



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:43 PM UTC

PDB ID : 6EWO / pdb_00006ewo
Title : Crystal structure of non-phosphorylated form of RTF PHOSPHOPEPTIDE
BOUND TO HLA-A2 in complex with LILRB1
Authors : Mohammed, F.; Stones, D.H.; Willcox, B.E.
Deposited on : 2017-11-06
Resolution : 2.30 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

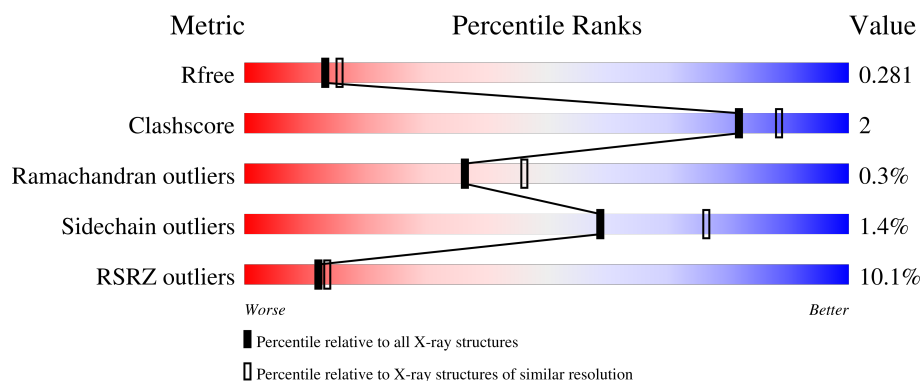
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	8% 96% .
1	E	276	6% 93% 6% .
2	B	99	3% 99% .
2	F	99	4% 95% . .
3	C	9	67% 78% 22%

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Mol	Chain	Length	Quality of chain
3	G	9	56% 56% 44%
4	D	195	13% 84% 11% 6%
4	H	195	17% 86% • 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9361 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	25	0	0
			2254	1408	410	427	9			
1	E	274	Total	C	N	O	S	5	0	0
			2237	1398	408	422	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	12	0	0
			829	528	140	158	3			
2	F	99	Total	C	N	O	S	3	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called Synemin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			74	48	12	14			
3	G	9	Total	C	N	O	0	0	0
			74	48	12	14			

- Molecule 4 is a protein called LIR-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	184	Total	C	N	O	S	16	0	0
			1446	920	249	271	6			
4	H	176	Total	C	N	O	S	3	0	0
			1391	887	238	260	6			

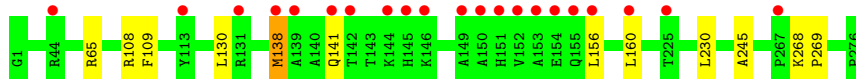
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	57	Total 57	O 57	0	0
5	B	36	Total 36	O 36	0	0
5	D	32	Total 32	O 32	0	0
5	E	32	Total 32	O 32	0	0
5	F	33	Total 33	O 33	0	0
5	H	37	Total 37	O 37	0	0

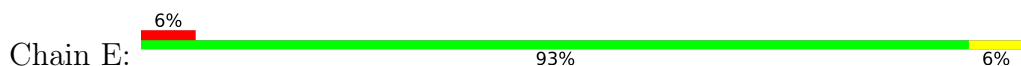
3 Residue-property plots [i](#)

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.

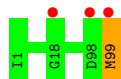
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



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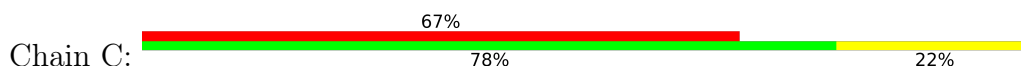
- Molecule 2: Beta-2-microglobulin



