Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2023 – 08:55 PM EDT

PDB ID	:	2F86
Title	:	The Association Domain of C. elegans CaMKII
Authors	:	Rosenberg, O.S.; Kuriyan, J.
Deposited on	:	2005-12-01
Resolution	:	2.64 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 (i) 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 (1)) were used in the production of this report:

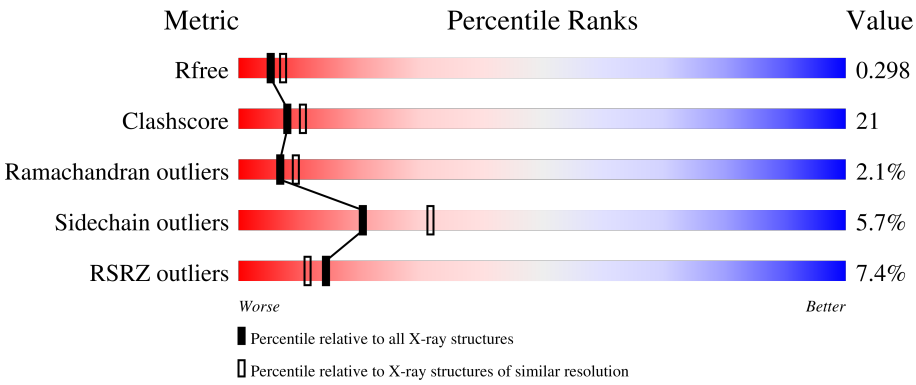
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	B	143	8% 60% 27% • 10%
1	D	143	6% 54% 32% • 10%
1	F	143	6% 55% 32% • 10%
1	H	143	6% 52% 35% • 10%
1	J	143	9% 57% 29% • 10%

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Mol	Chain	Length	Quality of chain
1	L	143	6% 63% 22% 5% 10%
1	N	143	4% 55% 34% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7335 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 Hypothetical protein K11E8.1d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	129	1045	647	192	199	7	0	0	0
1	D	129	1045	647	192	199	7	0	0	0
1	F	129	1045	647	192	199	7	0	0	0
1	H	129	1045	647	192	199	7	0	0	0
1	J	129	1045	647	192	199	7	0	0	0
1	L	129	1045	647	192	199	7	0	0	0
1	N	129	1045	647	192	199	7	0	0	0

- Molecule 2 is water.

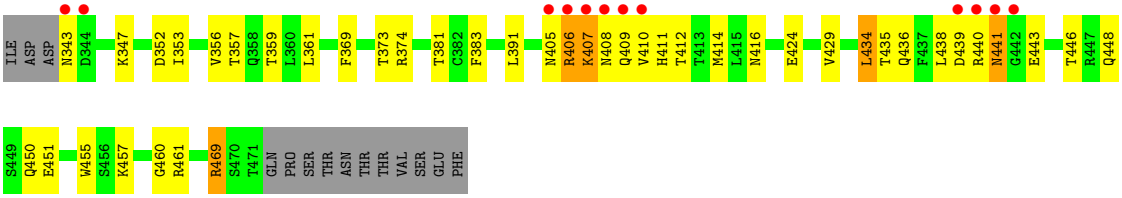
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	3	3	3	0	0
2	D	2	2	2	0	0
2	F	1	1	1	0	0
2	H	3	3	3	0	0
2	J	3	3	3	0	0
2	L	5	5	5	0	0
2	N	3	3	3	0	0

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.

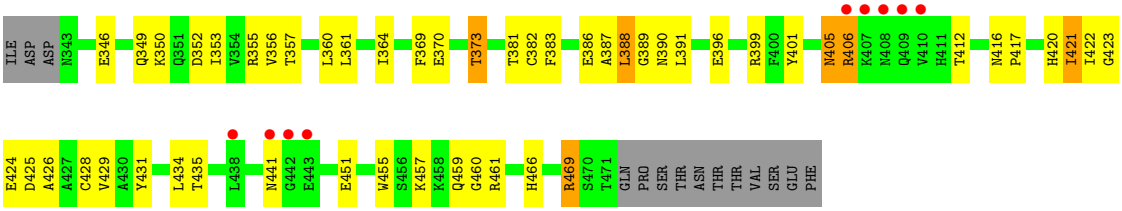
• Molecule 1: Hypothetical protein K11E8.1d

Chain B:



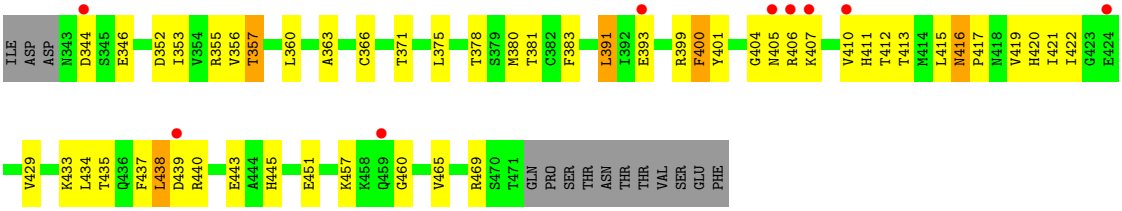
• Molecule 1: Hypothetical protein K11E8.1d

Chain D:



