



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:32 PM UTC

PDB ID : 8DW9 / pdb_00008dw9
Title : Crystal structure of neutralizing antibody D29 Fab in complex with SARS-CoV-2 spike receptor binding domain (RBD)
Authors : Reddem, E.R.; Shapiro, L.
Deposited on : 2022-08-01
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 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

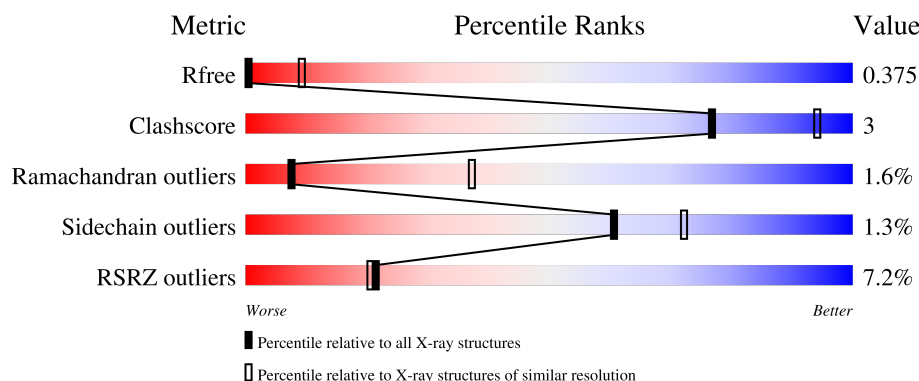
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	195	5% 81% 8% 11%
1	B	195	8% 82% 7% 11%
2	C	219	10% 89% 10%
2	H	219	5% 89% 11%
3	D	211	5% 92% 7%

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Mol	Chain	Length	Quality of chain
3	L	211	9% 91% 8% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9236 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	1	0
			1378	886	232	254	6			
1	B	174	Total	C	N	O	S	0	1	0
			1378	886	232	254	6			

- Molecule 2 is a protein called D29 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	219	Total	C	N	O	S	0	3	0
			1640	1043	265	326	6			
2	H	219	Total	C	N	O	S	0	3	0
			1640	1043	265	326	6			

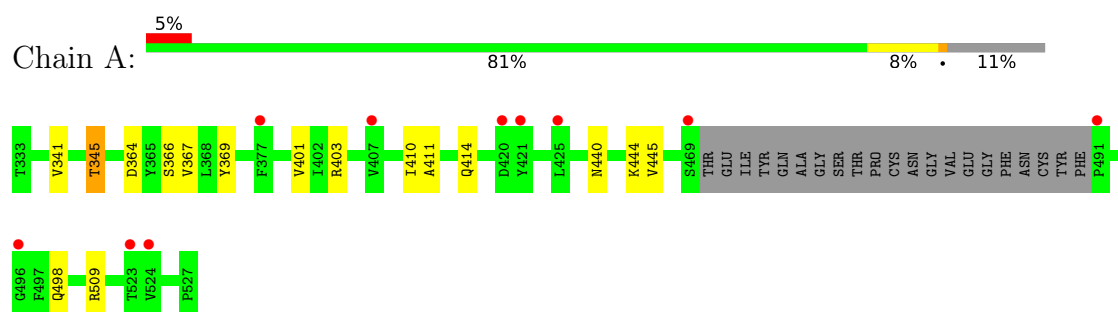
- Molecule 3 is a protein called D29 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	211	Total	C	N	O	S	0	2	0
			1600	1010	269	317	4			
3	L	211	Total	C	N	O	S	0	2	0
			1600	1010	269	317	4			

