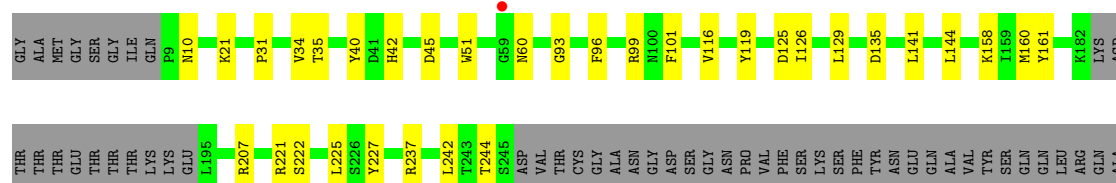
- Molecule 1: ADDobody



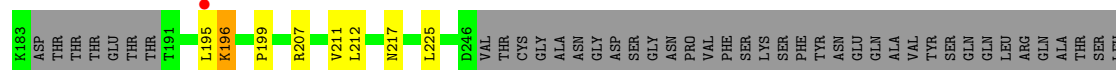
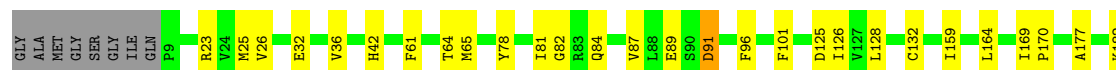
- Molecule 1: ADDobody

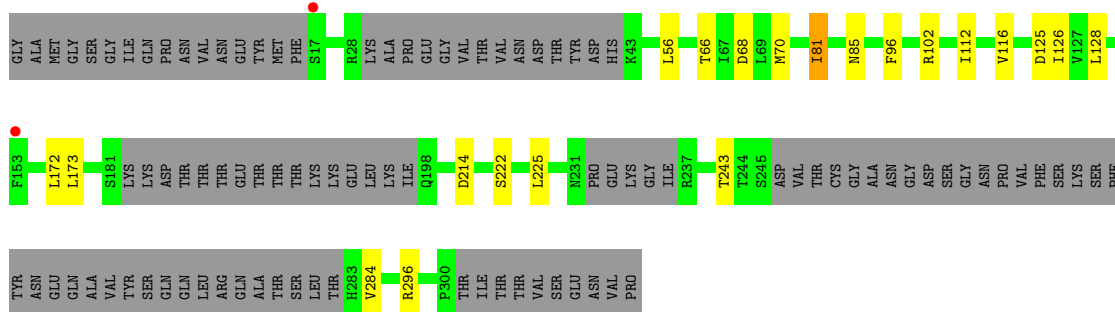


- Molecule 1: ADDobody



- Molecule 1: ADDobody





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.85Å 104.63Å 180.49Å 92.03° 95.65° 112.61°	Depositor
Resolution (Å)	19.97 – 3.17 19.97 – 3.17	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.97-3.17) 98.6 (19.97-3.17)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.15Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.213 , 0.261 0.213 , 0.261	Depositor DCC
R_{free} test set	5852 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	37335	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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	0.10	0/1975	0.31	1/2687 (0.0%)
1	B	0.09	0/2004	0.26	0/2723
1	C	0.10	0/1982	0.29	0/2698
1	D	0.10	0/1985	0.28	0/2695
1	E	0.09	0/1863	0.26	0/2528
1	F	0.11	0/1989	0.30	0/2694
1	G	0.09	0/1967	0.27	0/2671
1	H	0.10	0/1978	0.27	0/2681
1	I	0.10	0/2012	0.28	0/2737
1	J	0.10	0/1966	0.27	0/2673
1	K	0.11	0/2034	0.28	0/2763
1	L	0.10	0/1976	0.28	0/2685
1	M	0.09	0/1928	0.26	0/2618
1	N	0.08	0/1882	0.26	0/2556
1	O	0.09	0/1829	0.27	0/2485
1	P	0.11	0/1899	0.29	0/2585
1	Q	0.08	0/1838	0.24	0/2502
1	R	0.09	0/1816	0.26	0/2466
1	S	0.10	0/1686	0.27	0/2317
1	T	0.09	0/1636	0.26	0/2233
All	All	0.10	0/38245	0.28	1/51997 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	GLU	CB-CA-C	-5.92	109.73	116.54

There are no chirality outliers.

