



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 04:47 PM EDT

PDB ID : 4GRM
Title : The crystal structure of the high affinity TCR A6
Authors : Borbulevych, O.Y.; Scott, D.R.; Baker, B.M.
Deposited on : 2012-08-25
Resolution : 2.00 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 : 4.02b-467
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

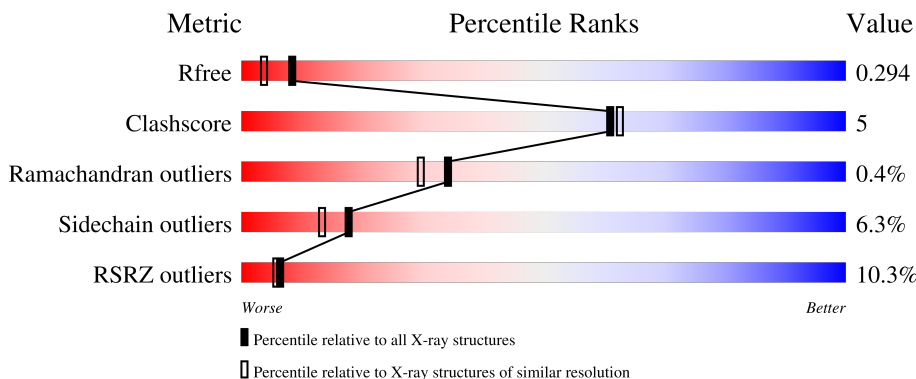
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	194	
1	C	194	
2	B	245	
2	D	245	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6612 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 A6 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	184	1375	856	224	287	8	0	0	0
1	C	187	1405	872	231	294	8	0	0	0

- Molecule 2 is a protein called A6 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	240	1880	1185	326	360	9	0	0	0
2	D	243	1893	1192	330	362	9	0	0	0

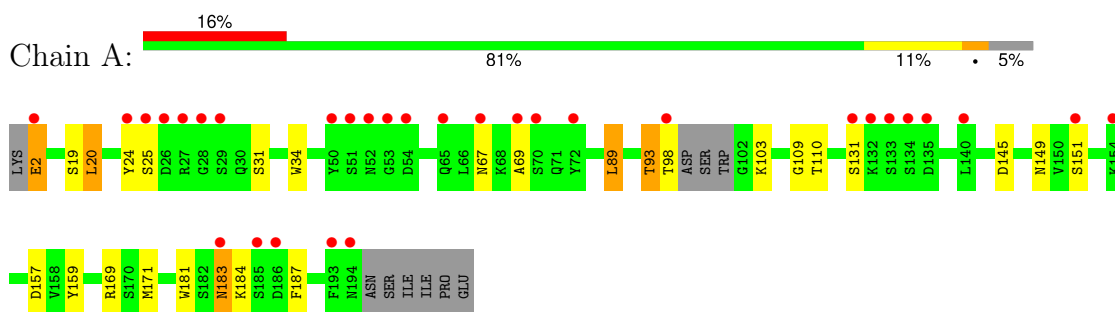
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	23	Total	O	0	0
			23	23		
3	C	15	Total	O	0	0
			15	15		
3	D	11	Total	O	0	0
			11	11		

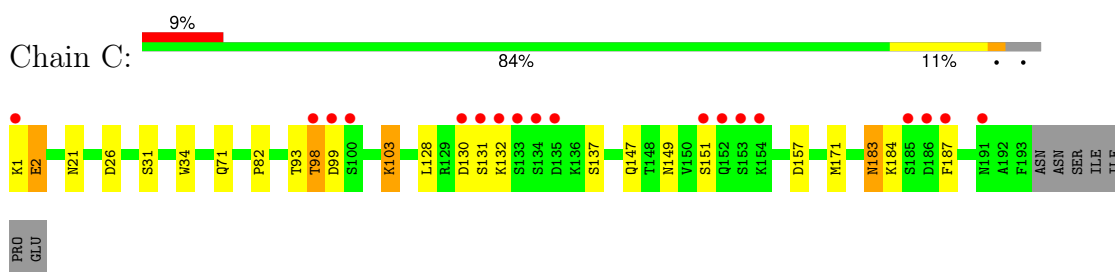
3 Residue-property plots [i](#)

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.

