



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:26 AM UTC

PDB ID : 5HHO / pdb_00005hho
Title : Crystal Structure of the JM22 TCR in complex with HLA-A*0201 in complex with M1-G4E
Authors : Gras, S.; Josephs, T.M.; Rossjohn, J.
Deposited on : 2016-01-11
Resolution : 2.95 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

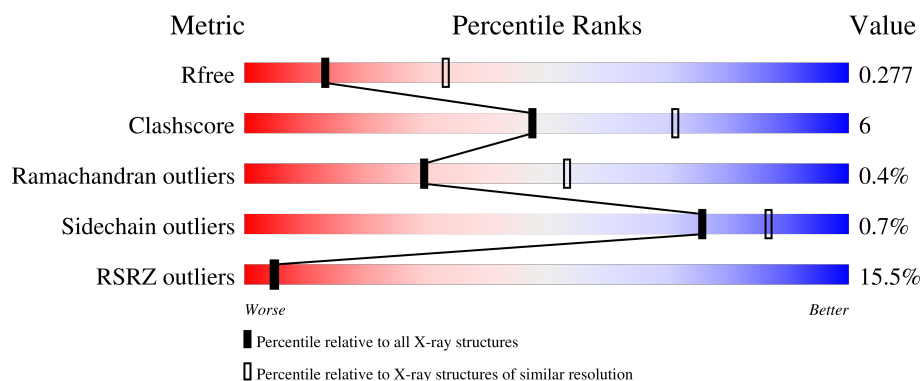
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	276	12% 85% 14% .
2	B	100	4% 89% 11%
3	D	199	24% 77% 21% .
4	E	241	17% 84% 15%
5	C	9	11% 89% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6592 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2253	1408	410	426	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called JM22 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	195	Total	C	N	O	S	0	1	0
			1500	936	252	305	7			

- Molecule 4 is a protein called JM22 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	240	Total	C	N	O	S	0	0	0
			1929	1219	333	371	6			

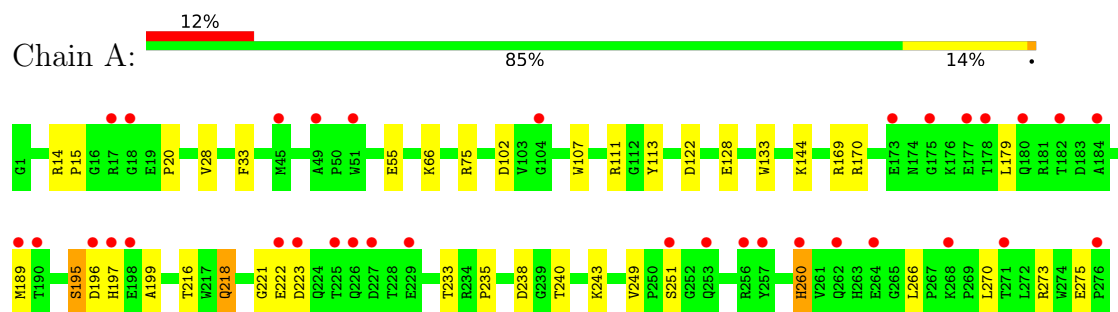
- Molecule 5 is a protein called M1-G4E, GILEFVFTL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	9	Total	C	N	O	0	0	0
			74	52	9	13			

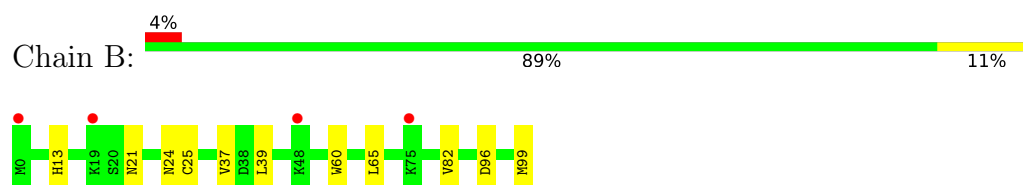
3 Residue-property plots

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.

