



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 27, 2025 – 12:25 PM EST

PDB ID : 8TQ4
Title : Crystal structure of Fab M142 in complex with MHC-I (H2-Dd)
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Deposited on : 2023-08-06
Resolution : 3.59 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	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

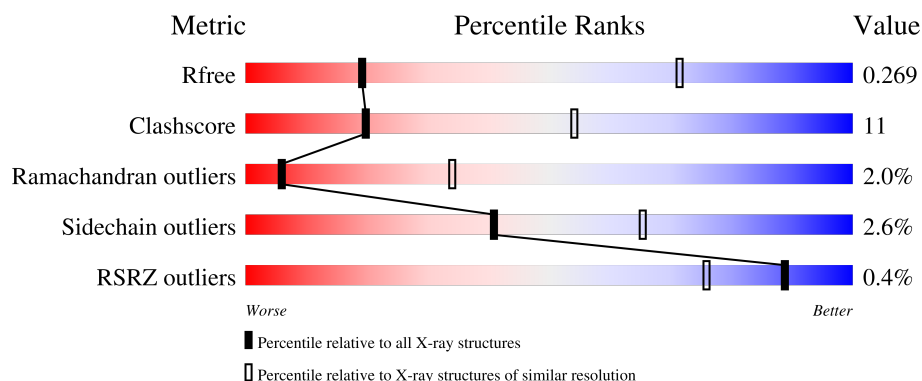
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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}	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)

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	273	<div> <div></div> <div>69%29%.</div> </div>
1	E	273	<div> <div>%</div> <div>80%20%</div> </div>
2	B	98	<div> <div></div> <div>76%22%.</div> </div>
2	F	98	<div> <div>3%</div> <div>78%20%.</div> </div>
3	C	222	<div> <div></div> <div>74%23%.</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	222	 73% 27%
4	D	213	 74% 24% •
4	L	213	 67% 30% •
5	G	10	 60% 30% 10%
5	P	10	 70% 30%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12671 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 H2 class I histocompatibility antigen D-d alpha chain (H2-Dd).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2220	1397	403	411	9			
1	E	273	Total	C	N	O	S	0	0	0
			2200	1386	390	416	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			809	518	137	148	6			
2	F	98	Total	C	N	O	S	0	0	0
			752	483	130	134	5			

- Molecule 3 is a protein called Fab M142 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	222	Total	C	N	O	S	0	0	0
			1642	1044	265	326	7			
3	H	222	Total	C	N	O	S	0	0	0
			1640	1040	270	323	7			

- Molecule 4 is a protein called Fab M142 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	213	Total	C	N	O	S	0	0	0
			1631	1013	269	340	9			
4	L	213	Total	C	N	O	S	0	0	0
			1625	1012	268	336	9			

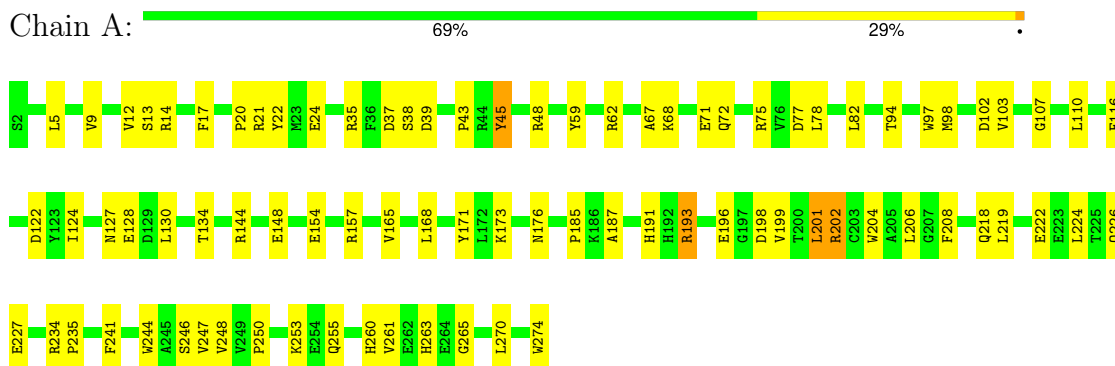
- Molecule 5 is a protein called HV1: HIV-1 P18-I10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	10	Total	C	N	O	0	0	0
			76	48	16	12			
5	P	10	Total	C	N	O	0	0	0
			76	48	16	12			