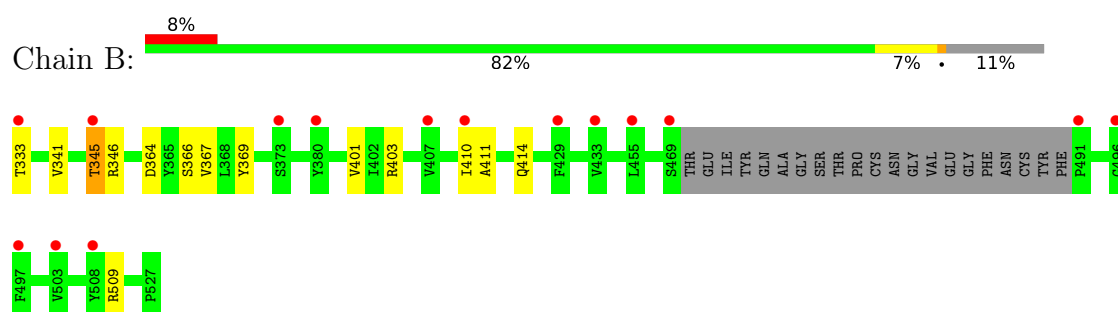
3 Residue-property plots [i](#)

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.

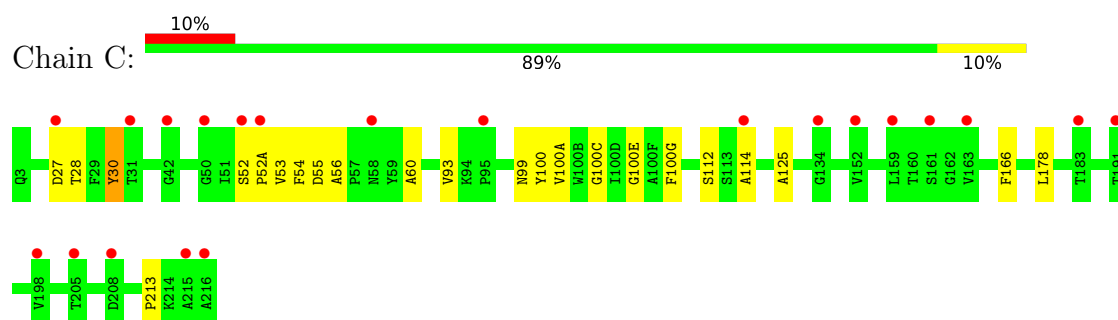
- Molecule 1: Spike protein S1



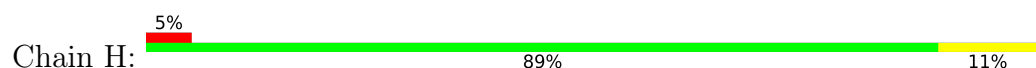
- Molecule 1: Spike protein S1



- Molecule 2: D29 Heavy chain

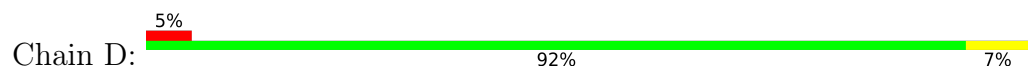


- Molecule 2: D29 Heavy chain

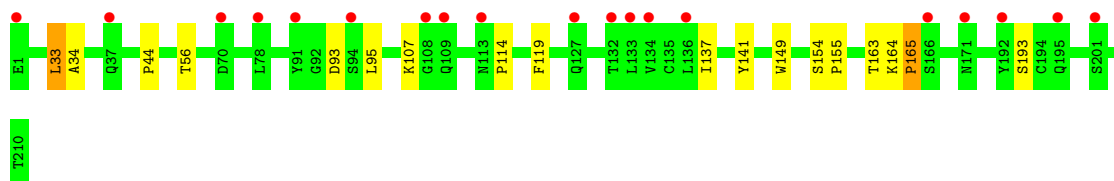
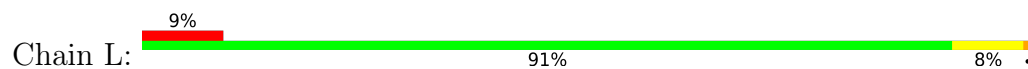