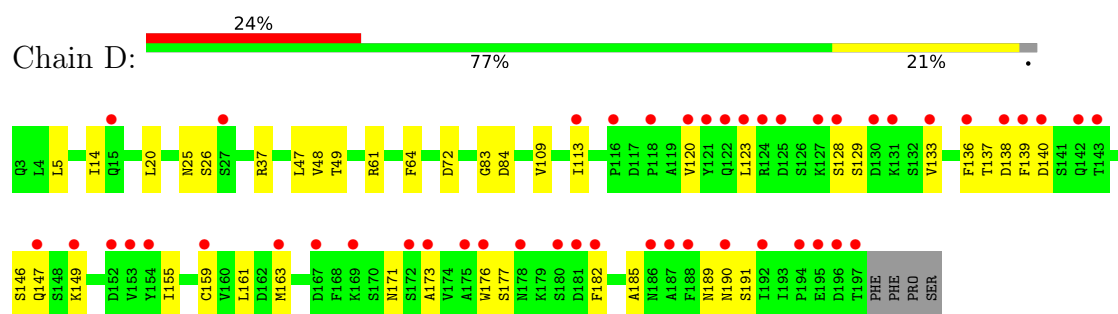
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



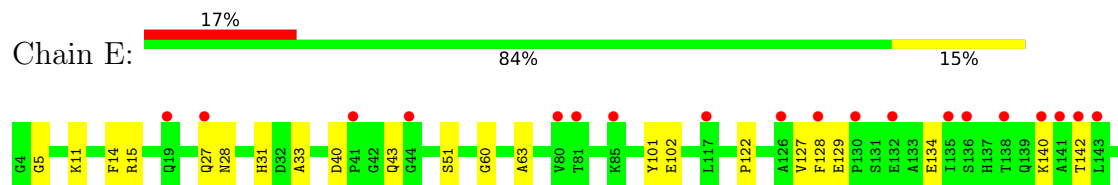
- Molecule 2: Beta-2-microglobulin

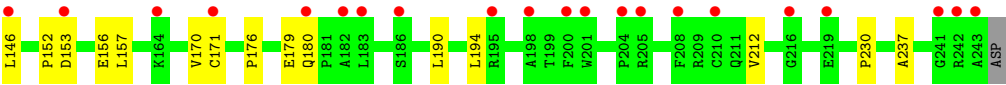


- Molecule 3: JM22 TCR alpha chain

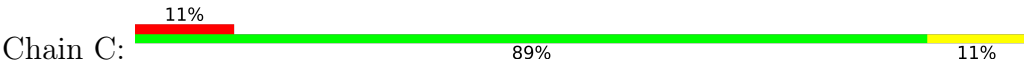


- Molecule 4: JM22 TCR beta chain





● Molecule 5: M1-G4E, GILEFVFTL



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.66Å 49.03Å 113.04Å 90.00° 115.95° 90.00°	Depositor
Resolution (Å)	40.06 – 2.95 40.06 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.06-2.95) 99.9 (40.06-2.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.236 , 0.279 0.239 , 0.277	Depositor DCC
R_{free} test set	1263 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	1.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6592	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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	0/2319	0.66	0/3149
2	B	0.23	0/859	0.66	0/1162
3	D	0.25	0/1530	0.72	0/2071
4	E	0.26	0/1982	0.71	2/2696 (0.1%)
5	C	0.20	0/75	0.58	0/99
All	All	0.26	0/6765	0.69	2/9177 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	129	GLU	CA-C-N	5.59	125.91	119.93
4	E	129	GLU	C-N-CA	5.59	125.91	119.93

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	2253	0	2103	25	0
2	B	836	0	803	7	0
3	D	1500	0	1458	25	0
4	E	1929	0	1832	22	0
5	C	74	0	78	1	0
All	All	6592	0	6274	72	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 6.