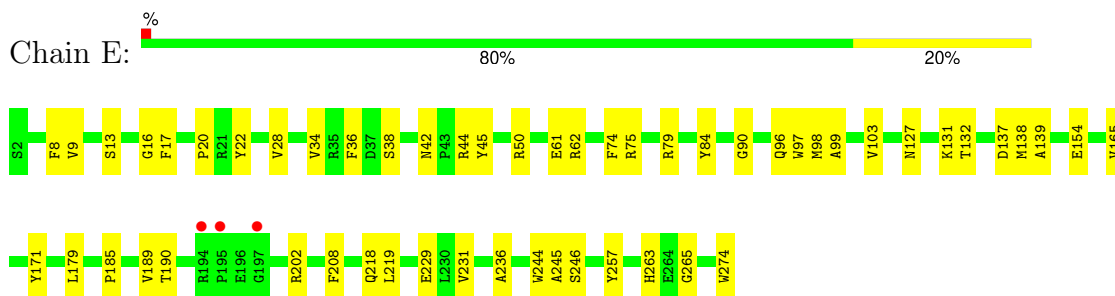
3 Residue-property plots [i](#)

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.

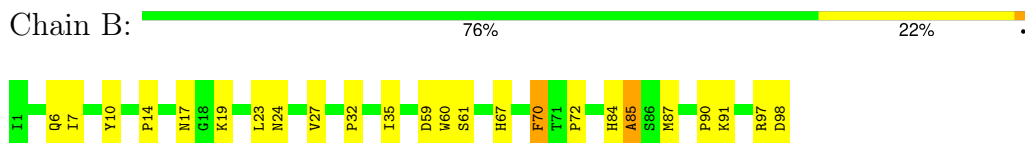
- Molecule 1: H2 class I histocompatibility antigen D-d alpha chain (H2-Dd)



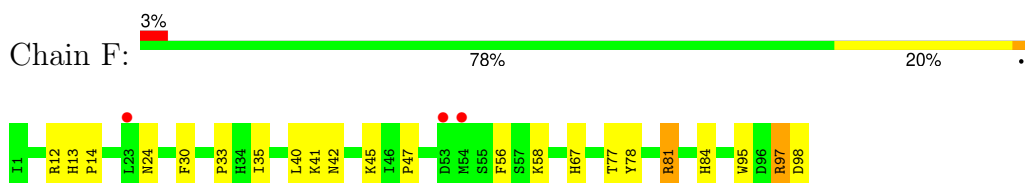
- Molecule 1: H2 class I histocompatibility antigen D-d alpha chain (H2-Dd)