There are no planarity outliers.

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	1927	0	1823	15	0
1	B	1956	0	1863	14	0
1	C	1935	0	1800	18	0
1	D	1938	0	1842	18	0
1	E	1818	0	1723	12	0
1	F	1941	0	1874	13	0
1	G	1920	0	1806	10	0
1	H	1931	0	1831	9	0
1	I	1964	0	1847	10	0
1	J	1917	0	1812	24	0
1	K	1985	0	1884	18	0
1	L	1928	0	1823	18	0
1	M	1882	0	1776	15	0
1	N	1838	0	1746	13	0
1	O	1788	0	1671	15	0
1	P	1855	0	1704	16	0
1	Q	1796	0	1658	8	0
1	R	1774	0	1668	19	0
1	S	1645	0	1372	19	0
1	T	1597	0	1402	13	0
All	All	37335	0	34925	283	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 4.

The worst 5 of 283 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:D:58:GLU:OE2	1:J:237:ARG:NH2	2.19	0.75
1:R:125:ASP:OD2	1:R:222:SER:OG	2.05	0.72
1:J:99:ARG:NH2	1:J:292:GLN:O	2.21	0.72
1:H:89:GLU:OE1	1:H:207:ARG:NH1	2.23	0.71
1:K:177:ALA:HB1	1:K:196:LYS:HD2	1.75	0.69

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	239/310 (77%)	215 (90%)	24 (10%)	0	100	100
1	B	240/310 (77%)	227 (95%)	13 (5%)	0	100	100
1	C	243/310 (78%)	228 (94%)	13 (5%)	2 (1%)	16	47
1	D	238/310 (77%)	222 (93%)	16 (7%)	0	100	100
1	E	220/310 (71%)	203 (92%)	17 (8%)	0	100	100
1	F	232/310 (75%)	212 (91%)	19 (8%)	1 (0%)	30	60
1	G	237/310 (76%)	213 (90%)	23 (10%)	1 (0%)	30	60
1	H	235/310 (76%)	213 (91%)	22 (9%)	0	100	100
1	I	243/310 (78%)	228 (94%)	15 (6%)	0	100	100
1	J	237/310 (76%)	219 (92%)	18 (8%)	0	100	100
1	K	244/310 (79%)	227 (93%)	17 (7%)	0	100	100
1	L	238/310 (77%)	220 (92%)	17 (7%)	1 (0%)	30	60
1	M	229/310 (74%)	209 (91%)	20 (9%)	0	100	100
1	N	224/310 (72%)	208 (93%)	16 (7%)	0	100	100
1	O	221/310 (71%)	201 (91%)	20 (9%)	0	100	100
1	P	237/310 (76%)	217 (92%)	19 (8%)	1 (0%)	30	60
1	Q	224/310 (72%)	209 (93%)	15 (7%)	0	100	100
1	R	219/310 (71%)	194 (89%)	24 (11%)	1 (0%)	24	57
1	S	222/310 (72%)	199 (90%)	22 (10%)	1 (0%)	24	57
1	T	202/310 (65%)	187 (93%)	15 (7%)	0	100	100
All	All	4624/6200 (75%)	4251 (92%)	365 (8%)	8 (0%)	43	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	42	HIS

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Mol	Chain	Res	Type
1	F	247	VAL
1	L	61	PHE
1	S	216	ILE
1	C	37	ASN

