



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:55 AM GMT

PDB ID : 3B71
Title : CD4 endocytosis motif bound to the Focal Adhesion Targeting (FAT) domain
of the Focal Adhesion Kinase
Authors : Garron, M.-L.; Arold, S.T.
Deposited on : 2007-10-30
Resolution : 2.82 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

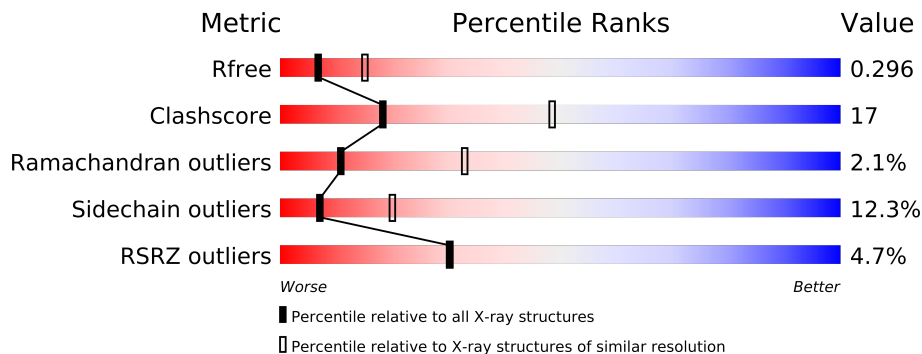
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.82 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}	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	162	
1	B	162	
1	C	162	
2	D	23	
2	E	23	
2	F	23	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3454 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Focal adhesion kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	1	0
			1048	662	178	201	7			
1	B	139	Total	C	N	O	S	0	0	0
			1073	680	180	206	7			
1	C	139	Total	C	N	O	S	0	0	0
			1073	680	180	206	7			

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

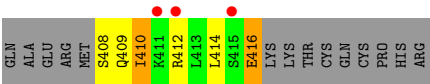
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	S	0	0	0
			93	57	19	16	1			
2	E	11	Total	C	N	O	S	0	0	0
			93	57	19	16	1			
2	F	9	Total	C	N	O		0	0	0
			74	46	14	14				

Chain E: 