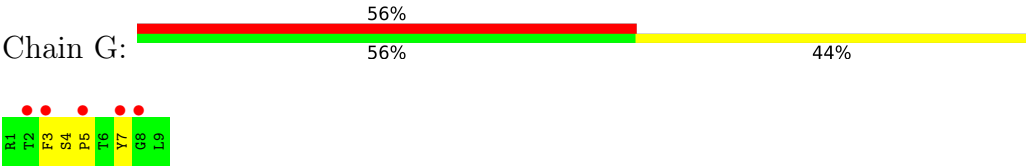
- Molecule 2: Beta-2-microglobulin



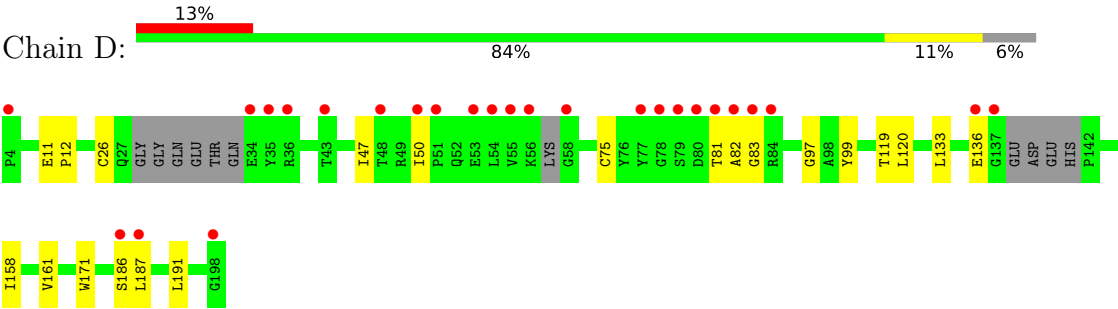
- Molecule 3: Synemin



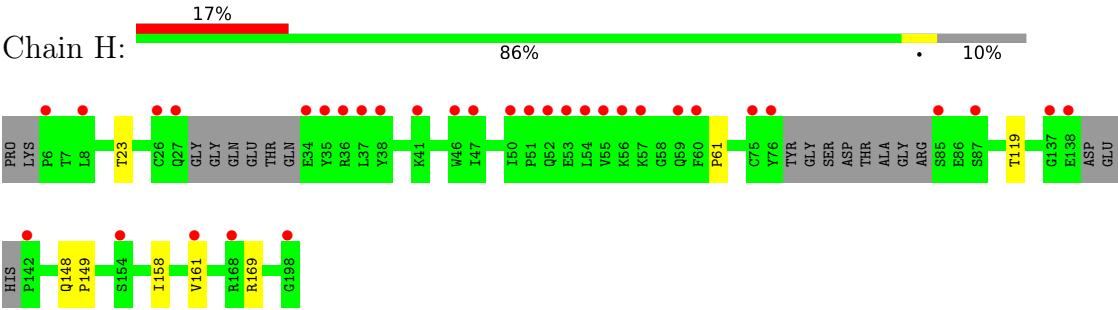
- Molecule 3: Synemin



● Molecule 4: LIR-1



● Molecule 4: LIR-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.30Å 116.30Å 192.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.70 – 2.30 19.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.70-2.30) 99.4 (19.70-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.276 0.239 , 0.281	Depositor DCC
R_{free} test set	3401 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9361	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.25 % 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 3.9743e-03. 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	0.57	0/2320	0.80	0/3149
1	E	0.59	0/2302	0.80	0/3125
2	B	0.52	0/852	0.73	0/1152
2	F	0.59	0/852	0.77	0/1152
3	C	1.04	0/76	1.13	0/101
3	G	0.86	0/76	0.94	0/101
4	D	0.56	0/1488	0.71	0/2026
4	H	0.61	0/1431	0.73	1/1948 (0.1%)
All	All	0.58	0/9397	0.77	1/12754 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	161	VAL	N-CA-C	6.45	119.85	113.53

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	2254	0	2103	7	0
1	E	2237	0	2090	11	0
2	B	829	0	794	2	0
2	F	829	0	794	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	74	0	73	1	0
3	G	74	0	73	3	0
4	D	1446	0	1401	17	0
4	H	1391	0	1351	4	0
5	A	57	0	0	0	0
5	B	36	0	0	1	0
5	D	32	0	0	1	0
5	E	32	0	0	0	0
5	F	33	0	0	0	0
5	H	37	0	0	0	0
All	All	9361	0	8679	44	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 2.