All (72) 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)
3:D:161:LEU:HB3	4:E:171:CYS:HB2	1.76	0.66
3:D:5:LEU:HD23	3:D:26:SER:HB2	1.79	0.65
1:A:216:THR:O	1:A:218:GLN:NE2	2.33	0.61
1:A:273:ARG:NH1	1:A:275:GLU:OE1	2.34	0.61
3:D:37:ARG:NH2	3:D:83:GLY:O	2.35	0.59
1:A:122:ASP:OD1	2:B:60:TRP:NE1	2.34	0.58
4:E:122:PRO:HD3	4:E:230:PRO:HB3	1.85	0.58
1:A:20:PRO:HG2	1:A:75:ARG:HG3	1.88	0.55
3:D:185:ALA:O	3:D:189:ASN:ND2	2.39	0.55
4:E:27:GLN:NE2	4:E:31:HIS:O	2.37	0.54
3:D:133:VAL:HG12	3:D:176:TRP:HB3	1.89	0.54
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.90	0.54
1:A:218:GLN:HE22	1:A:260:HIS:N	2.06	0.53
3:D:159:CYS:HB3	4:E:171:CYS:SG	2.48	0.53
1:A:199:ALA:N	1:A:249:VAL:O	2.41	0.53
3:D:113:ILE:HD11	3:D:140:ASP:HA	1.90	0.53
4:E:157:LEU:HG	4:E:212:VAL:HG22	1.91	0.52
1:A:218:GLN:HE22	1:A:260:HIS:H	1.57	0.52
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.92	0.52
4:E:14:PHE:O	4:E:15:ARG:NH1	2.40	0.51
1:A:218:GLN:OE1	1:A:260:HIS:ND1	2.45	0.50
1:A:28:VAL:HG11	1:A:179:LEU:HD13	1.92	0.50
1:A:111:ARG:NH1	1:A:113:TYR:OH	2.44	0.49
4:E:153:ASP:OD1	4:E:176:PRO:HG2	2.12	0.49
3:D:25:ASN:ND2	3:D:72:ASP:OD1	2.39	0.49
2:B:96:ASP:HB3	2:B:99:MET:HB3	1.93	0.49
3:D:163:MET:HE1	4:E:140:LYS:HD3	1.96	0.48
3:D:147:GLN:NE2	3:D:155:ILE:O	2.40	0.48
1:A:197:HIS:O	1:A:251:SER:N	2.46	0.48
2:B:13:HIS:O	2:B:21:ASN:ND2	2.39	0.48
3:D:128:SER:OG	3:D:129:SER:N	2.40	0.47
1:A:238:ASP:OD1	1:A:240:THR:OG1	2.33	0.46
1:A:111:ARG:HE	1:A:128:GLU:HG3	1.79	0.46
4:E:60:GLY:H	4:E:63:ALA:HB2	1.81	0.46
3:D:37:ARG:HB2	3:D:47:LEU:HD11	1.99	0.46
1:A:195:SER:OG	1:A:196:ASP:N	2.50	0.45
3:D:61:ARG:NH2	3:D:84:ASP:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:40:ASP:HB2	4:E:43:GLN:HG3	1.99	0.45
3:D:123:LEU:HB3	4:E:128:PHE:HB3	1.98	0.44
3:D:136:PHE:O	3:D:173:ALA:N	2.50	0.44
