Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 11:09 AM EDT

PDB ID	:	6QK9
Title	:	A dimeric ubiquitin formed by a single amino acid substitution
Authors	:	Gabrielsen, M.; Kowalczyk, D.; Buetow, L.; Huang, D.T.
Deposited on	:	2019-01-28
Resolution	:	2.23 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:

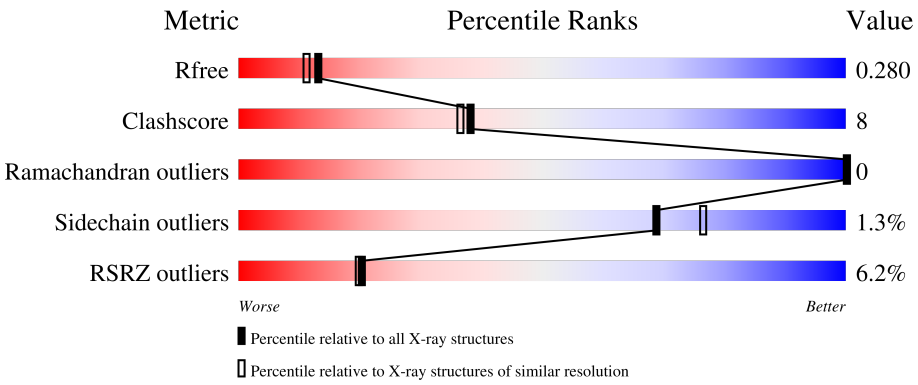
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.23 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	A	79	89% 5% 6%
1	B	79	% 82% 11% 6%
1	C	79	3% 76% 18% 6%
1	D	79	32% 66% 27% 8%
1	E	79	3% 68% 27% 5%

