



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2016 – 08:33 AM EST

PDB ID : 1Y19
Title : Structural basis for phosphatidylinositol phosphate kinase type I-gamma binding to talin at focal adhesions
Authors : de Pereda, J.M.; Wegener, K.; Santelli, E.; Bate, N.; Ginsberg, M.H.; Critchley, D.R.; Campbell, I.D.; Liddington, R.C.
Deposited on : 2004-11-17
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

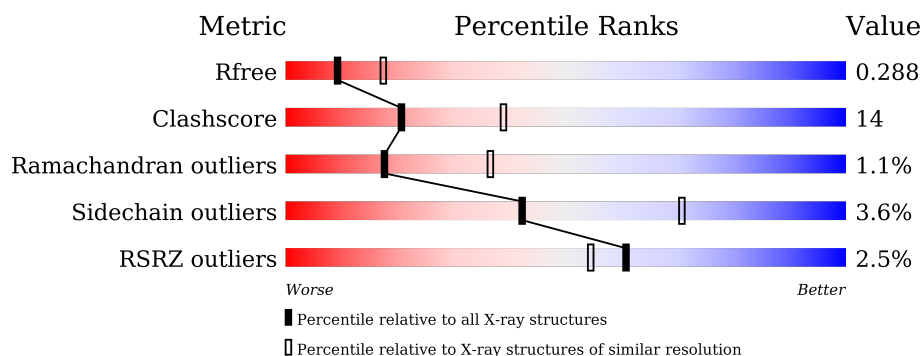
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	14	<div> <div>57%</div> <div>21%</div> <div>21%</div> </div>
1	C	14	<div> <div>36%</div> <div>43%</div> <div>21%</div> </div>
1	E	14	<div> <div>7%</div> <div>50%</div> <div>29%</div> <div>21%</div> </div>
1	G	14	<div> <div>43%</div> <div>36%</div> <div>21%</div> </div>
1	I	14	<div> <div>64%</div> <div>14%</div> <div>21%</div> </div>
1	K	14	<div> <div>50%</div> <div>29%</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	202	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>63%</div><div>29%</div><div>• 5%</div></div></div>
2	D	202	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>65%</div><div>26%</div><div>• 5%</div></div></div>
2	F	202	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>63%</div><div>29%</div><div>• 5%</div></div></div>
2	H	202	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>64%</div><div>29%</div><div>• 5%</div></div></div>
2	J	202	<div><div><div></div><div></div><div></div></div><div><div>5%</div><div>70%</div><div>23%</div><div>• 5%</div></div></div>
2	L	202	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>64%</div><div>28%</div><div>• 5%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10348 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 Phosphatidylinositol-4-phosphate 5-kinase, type 1 gamma.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	11	Total	C	N	O	0	0	0
			93	63	14	16			
1	C	11	Total	C	N	O	0	0	0
			93	63	14	16			
1	E	11	Total	C	N	O	0	0	0
			93	63	14	16			
1	G	11	Total	C	N	O	0	0	0
			93	63	14	16			
1	I	11	Total	C	N	O	0	0	0
			93	63	14	16			
1	K	11	Total	C	N	O	0	0	0
			93	63	14	16			

- Molecule 2 is a protein called Talin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	192	Total	C	N	O	S	0	0	0
			1554	1000	265	282	7			
2	D	192	Total	C	N	O	S	0	0	0
			1554	1000	265	282	7			
2	F	192	Total	C	N	O	S	0	0	0
			1554	1000	265	282	7			
2	H	192	Total	C	N	O	S	0	0	0
			1554	1000	265	282	7			
2	J	192	Total	C	N	O	S	0	0	0
			1554	1000	265	282	7			
2	L	192	Total	C	N	O	S	0	0	0
			1554	1000	265	282	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total 14	O 14	0	0
3	B	72	Total 72	O 72	0	0
3	C	5	Total 5	O 5	0	0
3	D	81	Total 81	O 81	0	0
3	E	7	Total 7	O 7	0	0
3	F	71	Total 71	O 71	0	0
3	G	8	Total 8	O 8	0	0
3	H	74	Total 74	O 74	0	0
3	I	6	Total 6	O 6	0	0
3	J	73	Total 73	O 73	0	0
3	K	10	Total 10	O 10	0	0
3	L	45	Total 45	O 45	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Phosphatidylinositol-4-phosphate 5-kinase, type 1 gamma

Chain A: 



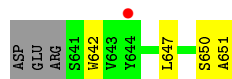
- Molecule 1: Phosphatidylinositol-4-phosphate 5-kinase, type 1 gamma

Chain C: 



- Molecule 1: Phosphatidylinositol-4-phosphate 5-kinase, type 1 gamma

Chain E: 



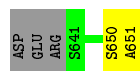
- Molecule 1: Phosphatidylinositol-4-phosphate 5-kinase, type 1 gamma

Chain G: 



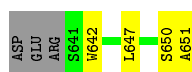
- Molecule 1: Phosphatidylinositol-4-phosphate 5-kinase, type 1 gamma

Chain I: 