1:A:66:LYS:HD3	5:C:4:GLU:HG3	2.00	0.44
1:A:266:LEU:HD13	1:A:270:LEU:HG	2.00	0.44
3:D:14:ILE:HD11	3:D:20:LEU:HD23	2.00	0.44
4:E:101:TYR:CD2	4:E:102:GLU:HG2	2.54	0.43
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.53	0.43
4:E:127:VAL:HG23	4:E:237:ALA:HB3	1.99	0.43
4:E:11:LYS:NZ	4:E:156:GLU:OE2	2.43	0.43
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.01	0.43
1:A:55:GLU:OE1	1:A:170:ARG:NH2	2.53	0.42
1:A:107:TRP:O	1:A:169:ARG:NH1	2.52	0.42
3:D:149:LYS:HA	3:D:149:LYS:HD2	1.88	0.42
3:D:177:SER:HB2	3:D:182:PHE:CG	2.55	0.42
3:D:137:THR:OG1	3:D:138:ASP:N	2.51	0.42
4:E:179:GLU:O	4:E:180:GLN:NE2	2.52	0.42
1:A:14:ARG:HA	1:A:15:PRO:HD3	1.90	0.41
2:B:37:VAL:HG22	2:B:82:VAL:HG22	2.01	0.41
3:D:49:THR:OG1	4:E:102:GLU:OE2	2.32	0.41
3:D:139:PHE:CZ	3:D:171:ASN:HB3	2.56	0.41
3:D:84:ASP:HB2	3:D:109:VAL:HG21	2.02	0.41
3:D:120:VAL:HG22	3:D:136:PHE:HD1	1.85	0.41
1:A:102:ASP:HB2	1:A:111:ARG:HB3	2.03	0.41
3:D:146:SER:H	3:D:191:SER:HB3	1.85	0.41
4:E:33:ALA:HA	4:E:51:SER:O	2.21	0.41
4:E:170:VAL:HG22	4:E:194:LEU:HD13	2.02	0.41
4:E:14:PHE:CD1	4:E:152:PRO:HG3	2.56	0.41
4:E:176:PRO:HG3	4:E:190:LEU:HD13	2.04	0.40
3:D:48:VAL:HG11	3:D:64:PHE:CG	2.56	0.40
1:A:133:TRP:HB2	1:A:144:LYS:HG3	2.03	0.40
1:A:233:THR:OG1	1:A:243:LYS:HD2	2.21	0.40
1:A:189:MET:HE3	1:A:189:MET:HB2	1.95	0.40
4:E:5:GLY:N	4:E:28:ASN:OD1	2.42	0.40
4:E:134:GLU:OE1	4:E:142:THR:OG1	2.38	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	274/276 (99%)	259 (94%)	12 (4%)	3 (1%)	11	29
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	D	194/199 (98%)	181 (93%)	13 (7%)	0	100	100
4	E	238/241 (99%)	229 (96%)	9 (4%)	0	100	100
5	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	811/825 (98%)	770 (95%)	38 (5%)	3 (0%)	30	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	A	195	SER
1	A	221	GLY