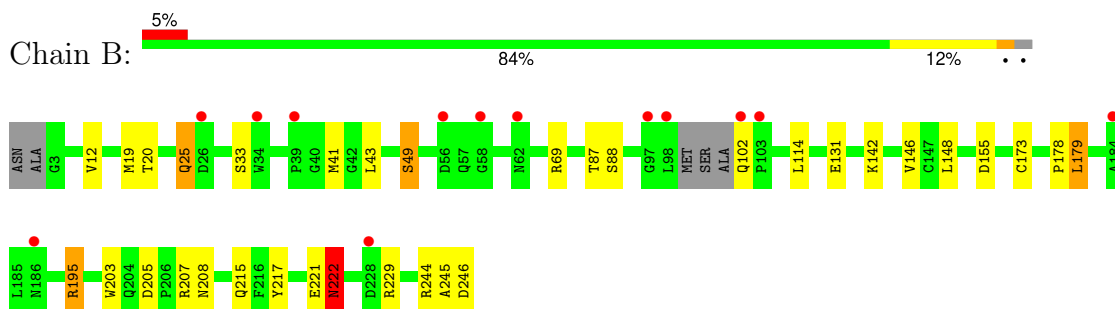
- Molecule 1: A6 alpha chain



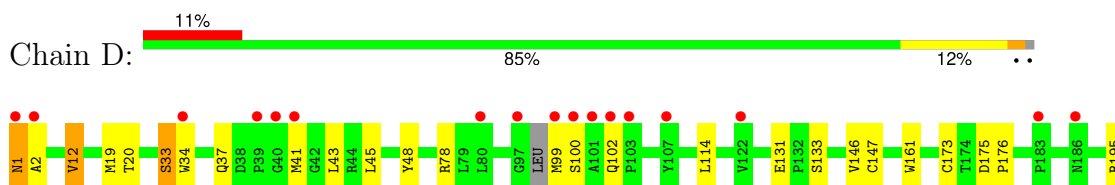
- Molecule 1: A6 alpha chain



- Molecule 2: A6 beta chain



- Molecule 2: A6 beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.49Å 51.97Å 95.22Å 90.00° 104.94° 90.00°	Depositor
Resolution (Å)	18.84 – 2.00 18.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (18.84-2.00) 98.8 (18.84-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.234 , 0.295 0.233 , 0.294	Depositor DCC
R_{free} test set	2918 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6612	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.93 % 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 1.8982e-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

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	0.93	2/1401 (0.1%)	0.89	3/1906 (0.2%)
1	C	0.94	1/1432 (0.1%)	0.92	0/1947
2	B	0.93	1/1932 (0.1%)	0.99	5/2636 (0.2%)
2	D	0.89	4/1945 (0.2%)	0.91	4/2653 (0.2%)
All	All	0.92	8/6710 (0.1%)	0.93	12/9142 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	TRP	CD2-CE2	7.60	1.50	1.41
1	C	34	TRP	CD2-CE2	6.57	1.49	1.41
2	D	203	TRP	CD2-CE2	6.45	1.49	1.41
2	D	242	TRP	CD2-CE2	6.38	1.49	1.41
1	A	181	TRP	CD2-CE2	6.14	1.48	1.41
2	B	203	TRP	CD2-CE2	5.70	1.48	1.41
2	D	225	TRP	CD2-CE2	5.34	1.47	1.41
2	D	34	TRP	CD2-CE2	5.09	1.47	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	146	VAL	CG1-CB-CG2	-8.80	96.83	110.90
2	D	12	VAL	CG1-CB-CG2	-8.51	97.28	110.90
2	D	207	ARG	NE-CZ-NH2	8.50	124.55	120.30
2	B	12	VAL	CG1-CB-CG2	-7.54	98.83	110.90
2	D	146	VAL	CG1-CB-CG2	-7.11	99.52	110.90
2	B	25	GLN	CA-CB-CG	6.81	128.39	113.40
2	D	207	ARG	NE-CZ-NH1	-6.78	116.91	120.30
2	B	148	LEU	CA-CB-CG	6.12	129.39	115.30
1	A	145	ASP	CB-CG-OD2	-5.54	113.31	118.30
2	B	229	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	169	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	169	ARG	NE-CZ-NH2	-5.07	117.76	120.30

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	1375	0	1250	17	0
1	C	1405	0	1290	11	0
2	B	1880	0	1770	21	0
2	D	1893	0	1786	15	0
3	A	10	0	0	0	0
3	B	23	0	0	0	0
3	C	15	0	0	0	0
3	D	11	0	0	0	0
All	All	6612	0	6096	57	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 5.

