Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2016 – 12:11 PM EDT

PDB ID	:	5JRB
Title	:	Rad52(1-212) K102A/K133A/E202A mutant
Authors	:	Saotome, M.; Saito, K.; Kurumizaka, H.; Kagawa, W.
Deposited on	:	2016-05-06
Resolution	:	2.40 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:

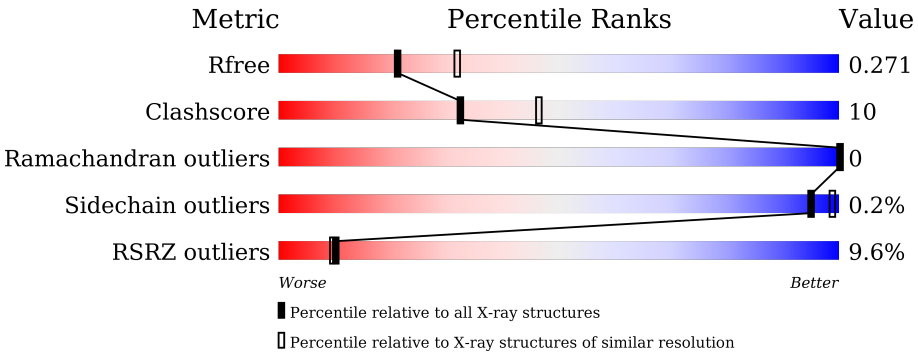
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	215	3% 75% 11% 14%
1	B	215	6% 73% 13% 14%
1	C	215	6% 73% 11% 14%
1	D	215	6% 73% 12% 14%
1	E	215	5% 68% 17% 14%
1	F	215	9% 69% 16% 14%

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Mol	Chain	Length	Quality of chain
1	G	215	15% 63% 23% 14%
1	H	215	15% 60% 26% 14%
1	I	215	10% 60% 26% 14%
1	J	215	10% 67% 18% 14%
1	K	215	5% 70% 16% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16252 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 DNA repair protein RAD52 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1438	899	259	272	8			
1	B	184	Total	C	N	O	S	0	0	0
			1438	899	259	272	8			
1	C	184	Total	C	N	O	S	0	0	0
			1438	899	259	272	8			
1	D	184	Total	C	N	O	S	0	0	0
			1438	899	259	272	8			
1	E	184	Total	C	N	O	S	0	0	0
			1438	899	259	272	8			
1	F	184	Total	C	N	O	S	0	0	0
			1438	899	259	272	8			
1	G	184	Total	C	N	O	S	0	0	0
			1438	899	259	272	8			
1	H	184	Total	C	N	O	S	0	0	0
			1438	899	259	272	8			
1	I	184	Total	C	N	O	S	0	0	0
			1438	899	259	272	8			
1	J	184	Total	C	N	O	S	0	0	0
			1438	899	259	272	8			
1	K	188	Total	C	N	O	S	0	0	0
			1472	919	267	277	9			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P43351
A	-1	SER	-	expression tag	UNP P43351
A	0	HIS	-	expression tag	UNP P43351
A	102	ALA	LYS	engineered mutation	UNP P43351
A	133	ALA	LYS	engineered mutation	UNP P43351
A	202	ALA	GLU	engineered mutation	UNP P43351
B	-2	GLY	-	expression tag	UNP P43351