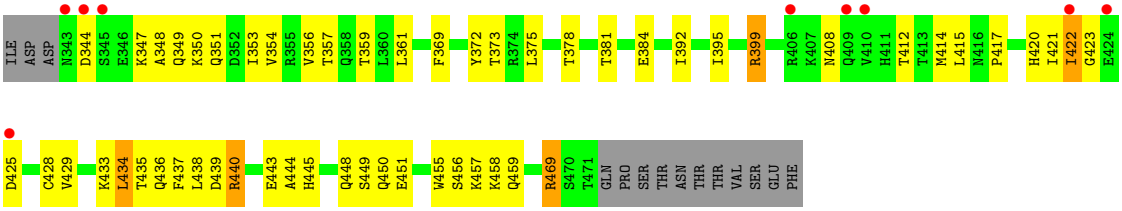
• Molecule 1: Hypothetical protein K11E8.1d

Chain F:



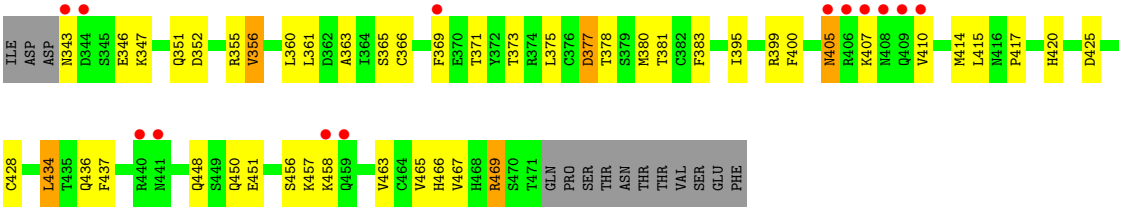
• Molecule 1: Hypothetical protein K11E8.1d

Chain H:



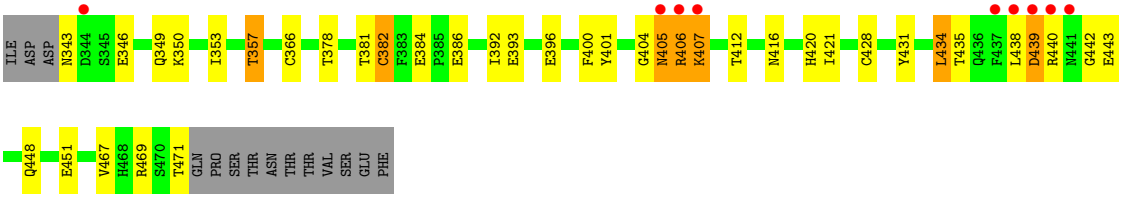
- Molecule 1: Hypothetical protein K11E8.1d

Chain J:



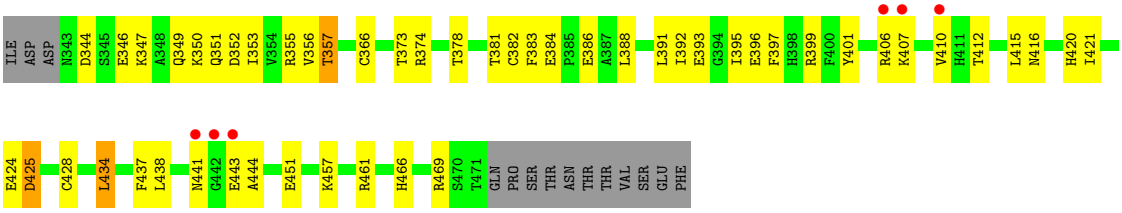
- Molecule 1: Hypothetical protein K11E8.1d

Chain L:



- Molecule 1: Hypothetical protein K11E8.1d

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	70.87Å 186.93Å 182.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 2.64 46.80 – 2.64	Depositor EDS
% Data completeness (in resolution range)	93.0 (46.80-2.64) 93.1 (46.80-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.65Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.301 0.248 , 0.298	Depositor DCC
R_{free} test set	3558 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7335	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	B	0.43	0/1065	0.70	0/1438
1	D	0.42	0/1065	0.65	0/1438
1	F	0.38	0/1065	0.64	0/1438
1	H	0.47	0/1065	0.71	0/1438
1	J	0.39	0/1065	0.64	0/1438
1	L	0.43	0/1065	0.65	0/1438
1	N	0.44	0/1065	0.64	0/1438
All	All	0.42	0/7455	0.66	0/10066

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	B	1045	0	1008	46	0
1	D	1045	0	1008	48	0
1	F	1045	0	1008	43	0
1	H	1045	0	1008	50	0
1	J	1045	0	1008	45	0
1	L	1045	0	1008	34	0
1	N	1045	0	1008	51	0
2	B	3	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1	0	0	0	0
2	H	3	0	0	0	0
2	J	3	0	0	0	0
2	L	5	0	0	0	0
2	N	3	0	0	0	0
All	All	7335	0	7056	308	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 21.