- Molecule 3: D29 Fab light chain



- Molecule 3: D29 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.17Å 106.71Å 207.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.09 – 4.00 95.09 – 4.00	Depositor EDS
% Data completeness (in resolution range)	82.0 (95.09-4.00) 82.0 (95.09-4.00)	Depositor EDS
R_{merge}	0.96	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 4.01Å)	Xtriage
Refinement program	PHENIX Refine	Depositor
R, R_{free}	0.300 , 0.381 0.346 , 0.375	Depositor DCC
R_{free} test set	639 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å ²)	88.9	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 18.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	9236	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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	0.57	0/1416	0.85	0/1925
1	B	0.57	0/1416	0.85	0/1925
2	C	0.58	0/1684	0.82	0/2298
2	H	0.58	0/1684	0.84	0/2298
3	D	0.56	0/1642	0.84	0/2238
3	L	0.55	0/1642	0.83	0/2238
All	All	0.57	0/9484	0.84	0/12922

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

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	1378	0	1314	8	0
1	B	1378	0	1314	7	0
2	C	1640	0	1592	14	0
2	H	1640	0	1592	17	0
3	D	1600	0	1556	9	0
3	L	1600	0	1556	9	0
All	All	9236	0	8924	52	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 3.

All (52) 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:445:VAL:HG21	2:H:64:GLN:HE22	1.38	0.88
1:B:333:THR:N	2:H:28:THR:HG1	1.75	0.85
2:C:93:VAL:HG11	2:C:100(G):PHE:HB3	1.67	0.76
1:A:345:THR:HG21	2:H:32:PHE:CE2	2.42	0.55
2:H:11:VAL:HG13	2:H:110:THR:OG1	2.06	0.55
2:H:93:VAL:HG11	2:H:100(G):PHE:HB3	1.89	0.54
2:H:100:TYR:HB3	2:H:100(C):GLY:HA3	1.89	0.54
2:H:93:VAL:HG11	2:H:100(G):PHE:CD2	2.43	0.53
2:H:54:PHE:O	2:H:56:ALA:N	2.42	0.53
2:H:166:PHE:HB3	3:L:163:THR:HG21	1.91	0.52
3:L:114:PRO:HB2	3:L:137:ILE:HG23	1.92	0.51
2:C:54:PHE:O	2:C:56:ALA:N	2.43	0.50
2:H:112:SER:O	2:H:114:ALA:N	2.44	0.50
2:C:112:SER:O	2:C:114:ALA:N	2.45	0.50
3:D:33:LEU:HD23	3:D:89:GLN:O	2.12	0.49
2:C:100(E):GLY:HA3	3:D:91:TYR:CD1	2.47	0.49
3:D:114:PRO:HB2	3:D:137:ILE:HG23	1.94	0.49
1:B:345:THR:HG22	2:C:99:ASN:HB3	1.94	0.48
3:D:164:LYS:HB3	3:D:165:PRO:HD2	1.93	0.48
1:B:411:ALA:HB3	1:B:414:GLN:HG2	1.95	0.48
3:L:107:LYS:HA	3:L:141:TYR:OH	2.14	0.48
3:D:107:LYS:HA	3:D:141:TYR:OH	2.14	0.47
1:B:366:SER:HA	1:B:369:TYR:CE2	2.50	0.47
2:C:100:TYR:HB3	2:C:100(C):GLY:HA3	1.97	0.47
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.98	0.46
3:L:164:LYS:HB3	3:L:165:PRO:HD2	1.98	0.46
2:C:166:PHE:HB3	3:D:163:THR:HG21	1.97	0.46
1:A:366:SER:HA	1:A:369:TYR:CE2	2.50	0.45
3:L:33:LEU:HD23	3:L:34:ALA:N	2.31	0.45
2:C:100:TYR:CG	2:C:100(A):VAL:N	2.85	0.45
1:A:444:LYS:HE2	2:H:56:ALA:HB1	1.98	0.44
2:H:125:ALA:HB1	2:H:213:PRO:HA	1.98	0.44
2:C:30:TYR:C	2:C:53:VAL:HG23	2.43	0.44
2:C:125:ALA:HB1	2:C:213:PRO:HA	2.00	0.44
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.99	0.44
3:D:164:LYS:HB3	3:D:165:PRO:CD	2.48	0.43
1:A:364:ASP:O	1:A:367:VAL:HG12	2.18	0.43
2:H:100:TYR:CG	2:H:100(A):VAL:N	2.86	0.42
2:C:93:VAL:CG1	2:C:100(G):PHE:HB3	2.42	0.42
2:C:60:ALA:HA	3:D:95:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ASP:O	1:B:367:VAL:HG12	2.19	0.42
1:B:346:ARG:HD2	2:C:54:PHE:CE2	2.54	0.42
1:B:401:VAL:HG22	1:B:509:ARG:HG2	2.01	0.41
2:C:178:LEU:C	2:C:178:LEU:HD12	2.45	0.41
3:L:164:LYS:HB3	3:L:165:PRO:CD	2.51	0.41
2:H:32:PHE:O	2:H:52(A):PRO:HD2	2.21	0.41
3:L:149:TRP:O	3:L:155:PRO:HA	2.20	0.41
3:D:149:TRP:O	3:D:155:PRO:HA	2.20	0.41
2:H:178:LEU:C	2:H:178:LEU:HD12	2.45	0.41
2:H:124:LEU:HB3	3:L:119:PHE:CD2	2.56	0.41
1:A:440:ASN:HB3	3:L:93:ASP:HA	2.03	0.40
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.02	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	170/195 (87%)	148 (87%)	18 (11%)	4 (2%)	4	30
1	B	170/195 (87%)	148 (87%)	18 (11%)	4 (2%)	4	30
2	C	214/219 (98%)	194 (91%)	17 (8%)	3 (1%)	9	39
2	H	214/219 (98%)	194 (91%)	18 (8%)	2 (1%)	14	48
3	D	208/211 (99%)	192 (92%)	13 (6%)	3 (1%)	9	39
3	L	208/211 (99%)	191 (92%)	14 (7%)	3 (1%)	9	39
All	All	1184/1250 (95%)	1067 (90%)	98 (8%)	19 (2%)	7	37