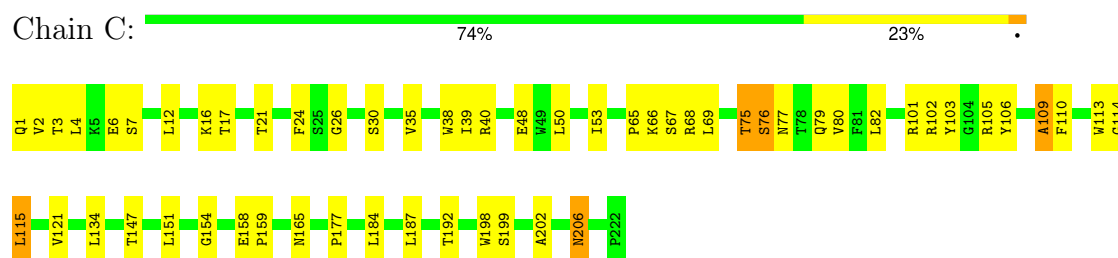
- Molecule 2: Beta-2-microglobulin



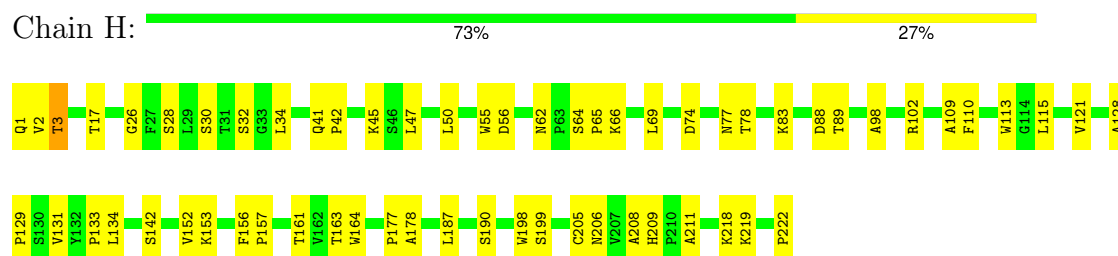
- Molecule 2: Beta-2-microglobulin



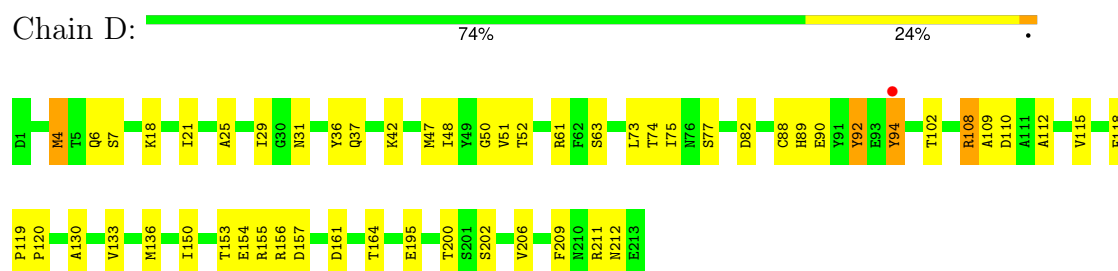
- Molecule 3: Fab M142 Heavy Chain



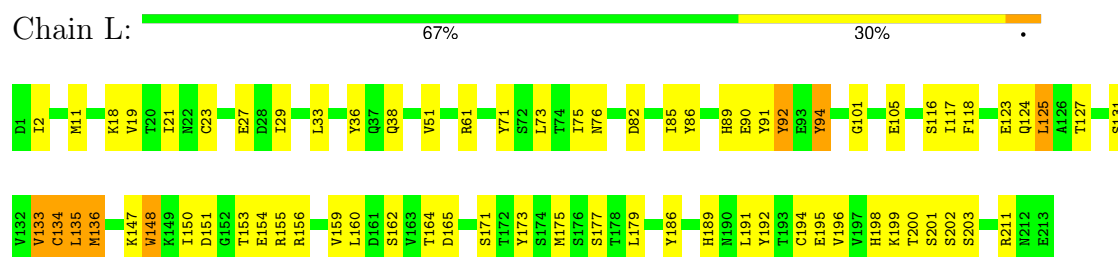
- Molecule 3: Fab M142 Heavy Chain



- Molecule 4: Fab M142 Light Chain



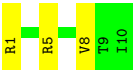
- Molecule 4: Fab M142 Light Chain



- Molecule 5: HV1: HIV-1 P18-I10



- Molecule 5: HV1: HIV-1 P18-I10



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.55Å 121.55Å 327.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.57 – 3.59 97.57 – 3.59	Depositor EDS
% Data completeness (in resolution range)	95.0 (97.57-3.59) 95.0 (97.57-3.59)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.221 , 0.270 0.221 , 0.269	Depositor DCC
R_{free} test set	1403 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	91.7	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 98.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12671	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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	0.26	0/2283	0.55	0/3102
1	E	0.27	0/2263	0.55	0/3080
2	B	0.27	0/835	0.54	0/1134
2	F	0.26	0/777	0.52	0/1064
3	C	0.28	0/1684	0.56	0/2311
3	H	0.28	0/1682	0.57	0/2306
4	D	0.29	0/1667	0.54	0/2263
4	L	0.35	0/1661	0.63	0/2255
5	G	0.36	0/77	0.68	0/101
5	P	0.26	0/77	0.64	0/101
All	All	0.29	0/13006	0.56	0/17717

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	2220	0	2082	58	0
1	E	2200	0	2035	41	0
2	B	809	0	788	18	0
2	F	752	0	691	16	0
3	C	1642	0	1592	36	0
3	H	1640	0	1590	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1631	0	1530	32	0
4	L	1625	0	1520	61	0
5	G	76	0	82	10	0
5	P	76	0	82	5	0
All	All	12671	0	11992	279	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 11.