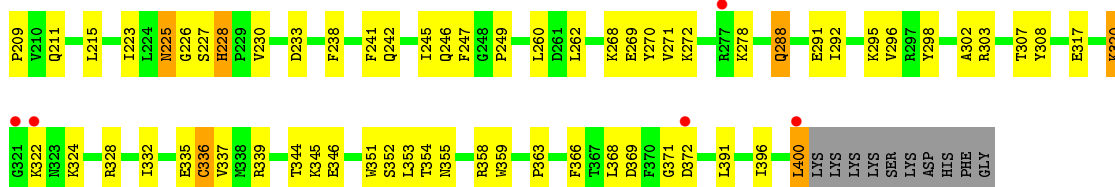


- Molecule 1: Phosphatidylinositol-4-phosphate 5-kinase, type 1 gamma

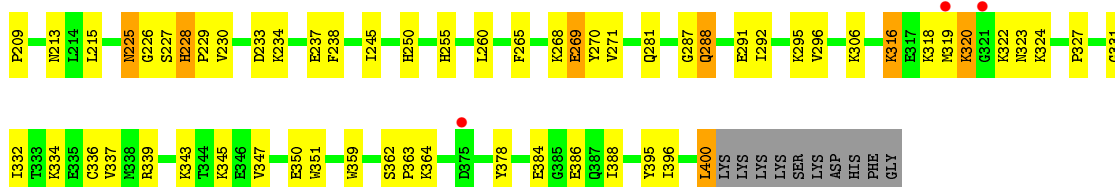
Chain K: 



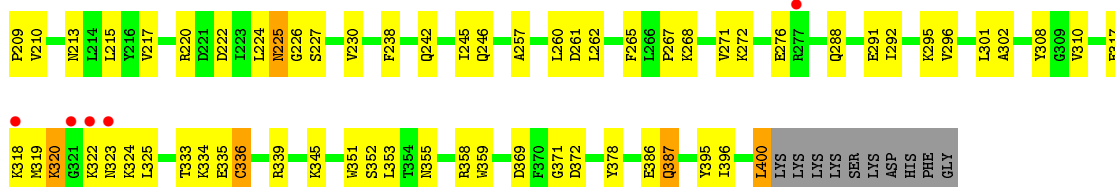
• Molecule 2: Talin 1



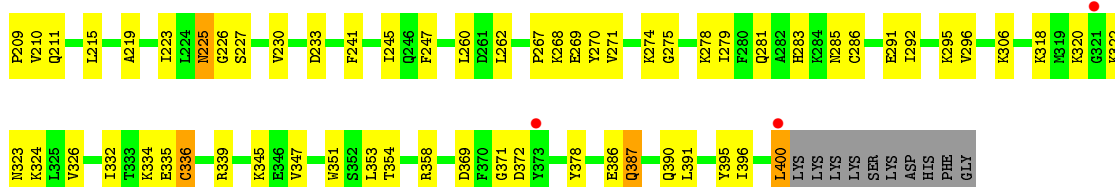
• Molecule 2: Talin 1



• Molecule 2: Talin 1

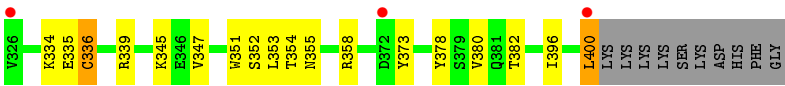


• Molecule 2: Talin 1

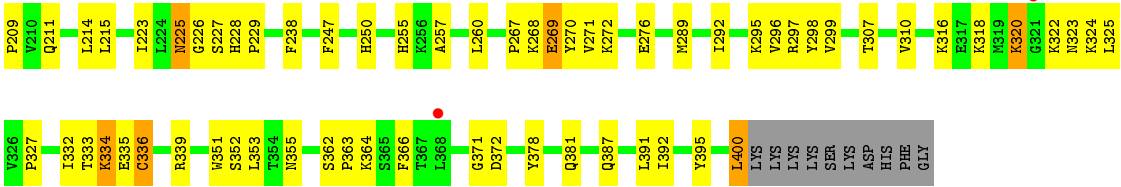


• Molecule 2: Talin 1





● Molecule 2: Talin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	118.10 Å 118.10 Å 93.31 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 42.45 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-2.60) 96.5 (42.45-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.61 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.253 , 0.286 0.253 , 0.288	Depositor DCC
R_{free} test set	2175 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.106 for -h,-k,l 0.106 for h,-h-k,-l 0.296 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10348	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.34	0/98	0.61	0/135
1	C	0.33	0/98	0.58	0/135
1	E	0.34	0/98	0.60	0/135
1	G	0.34	0/98	0.60	0/135
1	I	0.34	0/98	0.63	0/135
1	K	0.34	0/98	0.56	0/135
2	B	0.35	0/1586	0.54	0/2129
2	D	0.34	0/1586	0.55	0/2129
2	F	0.33	0/1586	0.53	0/2129
2	H	0.33	0/1586	0.52	0/2129
2	J	0.33	0/1586	0.53	0/2129
2	L	0.33	0/1586	0.55	0/2129
All	All	0.33	0/10104	0.54	0/13584

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	93	0	81	6	0
1	C	93	0	81	9	0
1	E	93	0	81	6	0
1	G	93	0	81	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	93	0	81	2	0
1	K	93	0	81	6	0
2	B	1554	0	1575	63	0
2	D	1554	0	1575	50	0
2	F	1554	0	1575	45	0
2	H	1554	0	1575	49	0
2	J	1554	0	1575	41	0
2	L	1554	0	1575	46	0
3	A	14	0	0	0	0
3	B	72	0	0	7	0
3	C	5	0	0	0	0
3	D	81	0	0	5	0
3	E	7	0	0	0	0
3	F	71	0	0	1	0
3	G	8	0	0	0	0
3	H	74	0	0	3	0
3	I	6	0	0	0	0
3	J	73	0	0	7	0
3	K	10	0	0	0	0
3	L	45	0	0	4	0
All	All	10348	0	9936	287	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 14.