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Mol	Chain	Length	Quality of chain
1	F	79	4% 67% 22% • 9%
1	G	79	% 78% 11% • 9%
1	H	79	18% 76% 18% • 5%
1	I	79	5% 80% 10% • 8%
1	J	79	90% 5% 5%
1	K	79	% 76% 19% 5%
1	L	79	3% 72% 19% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14066 atoms, of which 6988 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 Polyubiquitin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	74	1166	365	588	98	114	1	0	0	0
1	B	74	1198	372	610	99	116	1	0	0	0
1	C	74	1158	364	585	96	112	1	0	0	0
1	D	73	1081	348	536	86	110	1	0	0	0
1	E	75	1198	373	609	100	115	1	0	1	0
1	F	72	1106	351	554	88	112	1	0	0	0
1	G	72	1159	362	589	96	112		0	0	0
1	H	75	1156	365	580	97	113	1	0	0	0
1	I	73	1127	355	565	93	113	1	0	0	0
1	J	75	1207	374	615	103	114	1	0	0	0
1	K	75	1206	375	612	100	118	1	0	0	0
1	L	74	1101	353	545	91	111	1	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P0CG47
A	-3	SER	-	expression tag	UNP P0CG47
A	-2	GLY	-	expression tag	UNP P0CG47
A	-1	GLY	-	expression tag	UNP P0CG47
A	0	SER	-	expression tag	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
A	10	VAL	GLY	engineered mutation	UNP P0CG47
B	-4	GLY	-	expression tag	UNP P0CG47
B	-3	SER	-	expression tag	UNP P0CG47
B	-2	GLY	-	expression tag	UNP P0CG47
B	-1	GLY	-	expression tag	UNP P0CG47
B	0	SER	-	expression tag	UNP P0CG47
B	10	VAL	GLY	engineered mutation	UNP P0CG47
C	-4	GLY	-	expression tag	UNP P0CG47
C	-3	SER	-	expression tag	UNP P0CG47
C	-2	GLY	-	expression tag	UNP P0CG47
C	-1	GLY	-	expression tag	UNP P0CG47
C	0	SER	-	expression tag	UNP P0CG47
C	10	VAL	GLY	engineered mutation	UNP P0CG47
D	-4	GLY	-	expression tag	UNP P0CG47
D	-3	SER	-	expression tag	UNP P0CG47
D	-2	GLY	-	expression tag	UNP P0CG47
D	-1	GLY	-	expression tag	UNP P0CG47
D	0	SER	-	expression tag	UNP P0CG47
D	10	VAL	GLY	engineered mutation	UNP P0CG47
E	-4	GLY	-	expression tag	UNP P0CG47
E	-3	SER	-	expression tag	UNP P0CG47
E	-2	GLY	-	expression tag	UNP P0CG47
E	-1	GLY	-	expression tag	UNP P0CG47
E	0	SER	-	expression tag	UNP P0CG47
E	10	VAL	GLY	engineered mutation	UNP P0CG47
F	-4	GLY	-	expression tag	UNP P0CG47
F	-3	SER	-	expression tag	UNP P0CG47
F	-2	GLY	-	expression tag	UNP P0CG47
F	-1	GLY	-	expression tag	UNP P0CG47
F	0	SER	-	expression tag	UNP P0CG47
F	10	VAL	GLY	engineered mutation	UNP P0CG47
G	-4	GLY	-	expression tag	UNP P0CG47
G	-3	SER	-	expression tag	UNP P0CG47
G	-2	GLY	-	expression tag	UNP P0CG47
G	-1	GLY	-	expression tag	UNP P0CG47
G	0	SER	-	expression tag	UNP P0CG47
G	10	VAL	GLY	engineered mutation	UNP P0CG47
H	-4	GLY	-	expression tag	UNP P0CG47
H	-3	SER	-	expression tag	UNP P0CG47
H	-2	GLY	-	expression tag	UNP P0CG47
H	-1	GLY	-	expression tag	UNP P0CG47
H	0	SER	-	expression tag	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
H	10	VAL	GLY	engineered mutation	UNP P0CG47
I	-4	GLY	-	expression tag	UNP P0CG47
I	-3	SER	-	expression tag	UNP P0CG47
I	-2	GLY	-	expression tag	UNP P0CG47
I	-1	GLY	-	expression tag	UNP P0CG47
I	0	SER	-	expression tag	UNP P0CG47
I	10	VAL	GLY	engineered mutation	UNP P0CG47
J	-4	GLY	-	expression tag	UNP P0CG47
J	-3	SER	-	expression tag	UNP P0CG47
J	-2	GLY	-	expression tag	UNP P0CG47
J	-1	GLY	-	expression tag	UNP P0CG47
J	0	SER	-	expression tag	UNP P0CG47
J	10	VAL	GLY	engineered mutation	UNP P0CG47
K	-4	GLY	-	expression tag	UNP P0CG47
K	-3	SER	-	expression tag	UNP P0CG47
K	-2	GLY	-	expression tag	UNP P0CG47
K	-1	GLY	-	expression tag	UNP P0CG47
K	0	SER	-	expression tag	UNP P0CG47
K	10	VAL	GLY	engineered mutation	UNP P0CG47
L	-4	GLY	-	expression tag	UNP P0CG47
L	-3	SER	-	expression tag	UNP P0CG47
L	-2	GLY	-	expression tag	UNP P0CG47
L	-1	GLY	-	expression tag	UNP P0CG47
L	0	SER	-	expression tag	UNP P0CG47
L	10	VAL	GLY	engineered mutation	UNP P0CG47

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	31	31	31	0	0
2	B	18	18	18	0	0
2	C	27	27	27	0	0
2	D	6	6	6	0	0
2	E	17	17	17	0	0
2	F	3	3	3	0	0
2	G	34	34	34	0	0

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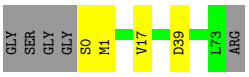
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	H	9	9	9	0	0
			Total	O		
2	I	9	9	9	0	0
			Total	O		
2	J	18	18	18	0	0
			Total	O		
2	K	14	14	14	0	0
			Total	O		
2	L	17	17	17	0	0

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.