All (308) 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:N:353:ILE:O	1:N:357:THR:HG22	1.56	1.05
1:H:425:ASP:HB3	1:H:457:LYS:HB3	1.03	1.02
1:H:425:ASP:HB3	1:H:457:LYS:CB	1.92	0.99
1:D:350:LYS:HE2	1:D:421:ILE:HD11	1.42	0.98
1:H:425:ASP:CB	1:H:457:LYS:HB3	1.94	0.97
1:F:451:GLU:HG2	1:F:469:ARG:HG2	1.45	0.97
1:J:469:ARG:HG3	1:J:469:ARG:HH11	1.32	0.93
1:L:353:ILE:O	1:L:357:THR:HG22	1.66	0.93
1:B:405:ASN:O	1:B:406:ARG:CB	2.16	0.93
1:D:421:ILE:H	1:D:421:ILE:HD12	1.32	0.92
1:H:412:THR:HG22	1:H:435:THR:HG23	1.51	0.91
1:L:407:LYS:H	1:L:407:LYS:HD2	1.35	0.91
1:J:366:CYS:HA	1:J:407:LYS:HG2	1.53	0.90
1:F:353:ILE:O	1:F:357:THR:HG23	1.74	0.88
1:H:348:ALA:HA	1:H:351:GLN:HE21	1.37	0.87
1:B:405:ASN:O	1:B:406:ARG:HB2	1.71	0.87
1:L:451:GLU:HG2	1:L:469:ARG:HG2	1.56	0.86
1:D:425:ASP:HB3	1:D:457:LYS:HB3	1.57	0.85
1:D:451:GLU:OE2	1:D:469:ARG:HD3	1.78	0.82
1:D:350:LYS:CE	1:D:421:ILE:HD11	2.12	0.80
1:F:381:THR:HG22	1:F:393:GLU:OE1	1.81	0.79
1:H:414:MET:HG2	1:H:417:PRO:HG3	1.64	0.78
1:F:352:ASP:HA	1:F:355:ARG:HH11	1.46	0.78
1:B:406:ARG:O	1:B:407:LYS:HG3	1.83	0.78
1:N:381:THR:CG2	1:N:391:LEU:HD11	2.14	0.77
1:H:469:ARG:HG3	1:H:469:ARG:HH11	1.50	0.76
1:B:353:ILE:O	1:B:357:THR:HG23	1.84	0.76
1:F:380:MET:HA	1:F:465:VAL:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:451:GLU:HG2	1:J:469:ARG:HG2	1.67	0.76
1:H:440:ARG:H	1:H:440:ARG:HD3	1.51	0.76
1:J:369:PHE:HB3	1:J:399:ARG:NH2	2.03	0.74
1:B:406:ARG:O	1:B:407:LYS:CG	2.35	0.74
1:D:357:THR:HG21	1:D:429:VAL:HG11	1.68	0.74
1:H:415:LEU:HD11	1:H:434:LEU:HD22	1.69	0.73
1:D:421:ILE:HD12	1:D:421:ILE:N	2.03	0.73
1:B:405:ASN:O	1:B:406:ARG:CG	2.36	0.73
1:L:407:LYS:HD2	1:L:407:LYS:N	2.04	0.72
1:J:469:ARG:HH11	1:J:469:ARG:CG	2.03	0.72
1:L:439:ASP:OD1	1:L:439:ASP:N	2.23	0.71
1:N:346:GLU:HG2	1:N:350:LYS:HE3	1.71	0.71
1:B:469:ARG:HG3	1:B:469:ARG:HH11	1.55	0.71
1:D:386:GLU:HB3	1:D:401:TYR:OH	1.91	0.70
1:D:451:GLU:HG2	1:D:469:ARG:HG2	1.74	0.70
1:J:380:MET:HA	1:J:465:VAL:O	1.91	0.69
1:D:396:GLU:OE1	1:D:399:ARG:NH2	2.24	0.69
1:L:440:ARG:O	1:L:443:GLU:HG2	1.92	0.69
1:H:448:GLN:HE21	1:H:450:GLN:HE21	1.37	0.69
1:H:349:GLN:HB3	1:H:421:ILE:HD11	1.73	0.69
1:B:369:PHE:O	1:B:373:THR:HG23	1.92	0.69
1:H:439:ASP:HB2	1:H:443:GLU:CG	2.23	0.69
1:B:405:ASN:O	1:B:406:ARG:HG3	1.92	0.69
1:D:420:HIS:HB2	1:D:428:CYS:SG	2.33	0.68
1:N:366:CYS:HB3	1:N:407:LYS:HE3	1.76	0.68
1:F:437:PHE:CE1	1:F:445:HIS:HB2	2.29	0.67
1:B:357:THR:HG22	1:B:455:TRP:CZ2	2.30	0.66
1:H:348:ALA:HA	1:H:351:GLN:NE2	2.10	0.66
1:N:352:ASP:OD1	1:N:355:ARG:NH2	2.28	0.66
1:F:357:THR:HG21	1:F:429:VAL:HG11	1.76	0.66
1:F:352:ASP:HA	1:F:355:ARG:NH1	2.11	0.66
1:D:357:THR:HG22	1:D:455:TRP:CZ2	2.31	0.65
1:L:400:PHE:CZ	1:N:438:LEU:HD22	2.31	0.65
1:N:386:GLU:HB3	1:N:401:TYR:OH	1.96	0.65