All (287) 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:D:306:LYS:HG2	2:D:347:VAL:HG21	1.35	1.07
2:B:249:PRO:CG	2:B:288:GLN:HE22	1.72	1.00
2:B:288:GLN:HA	2:B:288:GLN:NE2	1.77	0.97
2:B:288:GLN:HA	2:B:288:GLN:HE21	1.29	0.94
2:B:288:GLN:CA	2:B:288:GLN:HE21	1.76	0.92
2:B:249:PRO:HG2	2:B:288:GLN:HE22	1.40	0.87
2:F:268:LYS:O	2:F:271:VAL:HG22	1.74	0.86
2:B:249:PRO:HG3	2:B:288:GLN:HE22	1.46	0.81
2:J:400:LEU:HD12	2:L:215:LEU:HD21	1.62	0.80
2:B:268:LYS:HE2	3:B:459:HOH:O	1.81	0.80
1:E:647:LEU:HD13	2:H:396:ILE:HG23	1.61	0.80
2:D:288:GLN:N	2:D:288:GLN:HE21	1.82	0.77
2:D:268:LYS:O	2:D:271:VAL:HG22	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:320:LYS:H	2:J:320:LYS:HE2	1.51	0.75
2:H:292:ILE:O	2:H:296:VAL:HG23	1.85	0.75
2:B:271:VAL:HG23	2:B:272:LYS:N	2.04	0.73
2:B:225:ASN:ND2	2:B:227:SER:H	1.87	0.72
2:B:249:PRO:CG	2:B:288:GLN:NE2	2.52	0.72
2:L:271:VAL:HG23	2:L:272:LYS:H	1.54	0.71
2:B:320:LYS:HE2	2:B:320:LYS:N	2.06	0.71
2:L:271:VAL:HG23	2:L:272:LYS:N	2.06	0.70
2:B:268:LYS:HG3	3:B:432:HOH:O	1.91	0.70
2:B:245:ILE:HG23	2:B:291:GLU:HG3	1.75	0.69
2:F:320:LYS:HE2	2:F:320:LYS:N	2.08	0.69
2:D:336:CYS:HB2	2:D:351:TRP:O	1.93	0.69
2:L:352:SER:HB2	3:L:432:HOH:O	1.93	0.68
2:D:322:LYS:HD2	2:D:324:LYS:HB3	1.75	0.68
2:H:268:LYS:O	2:H:271:VAL:HG23	1.93	0.68
2:J:320:LYS:N	2:J:320:LYS:HE2	2.08	0.68
2:J:352:SER:HB3	2:J:355:ASN:OD1	1.94	0.67
2:F:322:LYS:HD2	2:F:324:LYS:HB3	1.77	0.66
2:D:306:LYS:HG2	2:D:347:VAL:CG2	2.21	0.66
2:H:245:ILE:HG23	2:H:291:GLU:HG3	1.78	0.66
2:L:327:PRO:HG2	3:L:450:HOH:O	1.95	0.66
2:H:390:GLN:HG2	3:H:484:HOH:O	1.95	0.66
2:B:215:LEU:HD21	2:D:400:LEU:HD12	1.78	0.66
2:B:271:VAL:HG23	2:B:272:LYS:H	1.61	0.66
2:B:320:LYS:H	2:B:320:LYS:HE2	1.61	0.65
2:J:261:ASP:OD2	2:J:263:LYS:HG2	1.97	0.64
2:D:230:VAL:C	2:D:345:LYS:HG3	2.17	0.64
2:F:225:ASN:ND2	2:F:227:SER:H	1.96	0.64
2:J:336:CYS:HB2	2:J:351:TRP:O	1.99	0.63
2:H:326:VAL:HG13	3:H:471:HOH:O	1.99	0.63
2:D:324:LYS:HB2	2:D:324:LYS:NZ	2.14	0.62
2:L:364:LYS:NZ	2:L:381:GLN:HE21	1.96	0.62
2:B:249:PRO:HG3	2:B:288:GLN:NE2	2.13	0.62
2:B:354:THR:HG22	1:C:647:LEU:HD23	1.80	0.62
2:L:268:LYS:O	2:L:271:VAL:HG22	1.99	0.61
2:B:225:ASN:HD22	2:B:226:GLY:N	1.98	0.61
2:L:316:LYS:HD3	2:L:381:GLN:OE1	2.00	0.61
2:B:354:THR:HA	1:C:647:LEU:HD23	1.80	0.61
2:L:225:ASN:HD22	2:L:226:GLY:N	1.98	0.61
2:L:225:ASN:ND2	2:L:227:SER:H	1.99	0.61
2:B:396:ILE:HG23	1:C:647:LEU:HD13	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:ALA:N	2:B:209:PRO:HD2	2.16	0.60
1:A:645:SER:HB2	2:D:359:TRP:HZ3	1.66	0.60
1:I:651:ALA:N	2:J:209:PRO:HD2	2.16	0.60
1:C:651:ALA:N	2:D:209:PRO:HD2	2.18	0.59
2:J:230:VAL:C	2:J:345:LYS:HG3	2.23	0.59
2:B:322:LYS:HD2	2:B:324:LYS:HB3	1.85	0.59
2:D:316:LYS:NZ	2:D:327:PRO:HG3	2.17	0.59
1:K:651:ALA:N	2:L:209:PRO:HD2	2.17	0.59
2:H:225:ASN:ND2	2:H:227:SER:H	2.00	0.59
1:E:647:LEU:HD23	2:H:354:THR:HA	1.85	0.58
2:B:225:ASN:HD22	2:B:225:ASN:C	2.06	0.58
2:F:386:GLU:HG3	2:F:387:GLN:OE1	2.03	0.58
2:J:354:THR:HG23	3:J:422:HOH:O	2.03	0.58
2:D:339:ARG:HD3	2:D:378:TYR:CE1	2.39	0.58
2:F:318:LYS:HE2	2:F:323:ASN:O	2.04	0.57
2:F:320:LYS:HE2	2:F:320:LYS:H	1.69	0.57
2:F:359:TRP:HZ3	1:G:645:SER:HB2	1.70	0.57
1:E:651:ALA:N	2:F:209:PRO:HD2	2.19	0.57
2:F:339:ARG:HD3	2:F:378:TYR:CE1	2.40	0.56
2:J:396:ILE:HG23	1:K:647:LEU:HD13	1.85	0.56