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP P43351
B	0	HIS	-	expression tag	UNP P43351
B	102	ALA	LYS	engineered mutation	UNP P43351
B	133	ALA	LYS	engineered mutation	UNP P43351
B	202	ALA	GLU	engineered mutation	UNP P43351
C	-2	GLY	-	expression tag	UNP P43351
C	-1	SER	-	expression tag	UNP P43351
C	0	HIS	-	expression tag	UNP P43351
C	102	ALA	LYS	engineered mutation	UNP P43351
C	133	ALA	LYS	engineered mutation	UNP P43351
C	202	ALA	GLU	engineered mutation	UNP P43351
D	-2	GLY	-	expression tag	UNP P43351
D	-1	SER	-	expression tag	UNP P43351
D	0	HIS	-	expression tag	UNP P43351
D	102	ALA	LYS	engineered mutation	UNP P43351
D	133	ALA	LYS	engineered mutation	UNP P43351
D	202	ALA	GLU	engineered mutation	UNP P43351
E	-2	GLY	-	expression tag	UNP P43351
E	-1	SER	-	expression tag	UNP P43351
E	0	HIS	-	expression tag	UNP P43351
E	102	ALA	LYS	engineered mutation	UNP P43351
E	133	ALA	LYS	engineered mutation	UNP P43351
E	202	ALA	GLU	engineered mutation	UNP P43351
F	-2	GLY	-	expression tag	UNP P43351
F	-1	SER	-	expression tag	UNP P43351
F	0	HIS	-	expression tag	UNP P43351
F	102	ALA	LYS	engineered mutation	UNP P43351
F	133	ALA	LYS	engineered mutation	UNP P43351
F	202	ALA	GLU	engineered mutation	UNP P43351
G	-2	GLY	-	expression tag	UNP P43351
G	-1	SER	-	expression tag	UNP P43351
G	0	HIS	-	expression tag	UNP P43351
G	102	ALA	LYS	engineered mutation	UNP P43351
G	133	ALA	LYS	engineered mutation	UNP P43351
G	202	ALA	GLU	engineered mutation	UNP P43351
H	-2	GLY	-	expression tag	UNP P43351
H	-1	SER	-	expression tag	UNP P43351
H	0	HIS	-	expression tag	UNP P43351
H	102	ALA	LYS	engineered mutation	UNP P43351
H	133	ALA	LYS	engineered mutation	UNP P43351
H	202	ALA	GLU	engineered mutation	UNP P43351
I	-2	GLY	-	expression tag	UNP P43351

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	SER	-	expression tag	UNP P43351
I	0	HIS	-	expression tag	UNP P43351
I	102	ALA	LYS	engineered mutation	UNP P43351
I	133	ALA	LYS	engineered mutation	UNP P43351
I	202	ALA	GLU	engineered mutation	UNP P43351
J	-2	GLY	-	expression tag	UNP P43351
J	-1	SER	-	expression tag	UNP P43351
J	0	HIS	-	expression tag	UNP P43351
J	102	ALA	LYS	engineered mutation	UNP P43351
J	133	ALA	LYS	engineered mutation	UNP P43351
J	202	ALA	GLU	engineered mutation	UNP P43351
K	-2	GLY	-	expression tag	UNP P43351
K	-1	SER	-	expression tag	UNP P43351
K	0	HIS	-	expression tag	UNP P43351
K	102	ALA	LYS	engineered mutation	UNP P43351
K	133	ALA	LYS	engineered mutation	UNP P43351
K	202	ALA	GLU	engineered mutation	UNP P43351

- Molecule 2 is water.

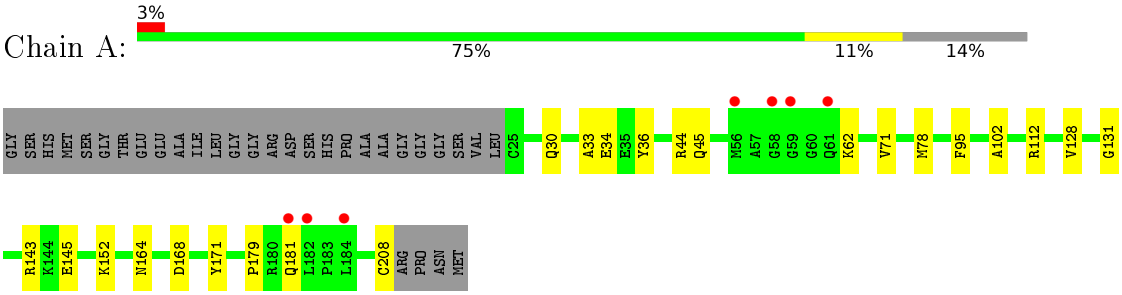
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	55	Total O 55 55	0	0
2	B	50	Total O 50 50	0	0
2	C	54	Total O 54 54	0	0
2	D	56	Total O 56 56	0	0
2	E	48	Total O 48 48	0	0
2	F	20	Total O 20 20	0	0
2	G	15	Total O 15 15	0	0
2	H	22	Total O 22 22	0	0
2	I	26	Total O 26 26	0	0
2	J	15	Total O 15 15	0	0
2	K	39	Total O 39 39	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.