All (44) 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:44:ARG:HG2	1:E:64:THR:HG21	1.37	1.04
4:D:97:GLY:HA2	4:D:187:LEU:HG	1.55	0.88
4:D:82:ALA:H	4:D:83:GLY:HA3	1.43	0.80
1:E:44:ARG:HG2	1:E:64:THR:CG2	2.12	0.79
3:C:4:SER:OG	3:C:5:PRO:HD3	1.89	0.73
4:D:97:GLY:HA2	4:D:187:LEU:CG	2.18	0.72
1:A:138:MET:SD	1:A:138:MET:N	2.65	0.69
4:D:82:ALA:N	4:D:83:GLY:HA3	2.09	0.66
1:E:14:ARG:HB3	1:E:17:ARG:HB2	1.78	0.64
4:D:97:GLY:HA2	4:D:187:LEU:CD2	2.31	0.61
4:D:119:THR:CG2	4:D:158:ILE:HG23	2.31	0.61
4:D:187:LEU:HD21	5:D:203:HOH:O	2.01	0.60
1:E:44:ARG:HA	1:E:64:THR:HG23	1.88	0.56
1:E:159:TYR:HB2	3:G:3:PHE:CE1	2.40	0.55
1:E:249:VAL:HG13	1:E:257:TYR:CE2	2.44	0.52
2:B:99:MET:SD	2:B:99:MET:N	2.83	0.51
4:H:148:GLN:HG3	4:H:149:PRO:HD2	1.93	0.51
1:A:268:LYS:HG2	1:A:269:PRO:N	2.25	0.50
4:D:119:THR:HG23	4:D:158:ILE:HG23	1.94	0.49
4:D:97:GLY:CA	4:D:187:LEU:HG	2.37	0.49
1:E:121:LYS:HE2	2:F:1:ILE:HD12	1.95	0.48
4:H:119:THR:HG23	4:H:158:ILE:HG23	1.94	0.48
1:E:159:TYR:HB2	3:G:3:PHE:CD1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:TYR:HB2	4:D:186:SER:HB2	1.97	0.47
4:D:99:TYR:HB2	4:D:186:SER:CB	2.45	0.47
1:E:81:LEU:HD23	1:E:118:TYR:CD1	2.49	0.47
4:D:97:GLY:HA2	4:D:187:LEU:HD23	1.96	0.46
4:D:11:GLU:HA	4:D:12:PRO:C	2.40	0.46
4:D:97:GLY:CA	4:D:187:LEU:CD2	2.94	0.46
4:D:171:TRP:HB3	4:D:191:LEU:HD11	1.98	0.46
1:E:43:GLN:O	1:E:44:ARG:HG3	2.17	0.44
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.53	0.43
2:B:99:MET:HE1	5:B:113:HOH:O	2.17	0.43
1:A:130:LEU:HD22	1:A:160:LEU:CD1	2.48	0.43
4:D:120:LEU:HD12	4:D:133:LEU:HD21	2.01	0.43
1:A:268:LYS:CG	1:A:269:PRO:HD2	2.49	0.42
2:F:46:ILE:HG22	2:F:47:GLU:O	2.19	0.42
4:D:47:ILE:HA	4:D:50:ILE:HD12	2.01	0.42
3:G:4:SER:HB2	3:G:5:PRO:HD3	2.01	0.42
1:A:108:ARG:O	1:A:109:PHE:C	2.62	0.41
4:H:23:THR:HA	4:H:61:PRO:HA	2.02	0.41
4:H:119:THR:CG2	4:H:158:ILE:HG23	2.51	0.41
1:A:138:MET:O	1:A:141:GLN:N	2.44	0.40
1:A:230:LEU:HD23	1:A:245:ALA:HB2	2.03	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	274/276 (99%)	265 (97%)	9 (3%)	0	100	100
1	E	272/276 (99%)	263 (97%)	7 (3%)	2 (1%)	18	23
2	B	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	F	97/99 (98%)	96 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
3	G	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
4	D	176/195 (90%)	168 (96%)	7 (4%)	1 (1%)	21	27
4	H	168/195 (86%)	162 (96%)	6 (4%)	0	100	100
All	All	1098/1158 (95%)	1057 (96%)	38 (4%)	3 (0%)	36	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	136	GLU
1	E	18	GLY
1	E	92	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	232/232 (100%)	229 (99%)	3 (1%)	61	77
1	E	230/232 (99%)	228 (99%)	2 (1%)	70	84
2	B	94/94 (100%)	93 (99%)	1 (1%)	65	81
2	F	94/94 (100%)	92 (98%)	2 (2%)	47	66
3	C	8/8 (100%)	8 (100%)	0	100	100
3	G	8/8 (100%)	7 (88%)	1 (12%)	4	5
4	D	160/169 (95%)	156 (98%)	4 (2%)	42	60
4	H	155/169 (92%)	154 (99%)	1 (1%)	78	89
All	All	981/1006 (98%)	967 (99%)	14 (1%)	59	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ARG

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Mol	Chain	Res	Type
1	A	138	MET
1	A	156	LEU
2	B	99	MET
4	D	26	CYS
4	D	75	CYS
4	D	81	THR
4	D	161	VAL
1	E	115	GLN
1	E	215	LEU
2	F	47	GLU
2	F	99	MET
3	G	7	TYR
4	H	169	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	96	GLN
1	A	192	HIS
1	A	197	HIS
1	A	253	GLN
2	B	13	HIS
4	D	18	GLN
4	D	150	HIS
1	E	87	GLN
1	E	141	GLN
2	F	13	HIS