2:D:291:GLU:O	2:D:295:LYS:HG3	2.05	0.56
2:J:225:ASN:HB3	3:J:418:HOH:O	2.05	0.56
2:L:324:LYS:HB2	2:L:324:LYS:NZ	2.20	0.56
2:B:344:THR:HG22	2:B:346:GLU:HG2	1.87	0.56
2:D:324:LYS:HZ2	2:D:324:LYS:HB2	1.69	0.55
1:G:651:ALA:N	2:H:209:PRO:HD2	2.22	0.55
2:B:230:VAL:C	2:B:345:LYS:HG3	2.27	0.55
2:F:324:LYS:NZ	2:F:324:LYS:HB2	2.21	0.55
2:D:288:GLN:CA	2:D:288:GLN:HE21	2.17	0.55
2:L:318:LYS:HE2	2:L:323:ASN:O	2.07	0.55
2:L:322:LYS:HD2	2:L:324:LYS:HB3	1.90	0.54
2:L:227:SER:O	2:L:229:PRO:HD3	2.06	0.54
2:F:292:ILE:O	2:F:296:VAL:HG23	2.08	0.54
2:B:271:VAL:CG2	2:B:272:LYS:N	2.71	0.54
2:D:332:ILE:HD12	2:D:337:VAL:HG22	1.89	0.54
2:B:324:LYS:NZ	2:B:324:LYS:HB2	2.23	0.53
2:F:336:CYS:HB2	2:F:351:TRP:O	2.07	0.53
2:F:225:ASN:HD22	2:F:225:ASN:C	2.11	0.53
2:J:324:LYS:NZ	2:J:324:LYS:HB2	2.24	0.53
2:D:227:SER:O	2:D:229:PRO:HD3	2.08	0.53
2:L:292:ILE:O	2:L:296:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:318:LYS:HE2	2:H:323:ASN:O	2.09	0.53
2:H:283:HIS:O	2:H:286:CYS:HB2	2.09	0.52
2:D:225:ASN:ND2	2:D:227:SER:H	2.07	0.52
1:I:650:SER:OG	2:J:209:PRO:HG2	2.10	0.52
2:D:322:LYS:CD	2:D:324:LYS:HB3	2.39	0.52
2:H:241:PHE:O	2:H:245:ILE:HG13	2.09	0.52
2:J:319:MET:HE3	3:J:471:HOH:O	2.09	0.52
2:L:339:ARG:HD3	2:L:378:TYR:CE1	2.45	0.52
2:L:334:LYS:HA	2:L:395:TYR:CG	2.45	0.52
2:H:336:CYS:HB2	2:H:351:TRP:O	2.10	0.52
2:J:223:ILE:O	2:J:267:PRO:HG3	2.10	0.52
2:L:292:ILE:HG12	3:L:429:HOH:O	2.08	0.52
2:D:318:LYS:HE2	2:D:323:ASN:O	2.10	0.51
2:F:400:LEU:CD1	2:H:215:LEU:HD11	2.39	0.51
2:J:247:PHE:HE1	2:J:260:LEU:HD21	1.75	0.51
2:J:225:ASN:ND2	2:J:227:SER:H	2.07	0.51
2:L:352:SER:HB3	2:L:355:ASN:ND2	2.26	0.51
2:J:306:LYS:HG2	2:J:347:VAL:HG21	1.92	0.51
2:J:302:ALA:O	2:J:308:TYR:HB2	2.11	0.51
2:D:228:HIS:HD2	3:D:426:HOH:O	1.92	0.51
2:L:225:ASN:HD22	2:L:225:ASN:C	2.13	0.51
2:B:269:GLU:HG3	2:B:270:TYR:CD2	2.46	0.51
2:B:336:CYS:HB2	2:B:351:TRP:O	2.10	0.50
2:J:292:ILE:O	2:J:296:VAL:HG23	2.12	0.50
2:D:269:GLU:HG3	2:D:270:TYR:CD2	2.47	0.50
2:B:400:LEU:HD12	2:D:215:LEU:HD21	1.94	0.50
2:H:324:LYS:NZ	2:H:324:LYS:HB2	2.26	0.50
2:L:295:LYS:O	2:L:299:VAL:HG23	2.12	0.50
2:B:363:PRO:HA	3:B:451:HOH:O	2.11	0.50
1:E:650:SER:OG	2:F:210:VAL:HG23	2.12	0.50
2:F:245:ILE:HG23	2:F:291:GLU:HG3	1.92	0.50
2:F:215:LEU:HD21	2:H:400:LEU:HD12	1.93	0.50
2:H:291:GLU:HG2	2:H:295:LYS:HE3	1.94	0.49
2:J:335:GLU:C	2:J:353:LEU:HG	2.32	0.49
2:D:245:ILE:HG23	2:D:291:GLU:HG3	1.93	0.49
2:H:387:GLN:N	2:H:387:GLN:OE1	2.46	0.49
2:H:291:GLU:O	2:H:295:LYS:HG3	2.12	0.49
2:B:228:HIS:HE1	2:B:307:THR:OG1	1.96	0.49
2:B:271:VAL:CG2	2:B:272:LYS:H	2.24	0.49
2:J:260:LEU:HD22	2:J:265:PHE:CE2	2.47	0.49
2:B:230:VAL:O	2:B:345:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:ARG:NH1	3:B:457:HOH:O	2.45	0.48
1:G:646:PRO:O	2:H:211:GLN:NE2	2.41	0.48
2:D:288:GLN:NE2	2:D:288:GLN:CA	2.75	0.48
2:F:291:GLU:HG2	2:F:295:LYS:HE3	1.95	0.48
2:H:322:LYS:HD2	2:H:324:LYS:HB3	1.94	0.48
2:J:230:VAL:O	2:J:345:LYS:HG3	2.13	0.48
2:B:233:ASP:OD1	2:B:278:LYS:NZ	2.47	0.48
2:L:238:PHE:HB3	2:L:298:TYR:CE1	2.49	0.48
2:L:336:CYS:HB2	2:L:351:TRP:O	2.13	0.48
2:B:247:PHE:HE1	2:B:260:LEU:HD21	1.79	0.48
2:D:250:HIS:CE1	2:D:255:HIS:HB2	2.49	0.48
2:H:334:LYS:HA	2:H:395:TYR:CG	2.49	0.48
2:B:292:ILE:O	2:B:296:VAL:HG23	2.13	0.48
2:D:225:ASN:HD22	2:D:226:GLY:N	2.12	0.48