All (57) 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)
2:B:244:ARG:HD3	2:B:246:ASP:HA	1.50	0.91
1:A:2:GLU:HA	1:A:2:GLU:OE1	1.68	0.91
2:B:221:GLU:O	2:B:222:ASN:HB3	1.75	0.87
1:C:2:GLU:HA	1:C:2:GLU:OE1	1.75	0.85
2:D:221:GLU:O	2:D:222:ASN:HB3	1.81	0.80
1:C:98:THR:OG1	1:C:99:ASP:N	2.14	0.79
2:B:19:MET:CE	2:B:20:THR:H	2.01	0.72
2:B:19:MET:HE2	2:B:20:THR:H	1.55	0.71
1:C:131:SER:HB2	2:D:131:GLU:OE2	1.91	0.71
2:B:244:ARG:O	2:B:244:ARG:HG3	1.93	0.69
1:C:128:LEU:O	1:C:137:SER:HB2	1.92	0.68
2:D:244:ARG:O	2:D:244:ARG:HG3	1.96	0.64
1:A:184:LYS:O	1:A:187:PHE:HB2	2.01	0.61
2:B:155:ASP:OD1	2:B:178:PRO:HG2	2.01	0.61
2:B:244:ARG:CD	2:B:246:ASP:HA	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TYR:HB3	2:B:179:LEU:HD23	1.85	0.58
2:B:49:SER:OG	2:B:69:ARG:NH1	2.37	0.53
1:A:2:GLU:N	1:A:25:SER:HG	2.08	0.52
1:A:131:SER:HB2	2:B:131:GLU:OE2	2.10	0.51
2:B:221:GLU:O	2:B:222:ASN:CB	2.53	0.51
2:B:19:MET:HE3	2:B:19:MET:HA	1.91	0.51
2:B:245:ALA:O	2:B:246:ASP:CB	2.58	0.51
1:A:31:SER:H	1:A:93:THR:HG22	1.76	0.51
1:A:31:SER:HB2	1:A:93:THR:CG2	2.41	0.50
2:D:37:GLN:HB2	2:D:43:LEU:HD23	1.93	0.50
1:C:184:LYS:O	1:C:187:PHE:HB2	2.13	0.49
2:D:222:ASN:C	2:D:222:ASN:OD1	2.52	0.48
2:B:222:ASN:OD1	2:B:222:ASN:C	2.52	0.48
2:D:221:GLU:O	2:D:222:ASN:CB	2.57	0.48
2:B:87:THR:O	2:B:88:SER:HB2	2.13	0.48
1:C:1:LYS:HD2	1:C:26:ASP:HB2	1.95	0.48
1:A:183:ASN:OD1	1:A:183:ASN:N	2.46	0.47
2:D:1:ASN:HB3	2:D:2:ALA:H	1.52	0.47
2:D:19:MET:CE	2:D:20:THR:H	2.28	0.46
2:D:19:MET:HE2	2:D:20:THR:H	1.82	0.45
2:B:19:MET:HE3	2:B:20:THR:H	1.82	0.45
2:D:99:MET:HA	2:D:100:SER:HA	1.64	0.45
1:A:67:ASN:OD1	1:A:69:ALA:HB3	2.16	0.45
1:C:130:ASP:OD1	1:C:132:LYS:HB3	2.17	0.45
1:C:31:SER:H	1:C:93:THR:HG22	1.82	0.45
1:C:183:ASN:OD1	1:C:183:ASN:N	2.51	0.44
2:D:33:SER:HB3	2:D:45:LEU:HD11	2.00	0.44
1:A:89:LEU:HD23	1:A:109:GLY:HA3	2.00	0.44
1:A:171:MET:SD	2:B:142:LYS:HE3	2.58	0.43
1:A:31:SER:HB2	1:A:93:THR:HG21	2.01	0.43
1:C:103:LYS:HE3	2:D:48:TYR:CE1	2.54	0.43
1:A:20:LEU:HD23	1:A:110:THR:HB	2.00	0.42
2:D:175:ASP:HA	2:D:176:PRO:HD3	1.95	0.41
1:A:2:GLU:O	1:A:24:TYR:HA	2.21	0.41
2:B:205:ASP:HB3	2:B:208:ASN:ND2	2.35	0.41
1:A:20:LEU:CD2	1:A:110:THR:HB	2.51	0.41
2:B:215:GLN:HG3	2:B:217:TYR:CE1	2.55	0.41
1:C:171:MET:CE	2:D:199:SER:HB3	2.51	0.41
1:A:89:LEU:HD23	1:A:109:GLY:CA	2.51	0.41
2:D:147:CYS:HB2	2:D:161:TRP:CZ2	2.56	0.41
2:B:195:ARG:HH11	2:B:195:ARG:HD2	1.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:SER:CB	2:B:131:GLU:OE2	2.69	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	180/194 (93%)	171 (95%)	9 (5%)	0	100	100
1	C	185/194 (95%)	173 (94%)	12 (6%)	0	100	100
2	B	236/245 (96%)	229 (97%)	6 (2%)	1 (0%)	34	30
2	D	239/245 (98%)	227 (95%)	10 (4%)	2 (1%)	19	13
All	All	840/878 (96%)	800 (95%)	37 (4%)	3 (0%)	34	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	222	ASN
2	D	222	ASN
2	D	102	GLN