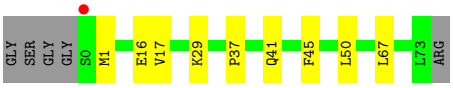
• Molecule 1: Polyubiquitin-B

Chain A:



• Molecule 1: Polyubiquitin-B

Chain B:

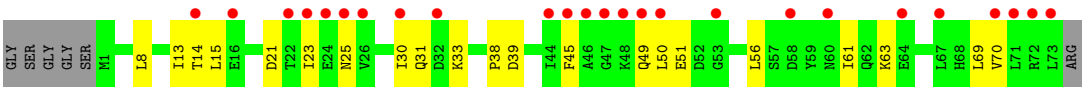


• Molecule 1: Polyubiquitin-B

Chain C:

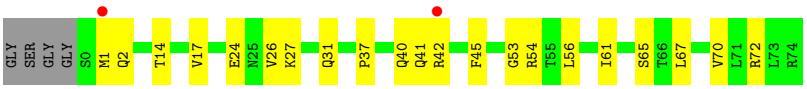
• Molecule 1: Polyubiquitin-B

Chain D:



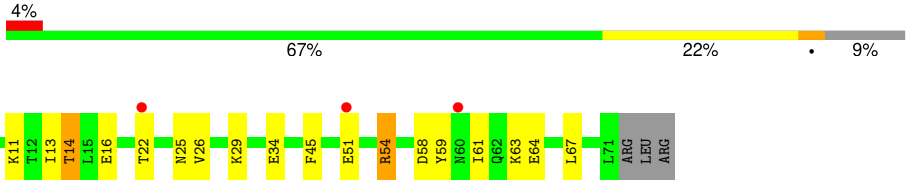
• Molecule 1: Polyubiquitin-B

Chain E:



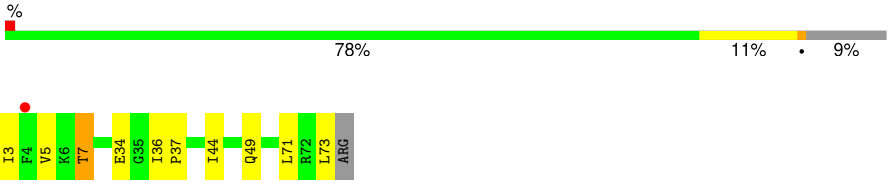
• Molecule 1: Polyubiquitin-B

Chain F:



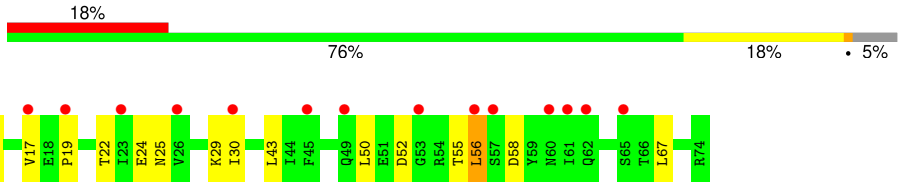
• Molecule 1: Polyubiquitin-B

Chain G:



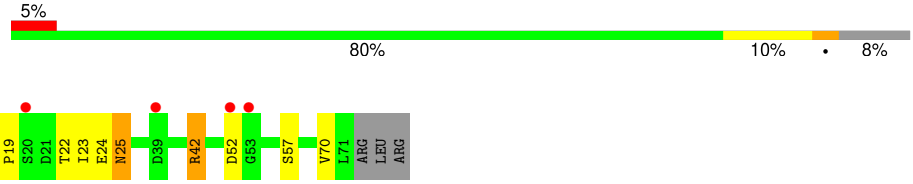
• Molecule 1: Polyubiquitin-B

Chain H:



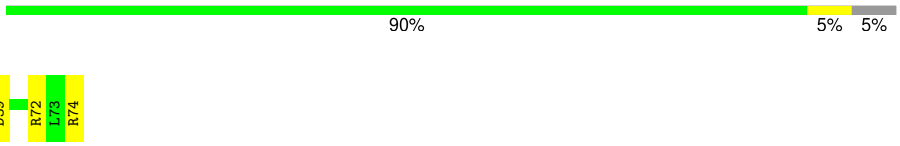
• Molecule 1: Polyubiquitin-B

Chain I:



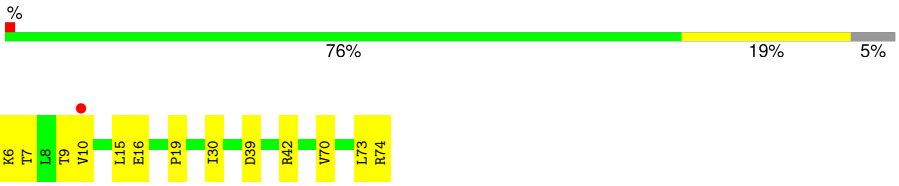
• Molecule 1: Polyubiquitin-B

Chain J:



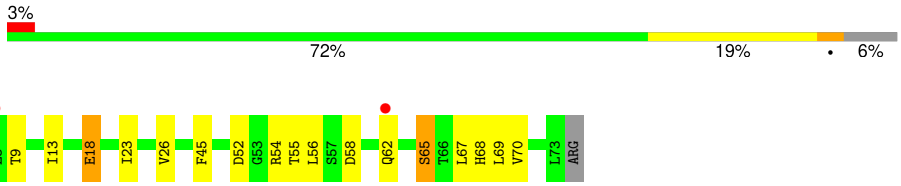
• Molecule 1: Polyubiquitin-B

Chain K:



• Molecule 1: Polyubiquitin-B

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.93Å 87.26Å 109.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.16 – 2.23 29.16 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.16-2.23) 93.6 (29.16-2.23)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.239 , 0.281 0.241 , 0.280	Depositor DCC
R_{free} test set	1995 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14066	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.33% 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	A	0.42	0/584	0.68	0/790
1	B	0.43	0/594	0.69	0/802
1	C	0.48	0/579	0.75	0/784
1	D	0.60	0/551	0.80	0/750
1	E	0.52	0/603	0.83	0/815
1	F	0.67	1/558 (0.2%)	1.00	3/757 (0.4%)
1	G	0.55	0/576	0.83	0/779
1	H	0.54	0/582	0.85	2/788 (0.3%)
1	I	0.58	1/568 (0.2%)	0.90	2/770 (0.3%)
1	J	0.42	0/598	0.69	0/806
1	K	0.51	0/600	0.76	1/809 (0.1%)
1	L	0.80	2/562 (0.4%)	0.74	0/765
All	All	0.55	4/6955 (0.1%)	0.80	8/9415 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	18	GLU	CD-OE2	10.27	1.36	1.25
1	L	18	GLU	CD-OE1	10.14	1.36	1.25
1	F	54	ARG	CZ-NH2	8.63	1.44	1.33
1	I	42	ARG	CZ-NH2	-5.09	1.26	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	42	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	F	54	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	F	54	ARG	NH1-CZ-NH2	9.36	129.70	119.40
1	F	54	ARG	NE-CZ-NH1	-8.73	115.93	120.30
1	H	56	LEU	CA-CB-CG	8.54	134.95	115.30
1	K	0	SER	N-CA-C	-6.53	93.37	111.00
1	H	56	LEU	CB-CG-CD2	-5.46	101.71	111.00
1	I	42	ARG	NH1-CZ-NH2	-5.25	113.62	119.40