2:H:225:ASN:HD22	2:H:225:ASN:C	2.15	0.48
1:E:647:LEU:HD23	2:H:354:THR:HG22	1.96	0.47
2:F:220:ARG:O	2:F:224:LEU:HG	2.14	0.47
2:H:225:ASN:HD22	2:H:226:GLY:N	2.11	0.47
2:F:310:VAL:HG22	2:F:333:THR:HG22	1.96	0.47
2:H:306:LYS:HG2	2:H:347:VAL:HG21	1.97	0.47
2:H:386:GLU:HB3	2:H:387:GLN:OE1	2.15	0.47
2:J:225:ASN:HD22	2:J:226:GLY:N	2.12	0.47
2:B:215:LEU:HD11	2:D:400:LEU:CD1	2.45	0.47
2:L:269:GLU:HG3	2:L:270:TYR:CD2	2.49	0.47
2:B:272:LYS:HG2	3:B:442:HOH:O	2.14	0.46
2:F:257:ALA:HA	2:F:276:GLU:OE1	2.15	0.46
2:F:325:LEU:N	2:F:325:LEU:HD12	2.30	0.46
2:D:234:LYS:O	2:D:238:PHE:CD1	2.69	0.46
2:H:274:LYS:NZ	3:H:462:HOH:O	2.48	0.46
2:B:223:ILE:HD13	2:B:238:PHE:CE1	2.50	0.46
2:D:213:ASN:OD1	2:D:295:LYS:NZ	2.44	0.46
2:H:274:LYS:NZ	2:H:274:LYS:HA	2.30	0.46
2:H:335:GLU:C	2:H:353:LEU:HG	2.36	0.46
2:F:396:ILE:HG23	1:G:647:LEU:HD13	1.96	0.46
2:J:245:ILE:HG23	2:J:291:GLU:HG3	1.98	0.46
2:J:256:LYS:HB3	3:J:459:HOH:O	2.15	0.46
2:F:317:GLU:OE1	2:F:339:ARG:HD2	2.16	0.46
2:L:320:LYS:HD3	3:L:418:HOH:O	2.15	0.46
1:A:647:LEU:HD13	2:D:396:ILE:HG23	1.98	0.46
2:H:358:ARG:HG3	2:H:369:ASP:HB3	1.96	0.46
2:J:339:ARG:HD3	2:J:378:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:PHE:O	2:B:245:ILE:HG13	2.16	0.45
2:B:358:ARG:HG3	2:B:369:ASP:HB3	1.97	0.45
2:F:322:LYS:CD	2:F:324:LYS:HB3	2.44	0.45
2:H:320:LYS:HB2	2:H:320:LYS:HE2	1.79	0.45
2:J:322:LYS:HD2	2:J:324:LYS:HB3	1.97	0.45
2:L:257:ALA:HA	2:L:276:GLU:OE1	2.16	0.45
2:L:362:SER:HB2	2:L:363:PRO:HD2	1.99	0.45
2:D:386:GLU:HG3	3:D:424:HOH:O	2.17	0.45
2:F:335:GLU:C	2:F:353:LEU:HG	2.36	0.45
2:L:364:LYS:HZ3	2:L:381:GLN:HE21	1.64	0.45
2:L:364:LYS:HZ1	2:L:381:GLN:HE21	1.62	0.45
2:D:225:ASN:HD22	2:D:225:ASN:C	2.20	0.45
2:J:306:LYS:HE2	3:J:417:HOH:O	2.16	0.45
1:K:650:SER:O	2:L:211:GLN:HG3	2.17	0.45
2:L:310:VAL:HG22	2:L:333:THR:HG22	1.99	0.45
2:D:234:LYS:HG3	3:D:423:HOH:O	2.16	0.45
2:F:225:ASN:C	2:F:225:ASN:ND2	2.70	0.45
1:G:650:SER:OG	2:H:210:VAL:HG23	2.17	0.44
1:A:645:SER:HB2	2:D:359:TRP:CZ3	2.50	0.44
2:B:335:GLU:C	2:B:353:LEU:HG	2.38	0.44
2:D:334:LYS:HA	2:D:395:TYR:CG	2.53	0.44
2:L:247:PHE:HE1	2:L:260:LEU:HD21	1.80	0.44
2:H:269:GLU:HG3	2:H:270:TYR:CD2	2.52	0.44
2:F:302:ALA:O	2:F:308:TYR:HB2	2.18	0.44
2:D:292:ILE:O	2:D:296:VAL:HG23	2.17	0.44
2:F:225:ASN:HD22	2:F:226:GLY:N	2.14	0.44
2:H:339:ARG:HD3	2:H:378:TYR:CE1	2.53	0.44
2:B:242:GLN:O	2:B:246:GLN:HG3	2.17	0.43
2:D:384:GLU:O	2:D:388:ILE:HG13	2.18	0.43
2:F:242:GLN:O	2:F:246:GLN:HG3	2.18	0.43
2:F:358:ARG:HG3	2:F:369:ASP:HB3	1.99	0.43
2:J:243:CYS:SG	2:J:260:LEU:HD11	2.58	0.43
2:J:315:VAL:HG12	2:J:382:THR:HB	2.00	0.43
2:D:281:GLN:NE2	3:D:447:HOH:O	2.51	0.43
2:H:281:GLN:O	2:H:285:ASN:ND2	2.51	0.43
2:L:223:ILE:O	2:L:267:PRO:HG3	2.19	0.43
2:F:319:MET:HB3	2:F:320:LYS:NZ	2.33	0.43
2:L:335:GLU:C	2:L:353:LEU:HG	2.38	0.43
2:F:238:PHE:CE2	2:F:301:LEU:HD23	2.53	0.43
2:H:245:ILE:HD13	2:H:295:LYS:HG2	1.99	0.43
2:J:215:LEU:HD21	2:L:400:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:GLU:O	2:B:295:LYS:HG3	2.19	0.43
2:B:328:ARG:HD3	3:B:474:HOH:O	2.17	0.43
2:J:354:THR:HA	1:K:647:LEU:HD23	1.99	0.43
2:D:362:SER:C	2:D:364:LYS:H	2.21	0.43
2:F:334:LYS:HA	2:F:395:TYR:CG	2.54	0.43
2:B:352:SER:HB3	2:B:355:ASN:ND2	2.34	0.43
2:B:366:PHE:CE2	2:B:368:LEU:HG	2.54	0.43