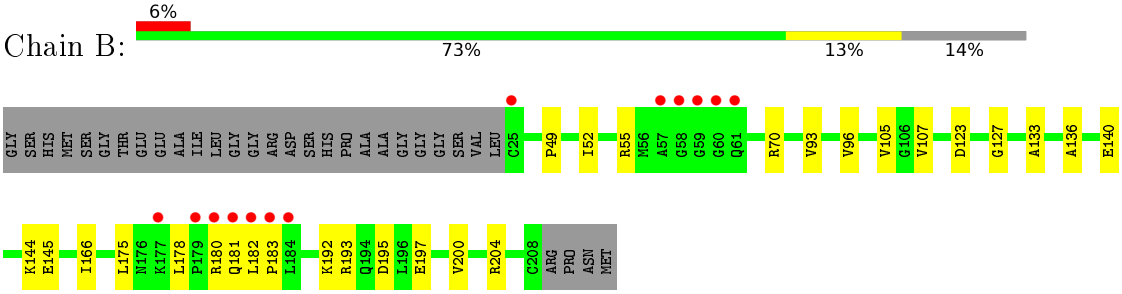
- Molecule 1: DNA repair protein RAD52 homolog

Chain A:



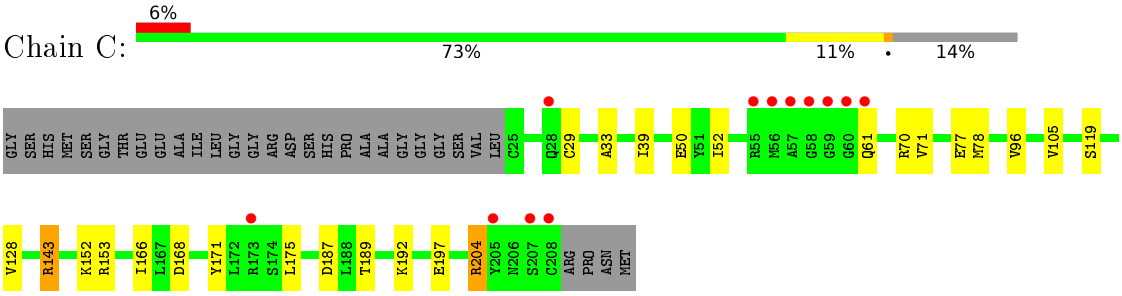
- Molecule 1: DNA repair protein RAD52 homolog

Chain B:



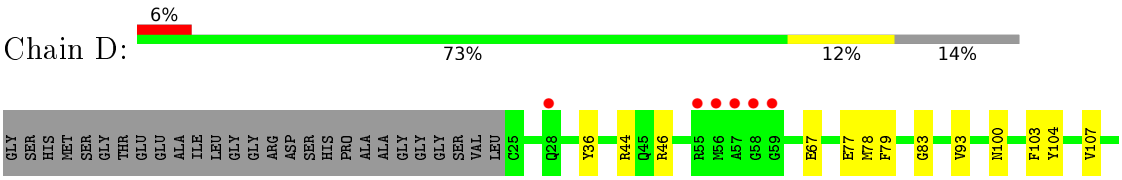
- Molecule 1: DNA repair protein RAD52 homolog

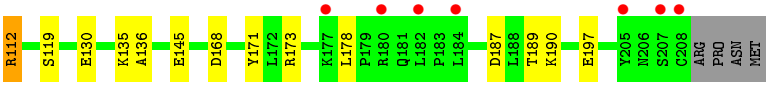
Chain C:



- Molecule 1: DNA repair protein RAD52 homolog

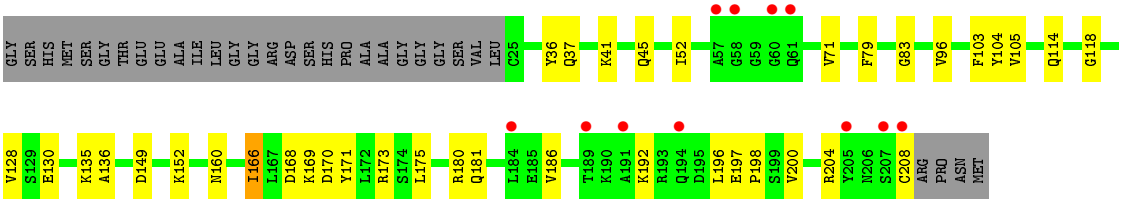
Chain D:





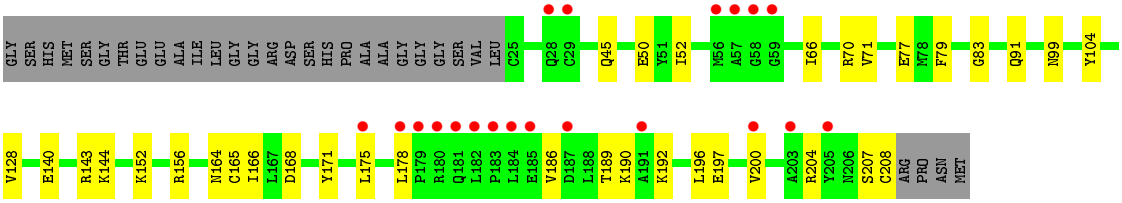
• Molecule 1: DNA repair protein RAD52 homolog

Chain E:



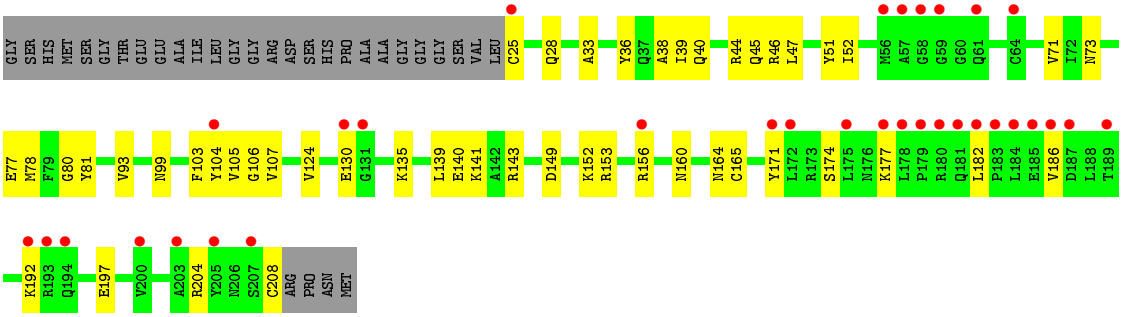
• Molecule 1: DNA repair protein RAD52 homolog

Chain F:



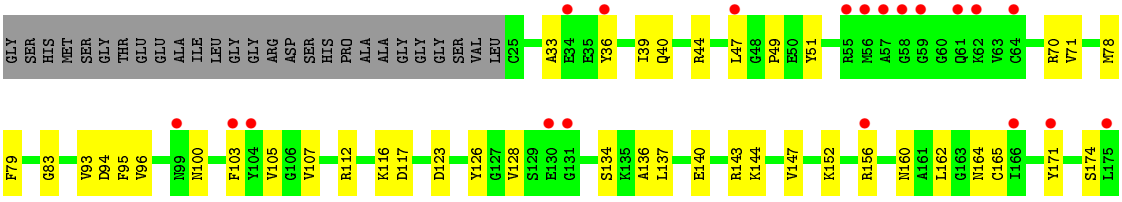
• Molecule 1: DNA repair protein RAD52 homolog

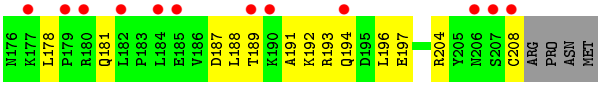
Chain G:



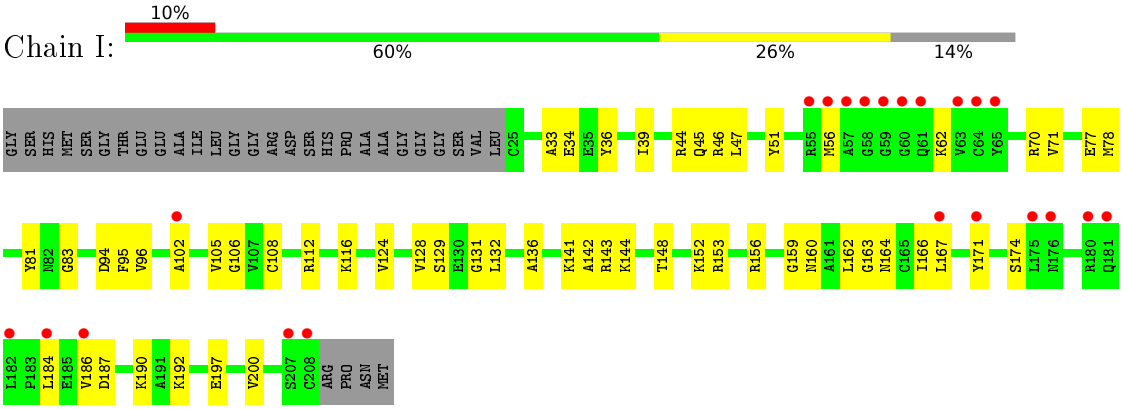
• Molecule 1: DNA repair protein RAD52 homolog

Chain H:

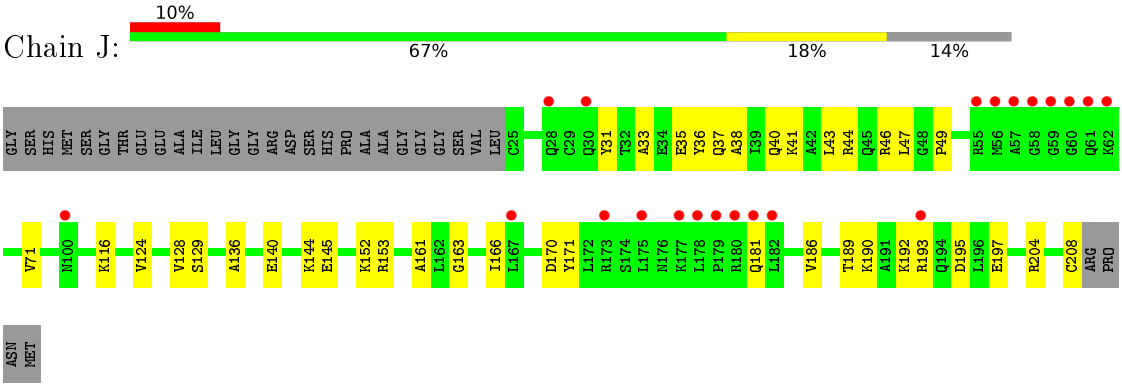




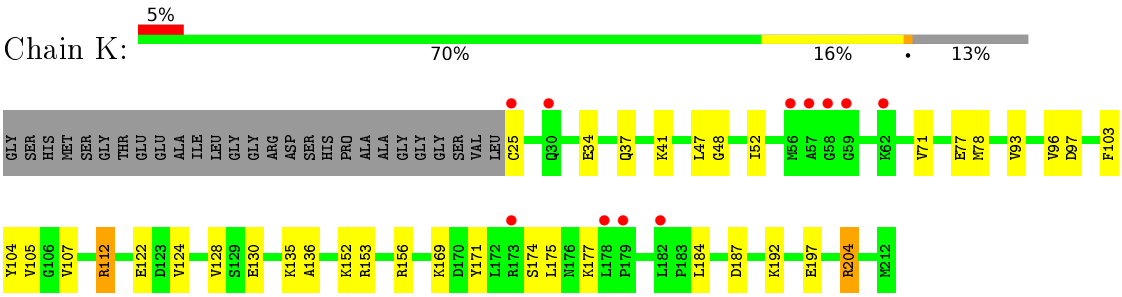
• Molecule 1: DNA repair protein RAD52 homolog



• Molecule 1: DNA repair protein RAD52 homolog



• Molecule 1: DNA repair protein RAD52 homolog



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	110.95Å 98.52Å 116.37Å 90.00° 91.99° 90.00°	Depositor
Resolution (Å)	49.26 – 2.40 46.16 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.26-2.40) 99.6 (46.16-2.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.224 , 0.273 0.222 , 0.271	Depositor DCC
R_{free} test set	4865 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	42.9	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.007 for l,k,-h 0.021 for h,-k,-l 0.014 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16252	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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