1:J:369:PHE:HD2	1:J:399:ARG:NE	1.95	0.65
1:L:366:CYS:HB2	1:L:407:LYS:HE2	1.80	0.64
1:F:366:CYS:HB3	1:F:407:LYS:CE	2.28	0.63
1:H:420:HIS:HB2	1:H:428:CYS:SG	2.39	0.63
1:J:415:LEU:HD11	1:J:434:LEU:HD22	1.78	0.63
1:F:419:VAL:HG12	1:F:420:HIS:N	2.14	0.63
1:H:349:GLN:HB3	1:H:421:ILE:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:377:ASP:OD1	1:J:378:THR:N	2.34	0.61
1:H:438:LEU:HA	1:H:443:GLU:O	2.00	0.61
1:D:386:GLU:HG2	1:D:401:TYR:OH	2.01	0.60
1:J:373:THR:HG23	1:J:399:ARG:HH22	1.64	0.60
1:J:410:VAL:HG13	1:J:436:GLN:O	2.01	0.60
1:H:469:ARG:HH11	1:H:469:ARG:CG	2.15	0.60
1:D:469:ARG:HH11	1:D:469:ARG:HG3	1.67	0.60
1:F:438:LEU:HA	1:F:443:GLU:O	2.00	0.60
1:L:400:PHE:HZ	1:N:438:LEU:HD22	1.66	0.60
1:J:373:THR:CG2	1:J:399:ARG:HH22	2.15	0.60
1:N:381:THR:HG22	1:N:466:HIS:CE1	2.37	0.59
1:F:443:GLU:HG3	1:F:445:HIS:NE2	2.16	0.59
1:L:386:GLU:HB3	1:L:401:TYR:OH	2.03	0.59
1:J:369:PHE:HB3	1:J:399:ARG:CZ	2.33	0.58
1:D:346:GLU:OE2	1:D:421:ILE:HD13	2.04	0.58
1:N:381:THR:HG23	1:N:391:LEU:HD11	1.84	0.58
1:B:352:ASP:O	1:B:356:VAL:HG22	2.04	0.58
1:D:381:THR:HG23	1:D:391:LEU:HD21	1.85	0.58
1:D:360:LEU:O	1:D:364:ILE:HG13	2.03	0.58
1:F:438:LEU:HD12	1:F:438:LEU:H	1.68	0.58
1:B:439:ASP:HB2	1:B:443:GLU:HG3	1.84	0.58
1:D:369:PHE:O	1:D:373:THR:HG23	2.04	0.57
1:L:382:CYS:HB2	1:L:467:VAL:HG13	1.85	0.57
1:D:412:THR:HG22	1:D:435:THR:OG1	2.03	0.57
1:H:369:PHE:O	1:H:373:THR:HG23	2.05	0.57
1:H:438:LEU:HD23	1:H:444:ALA:HA	1.86	0.57
1:L:431:TYR:CE1	1:L:451:GLU:HB2	2.39	0.57
1:N:381:THR:HB	1:N:466:HIS:ND1	2.21	0.56
1:J:410:VAL:HG13	1:J:437:PHE:HB3	1.87	0.56
1:D:386:GLU:HG2	1:D:401:TYR:CZ	2.40	0.56
1:J:352:ASP:O	1:J:356:VAL:HG22	2.06	0.56
1:N:469:ARG:HG3	1:N:469:ARG:HH11	1.71	0.56
1:B:357:THR:HG22	1:B:455:TRP:CE2	2.40	0.56
1:D:459:GLN:HA	1:D:459:GLN:OE1	2.06	0.56
1:N:451:GLU:HG3	1:N:469:ARG:HG3	1.88	0.56
1:B:411:HIS:O	1:B:435:THR:HA	2.06	0.56
1:H:439:ASP:HB2	1:H:443:GLU:HG2	1.87	0.56
1:N:373:THR:HG22	1:N:395:ILE:HG21	1.88	0.55
1:J:366:CYS:HA	1:J:407:LYS:CG	2.33	0.55
1:J:343:ASN:O	1:J:346:GLU:HB3	2.07	0.55
1:L:412:THR:HG22	1:L:435:THR:OG1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:451:GLU:CG	1:N:469:ARG:HG3	2.37	0.55
1:D:352:ASP:O	1:D:356:VAL:HG22	2.07	0.55
1:L:349:GLN:NE2	1:L:421:ILE:HD12	2.22	0.54
1:L:405:ASN:O	1:L:406:ARG:C	2.46	0.54
1:N:349:GLN:NE2	1:N:421:ILE:HD12	2.22	0.54
1:H:439:ASP:HB2	1:H:443:GLU:HG3	1.88	0.54
1:B:361:LEU:HD12	1:B:414:MET:HE2	1.89	0.54
1:B:405:ASN:C	1:B:406:ARG:HG3	2.28	0.54
1:B:374:ARG:HD2	1:B:461:ARG:NH1	2.22	0.54
1:J:373:THR:CG2	1:J:399:ARG:NH2	2.71	0.54
1:B:410:VAL:HA	1:B:436:GLN:O	2.07	0.54
1:D:425:ASP:CB	1:D:457:LYS:HB3	2.34	0.54
1:B:438:LEU:HA	1:B:443:GLU:O	2.07	0.54
1:L:384:GLU:OE2	1:L:469:ARG:NH1	2.41	0.54
1:D:381:THR:CG2	1:D:391:LEU:HD11	2.38	0.53