2:B:322:LYS:CD	2:B:324:LYS:HB3	2.48	0.43
1:C:650:SER:OG	2:D:209:PRO:HG2	2.19	0.43
2:D:306:LYS:HZ1	2:D:350:GLU:CD	2.21	0.43
2:F:271:VAL:HG23	2:F:272:LYS:N	2.34	0.43
2:L:289:MET:SD	2:L:297:ARG:HD2	2.58	0.43
2:F:230:VAL:C	2:F:345:LYS:HG3	2.39	0.43
2:H:332:ILE:HB	2:H:391:LEU:HD23	2.00	0.43
2:L:334:LYS:HA	2:L:395:TYR:CD1	2.54	0.42
2:D:287:GLY:C	2:D:288:GLN:HE21	2.22	0.42
2:D:319:MET:O	2:D:320:LYS:O	2.37	0.42
1:E:647:LEU:HD13	2:H:396:ILE:CG2	2.41	0.42
2:H:233:ASP:OD1	2:H:278:LYS:NZ	2.50	0.42
2:F:324:LYS:HZ2	2:F:324:LYS:HB2	1.83	0.42
2:B:225:ASN:ND2	2:B:225:ASN:C	2.70	0.42
2:L:228:HIS:HE1	2:L:307:THR:OG1	2.00	0.42
2:H:275:GLY:O	2:H:279:ILE:HG13	2.19	0.42
2:H:230:VAL:C	2:H:345:LYS:HG3	2.40	0.42
2:L:366:PHE:HZ	2:L:392:ILE:HD12	1.85	0.42
2:H:223:ILE:O	2:H:267:PRO:HG3	2.20	0.42
2:L:250:HIS:CE1	2:L:255:HIS:HB2	2.55	0.42
2:D:260:LEU:HD22	2:D:265:PHE:CE2	2.55	0.42
2:J:400:LEU:CD1	2:L:215:LEU:HD11	2.49	0.42
2:J:358:ARG:NH1	1:K:642:TRP:CD1	2.88	0.42
2:D:233:ASP:O	2:D:237:GLU:HG3	2.20	0.42
2:J:241:PHE:O	2:J:245:ILE:HG13	2.20	0.42
2:J:334:LYS:HE2	3:J:470:HOH:O	2.20	0.42
2:F:261:ASP:N	3:F:420:HOH:O	2.53	0.42
2:B:228:HIS:HD2	3:B:431:HOH:O	2.02	0.41
2:F:352:SER:HB3	2:F:355:ASN:ND2	2.35	0.41
2:H:247:PHE:HE1	2:H:260:LEU:HD21	1.83	0.41
2:L:325:LEU:N	2:L:325:LEU:HD12	2.34	0.41
2:J:317:GLU:OE1	2:J:339:ARG:HD2	2.20	0.41
2:H:336:CYS:N	2:H:353:LEU:HG	2.35	0.41
2:B:278:LYS:HE2	2:B:278:LYS:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:331:GLY:O	2:D:332:ILE:HD13	2.21	0.41
2:F:267:PRO:O	2:F:268:LYS:C	2.58	0.41
2:B:317:GLU:OE1	2:B:339:ARG:HD2	2.20	0.41
1:C:646:PRO:HA	1:C:649:TYR:CD1	2.55	0.41
2:F:213:ASN:O	2:F:217:VAL:HG23	2.21	0.41
1:K:651:ALA:N	2:L:209:PRO:CD	2.84	0.41
2:L:332:ILE:HB	2:L:391:LEU:HD23	2.03	0.41
2:J:315:VAL:HB	2:J:380:VAL:HB	2.03	0.41
1:A:651:ALA:N	2:B:209:PRO:CD	2.84	0.41
2:B:354:THR:HG22	1:C:647:LEU:CD2	2.47	0.41
2:D:343:LYS:HD2	3:D:476:HOH:O	2.21	0.41
2:H:225:ASN:C	2:H:225:ASN:ND2	2.74	0.41
2:J:325:LEU:N	2:J:325:LEU:HD12	2.36	0.41
1:A:647:LEU:HA	2:B:211:GLN:NE2	2.37	0.40
2:B:332:ILE:HD12	2:B:337:VAL:HG22	2.04	0.40
1:C:651:ALA:N	2:D:209:PRO:CD	2.83	0.40
2:H:219:ALA:O	2:H:223:ILE:HG13	2.21	0.40
2:B:302:ALA:O	2:B:308:TYR:HB2	2.20	0.40
1:G:647:LEU:HA	2:H:211:GLN:NE2	2.36	0.40
2:B:332:ILE:HB	2:B:391:LEU:HD23	2.03	0.40
2:F:260:LEU:HD22	2:F:265:PHE:CE2	2.56	0.40
2:L:267:PRO:O	2:L:268:LYS:C	2.58	0.40
2:B:359:TRP:HZ3	1:C:645:SER:HB2	1.86	0.40
2:F:320:LYS:CE	2:F:320:LYS:H	2.33	0.40
2:H:274:LYS:HA	2:H:274:LYS:HZ2	1.86	0.40
2:J:256:LYS:HD3	3:J:459:HOH:O	2.20	0.40
2:B:238:PHE:HB3	2:B:298:TYR:CE1	2.56	0.40
2:F:222:ASP:HA	2:F:225:ASN:HD21	1.87	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	9/14 (64%)	9 (100%)	0	0	100	100
1	C	9/14 (64%)	9 (100%)	0	0	100	100
1	E	9/14 (64%)	8 (89%)	0	1 (11%)	0	0
1	G	9/14 (64%)	9 (100%)	0	0	100	100
1	I	9/14 (64%)	8 (89%)	1 (11%)	0	100	100
1	K	9/14 (64%)	8 (89%)	1 (11%)	0	100	100
2	B	190/202 (94%)	177 (93%)	11 (6%)	2 (1%)	17	36
2	D	190/202 (94%)	171 (90%)	16 (8%)	3 (2%)	12	24
2	F	190/202 (94%)	171 (90%)	17 (9%)	2 (1%)	17	36
2	H	190/202 (94%)	174 (92%)	14 (7%)	2 (1%)	17	36
2	J	190/202 (94%)	176 (93%)	13 (7%)	1 (0%)	34	60
2	L	190/202 (94%)	177 (93%)	11 (6%)	2 (1%)	17	36
All	All	1194/1296 (92%)	1097 (92%)	84 (7%)	13 (1%)	17	36