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	149/172 (87%)	138 (93%)	11 (7%)	13	9
1	C	154/172 (90%)	143 (93%)	11 (7%)	14	10
2	B	203/211 (96%)	191 (94%)	12 (6%)	19	15
2	D	203/211 (96%)	192 (95%)	11 (5%)	22	18
All	All	709/766 (93%)	664 (94%)	45 (6%)	18	13

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	19	SER
1	A	20	LEU
1	A	89	LEU
1	A	93	THR
1	A	98	THR
1	A	103	LYS
1	A	149	ASN
1	A	151	SER
1	A	157	ASP
1	A	183	ASN
2	B	25	GLN
2	B	33	SER
2	B	41	MET
2	B	43	LEU
2	B	49	SER
2	B	102	GLN
2	B	114	LEU
2	B	173	CYS
2	B	179	LEU
2	B	195	ARG
2	B	207	ARG
2	B	222	ASN
1	C	2	GLU
1	C	21	ASN
1	C	71	GLN
1	C	82	PRO
1	C	98	THR
1	C	103	LYS
1	C	147	GLN
1	C	149	ASN
1	C	151	SER
1	C	157	ASP

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Mol	Chain	Res	Type
1	C	183	ASN
2	D	1	ASN
2	D	12	VAL
2	D	33	SER
2	D	41	MET
2	D	78	ARG
2	D	114	LEU
2	D	133	SER
2	D	173	CYS
2	D	195	ARG
2	D	207	ARG
2	D	222	ASN

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 [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	184/194 (94%)	0.76	31 (16%) 1 1	21, 41, 87, 106	0
1	C	187/194 (96%)	0.49	18 (9%) 8 7	20, 36, 85, 117	0
2	B	240/245 (97%)	0.34	13 (5%) 25 24	19, 36, 69, 125	0
2	D	243/245 (99%)	0.53	26 (10%) 6 5	21, 43, 89, 120	0
All	All	854/878 (97%)	0.52	88 (10%) 6 6	19, 39, 85, 125	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	185	SER	9.5
2	D	228	ASP	8.8
1	A	69	ALA	7.5
1	C	186	ASP	7.5
2	D	2	ALA	7.4
1	A	72	TYR	7.0
2	D	99	MET	6.6
1	C	154	LYS	6.6
2	D	1	ASN	6.5
2	D	97	GLY	6.0
1	A	27	ARG	5.9
1	C	135	ASP	5.9
1	A	185	SER	5.8
2	D	221	GLU	5.7
2	B	98	LEU	5.6
1	A	186	ASP	5.6
1	A	134	SER	5.5
1	C	98	THR	5.4
2	B	102	GLN	5.3
1	C	134	SER	5.0
1	C	187	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	70	SER	4.6
1	C	133	SER	4.5
1	A	98	THR	4.4
1	A	194	ASN	4.1
1	C	1	LYS	3.8
2	D	40	GLY	3.8
2	B	103	PRO	3.7
1	A	133	SER	3.6
1	C	153	SER	3.6
1	A	151	SER	3.5
2	D	230	ALA	3.5
2	D	226	THR	3.4
1	C	131	SER	3.4
1	A	51	SER	3.4
2	D	101	ALA	3.4
2	B	186	ASN	3.3
2	D	41	MET	3.3
2	D	223	ASP	3.2
2	D	222	ASN	3.2
1	A	25	SER	3.2
2	D	224	GLU	3.2
2	D	225	TRP	3.2
1	A	154	LYS	3.2
2	D	102	GLN	3.1
1	C	99	ASP	3.0
2	B	39	PRO	3.0
1	A	131	SER	2.9
1	C	151	SER	2.9
2	B	184	ALA	2.9
1	A	26	ASP	2.9
2	D	103	PRO	2.9
1	C	100	SER	2.8
2	D	186	ASN	2.8
2	B	97	GLY	2.7
2	D	100	SER	2.7
1	A	28	GLY	2.6
1	A	135	ASP	2.5
1	C	191	ASN	2.5
1	A	52	ASN	2.5
1	A	50	TYR	2.5
1	A	65	GLN	2.5
1	A	54	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	228	ASP	2.4
1	A	29	SER	2.4
2	B	62	ASN	2.3
1	A	183	ASN	2.3
2	B	26	ASP	2.3
1	A	67	ASN	2.3
1	C	152	GLN	2.2
2	B	34	TRP	2.2
2	B	58	GLY	2.2
2	D	80	LEU	2.2
2	D	227	GLN	2.2
2	D	34	TRP	2.2
1	C	130	ASP	2.2
1	A	53	GLY	2.1
1	A	2	GLU	2.1
1	A	132	LYS	2.1
1	A	193	PHE	2.1
2	D	183	PRO	2.1
1	A	24	TYR	2.1
2	D	39	PRO	2.0
1	C	132	LYS	2.0
2	B	56	ASP	2.0
1	A	140	LEU	2.0
2	D	107	TYR	2.0
2	D	122	VAL	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.