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	202/276 (73%)	198 (98%)	4 (2%)	48	69
1	B	209/276 (76%)	206 (99%)	3 (1%)	59	74
1	C	198/276 (72%)	192 (97%)	6 (3%)	36	63
1	D	206/276 (75%)	203 (98%)	3 (2%)	57	73
1	E	194/276 (70%)	192 (99%)	2 (1%)	68	78
1	F	211/276 (76%)	205 (97%)	6 (3%)	38	64
1	G	200/276 (72%)	198 (99%)	2 (1%)	68	78
1	H	203/276 (74%)	202 (100%)	1 (0%)	81	83
1	I	207/276 (75%)	201 (97%)	6 (3%)	37	64
1	J	201/276 (73%)	199 (99%)	2 (1%)	68	78
1	K	210/276 (76%)	198 (94%)	12 (6%)	18	48
1	L	204/276 (74%)	197 (97%)	7 (3%)	32	61
1	M	200/276 (72%)	193 (96%)	7 (4%)	32	61
1	N	196/276 (71%)	189 (96%)	7 (4%)	31	60
1	O	184/276 (67%)	178 (97%)	6 (3%)	33	62
1	P	188/276 (68%)	172 (92%)	16 (8%)	10	34
1	Q	185/276 (67%)	179 (97%)	6 (3%)	34	62
1	R	184/276 (67%)	175 (95%)	9 (5%)	22	52
1	S	145/276 (52%)	140 (97%)	5 (3%)	32	61
1	T	154/276 (56%)	149 (97%)	5 (3%)	34	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3881/5520 (70%)	3766 (97%)	115 (3%)	36 63

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	144	LEU
1	T	81	ILE
1	O	102	ARG
1	S	288	PHE
1	R	103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	R	210	ASN
1	S	283	HIS
1	T	217	ASN
1	F	72	ASN
1	E	210	ASN

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 ⓘ

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	245/310 (79%)	-0.17	2 (0%) 82 67	53, 77, 120, 159	0
1	B	246/310 (79%)	-0.31	2 (0%) 82 67	46, 66, 118, 137	0
1	C	249/310 (80%)	-0.19	3 (1%) 76 57	48, 69, 118, 160	0
1	D	244/310 (78%)	-0.34	2 (0%) 82 67	43, 62, 111, 170	0
1	E	228/310 (73%)	-0.26	2 (0%) 81 64	50, 75, 112, 146	0
1	F	240/310 (77%)	-0.29	1 (0%) 88 78	46, 72, 117, 153	0
1	G	243/310 (78%)	-0.15	2 (0%) 82 67	57, 80, 130, 165	0
1	H	243/310 (78%)	-0.20	0 100 100	54, 77, 126, 172	0
1	I	249/310 (80%)	-0.16	2 (0%) 82 67	50, 77, 125, 161	0
1	J	243/310 (78%)	-0.21	1 (0%) 88 78	49, 75, 127, 162	0
1	K	250/310 (80%)	-0.17	1 (0%) 88 78	64, 86, 129, 179	0
1	L	244/310 (78%)	-0.12	3 (1%) 76 57	61, 87, 141, 161	0
1	M	237/310 (76%)	-0.07	2 (0%) 82 67	64, 89, 127, 157	0
1	N	232/310 (74%)	-0.07	0 100 100	71, 99, 139, 177	0
1	O	229/310 (73%)	0.05	3 (1%) 75 55	72, 101, 133, 174	0
1	P	243/310 (78%)	0.13	3 (1%) 76 57	79, 110, 149, 176	0
1	Q	232/310 (74%)	-0.05	1 (0%) 88 78	80, 104, 135, 166	0
1	R	227/310 (73%)	0.10	3 (1%) 75 55	88, 112, 145, 167	0
1	S	230/310 (74%)	0.45	9 (3%) 43 25	94, 126, 154, 220	0
1	T	212/310 (68%)	0.26	2 (0%) 81 64	100, 126, 154, 180	0
All	All	4766/6200 (76%)	-0.09	44 (0%) 81 64	43, 89, 139, 220	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	93	GLY	5.3
1	O	60	ASN	3.9
1	J	59	GLY	3.6
1	R	91	ASP	3.3
1	E	60	ASN	3.1

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 oligosaccharides 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.