1:F:366:CYS:HB3	1:F:407:LYS:HE3	1.90	0.53
1:H:357:THR:HG21	1:H:429:VAL:HG11	1.90	0.53
1:H:369:PHE:CZ	1:H:399:ARG:HG3	2.43	0.53
1:B:357:THR:HG21	1:B:429:VAL:HG11	1.91	0.53
1:J:448:GLN:HE21	1:J:450:GLN:HE21	1.57	0.53
1:L:434:LEU:CD1	1:L:448:GLN:HG3	2.39	0.53
1:D:421:ILE:H	1:D:421:ILE:CD1	2.13	0.53
1:D:346:GLU:HG3	1:D:421:ILE:HG12	1.91	0.52
1:J:352:ASP:HA	1:J:355:ARG:NH2	2.24	0.52
1:N:346:GLU:O	1:N:350:LYS:HG3	2.08	0.52
1:J:369:PHE:HD2	1:J:399:ARG:CD	2.22	0.52
1:F:353:ILE:O	1:F:356:VAL:HG22	2.09	0.52
1:H:425:ASP:O	1:H:456:SER:HA	2.10	0.52
1:N:415:LEU:HD11	1:N:434:LEU:HD22	1.91	0.52
1:D:357:THR:HG22	1:D:455:TRP:HZ2	1.73	0.52
1:B:381:THR:HG23	1:B:391:LEU:HD21	1.91	0.52
1:J:347:LYS:O	1:J:351:GLN:HG3	2.10	0.51
1:B:374:ARG:HD2	1:B:461:ARG:HH12	1.74	0.51
1:N:425:ASP:OD2	1:N:457:LYS:HB3	2.10	0.51
1:D:386:GLU:CG	1:D:401:TYR:OH	2.59	0.51
1:F:415:LEU:O	1:F:417:PRO:HD3	2.10	0.51
1:F:404:GLY:O	1:F:406:ARG:N	2.43	0.51
1:J:373:THR:HG21	1:J:399:ARG:NH2	2.25	0.51
1:D:353:ILE:O	1:D:357:THR:HG23	2.11	0.51
1:H:353:ILE:O	1:H:357:THR:HG23	2.10	0.51
1:D:381:THR:HG21	1:D:391:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:LEU:HD23	1:N:397:PHE:HE2	1.76	0.50
1:D:381:THR:HG22	1:D:382:CYS:N	2.27	0.50
1:N:381:THR:CG2	1:N:466:HIS:CE1	2.95	0.50
1:F:346:GLU:HG3	1:F:421:ILE:HG13	1.94	0.49
1:J:420:HIS:HB2	1:J:428:CYS:SG	2.52	0.49
1:H:448:GLN:NE2	1:H:450:GLN:HE21	2.07	0.49
1:L:382:CYS:SG	1:L:384:GLU:HG2	2.52	0.49
1:F:451:GLU:HG2	1:F:469:ARG:CG	2.31	0.49
1:J:469:ARG:HG3	1:J:469:ARG:NH1	2.12	0.49
1:N:381:THR:CG2	1:N:466:HIS:ND1	2.74	0.49
1:D:355:ARG:HH12	1:D:356:VAL:HG13	1.77	0.49
1:L:405:ASN:O	1:L:406:ARG:O	2.31	0.49
1:F:353:ILE:HA	1:F:356:VAL:HG22	1.95	0.49
1:F:419:VAL:CG1	1:F:420:HIS:N	2.75	0.49
1:J:361:LEU:HD12	1:J:414:MET:HE3	1.94	0.49
1:D:386:GLU:CB	1:D:401:TYR:OH	2.59	0.49
1:N:382:CYS:HB3	1:N:392:ILE:HB	1.94	0.49
1:F:413:THR:HG22	1:F:415:LEU:HD23	1.94	0.49
1:B:451:GLU:HG3	1:B:469:ARG:HG3	1.95	0.48
1:D:350:LYS:HE2	1:D:421:ILE:CD1	2.29	0.48
1:N:441:ASN:HB2	1:N:443:GLU:HG3	1.94	0.48
1:B:446:THR:O	1:N:388:LEU:HD11	2.12	0.48
1:J:377:ASP:O	1:J:395:ILE:HD11	2.14	0.48
1:F:412:THR:HG22	1:F:435:THR:HG23	1.95	0.48
1:J:410:VAL:CG1	1:J:437:PHE:HB3	2.43	0.48
1:H:359:THR:HG22	1:H:375:LEU:HD11	1.96	0.48
1:F:437:PHE:CD1	1:F:437:PHE:C	2.87	0.47
1:H:469:ARG:CG	1:H:469:ARG:NH1	2.76	0.47
1:F:469:ARG:HG3	1:F:469:ARG:HH11	1.79	0.47
1:J:371:THR:HG22	1:J:375:LEU:HD12	1.97	0.47
1:L:343:ASN:O	1:L:346:GLU:N	2.48	0.47
1:L:382:CYS:HB2	1:L:467:VAL:CG1	2.43	0.47
1:N:366:CYS:CB	1:N:407:LYS:HE3	2.45	0.47
1:B:424:GLU:O	1:B:424:GLU:HG2	2.15	0.47
1:N:352:ASP:O	1:N:356:VAL:HG22	2.15	0.47
1:B:469:ARG:HH11	1:B:469:ARG:CG	2.25	0.47
1:H:422:ILE:HG22	1:H:423:GLY:N	2.29	0.47
1:J:360:LEU:O	1:J:363:ALA:HB3	2.15	0.47