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	232/232 (100%)	229 (99%)	3 (1%)	61	78
2	B	95/95 (100%)	95 (100%)	0	100	100
3	D	172/175 (98%)	171 (99%)	1 (1%)	78	89
4	E	210/211 (100%)	209 (100%)	1 (0%)	81	90
5	C	8/8 (100%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	717/721 (99%)	712 (99%)	5 (1%)	76	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
1	A	222	GLU
1	A	260	HIS
3	D	190	ASN
4	E	146	LEU

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

Mol	Chain	Res	Type
1	A	255	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 ⓘ

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	276/276 (100%)	0.91	34 (12%) 8 8	31, 57, 98, 116	26 (9%)
2	B	100/100 (100%)	0.59	4 (4%) 42 35	29, 48, 78, 89	14 (14%)
3	D	195/199 (97%)	1.16	48 (24%) 2 1	27, 52, 96, 115	40 (20%)
4	E	240/241 (99%)	1.03	40 (16%) 4 4	22, 60, 92, 112	22 (9%)
5	C	9/9 (100%)	0.62	1 (11%) 10 9	32, 34, 41, 47	1 (11%)
All	All	820/825 (99%)	0.96	127 (15%) 5 5	22, 56, 94, 116	103 (12%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	131	LYS	5.1
3	D	197	THR	4.8
3	D	196	ASP	4.6
3	D	192	ILE	4.5
3	D	136	PHE	4.5
4	E	140	LYS	4.3
4	E	200	PHE	4.2
3	D	122	GLN	4.0
4	E	132	GLU	3.9
3	D	139	PHE	3.8
3	D	143	THR	3.8
3	D	195	GLU	3.7
1	A	271	THR	3.6
1	A	175	GLY	3.6
3	D	149	LYS	3.5
4	E	242	ARG	3.5
3	D	176	TRP	3.5
3	D	142	GLN	3.5
3	D	120	VAL	3.5
1	A	268	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	75	LYS	3.5
4	E	164	LYS	3.5
1	A	251	SER	3.5
4	E	201	TRP	3.4
4	E	241	GLY	3.3
3	D	127	LYS	3.3
3	D	187	ALA	3.2
1	A	17	ARG	3.2
3	D	124	ARG	3.2
3	D	147	GLN	3.2
1	A	225	THR	3.2
3	D	194	PRO	3.2
4	E	135	ILE	3.2
1	A	257	TYR	3.2
4	E	198	ALA	3.2
3	D	123	LEU	3.1
4	E	19	GLN	3.1
4	E	136	SER	3.1
1	A	222	GLU	3.1
3	D	167	ASP	3.0
3	D	186	ASN	3.0
1	A	262	GLN	3.0
4	E	216	GLY	2.9
4	E	44	GLY	2.9
1	A	49	ALA	2.9
4	E	128	PHE	2.9
4	E	81	THR	2.9
3	D	173	ALA	2.8
3	D	125	ASP	2.8
1	A	276	PRO	2.8
1	A	177	GLU	2.8
4	E	205	ARG	2.8
4	E	143	LEU	2.8
1	A	178	THR	2.8
1	A	256	ARG	2.8
4	E	243	ALA	2.8
1	A	223	ASP	2.8
1	A	253	GLN	2.7
4	E	142	THR	2.7
3	D	188	PHE	2.7
4	E	219	GLU	2.7
3	D	180	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	175	ALA	2.6
3	D	178	ASN	2.6
2	B	0	MET	2.6
4	E	195	ARG	2.6
4	E	41	PRO	2.6
3	D	172	SER	2.6
3	D	182	PHE	2.6
3	D	133	VAL	2.5
4	E	141	ALA	2.5
3	D	140	ASP	2.5
1	A	226	GLN	2.5
3	D	152	ASP	2.5
3	D	116	PRO	2.5
1	A	264	GLU	2.5
4	E	126	ALA	2.5
4	E	138	THR	2.5
4	E	180	GLN	2.5
4	E	130	PRO	2.5
3	D	153	VAL	2.5
2	B	19	LYS	2.5
3	D	159	CYS	2.5
3	D	113	ILE	2.4
4	E	186	SER	2.4
3	D	190	ASN	2.4
4	E	171	CYS	2.4
4	E	80	VAL	2.4
3	D	27	SER	2.4
1	A	18	GLY	2.4
4	E	153	ASP	2.3
3	D	121	TYR	2.3
3	D	154	TYR	2.3
1	A	104	GLY	2.3
3	D	130	ASP	2.3
1	A	184	ALA	2.3
4	E	208	PHE	2.3
1	A	173	GLU	2.3
4	E	183	LEU	2.3
1	A	197	HIS	2.3
1	A	227	ASP	2.3
3	D	181	ASP	2.3
4	E	27	GLN	2.3
3	D	163	MET	2.2

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Mol	Chain	Res	Type	RSRZ
4	E	182	ALA	2.2
1	A	260	HIS	2.2
3	D	118	PRO	2.2
4	E	204	PRO	2.2
1	A	182	THR	2.2
4	E	85	LYS	2.2
1	A	180	GLN	2.2
3	D	138	ASP	2.1
4	E	210	CYS	2.1
5	C	4	GLU	2.1
3	D	169	LYS	2.1
1	A	198	GLU	2.1
1	A	229	GLU	2.1
3	D	15	GLN	2.1
1	A	45	MET	2.1
3	D	128	SER	2.1
4	E	117	LEU	2.0
2	B	48	LYS	2.0
1	A	189	MET	2.0
4	E	146	LEU	2.0
1	A	190	THR	2.0
1	A	196	ASP	2.0
1	A	51	TRP	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.