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	55	ASP

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Mol	Chain	Res	Type
2	H	55	ASP
1	A	345	THR
1	B	345	THR
2	H	30	TYR
1	A	403	ARG
1	B	403	ARG
2	C	30	TYR
2	C	27	ASP
3	D	56	THR
3	D	165	PRO
3	L	165	PRO
3	L	56	THR
1	B	341	VAL
1	A	341	VAL
1	A	410	ILE
1	B	410	ILE
3	L	44	PRO
3	D	44	PRO

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	149/168 (89%)	148 (99%)	1 (1%)	76	79
1	B	149/168 (89%)	149 (100%)	0	100	100
2	C	184/184 (100%)	181 (98%)	3 (2%)	55	70
2	H	184/184 (100%)	181 (98%)	3 (2%)	55	70
3	D	175/177 (99%)	173 (99%)	2 (1%)	65	74
3	L	175/177 (99%)	171 (98%)	4 (2%)	44	64
All	All	1016/1058 (96%)	1003 (99%)	13 (1%)	61	72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	498	GLN
2	C	28	THR
2	C	52	SER
2	C	52(A)	PRO
3	D	33	LEU
3	D	154	SER
2	H	28	THR
2	H	52	SER
2	H	52(A)	PRO
3	L	33	LEU
3	L	95	LEU
3	L	154	SER
3	L	193	SER

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

Mol	Chain	Res	Type
1	A	414	GLN
1	B	360	ASN
2	C	39	GLN
3	D	38	GLN
2	H	61	GLN
2	H	64	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	2
2	C	2
3	D	1
3	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	127:SER	C	134:GLY	N	13.16
1	C	127:SER	C	134:GLY	N	11.03
1	C	113:SER	C	114:ALA	N	4.75
1	H	113:SER	C	114:ALA	N	4.74
1	D	107:LYS	C	108:GLY	N	3.73
1	L	107:LYS	C	108:GLY	N	3.73