1:B:407:LYS:O	1:B:408:ASN:HB2	2.15	0.46
1:B:451:GLU:HG3	1:B:469:ARG:CG	2.46	0.46
1:H:347:LYS:O	1:H:351:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:458:LYS:HD2	1:J:463:VAL:HG21	1.97	0.46
1:N:469:ARG:HH11	1:N:469:ARG:CG	2.27	0.46
1:F:381:THR:HB	1:F:391:LEU:HD21	1.96	0.46
1:N:420:HIS:HB2	1:N:428:CYS:SG	2.55	0.46
1:D:349:GLN:NE2	1:D:421:ILE:HG23	2.31	0.46
1:H:350:LYS:O	1:H:354:VAL:HG23	2.16	0.46
1:B:356:VAL:HG23	1:B:357:THR:H	1.81	0.46
1:H:369:PHE:CE2	1:H:399:ARG:HG3	2.51	0.46
1:B:441:ASN:HD22	1:B:443:GLU:CD	2.18	0.46
1:H:373:THR:HG22	1:H:395:ILE:HD12	1.98	0.46
1:H:448:GLN:HG2	1:H:449:SER:N	2.31	0.46
1:N:438:LEU:HD13	1:N:444:ALA:HA	1.97	0.46
1:B:457:LYS:HE3	1:B:460:GLY:O	2.16	0.46
1:N:349:GLN:HE21	1:N:421:ILE:HD12	1.81	0.46
1:F:371:THR:O	1:F:375:LEU:HG	2.16	0.46
1:N:451:GLU:HG3	1:N:469:ARG:CG	2.46	0.46
1:B:439:ASP:HB3	1:B:440:ARG:H	1.62	0.45
1:N:347:LYS:HG2	1:N:347:LYS:O	2.15	0.45
1:N:374:ARG:HD2	1:N:461:ARG:HH12	1.81	0.45
1:L:440:ARG:C	1:L:442:GLY:H	2.19	0.45
1:H:357:THR:HG22	1:H:455:TRP:CZ2	2.51	0.45
1:B:356:VAL:O	1:B:359:THR:HB	2.16	0.45
1:F:366:CYS:HB3	1:F:407:LYS:HE2	1.99	0.45
1:H:433:LYS:HD3	1:H:451:GLU:OE2	2.17	0.45
1:D:412:THR:HA	1:D:434:LEU:O	2.17	0.45
1:D:405:ASN:O	1:D:406:ARG:C	2.55	0.44
1:B:448:GLN:NE2	1:B:450:GLN:NE2	2.65	0.44
1:F:360:LEU:O	1:F:363:ALA:HB3	2.18	0.44
1:F:410:VAL:HG12	1:F:411:HIS:N	2.32	0.44
1:D:422:ILE:O	1:D:426:ALA:HB3	2.17	0.44
1:H:451:GLU:HG2	1:H:469:ARG:HG3	2.00	0.44
1:N:346:GLU:CG	1:N:350:LYS:HE3	2.42	0.44
1:N:381:THR:HG22	1:N:382:CYS:N	2.32	0.44
1:B:391:LEU:C	1:B:391:LEU:HD23	2.38	0.44
1:H:381:THR:HA	1:H:392:ILE:O	2.17	0.44
1:J:434:LEU:HD12	1:J:434:LEU:HA	1.88	0.44
1:L:439:ASP:OD2	1:L:443:GLU:HG3	2.17	0.44
1:B:438:LEU:HD23	1:B:443:GLU:C	2.38	0.43
1:L:420:HIS:HB2	1:L:428:CYS:SG	2.58	0.43
1:D:370:GLU:HA	1:D:370:GLU:OE1	2.18	0.43
1:N:396:GLU:OE1	1:N:399:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ARG:O	1:B:407:LYS:HG2	2.18	0.43
1:F:399:ARG:O	1:F:400:PHE:C	2.55	0.43
1:H:357:THR:O	1:H:361:LEU:HG	2.18	0.43
1:L:406:ARG:HB3	1:L:407:LYS:HD2	2.01	0.43
1:F:356:VAL:HG23	1:F:357:THR:N	2.33	0.43
1:F:469:ARG:HG3	1:F:469:ARG:NH1	2.33	0.43
1:J:381:THR:O	1:J:466:HIS:HA	2.17	0.43
1:B:343:ASN:O	1:B:347:LYS:N	2.46	0.43
1:F:407:LYS:HE3	1:F:407:LYS:HB2	1.79	0.43
1:L:353:ILE:O	1:L:357:THR:CG2	2.51	0.43
1:F:457:LYS:HE2	1:F:460:GLY:O	2.18	0.43
1:D:422:ILE:O	1:D:423:GLY:C	2.57	0.43
1:H:384:GLU:OE2	1:H:469:ARG:NH2	2.52	0.43
1:N:410:VAL:HG22	1:N:437:PHE:HB2	2.00	0.43
1:D:417:PRO:HA	1:D:431:TYR:HB3	2.01	0.43
1:H:357:THR:HG22	1:H:455:TRP:NE1	2.33	0.43
1:J:369:PHE:CD2	1:J:399:ARG:HD3	2.54	0.42
1:J:425:ASP:HA	1:J:457:LYS:HB3	2.01	0.42
1:N:384:GLU:OE2	1:N:469:ARG:NH2	2.52	0.42
1:D:461:ARG:HH11	1:D:461:ARG:HG2	1.84	0.42
1:L:400:PHE:CZ	1:N:438:LEU:CD2	3.00	0.42