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	578	588	590	5	0
1	B	588	610	612	7	0
1	C	573	585	587	11	2
1	D	545	536	538	17	0
1	E	589	609	599	19	1
1	F	552	554	556	16	0
1	G	570	589	589	9	0
1	H	576	580	582	14	0
1	I	562	565	567	10	0
1	J	592	615	617	2	0
1	K	594	612	614	11	1
1	L	556	545	548	13	0
2	A	31	0	0	2	0
2	B	18	0	0	0	0
2	C	27	0	0	0	0
2	D	6	0	0	1	0
2	E	17	0	0	2	2
2	F	3	0	0	1	0
2	G	34	0	0	0	0
2	H	9	0	0	0	0
2	I	9	0	0	3	0
2	J	18	0	0	0	0
2	K	14	0	0	0	0
2	L	17	0	0	0	0
All	All	7078	6988	6999	105	3

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 8.

All (105) 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:I:24:GLU:N	2:I:101:HOH:O	1.93	0.96
1:F:54:ARG:NH1	1:F:59:TYR:OH	2.03	0.91
1:E:1:MET:HB2	1:F:63:LYS:HB3	1.56	0.87
1:B:16:GLU:O	1:B:29:LYS:NZ	2.07	0.86
1:D:14:THR:O	1:D:33:LYS:NZ	2.09	0.85
1:D:49:GLN:NE2	2:D:101:HOH:O	2.11	0.83
1:L:55:THR:OG1	1:L:58:ASP:OD1	1.98	0.80
1:A:39:ASP:OD2	2:A:101:HOH:O	2.01	0.78
1:E:2:GLN:HG2	1:F:16:GLU:HG3	1.66	0.77
1:H:22:THR:HG23	1:H:25:ASN:H	1.49	0.77
1:A:0:SER:O	2:A:102:HOH:O	2.09	0.71
1:D:13:ILE:HD11	1:D:30:ILE:HD13	1.73	0.70
1:I:42:ARG:HH12	1:I:70:VAL:HG11	1.58	0.68
1:E:24:GLU:OE2	1:E:53:GLY:N	2.26	0.67
1:D:21:ASP:OD1	1:D:25:ASN:ND2	2.30	0.65
1:E:2:GLN:HG2	1:F:16:GLU:CG	2.27	0.65
1:H:24:GLU:OE2	1:H:52:ASP:HA	1.97	0.65
1:F:22:THR:OG1	1:F:25:ASN:N	2.26	0.64
1:C:5:VAL:HG21	1:D:30:ILE:HD11	1.82	0.62
1:C:7:THR:HG22	1:D:69:LEU:HB3	1.83	0.60
1:K:5:VAL:HB	1:L:13:ILE:HG13	1.84	0.60
1:E:42:ARG:NH2	2:E:101:HOH:O	2.28	0.59
1:D:56:LEU:HD22	1:D:61:ILE:HG21	1.84	0.59
1:H:24:GLU:OE1	1:H:24:GLU:N	2.31	0.59
1:G:5:VAL:HG21	1:H:30:ILE:HD11	1.84	0.58
1:C:1:MET:HG3	1:D:63:LYS:CG	2.34	0.57
1:C:11:LYS:NZ	1:C:34:GLU:OE1	2.25	0.57