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	174/195 (89%)	0.79	10 (5%)	29 26	41, 41, 41, 41	0
1	B	174/195 (89%)	0.73	15 (8%)	16 17	37, 41, 41, 41	1 (0%)
2	C	219/219 (100%)	0.78	21 (9%)	13 16	26, 41, 41, 41	1 (0%)
2	H	219/219 (100%)	0.77	12 (5%)	30 26	26, 41, 41, 41	1 (0%)
3	D	211/211 (100%)	0.70	10 (4%)	36 29	26, 41, 41, 41	1 (0%)
3	L	211/211 (100%)	0.79	19 (9%)	15 17	26, 41, 41, 41	1 (0%)
All	All	1208/1250 (96%)	0.76	87 (7%)	21 20	26, 41, 41, 41	5 (0%)

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	49	GLY	4.8
3	L	171	ASN	4.3
3	L	134	VAL	4.3
3	D	153	GLY	4.0
3	D	154	SER	3.9
1	B	455	LEU	3.6
1	B	345	THR	3.6
3	L	133	LEU	3.5
3	L	127	GLN	3.4
1	B	333	THR	3.3
3	L	113	ASN	3.3
2	H	48	MET	3.3
1	A	496	GLY	3.3
3	L	201	SER	3.3
2	C	134	GLY	3.3
2	C	58	ASN	3.2
2	C	191	THR	3.0
2	C	215	ALA	3.0
2	C	50	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	114	ALA	3.0
3	L	108	GLY	3.0
2	C	52	SER	3.0
3	L	195	GLN	3.0
2	H	63	PHE	2.9
2	H	55	ASP	2.9
2	C	198	VAL	2.9
1	B	407	VAL	2.8
1	B	508	TYR	2.8
2	C	95	PRO	2.8
1	A	407	VAL	2.8
2	C	31	THR	2.7
2	H	91	TYR	2.7
3	D	159	GLY	2.7
1	A	425	LEU	2.6
2	H	50	GLY	2.6
2	H	120	SER	2.6
1	A	421	TYR	2.6
3	L	192	TYR	2.6
2	C	216	ALA	2.6
1	B	433	VAL	2.6
1	B	380	TYR	2.6
3	L	166	SER	2.6
3	L	109	GLN	2.6
2	H	52(A)	PRO	2.6
3	L	70	ASP	2.5
3	L	1	GLU	2.5
1	A	524	VAL	2.5
2	C	205	THR	2.4
3	L	78	LEU	2.4
3	L	91	TYR	2.4
3	L	94	SER	2.4
3	L	37	GLN	2.4
1	A	491	PRO	2.4
3	D	158	ALA	2.4
2	H	28	THR	2.4
1	B	491	PRO	2.3
1	B	373	SER	2.3
2	H	119	PRO	2.3
2	C	114	ALA	2.3
2	C	52(A)	PRO	2.3
2	C	42	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	497	PHE	2.3
1	A	377	PHE	2.2
1	A	523	THR	2.2
3	D	165	PRO	2.2
1	A	469	SER	2.2
1	B	503	VAL	2.2
2	C	161	SER	2.2
2	C	152	VAL	2.2
2	C	208	ASP	2.2
3	D	118	LEU	2.2
1	A	420	ASP	2.1
1	B	429	PHE	2.1
2	C	183	THR	2.1
3	D	2	ILE	2.1
3	D	31	ILE	2.1
1	B	469	SER	2.1
2	C	159	LEU	2.1
3	L	132	THR	2.1
2	C	163	VAL	2.1
3	L	136	LEU	2.1
2	H	99	ASN	2.1
1	B	410	ILE	2.0
1	B	496	GLY	2.0
2	C	27	ASP	2.0
3	D	144	ALA	2.0
3	D	65	SER	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 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.