1:F:352:ASP:CA	1:F:355:ARG:NH1	2.81	0.42
1:J:369:PHE:CD2	1:J:399:ARG:CD	3.02	0.42
1:N:434:LEU:HD12	1:N:434:LEU:HA	1.83	0.42
1:F:421:ILE:C	1:F:422:ILE:HG13	2.39	0.42
1:L:346:GLU:O	1:L:350:LYS:HG3	2.19	0.42
1:N:347:LYS:O	1:N:351:GLN:HG3	2.19	0.42
1:B:406:ARG:C	1:B:407:LYS:HG3	2.39	0.42
1:B:408:ASN:C	1:B:409:GLN:HG3	2.40	0.42
1:D:457:LYS:HE2	1:D:460:GLY:O	2.19	0.42
1:B:356:VAL:HG23	1:B:357:THR:N	2.34	0.42
1:B:448:GLN:HE21	1:B:450:GLN:HE21	1.67	0.42
1:F:401:TYR:CE1	1:H:436:GLN:NE2	2.88	0.42
1:J:355:ARG:HB3	1:J:355:ARG:CZ	2.49	0.42
1:H:437:PHE:CZ	1:H:445:HIS:HB2	2.55	0.42
1:H:357:THR:HG22	1:H:455:TRP:CE2	2.54	0.42
1:H:369:PHE:HA	1:H:372:TYR:HB3	2.02	0.42
1:H:434:LEU:HD12	1:H:434:LEU:HA	1.84	0.42
1:N:441:ASN:HB2	1:N:443:GLU:CG	2.49	0.42
1:F:401:TYR:HE1	1:H:436:GLN:NE2	2.18	0.41
1:J:469:ARG:CG	1:J:469:ARG:NH1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:373:THR:HG22	1:N:395:ILE:HD13	2.01	0.41
1:B:434:LEU:HD23	1:N:397:PHE:CE2	2.54	0.41
1:H:353:ILE:O	1:H:356:VAL:HG22	2.20	0.41
1:L:381:THR:HA	1:L:392:ILE:O	2.19	0.41
1:N:374:ARG:HD2	1:N:461:ARG:NH1	2.35	0.41
1:N:424:GLU:HG2	1:N:424:GLU:O	2.20	0.41
1:J:410:VAL:HG22	1:J:437:PHE:HB2	2.03	0.41
1:L:434:LEU:HD12	1:L:434:LEU:HA	1.84	0.41
1:L:471:THR:O	1:L:471:THR:CG2	2.68	0.41
1:B:412:THR:HG22	1:B:435:THR:HG23	2.01	0.41
1:H:443:GLU:HG2	1:H:443:GLU:H	1.68	0.41
1:L:404:GLY:O	1:L:406:ARG:N	2.54	0.41
1:F:352:ASP:O	1:F:356:VAL:HG13	2.21	0.41
1:F:404:GLY:C	1:F:406:ARG:H	2.23	0.41
1:J:369:PHE:HD2	1:J:399:ARG:CZ	2.34	0.41
1:J:456:SER:O	1:J:463:VAL:HG22	2.20	0.41
1:F:433:LYS:HD3	1:F:451:GLU:OE2	2.20	0.41
1:N:381:THR:CG2	1:N:382:CYS:N	2.83	0.41
1:N:392:ILE:HG22	1:N:393:GLU:N	2.36	0.41
1:D:357:THR:O	1:D:361:LEU:HG	2.21	0.41
1:D:383:PHE:CE2	1:D:391:LEU:HB2	2.56	0.41
1:B:434:LEU:HA	1:B:434:LEU:HD12	1.90	0.41
1:J:414:MET:HG2	1:J:417:PRO:HG3	2.02	0.41
1:N:412:THR:HA	1:N:434:LEU:O	2.20	0.41
1:D:387:ALA:O	1:D:390:ASN:HB2	2.21	0.40
1:J:369:PHE:H	1:J:369:PHE:HD1	1.65	0.40
1:J:451:GLU:OE2	1:J:469:ARG:HD3	2.20	0.40
1:J:400:PHE:CZ	1:L:438:LEU:HG	2.57	0.40
1:N:349:GLN:NE2	1:N:421:ILE:HG23	2.37	0.40
1:D:469:ARG:HG3	1:D:469:ARG:NH1	2.33	0.40
1:F:415:LEU:O	1:F:416:ASN:C	2.59	0.40
1:L:381:THR:HG22	1:L:393:GLU:HG2	2.03	0.40
1:D:381:THR:HB	1:D:466:HIS:ND1	2.37	0.40
1:H:458:LYS:HB3	1:H:459:GLN:OE1	2.22	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	B	127/143 (89%)	116 (91%)	9 (7%)	2 (2%)	9 13
1	D	127/143 (89%)	117 (92%)	5 (4%)	5 (4%)	3 3
1	F	127/143 (89%)	116 (91%)	7 (6%)	4 (3%)	4 5
1	H	127/143 (89%)	117 (92%)	9 (7%)	1 (1%)	19 28
1	J	127/143 (89%)	115 (91%)	10 (8%)	2 (2%)	9 13
1	L	127/143 (89%)	112 (88%)	12 (9%)	3 (2%)	6 7
1	N	127/143 (89%)	120 (94%)	5 (4%)	2 (2%)	9 13
All	All	889/1001 (89%)	813 (92%)	57 (6%)	19 (2%)	7 9