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	0.49	0/1462	0.67	1/1968 (0.1%)
1	B	0.49	0/1462	0.68	0/1968
1	C	0.46	0/1462	0.69	2/1968 (0.1%)
1	D	0.46	0/1462	0.65	1/1968 (0.1%)
1	E	0.46	0/1462	0.65	0/1968
1	F	0.42	0/1462	0.63	0/1968
1	G	0.38	0/1462	0.57	0/1968
1	H	0.40	0/1462	0.60	0/1968
1	I	0.39	0/1462	0.58	0/1968
1	J	0.40	0/1462	0.59	0/1968
1	K	0.43	0/1497	0.66	2/2015 (0.1%)
All	All	0.44	0/16117	0.63	6/21695 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	143	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	K	112	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	143	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	D	112	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	204	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	K	204	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	1438	0	1416	20	0
1	B	1438	0	1416	24	0
1	C	1438	0	1416	24	0
1	D	1438	0	1416	24	0
1	E	1438	0	1416	32	0
1	F	1438	0	1416	36	0
1	G	1438	0	1416	56	0
1	H	1438	0	1416	58	0
1	I	1438	0	1416	59	0
1	J	1438	0	1416	33	0
1	K	1472	0	1451	33	0
2	A	55	0	0	6	0
2	B	50	0	0	6	0
2	C	54	0	0	3	0
2	D	56	0	0	7	0
2	E	48	0	0	8	0
2	F	20	0	0	6	0
2	G	15	0	0	7	0
2	H	22	0	0	13	0
2	I	26	0	0	20	0
2	J	15	0	0	6	0
2	K	39	0	0	7	0
All	All	16252	0	15611	329	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 10.