● Molecule 2: T-cell surface glycoprotein CD4

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	88.07Å 220.47Å 97.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.82 29.35 – 2.82	Depositor EDS
% Data completeness (in resolution range)	93.8 (29.00-2.82) 93.9 (29.35-2.82)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.241 , 0.307 0.233 , 0.296	Depositor DCC
R_{free} test set	459 reflections (2.14%)	DCC
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 21922 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3454	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.86	0/1064	0.90	1/1439 (0.1%)
1	B	0.87	0/1087	0.90	0/1474
1	C	0.73	0/1087	0.89	1/1474 (0.1%)
2	D	0.54	0/92	0.92	0/119
2	E	0.78	0/92	0.74	0/119
2	F	1.05	0/73	0.74	0/95
All	All	0.82	0/3495	0.89	2/4720 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	917	LEU	CB-CG-CD1	-5.76	101.20	111.00
1	C	962	ARG	NE-CZ-NH1	5.28	122.94	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1048	0	1096	23	0
1	B	1073	0	1127	41	0
1	C	1073	0	1127	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	93	0	104	10	0
2	E	93	0	104	10	0
2	F	74	0	82	4	0
All	All	3454	0	3640	120	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (120) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:942:ILE:HG23	1:C:943:GLN:N	1.82	0.94
1:B:950:TYR:HA	1:B:953:MET:HE2	1.51	0.92
1:C:977:ALA:HA	1:C:980:HIS:NE2	1.84	0.91
1:C:1003:LEU:O	1:C:1006:GLN:HB2	1.71	0.91
1:B:950:TYR:HA	1:B:953:MET:CE	2.00	0.90
1:B:1008:VAL:HA	1:B:1013:GLN:OE1	1.74	0.85
1:C:942:ILE:CG2	1:C:943:GLN:H	1.90	0.83
1:C:942:ILE:HG23	1:C:943:GLN:H	1.37	0.83
2:F:412:ARG:O	2:F:416:GLU:HB3	1.82	0.79
1:B:956:GLU:OE2	1:B:956:GLU:HA	1.82	0.79
1:C:942:ILE:CG2	1:C:943:GLN:N	2.47	0.78
1:B:943:GLN:HB3	1:B:944:PRO:HD3	1.66	0.78
1:C:977:ALA:HA	1:C:980:HIS:CD2	2.19	0.77
1:C:968:VAL:O	1:C:972:ILE:HG13	1.86	0.76
2:E:406:ARG:O	2:E:410:ILE:HG22	1.86	0.76
2:D:406:ARG:HB3	2:D:406:ARG:HH11	1.49	0.76
2:D:413:LEU:HA	2:D:416:GLU:CD	2.06	0.75
1:C:980:HIS:O	1:C:984:GLU:HG2	1.92	0.70
2:E:408:SER:OG	2:E:412:ARG:NH1	2.24	0.69
1:B:995:GLY:HA3	2:E:406:ARG:HH21	1.58	0.69
1:A:1043:LEU:HD13	1:A:1048:GLN:HG2	1.76	0.68
1:A:998:ILE:CG2	1:A:1002:LYS:HE3	2.25	0.67
1:A:998:ILE:HG22	1:A:1002:LYS:HE3	1.78	0.66
1:A:942:ILE:HG21	1:A:1021:LEU:HD11	1.80	0.64
1:A:1025[A]:HIS:CE1	2:D:406:ARG:HH12	2.16	0.64
1:B:950:TYR:HA	1:B:953:MET:HE3	1.79	0.64
1:C:977:ALA:HA	1:C:980:HIS:HE2	1.62	0.63
1:B:979:THR:O	1:B:983:ILE:HD12	1.99	0.63
1:C:1007:TYR:O	1:C:1013:GLN:HB3	1.98	0.63
1:B:937:GLU:HA	1:B:937:GLU:OE1	1.99	0.62
1:C:962:ARG:HG3	1:C:962:ARG:HH11	1.63	0.62
1:B:976:PRO:HB2	1:B:979:THR:HG23	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:938:MET:O	1:C:942:ILE:HB	2.01	0.60
2:D:414:LEU:O	2:D:414:LEU:HD22	2.01	0.60
2:D:412:ARG:NH1	2:D:412:ARG:HB2	2.17	0.60
1:C:938:MET:HE1	1:C:954:VAL:HG22	1.82	0.60
1:C:951:VAL:HB	1:C:952:PRO:HD3	1.84	0.59
1:B:998:ILE:HD13	2:E:409:GLN:HB3	1.84	0.59
1:B:950:TYR:HE2	1:B:1013:GLN:NE2	1.99	0.59
1:B:950:TYR:CA	1:B:953:MET:HE2	2.28	0.59
1:C:969:ASP:O	1:C:973:PRO:HD3	2.04	0.58
2:D:409:GLN:HA	2:D:412:ARG:NH2	2.19	0.58
1:A:1012:LEU:O	1:A:1013:GLN:C	2.42	0.57
1:B:949:GLU:O	1:B:952:PRO:HD2	2.05	0.57
1:C:979:THR:HG23	1:C:979:THR:O	2.05	0.56
1:C:910:SER:HB2	1:C:911:PRO:HD2	1.88	0.55
1:B:985:MET:HE2	1:B:988:LYS:HD3	1.88	0.55
1:B:980:HIS:O	1:B:984:GLU:HG3	2.06	0.55
1:B:949:GLU:C	1:B:952:PRO:HD2	2.27	0.55
2:F:408:SER:N	2:F:410:ILE:HG23	2.22	0.55