The worst 5 of 279 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:E:74:PHE:CE1	5:G:5:ARG:NH1	2.49	0.80
4:D:4:MET:HE2	4:D:25:ALA:HB2	1.64	0.79
4:L:118:PHE:HE2	4:L:135:LEU:HD11	1.46	0.79
5:G:5:ARG:HG2	5:G:5:ARG:HH11	1.50	0.77
4:L:136:MET:HG3	4:L:175:MET:HB3	1.70	0.73

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	271/273 (99%)	254 (94%)	13 (5%)	4 (2%)	8	39
1	E	271/273 (99%)	256 (94%)	15 (6%)	0	100	100
2	B	96/98 (98%)	87 (91%)	8 (8%)	1 (1%)	13	46
2	F	96/98 (98%)	85 (88%)	10 (10%)	1 (1%)	13	46
3	C	220/222 (99%)	195 (89%)	17 (8%)	8 (4%)	3	23
3	H	220/222 (99%)	192 (87%)	19 (9%)	9 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	211/213 (99%)	192 (91%)	15 (7%)	4 (2%)	6	35
4	L	211/213 (99%)	190 (90%)	16 (8%)	5 (2%)	5	30
5	G	8/10 (80%)	8 (100%)	0	0	100	100
5	P	8/10 (80%)	8 (100%)	0	0	100	100
All	All	1612/1632 (99%)	1467 (91%)	113 (7%)	32 (2%)	6	34

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	GLU
3	C	30	SER
3	C	66	LYS
3	C	68	ARG
3	C	76	SER

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	223/229 (97%)	217 (97%)	6 (3%)	40	65
1	E	220/229 (96%)	219 (100%)	1 (0%)	86	93
2	B	92/92 (100%)	89 (97%)	3 (3%)	33	61
2	F	77/92 (84%)	75 (97%)	2 (3%)	41	65
3	C	184/192 (96%)	182 (99%)	2 (1%)	70	83
3	H	183/192 (95%)	181 (99%)	2 (1%)	70	83
4	D	185/190 (97%)	178 (96%)	7 (4%)	28	57
4	L	182/190 (96%)	170 (93%)	12 (7%)	14	42
5	G	7/7 (100%)	6 (86%)	1 (14%)	2	17
5	P	7/7 (100%)	7 (100%)	0	100	100
All	All	1360/1420 (96%)	1324 (97%)	36 (3%)	41	65

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	124	GLN
4	L	191	LEU
4	L	125	LEU
4	L	134	CYS
4	D	42	LYS

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 [i](#)

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	273/273 (100%)	-0.36	0 100 100	45, 75, 112, 141	0
1	E	273/273 (100%)	-0.21	3 (1%) 77 57	50, 86, 166, 184	4 (1%)
2	B	98/98 (100%)	-0.38	0 100 100	47, 64, 100, 115	0
2	F	98/98 (100%)	-0.10	3 (3%) 51 33	56, 87, 133, 155	0
3	C	222/222 (100%)	-0.24	0 100 100	52, 90, 142, 175	0
3	H	222/222 (100%)	-0.18	0 100 100	41, 79, 123, 171	0
4	D	213/213 (100%)	-0.20	1 (0%) 87 72	53, 93, 140, 164	0
4	L	213/213 (100%)	-0.27	0 100 100	47, 80, 122, 174	0
5	G	10/10 (100%)	-0.19	0 100 100	71, 78, 94, 98	0
5	P	10/10 (100%)	-0.53	0 100 100	63, 74, 85, 96	0
All	All	1632/1632 (100%)	-0.25	7 (0%) 89 76	41, 83, 140, 184	4 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	195	PRO	5.1
1	E	197	GLY	4.2
2	F	53	ASP	3.3
1	E	194	ARG	3.1
4	D	94	TYR	2.2

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.