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	320	LYS
1	E	642	TRP
2	F	262	LEU
2	J	373	TYR
2	L	371	GLY
2	B	262	LEU
2	B	371	GLY
2	D	269	GLU
2	H	262	LEU
2	H	371	GLY
2	L	269	GLU
2	D	363	PRO
2	F	371	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	10/13 (77%)	10 (100%)	0	100	100
1	C	10/13 (77%)	10 (100%)	0	100	100
1	E	10/13 (77%)	10 (100%)	0	100	100
1	G	10/13 (77%)	10 (100%)	0	100	100
1	I	10/13 (77%)	10 (100%)	0	100	100
1	K	10/13 (77%)	10 (100%)	0	100	100
2	B	168/177 (95%)	161 (96%)	7 (4%)	36	65
2	D	168/177 (95%)	163 (97%)	5 (3%)	48	76
2	F	168/177 (95%)	161 (96%)	7 (4%)	36	65
2	H	168/177 (95%)	163 (97%)	5 (3%)	48	76
2	J	168/177 (95%)	162 (96%)	6 (4%)	42	71
2	L	168/177 (95%)	160 (95%)	8 (5%)	31	58
All	All	1068/1140 (94%)	1030 (96%)	38 (4%)	42	71

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	225	ASN
2	B	228	HIS
2	B	288	GLN
2	B	320	LYS
2	B	336	CYS
2	B	372	ASP
2	B	400	LEU
2	D	225	ASN
2	D	228	HIS
2	D	288	GLN
2	D	316	LYS
2	D	400	LEU
2	F	225	ASN
2	F	288	GLN
2	F	320	LYS
2	F	336	CYS
2	F	372	ASP
2	F	387	GLN
2	F	400	LEU
2	H	225	ASN
2	H	336	CYS
2	H	372	ASP