1:G:36:ILE:HD13	1:G:71:LEU:HD21	1.87	0.56
1:L:45:PHE:HB2	1:L:67:LEU:HD22	1.87	0.56
1:H:55:THR:OG1	1:H:58:ASP:OD1	2.22	0.56
1:H:22:THR:OG1	1:H:24:GLU:OE1	2.24	0.55
1:H:24:GLU:OE2	1:H:52:ASP:CA	2.54	0.55
1:A:1:MET:HE3	1:B:17:VAL:HG23	1.89	0.55
1:C:9:THR:O	1:D:8:LEU:HD12	2.06	0.54
1:I:22:THR:CB	2:I:101:HOH:O	2.56	0.54
1:E:2:GLN:O	1:F:64:GLU:N	2.28	0.53
1:G:34:GLU:OE1	1:K:6:LYS:NZ	2.41	0.53
1:G:37:PRO:HD3	1:L:70:VAL:HG11	1.90	0.53
1:K:73:LEU:O	1:K:74:ARG:CB	2.56	0.52
1:I:42:ARG:NH1	1:I:70:VAL:CG1	2.73	0.52
1:K:9:THR:HB	1:L:9:THR:HG23	1.91	0.52
1:G:44:ILE:HD13	1:G:49:GLN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ILE:HD13	1:C:71:LEU:HD21	1.92	0.52
1:I:22:THR:OG1	2:I:101:HOH:O	2.19	0.51
1:I:23:ILE:HB	1:I:52:ASP:HA	1.91	0.51
1:E:42:ARG:NH2	1:E:70:VAL:HG11	2.25	0.51
1:K:6:LYS:HD3	1:L:68:HIS:CE1	2.46	0.51
1:F:51:GLU:OE2	2:F:101:HOH:O	2.19	0.51
1:H:50:LEU:HD11	1:H:67:LEU:HD22	1.94	0.50
1:A:17:VAL:HG23	1:B:1:MET:HG3	1.94	0.50
1:H:24:GLU:OE2	1:H:52:ASP:CB	2.60	0.49
1:H:25:ASN:O	1:H:29:LYS:HG3	2.12	0.49
1:L:26:VAL:HG21	1:L:56:LEU:HD21	1.95	0.49
1:E:2:GLN:OE1	1:F:14:THR:CG2	2.61	0.49
1:I:42:ARG:HH12	1:I:70:VAL:CG1	2.24	0.48
1:E:45:PHE:HB2	1:E:67:LEU:HD22	1.96	0.48
1:K:7:THR:HG22	1:L:69:LEU:HB3	1.95	0.47
1:D:23:ILE:HB	1:D:51:GLU:O	2.15	0.47
1:F:45:PHE:HB2	1:F:67:LEU:HD22	1.96	0.47
1:F:11:LYS:CE	1:F:34:GLU:OE1	2.63	0.47
1:C:37:PRO:HG2	1:C:40:GLN:OE1	2.13	0.47
1:E:24:GLU:H	1:E:24:GLU:CD	2.17	0.47
1:G:73:LEU:HD21	1:K:10:VAL:HG12	1.97	0.47
1:I:18:GLU:OE2	1:J:0:SER:N	2.48	0.46
1:E:37:PRO:HG2	1:E:40:GLN:HE21	1.80	0.46
1:E:26:VAL:HG21	1:E:56:LEU:HD21	1.98	0.46
1:H:43:LEU:HB3	1:H:50:LEU:HD12	1.98	0.46
1:F:26:VAL:HA	1:F:29:LYS:HD2	1.97	0.46