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	406	ARG
1	D	406	ARG
1	F	405	ASN
1	F	440	ARG
1	L	405	ASN
1	L	406	ARG
1	N	406	ARG
1	B	407	LYS
1	D	388	LEU
1	D	405	ASN
1	J	377	ASP
1	J	405	ASN
1	F	400	PHE
1	L	416	ASN
1	N	416	ASN
1	D	416	ASN
1	F	416	ASN
1	H	422	ILE
1	D	389	GLY

5.3.2 Protein sidechains (i)

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	B	116/130 (89%)	111 (96%)	5 (4%)	29	45
1	D	116/130 (89%)	110 (95%)	6 (5%)	23	36
1	F	116/130 (89%)	108 (93%)	8 (7%)	15	23
1	H	116/130 (89%)	109 (94%)	7 (6%)	19	29
1	J	116/130 (89%)	109 (94%)	7 (6%)	19	29
1	L	116/130 (89%)	109 (94%)	7 (6%)	19	29
1	N	116/130 (89%)	110 (95%)	6 (5%)	23	36
All	All	812/910 (89%)	766 (94%)	46 (6%)	20	31

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	383	PHE
1	B	416	ASN
1	B	434	LEU
1	B	441	ASN
1	B	469	ARG
1	D	373	THR
1	D	388	LEU
1	D	421	ILE
1	D	424	GLU
1	D	441	ASN
1	D	469	ARG
1	F	344	ASP
1	F	357	THR
1	F	378	THR
1	F	383	PHE
1	F	391	LEU
1	F	434	LEU
1	F	438	LEU
1	F	439	ASP
1	H	344	ASP

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Mol	Chain	Res	Type
1	H	378	THR
1	H	399	ARG
1	H	408	ASN
1	H	434	LEU
1	H	440	ARG
1	H	469	ARG
1	J	356	VAL
1	J	365	SER
1	J	383	PHE
1	J	405	ASN
1	J	434	LEU
1	J	467	VAL
1	J	469	ARG
1	L	357	THR
1	L	378	THR
1	L	382	CYS
1	L	396	GLU
1	L	407	LYS
1	L	434	LEU
1	L	439	ASP
1	N	344	ASP
1	N	357	THR
1	N	378	THR
1	N	383	PHE
1	N	425	ASP
1	N	434	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	351	GLN
1	B	390	ASN
1	B	398	HIS
1	B	411	HIS
1	B	441	ASN
1	B	445	HIS
1	B	448	GLN
1	D	349	GLN
1	D	351	GLN
1	D	390	ASN
1	D	441	ASN
1	D	448	GLN

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Mol	Chain	Res	Type
1	D	468	HIS
1	F	349	GLN
1	F	351	GLN
1	F	468	HIS
1	H	351	GLN
1	H	358	GLN
1	H	390	ASN
1	H	411	HIS
1	H	436	GLN
1	H	448	GLN
1	J	349	GLN
1	J	390	ASN
1	J	436	GLN
1	J	450	GLN
1	J	468	HIS
1	L	349	GLN
1	L	351	GLN
1	L	390	ASN
1	L	436	GLN
1	L	445	HIS
1	L	448	GLN
1	L	468	HIS
1	N	351	GLN
1	N	358	GLN
1	N	398	HIS
1	N	416	ASN
1	N	468	HIS

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 monosaccharides 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	B	129/143 (90%)	0.41	12 (9%)	8	6	23, 42, 93, 102	0
1	D	129/143 (90%)	0.40	9 (6%)	16	13	26, 42, 92, 103	0
1	F	129/143 (90%)	0.43	9 (6%)	16	13	31, 54, 93, 107	0
1	H	129/143 (90%)	0.26	9 (6%)	16	13	20, 37, 88, 95	0
1	J	129/143 (90%)	0.35	13 (10%)	7	5	30, 55, 94, 102	0
1	L	129/143 (90%)	0.33	9 (6%)	16	13	25, 42, 95, 102	0
1	N	129/143 (90%)	0.22	6 (4%)	31	27	23, 42, 93, 107	0
All	All	903/1001 (90%)	0.34	67 (7%)	14	11	20, 45, 94, 107	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	ARG	6.3
1	L	438	LEU	6.0
1	N	407	LYS	5.4
1	B	407	LYS	5.3
1	H	424	GLU	4.5
1	L	439	ASP	4.5
1	B	409	GLN	4.4
1	L	406	ARG	4.3
1	F	405	ASN	4.2
1	N	406	ARG	4.0
1	D	408	ASN	4.0
1	N	441	ASN	3.9
1	H	425	ASP	3.9
1	B	408	ASN	3.9
1	F	344	ASP	3.8
1	F	439	ASP	3.7
1	B	442	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	J	407	LYS	3.6
1	J	369	PHE	3.6
1	B	439	ASP	3.5
1	F	424	GLU	3.5
1	L	437	PHE	3.5
1	D	406	ARG	3.5
1	B	343	ASN	3.3
1	J	406	ARG	3.3
1	B	405	ASN	3.3
1	B	440	ARG	3.3
1	B	441	ASN	3.3
1	F	459	GLN	3.2
1	B	410	VAL	3.2
1	F	406	ARG	3.0
1	D	442	GLY	3.0
1	H	409	GLN	2.9
1	D	407	LYS	2.9
1	D	438	LEU	2.9
1	F	410	VAL	2.8
1	B	344	ASP	2.8
1	J	459	GLN	2.8
1	N	410	VAL	2.8
1	D	410	VAL	2.6
1	D	409	GLN	2.6
1	D	441	ASN	2.6
1	L	440	ARG	2.6
1	D	443	GLU	2.5
1	J	441	ASN	2.5
1	J	410	VAL	2.5
1	F	393	GLU	2.4
1	N	442	GLY	2.3
1	J	458	LYS	2.3
1	H	406	ARG	2.3
1	L	407	LYS	2.3
1	L	441	ASN	2.3
1	J	408	ASN	2.2
1	H	422	ILE	2.2
1	H	345	SER	2.2
1	J	405	ASN	2.2
1	N	443	GLU	2.1
1	J	409	GLN	2.1
1	F	407	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	343	ASN	2.1
1	H	344	ASP	2.1
1	J	440	ARG	2.1
1	L	405	ASN	2.1
1	L	344	ASP	2.1
1	J	343	ASN	2.0
1	J	344	ASP	2.0
1	H	410	VAL	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 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.