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

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%)	0.47	21 (7%)	20 21	12, 34, 63, 79	5 (1%)
1	E	274/276 (99%)	0.46	16 (5%)	29 31	18, 37, 64, 81	1 (0%)
2	B	99/99 (100%)	0.08	3 (3%)	52 54	15, 26, 47, 52	3 (3%)
2	F	99/99 (100%)	-0.02	4 (4%)	42 44	19, 26, 44, 52	1 (1%)
3	C	9/9 (100%)	2.05	6 (66%)	0 0	41, 54, 73, 76	0
3	G	9/9 (100%)	2.03	5 (55%)	0 0	37, 47, 70, 73	0
4	D	184/195 (94%)	0.65	26 (14%)	6 7	19, 36, 77, 93	5 (2%)
4	H	176/195 (90%)	0.83	33 (18%)	3 4	18, 39, 77, 96	1 (0%)
All	All	1126/1158 (97%)	0.50	114 (10%)	12 14	12, 35, 68, 96	16 (1%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	37	LEU	6.3
1	E	225	THR	6.2
1	E	17	ARG	5.9
4	H	76	TYR	5.4
4	H	6	PRO	4.9
4	H	75	CYS	4.8
4	H	85	SER	4.8
1	A	138	MET	4.7
1	A	149	ALA	4.7
4	D	81	THR	4.6
4	D	53	GLU	4.3
3	G	7	TYR	4.3
4	H	54	LEU	4.2
4	D	55	VAL	4.2
1	A	154	GLU	4.1
4	D	58	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
4	H	35	TYR	4.0
1	A	145	HIS	3.9
1	A	146	LYS	3.9
4	D	79	SER	3.8
1	A	150	ALA	3.8
4	H	34	GLU	3.8
4	H	26	CYS	3.7
2	B	18	GLY	3.7
4	D	35	TYR	3.7
2	B	99	MET	3.6
4	D	4	PRO	3.6
4	D	50	ILE	3.6
4	H	50	ILE	3.6
1	E	16	GLY	3.6
1	A	139	ALA	3.6
4	D	54	LEU	3.5
1	A	153	ALA	3.4
4	D	137	GLY	3.4
4	H	36	ARG	3.4
4	D	78	GLY	3.4
4	D	187	LEU	3.3
1	A	142	THR	3.2
3	C	7	TYR	3.2
4	D	83	GLY	3.1
4	D	198	GLY	3.1
4	H	8	LEU	3.1
4	D	80	ASP	3.1
4	H	137	GLY	3.1
4	H	55	VAL	3.1
4	D	56	LYS	2.9
4	H	52	GLN	2.9
4	D	34	GLU	2.9
4	D	48	THR	2.9
4	H	57	LYS	2.9
4	H	142	PRO	2.8
4	H	60	PHE	2.8
4	D	136	GLU	2.8
4	D	186	SER	2.8
4	D	84	ARG	2.8
1	E	255	GLN	2.7
4	H	38	TYR	2.7
4	D	82	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	141	GLN	2.7
3	C	4	SER	2.7
1	A	156	LEU	2.7
1	A	155	GLN	2.6
1	E	89	GLU	2.6
4	H	161	VAL	2.6
4	D	51	PRO	2.6
2	F	99	MET	2.6
3	G	3	PHE	2.6
4	H	47	ILE	2.6
1	E	249	VAL	2.6
4	H	51	PRO	2.6
4	D	77	TYR	2.6
3	C	8	GLY	2.5
4	H	168	ARG	2.5
1	E	252	GLY	2.5
3	G	8	GLY	2.5
4	D	43	THR	2.5
4	H	27	GLN	2.5
1	E	44	ARG	2.4
4	H	138	GLU	2.4
1	E	88	SER	2.4
1	E	274	TRP	2.4
3	C	3	PHE	2.4
4	H	87	SER	2.4
1	E	197	HIS	2.4
3	C	5	PRO	2.4
1	E	91	GLY	2.4
4	H	198	GLY	2.4
1	A	160	LEU	2.4
1	A	144	LYS	2.3
2	B	98	ASP	2.3
1	A	151	HIS	2.3
2	F	17	ASN	2.3
4	H	59	GLN	2.3
2	F	48	LYS	2.3
1	E	82	ARG	2.2
3	C	6	THR	2.2
3	G	2	THR	2.2
1	E	105	SER	2.2
4	H	41	LYS	2.2
4	H	56	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
4	H	46	TRP	2.2
1	A	152	VAL	2.2
1	A	225	THR	2.2
1	E	227	ASP	2.2
1	A	131	ARG	2.1
3	G	5	PRO	2.1
1	A	44	ARG	2.1
4	H	53	GLU	2.1
1	E	86	ASN	2.1
1	A	113	TYR	2.1
2	F	18	GLY	2.1
4	D	36	ARG	2.1
4	H	154	SER	2.0
1	A	267	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.