1:C:950:TYR:O	1:C:954:VAL:HG23	2.07	0.55
1:C:950:TYR:HA	1:C:953:MET:HB2	1.89	0.54
2:D:412:ARG:HH11	2:D:412:ARG:HB2	1.71	0.54
1:B:931:LEU:O	1:B:931:LEU:HD12	2.07	0.54
1:A:943:GLN:OE1	1:A:1014:GLN:HG3	2.08	0.53
1:B:943:GLN:HB3	1:B:944:PRO:CD	2.37	0.53
1:C:982:GLU:HG2	1:C:1037:VAL:HG11	1.91	0.52
1:A:1033:ASN:O	1:A:1037:VAL:HG23	2.10	0.51
2:E:407:MET:HA	2:E:410:ILE:CG2	2.41	0.51
1:B:1008:VAL:O	1:B:1008:VAL:HG22	2.10	0.51
2:F:409:GLN:HA	2:F:412:ARG:HB2	1.94	0.50
1:B:1018:LYS:HA	1:B:1021:LEU:HD12	1.94	0.49
1:A:972:ILE:HB	1:A:973:PRO:HD3	1.95	0.49
1:B:919:ARG:HD2	1:B:925:TYR:CD2	2.48	0.49
1:C:977:ALA:O	1:C:979:THR:N	2.46	0.48
1:C:977:ALA:C	1:C:979:THR:H	2.16	0.48
1:A:961:LEU:HD23	1:A:994:LEU:HD22	1.95	0.48
1:B:950:TYR:CA	1:B:953:MET:CE	2.85	0.48
2:E:406:ARG:N	2:E:406:ARG:HE	2.12	0.48
2:E:406:ARG:C	2:E:410:ILE:HG22	2.33	0.48
1:A:937:GLU:OE2	1:A:941:LYS:HE3	2.13	0.48
1:A:971:THR:HG22	1:A:975:LEU:HD11	1.96	0.48
2:F:410:ILE:HG13	2:F:414:LEU:HD12	1.96	0.47
1:B:942:ILE:O	1:B:943:GLN:C	2.52	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:931:LEU:HD23	1:C:1031:ALA:HB2	1.96	0.47
1:B:1003:LEU:O	1:B:1007:TYR:HD1	1.97	0.47
1:A:993:ASP:CB	1:A:1027:LEU:HD13	2.45	0.47
1:A:986:ALA:HB3	1:A:1034:LEU:HD13	1.96	0.47
1:B:909:ILE:HG23	1:B:909:ILE:O	2.15	0.46
1:A:971:THR:O	1:A:972:ILE:C	2.54	0.45
1:B:990:LEU:HD22	1:B:1027:LEU:HD12	1.98	0.45
1:B:950:TYR:CE2	1:B:1013:GLN:NE2	2.81	0.45
1:B:994:LEU:HD23	2:E:410:ILE:HB	1.98	0.45
1:C:990:LEU:HD12	1:C:990:LEU:N	2.32	0.45
1:C:983:ILE:O	1:C:984:GLU:C	2.55	0.45
1:A:993:ASP:HB2	1:A:1027:LEU:CD1	2.47	0.45
1:A:965:LEU:HD22	1:A:987:GLN:HG2	1.99	0.45
1:C:942:ILE:HG21	1:C:1021:LEU:HD21	1.99	0.45
1:A:976:PRO:HD3	1:A:1045:MET:SD	2.57	0.45
1:B:1034:LEU:O	1:B:1035:LEU:C	2.54	0.45
1:C:964:LEU:O	1:C:968:VAL:HG23	2.17	0.45
1:C:972:ILE:HG22	1:C:980:HIS:ND1	2.33	0.44
2:E:407:MET:CA	2:E:410:ILE:HG22	2.47	0.44
1:A:918:ASP:HB3	1:B:1045:MET:SD	2.58	0.44
1:A:1042:ARG:O	1:A:1046:LEU:N	2.46	0.44
1:A:976:PRO:HD3	1:A:1045:MET:HB2	2.00	0.44
1:C:1034:LEU:O	1:C:1037:VAL:HG23	2.18	0.44
1:B:961:LEU:O	1:B:961:LEU:HD12	2.18	0.43
1:C:972:ILE:N	1:C:973:PRO:HD2	2.33	0.42
1:B:1001:MET:O	1:B:1005:GLN:HG3	2.19	0.42
1:B:910:SER:HB2	1:B:911:PRO:HD2	2.00	0.42
1:A:1038:ILE:O	1:A:1041:ALA:HB3	2.19	0.42
1:C:971:THR:C	1:C:973:PRO:HD2	2.40	0.42
1:C:969:ASP:O	1:C:973:PRO:CD	2.67	0.42
1:B:959:LEU:HA	1:B:959:LEU:HD23	1.92	0.42
1:C:1013:GLN:HG3	1:C:1014:GLN:N	2.35	0.42
1:C:1037:VAL:O	1:C:1038:ILE:C	2.57	0.42
1:B:929:THR:O	1:B:933:LYS:HG2	2.19	0.42
1:C:1045:MET:O	1:C:1045:MET:HG2	2.20	0.42
2:D:410:ILE:H	2:D:410:ILE:HG13	1.74	0.41
2:D:412:ARG:HH11	2:D:412:ARG:CB	2.32	0.41
1:C:981:ARG:HB3	1:C:981:ARG:HE	1.61	0.41
1:B:1010:THR:HB	1:C:981:ARG:HH22	1.85	0.41
1:B:945:ALA:HA	1:B:946:PRO:HD3	1.89	0.41
2:E:409:GLN:O	2:E:413:LEU:N	2.32	0.40
1:A:916:ASN:HB3	1:A:917:LEU:H	1.63	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1044:LYS:HE2	1:B:1044:LYS:HB3	1.81	0.40
1:B:942:ILE:HG21	1:B:1021:LEU:HD21	2.03	0.40
1:B:948:GLU:HG3	1:B:948:GLU:H	1.41	0.40
2:D:406:ARG:CB	2:D:406:ARG:HH11	2.27	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	133/162 (82%)	123 (92%)	8 (6%)	2 (2%)	15	45
1	B	137/162 (85%)	125 (91%)	11 (8%)	1 (1%)	30	68
1	C	137/162 (85%)	115 (84%)	16 (12%)	6 (4%)	4	11
2	D	9/23 (39%)	9 (100%)	0	0	100	100
2	E	9/23 (39%)	3 (33%)	6 (67%)	0	100	100
2	F	7/23 (30%)	4 (57%)	3 (43%)	0	100	100
All	All	432/555 (78%)	379 (88%)	44 (10%)	9 (2%)	11	33