All (329) 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:143:ARG:NH2	2:I:304:HOH:O	2.01	0.93
1:G:165:CYS:SG	2:G:310:HOH:O	2.28	0.91
1:I:144:LYS:O	2:I:301:HOH:O	1.86	0.91
1:H:112:ARG:NH1	2:H:304:HOH:O	2.04	0.90
1:J:192:LYS:NZ	1:J:197:GLU:OE2	2.05	0.90
1:G:47:LEU:N	2:G:302:HOH:O	2.06	0.85
1:E:170:ASP:OD2	2:E:301:HOH:O	1.95	0.85
1:I:108:CYS:SG	2:I:314:HOH:O	2.34	0.84
1:I:112:ARG:NH1	2:I:307:HOH:O	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:192:LYS:O	2:J:301:HOH:O	1.95	0.84
1:I:159:GLY:O	2:I:302:HOH:O	1.94	0.83
1:G:106:GLY:O	2:G:301:HOH:O	1.97	0.83
1:A:62:LYS:NZ	2:A:301:HOH:O	1.98	0.83
1:F:66:ILE:HG13	1:F:166:ILE:HD11	1.63	0.80
1:F:77:GLU:OE1	1:G:44:ARG:NH1	2.14	0.80
1:H:143:ARG:HD2	2:I:303:HOH:O	1.80	0.80
1:I:94:ASP:OD2	2:I:303:HOH:O	2.01	0.79
1:K:187:ASP:O	2:K:301:HOH:O	2.01	0.78
1:J:37:GLN:HG2	1:J:41:LYS:HE2	1.65	0.78
1:I:77:GLU:OE2	2:I:305:HOH:O	2.02	0.78
1:G:25:CYS:SG	1:G:28:GLN:NE2	2.56	0.77
1:H:40:GLN:O	2:H:302:HOH:O	2.02	0.77
1:A:44:ARG:NH2	2:A:302:HOH:O	2.12	0.77
1:G:192:LYS:NZ	1:G:197:GLU:OE2	2.18	0.77
1:F:178:LEU:O	2:F:301:HOH:O	2.01	0.77
1:K:130:GLU:OE2	2:K:302:HOH:O	2.02	0.77
1:H:137:LEU:N	2:H:305:HOH:O	2.18	0.76
1:H:192:LYS:NZ	1:H:197:GLU:OE1	2.19	0.76
1:B:204:ARG:NH2	1:C:78:MET:O	2.18	0.75
1:E:180:ARG:HD2	1:E:181:GLN:H	1.52	0.74
1:I:71:VAL:HG21	1:I:152:LYS:HG2	1.70	0.74
1:H:193:ARG:O	2:H:303:HOH:O	2.04	0.73
1:I:45:GLN:HG3	2:I:306:HOH:O	1.87	0.73
1:A:78:MET:O	1:K:204:ARG:NH2	2.23	0.71
1:E:52:ILE:HD12	1:E:166:ILE:HD11	1.72	0.71
1:I:148:THR:OG1	2:I:301:HOH:O	2.07	0.71
1:H:134:SER:O	2:H:305:HOH:O	2.06	0.71
1:B:49:PRO:HG3	1:B:178:LEU:HD23	1.73	0.71
1:I:186:VAL:HG11	1:J:171:TYR:HA	1.71	0.71
1:K:34:GLU:O	2:K:303:HOH:O	2.08	0.70
1:J:204:ARG:NH2	1:K:78:MET:O	2.24	0.70
1:D:77:GLU:OE2	2:D:301:HOH:O	2.09	0.70
1:G:204:ARG:NH2	1:H:78:MET:O	2.23	0.70
1:D:112:ARG:NH1	2:D:304:HOH:O	2.24	0.70
1:K:122:GLU:OE2	2:K:304:HOH:O	2.09	0.70
1:E:149:ASP:OD1	2:E:302:HOH:O	2.09	0.69
1:B:182:LEU:HG	1:B:183:PRO:HD2	1.74	0.69
1:H:181:GLN:NE2	2:H:308:HOH:O	2.27	0.68
1:J:145:GLU:OE1	2:J:302:HOH:O	2.10	0.68
1:C:187:ASP:OD1	1:C:189:THR:OG1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:LEU:HD11	1:I:174:SER:HB3	1.76	0.68
1:B:192:LYS:NZ	1:B:197:GLU:OE2	2.25	0.67
1:J:47:LEU:O	1:J:171:TYR:OH	2.08	0.67
1:B:204:ARG:HD2	1:D:36:TYR:OH	1.94	0.67
1:I:56:MET:HA	1:I:62:LYS:HA	1.76	0.67
1:B:133:ALA:N	2:B:302:HOH:O	2.19	0.67
1:H:194:GLN:HE21	1:H:196:LEU:HB2	1.60	0.67
1:E:114:GLN:HE21	1:E:118:GLY:HA2	1.61	0.66
1:I:106:GLY:O	2:I:308:HOH:O	2.12	0.66
1:B:123:ASP:OD2	2:B:301:HOH:O	2.12	0.66
1:D:189:THR:HG23	1:D:190:LYS:HG3	1.77	0.65
1:C:204:ARG:HD2	1:E:36:TYR:OH	1.96	0.65