1:L:23:ILE:HG12	1:L:54:ARG:O	2.16	0.46
1:A:1:MET:CE	1:B:17:VAL:HG23	2.46	0.45
1:H:19:PRO:HA	1:H:56:LEU:HD22	1.99	0.45
1:C:42:ARG:HE	1:C:72:ARG:HH11	1.64	0.45
1:E:42:ARG:HE	1:E:72:ARG:CG	2.30	0.45
1:G:36:ILE:HG21	1:G:71:LEU:HD22	1.99	0.45
1:D:31:GLN:O	1:K:19:PRO:HG2	2.17	0.44
1:B:67:LEU:HD12	1:B:67:LEU:N	2.32	0.44
1:D:31:GLN:OE1	1:D:38:PRO:HD3	2.17	0.44
1:D:45:PHE:CG	1:D:61:ILE:HD11	2.52	0.44
1:C:73:LEU:HD23	1:C:73:LEU:H	1.83	0.44
1:I:22:THR:O	1:I:25:ASN:HB2	2.18	0.44
1:E:61:ILE:HG23	1:E:65:SER:CB	2.48	0.44
1:G:7:THR:O	1:H:10:VAL:HA	2.18	0.44
1:F:11:LYS:HE2	1:F:34:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3:ILE:HG12	1:H:17:VAL:HG21	2.00	0.43
1:C:2:GLN:HA	1:D:15:LEU:O	2.18	0.43
1:B:45:PHE:HB3	1:B:50:LEU:HD21	2.01	0.43
1:K:15:LEU:HD11	1:K:30:ILE:CG1	2.49	0.43
1:F:13:ILE:HG21	1:F:34:GLU:OE2	2.19	0.43
1:E:2:GLN:OE1	1:F:14:THR:HG22	2.19	0.43
1:E:31:GLN:NE2	2:E:102:HOH:O	2.47	0.43
1:L:62:GLN:HG2	1:L:65:SER:OG	2.19	0.42
1:D:45:PHE:HB2	1:D:50:LEU:HD11	2.01	0.42
1:J:39:ASP:O	1:J:72:ARG:NH1	2.52	0.42
1:K:5:VAL:HB	1:L:13:ILE:CG1	2.50	0.42
1:L:23:ILE:HB	1:L:52:ASP:HA	2.02	0.42
1:E:61:ILE:HG23	1:E:65:SER:HB2	2.00	0.42
1:L:18:GLU:HA	1:L:18:GLU:OE1	2.19	0.42
1:E:27:LYS:HD2	1:E:41:GLN:HB2	2.02	0.41
1:E:17:VAL:O	1:F:1:MET:HG3	2.21	0.40
1:K:42:ARG:HB2	1:K:70:VAL:HB	2.04	0.40
1:B:37:PRO:O	1:B:41:GLN:HG3	2.21	0.40
1:I:19:PRO:O	1:I:57:SER:N	2.53	0.40
1:C:1:MET:HG3	1:D:63:LYS:HA	2.03	0.40
1:F:61:ILE:HD13	1:F:67:LEU:HD21	2.03	0.40
1:D:45:PHE:CG	1:D:61:ILE:CD1	3.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ARG:NH2	2:E:101:HOH:O[2_455]	2.14	0.06
1:E:54:ARG:HH12	1:K:39:ASP:OD2[4_545]	1.57	0.03
1:C:72:ARG:HH21	2:E:101:HOH:O[2_455]	1.58	0.02