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	942	ILE
1	C	978	SER
1	A	1013	GLN
1	C	970	GLU
1	C	923	LYS
1	C	941	LYS
1	C	1035	LEU
1	A	1011	SER
1	B	1034	LEU

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	118/142 (83%)	110 (93%)	8 (7%)	22	54
1	B	121/142 (85%)	108 (89%)	13 (11%)	10	26
1	C	121/142 (85%)	103 (85%)	18 (15%)	4	12
2	D	11/22 (50%)	7 (64%)	4 (36%)	0	0
2	E	11/22 (50%)	8 (73%)	3 (27%)	0	1
2	F	9/22 (41%)	7 (78%)	2 (22%)	1	3
All	All	391/492 (80%)	343 (88%)	48 (12%)	7	20

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	940	SER
1	A	978	SER
1	A	988	LYS
1	A	1011	SER
1	A	1013	GLN
1	A	1021	LEU
1	A	1032	LYS
1	A	1049	THR
1	B	921	ASN
1	B	923	LYS
1	B	939	SER
1	B	940	SER
1	B	941	LYS
1	B	948	GLU
1	B	963	THR
1	B	978	SER
1	B	979	THR
1	B	988	LYS
1	B	992	SER
1	B	1021	LEU
1	B	1044	LYS
1	C	927	ASN
1	C	936	ILE

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Mol	Chain	Res	Type
1	C	939	SER
1	C	940	SER
1	C	941	LYS
1	C	942	ILE
1	C	955	LYS
1	C	959	LEU
1	C	962	ARG
1	C	970	GLU
1	C	974	LEU
1	C	979	THR
1	C	988	LYS
1	C	991	ASN
1	C	992	SER
1	C	1032	LYS
1	C	1037	VAL
1	C	1046	LEU
2	D	406	ARG
2	D	409	GLN
2	D	410	ILE
2	D	414	LEU
2	E	406	ARG
2	E	407	MET
2	E	416	GLU
2	F	410	ILE
2	F	416	GLU

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

Mol	Chain	Res	Type
2	D	409	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	134/162 (82%)	-0.40	1 (0%)	84 86	20, 36, 48, 53	0
1	B	139/162 (85%)	-0.38	2 (1%)	72 72	26, 35, 43, 49	0
1	C	139/162 (85%)	-0.23	7 (5%)	28 28	26, 37, 48, 56	0
2	D	11/23 (47%)	1.88	4 (36%)	1 0	75, 78, 83, 83	11 (100%)
2	E	11/23 (47%)	1.61	4 (36%)	1 0	57, 63, 69, 69	11 (100%)
2	F	9/23 (39%)	1.17	3 (33%)	1 1	49, 51, 55, 57	9 (100%)
All	All	443/555 (79%)	-0.20	21 (4%)	30 30	20, 37, 56, 83	31 (6%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	408	SER	6.9
2	E	416	GLU	3.6
2	F	415	SER	3.3
1	C	1008	VAL	3.0
1	C	944	PRO	2.9
1	C	948	GLU	2.8
2	E	406	ARG	2.8
2	D	415	SER	2.7
1	B	943	GLN	2.7
1	C	1009	MET	2.7
1	C	1014	GLN	2.6
2	F	412	ARG	2.5
1	A	981	ARG	2.4
2	E	415	SER	2.4
2	D	412	ARG	2.4
1	C	1013	GLN	2.3
1	B	1014	GLN	2.3
2	E	412	ARG	2.2
2	F	411	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	414	LEU	2.1
1	C	941	LYS	2.1

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 carbohydrates 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.