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Mol	Chain	Res	Type
2	H	387	GLN
2	H	400	LEU
2	J	225	ASN
2	J	228	HIS
2	J	253	GLN
2	J	320	LYS
2	J	336	CYS
2	J	400	LEU
2	L	214	LEU
2	L	225	ASN
2	L	320	LYS
2	L	334	LYS
2	L	336	CYS
2	L	372	ASP
2	L	387	GLN
2	L	400	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	211	GLN
2	B	225	ASN
2	B	228	HIS
2	B	288	GLN
2	B	355	ASN
2	B	374	GLN
2	D	218	GLN
2	D	225	ASN
2	D	228	HIS
2	D	288	GLN
2	D	355	ASN
2	F	225	ASN
2	F	355	ASN
2	F	374	GLN
2	H	225	ASN
2	H	285	ASN
2	H	355	ASN
2	H	374	GLN
2	J	225	ASN
2	J	228	HIS
2	J	374	GLN
2	L	225	ASN

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Mol	Chain	Res	Type
2	L	228	HIS
2	L	250	HIS
2	L	355	ASN
2	L	374	GLN
2	L	381	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 carbohydrates 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	11/14 (78%)	0.01	0 100 100	35, 41, 54, 56	0
1	C	11/14 (78%)	-0.15	0 100 100	29, 49, 67, 69	0
1	E	11/14 (78%)	0.40	1 (9%) 11 7	46, 57, 70, 75	0
1	G	11/14 (78%)	-0.13	0 100 100	44, 54, 71, 74	0
1	I	11/14 (78%)	0.07	0 100 100	39, 52, 71, 74	0
1	K	11/14 (78%)	-0.05	0 100 100	40, 53, 67, 71	0
2	B	192/202 (95%)	0.05	5 (2%) 59 53	22, 47, 87, 99	0
2	D	192/202 (95%)	0.03	3 (1%) 74 69	26, 46, 84, 96	0
2	F	192/202 (95%)	0.02	5 (2%) 59 53	32, 56, 88, 98	0
2	H	192/202 (95%)	-0.12	3 (1%) 74 69	33, 56, 90, 100	0
2	J	192/202 (95%)	0.01	11 (5%) 27 20	32, 53, 89, 100	0
2	L	192/202 (95%)	-0.05	2 (1%) 84 81	32, 56, 91, 98	0
All	All	1218/1296 (93%)	-0.01	30 (2%) 61 54	22, 53, 89, 100	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	321	GLY	6.2
2	F	321	GLY	6.1
2	J	320	LYS	4.6
2	J	319	MET	4.4
2	F	322	LYS	4.3
2	D	319	MET	3.7
2	J	322	LYS	3.5
2	J	321	GLY	3.5
2	H	321	GLY	3.4
2	H	373	TYR	3.3
2	B	322	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	J	324	LYS	3.1
2	F	323	ASN	2.8
1	E	644	TYR	2.8
2	J	277	ARG	2.8
2	B	372	ASP	2.7
2	F	318	LYS	2.7
2	J	272	LYS	2.6
2	B	277	ARG	2.6
2	J	325	LEU	2.6
2	J	372	ASP	2.6
2	D	321	GLY	2.5
2	L	321	GLY	2.5
2	B	400	LEU	2.4
2	H	400	LEU	2.4
2	F	277	ARG	2.3
2	J	400	LEU	2.3
2	J	326	VAL	2.2
2	L	368	LEU	2.1
2	D	375	ASP	2.1

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 carbohydrates 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.