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	72/79 (91%)	72 (100%)	0	0	100	100
1	B	72/79 (91%)	72 (100%)	0	0	100	100
1	C	72/79 (91%)	72 (100%)	0	0	100	100
1	D	71/79 (90%)	70 (99%)	1 (1%)	0	100	100
1	E	74/79 (94%)	74 (100%)	0	0	100	100
1	F	70/79 (89%)	70 (100%)	0	0	100	100
1	G	70/79 (89%)	70 (100%)	0	0	100	100
1	H	73/79 (92%)	72 (99%)	1 (1%)	0	100	100
1	I	71/79 (90%)	71 (100%)	0	0	100	100
1	J	73/79 (92%)	72 (99%)	1 (1%)	0	100	100
1	K	73/79 (92%)	73 (100%)	0	0	100	100
1	L	72/79 (91%)	72 (100%)	0	0	100	100
All	All	863/948 (91%)	860 (100%)	3 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	A	65/71 (92%)	65 (100%)	0	100	100
1	B	68/71 (96%)	68 (100%)	0	100	100
1	C	64/71 (90%)	64 (100%)	0	100	100
1	D	59/71 (83%)	57 (97%)	2 (3%)	37	42
1	E	68/71 (96%)	67 (98%)	1 (2%)	65	72
1	F	62/71 (87%)	60 (97%)	2 (3%)	39	44
1	G	65/71 (92%)	64 (98%)	1 (2%)	65	72
1	H	63/71 (89%)	63 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	63/71 (89%)	62 (98%)	1 (2%)	62	70
1	J	67/71 (94%)	66 (98%)	1 (2%)	65	72
1	K	68/71 (96%)	67 (98%)	1 (2%)	65	72
1	L	60/71 (84%)	59 (98%)	1 (2%)	60	68
All	All	772/852 (91%)	762 (99%)	10 (1%)	69	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	39	ASP
1	D	70	VAL
1	E	14	THR
1	F	14	THR
1	F	58	ASP
1	G	7	THR
1	I	25	ASN
1	J	74	ARG
1	K	16	GLU
1	L	65	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	40	GLN
1	E	68	HIS
1	K	49	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 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	A	74/79 (93%)	0.03	0 100 100	25, 32, 42, 66	0
1	B	74/79 (93%)	0.14	1 (1%) 75 76	28, 39, 48, 54	0
1	C	74/79 (93%)	0.30	2 (2%) 54 55	33, 40, 52, 58	0
1	D	73/79 (92%)	1.43	25 (34%) 0 0	33, 51, 66, 71	0
1	E	75/79 (94%)	0.19	2 (2%) 54 55	29, 37, 52, 68	0
1	F	72/79 (91%)	0.51	3 (4%) 36 35	33, 45, 58, 61	0
1	G	72/79 (91%)	0.15	1 (1%) 75 76	24, 30, 43, 55	0
1	H	75/79 (94%)	0.94	14 (18%) 1 1	27, 47, 67, 83	0
1	I	73/79 (92%)	0.52	4 (5%) 25 24	30, 43, 61, 72	0
1	J	75/79 (94%)	0.15	0 100 100	33, 39, 50, 56	0
1	K	75/79 (94%)	0.16	1 (1%) 77 78	27, 35, 49, 58	0
1	L	74/79 (93%)	0.40	2 (2%) 54 55	32, 43, 56, 66	0
All	All	886/948 (93%)	0.41	55 (6%) 20 20	24, 40, 59, 83	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	LEU	5.6
1	D	45	PHE	5.0
1	H	60	ASN	4.6
1	I	20	SER	4.3
1	I	53	GLY	4.0
1	H	65	SER	3.8
1	H	26	VAL	3.8
1	D	60	ASN	3.8
1	F	51	GLU	3.7
1	F	60	ASN	3.6
1	D	64	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	56	LEU	3.3
1	H	57	SER	3.3
1	H	49	GLN	3.3
1	D	46	ALA	3.2
1	D	47	GLY	3.1
1	D	48	LYS	3.1
1	D	23	ILE	3.1
1	E	1	MET	3.0
1	C	72	ARG	3.0
1	D	67	LEU	2.9
1	G	4	PHE	2.9
1	H	19	PRO	2.9
1	H	53	GLY	2.9
1	D	71	LEU	2.8
1	H	61	ILE	2.8
1	D	73	LEU	2.8
1	D	25	ASN	2.8
1	D	32	ASP	2.8
1	I	52	ASP	2.6
1	D	24	GLU	2.6
1	D	16	GLU	2.6
1	H	23	ILE	2.6
1	D	49	GLN	2.6
1	I	39	ASP	2.6
1	C	0	SER	2.5
1	L	62	GLN	2.5
1	D	22	THR	2.5
1	D	58	ASP	2.5
1	H	17	VAL	2.5
1	D	44	ILE	2.4
1	D	70	VAL	2.4
1	H	62	GLN	2.4
1	D	26	VAL	2.4
1	F	22	THR	2.3
1	L	8	LEU	2.3
1	B	0	SER	2.3
1	K	10	VAL	2.2
1	D	72	ARG	2.2
1	H	45	PHE	2.2
1	D	14	THR	2.1
1	H	30	ILE	2.1
1	E	42	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	30	ILE	2.0
1	D	53	GLY	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.