1:I:81:TYR:O	2:I:309:HOH:O	2.12	0.65
1:K:47:LEU:O	1:K:171:TYR:OH	2.12	0.65
1:F:70:ARG:NH1	2:F:304:HOH:O	2.29	0.65
1:I:95:PHE:O	2:I:308:HOH:O	2.13	0.65
1:E:186:VAL:HG21	1:F:171:TYR:HA	1.79	0.65
1:G:47:LEU:HB3	1:G:51:TYR:HD2	1.61	0.65
1:J:124:VAL:O	1:J:153:ARG:NH1	2.30	0.65
1:J:195:ASP:HB3	1:K:77:GLU:HG3	1.78	0.65
1:C:52:ILE:HD12	1:C:166:ILE:HD11	1.78	0.64
1:E:192:LYS:NZ	1:E:197:GLU:OE1	2.26	0.64
1:J:71:VAL:HG21	1:J:152:LYS:HG2	1.78	0.64
1:I:51:TYR:HD1	1:I:70:ARG:HD3	1.62	0.64
1:I:163:GLY:N	2:I:302:HOH:O	2.30	0.64
1:I:45:GLN:N	2:I:306:HOH:O	2.08	0.63
2:B:319:HOH:O	1:C:119:SER:HB2	1.99	0.63
1:I:192:LYS:NZ	1:I:197:GLU:OE1	2.31	0.63
1:F:208:CYS:HB2	1:H:33:ALA:HA	1.81	0.63
1:F:196:LEU:HA	1:G:77:GLU:HG2	1.81	0.62
1:H:204:ARG:NH2	1:I:78:MET:O	2.28	0.62
1:E:196:LEU:HG	2:E:311:HOH:O	1.98	0.61
1:F:156:ARG:NH2	2:F:305:HOH:O	2.34	0.61
1:C:70:ARG:NH2	2:C:301:HOH:O	2.26	0.61
1:A:208:CYS:HB2	1:C:33:ALA:HB2	1.82	0.61
1:I:187:ASP:OD2	1:I:190:LYS:NZ	2.33	0.61
1:A:128:VAL:HG22	1:K:136:ALA:HB1	1.83	0.60
1:A:164:ASN:OD1	2:A:303:HOH:O	2.17	0.60
1:E:197:GLU:N	2:E:311:HOH:O	2.33	0.60
1:I:144:LYS:HE3	1:J:153:ARG:NH1	2.16	0.60
1:D:100:ASN:ND2	1:D:100:ASN:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:TYR:CE1	1:J:116:LYS:HE3	2.37	0.59
1:H:160:ASN:HA	1:H:164:ASN:HB3	1.83	0.59
1:H:147:VAL:HG21	1:I:124:VAL:HG23	1.82	0.59
1:I:136:ALA:HB1	1:J:128:VAL:HG22	1.83	0.59
1:I:83:GLY:HA2	1:I:116:LYS:HD3	1.84	0.59
1:A:112:ARG:NH1	2:A:304:HOH:O	2.21	0.59
1:K:169:LYS:HB2	2:K:309:HOH:O	2.03	0.58
1:A:36:TYR:OH	1:J:204:ARG:HD2	2.03	0.58
1:F:144:LYS:HG2	1:G:153:ARG:NH1	2.19	0.58
1:J:40:GLN:NE2	2:J:307:HOH:O	2.36	0.58
1:E:103:PHE:CZ	1:E:135:LYS:HB2	2.39	0.58
1:H:78:MET:HG3	1:H:162:LEU:HD11	1.85	0.58
1:H:147:VAL:HG21	1:I:124:VAL:CG2	2.34	0.58
1:D:112:ARG:NH2	2:D:302:HOH:O	2.16	0.58
1:G:141:LYS:NZ	2:G:304:HOH:O	2.31	0.58
1:G:71:VAL:HG21	1:G:152:LYS:HG2	1.85	0.57
1:G:99:ASN:HB2	1:G:104:TYR:HE1	1.67	0.57
1:D:67:GLU:OE2	1:E:169:LYS:NZ	2.37	0.57
1:H:100:ASN:O	1:H:100:ASN:ND2	2.37	0.57
1:H:160:ASN:HB3	1:H:165:CYS:SG	2.43	0.57
1:H:51:TYR:HD1	1:H:70:ARG:HD3	1.70	0.57
1:J:46:ARG:HB3	1:J:171:TYR:HE2	1.70	0.57
1:H:44:ARG:N	2:H:302:HOH:O	2.30	0.56
1:I:129:SER:HB2	1:I:141:LYS:HD3	1.87	0.56
1:I:77:GLU:OE1	1:J:44:ARG:NE	2.32	0.56
1:A:30:GLN:OE1	1:K:25:CYS:HA	2.05	0.56
1:I:47:LEU:O	1:I:171:TYR:OH	2.21	0.56
1:B:136:ALA:HB1	1:C:128:VAL:HG22	1.87	0.56
1:F:52:ILE:HG13	1:F:175:LEU:HD11	1.87	0.56
1:H:49:PRO:HG3	1:H:178:LEU:HD13	1.88	0.56
1:H:187:ASP:OD2	1:H:189:THR:OG1	2.24	0.56
1:H:136:ALA:HB1	1:I:128:VAL:HG22	1.88	0.56
1:I:83:GLY:HA2	1:I:116:LYS:HG2	1.87	0.55
1:B:180:ARG:N	2:B:303:HOH:O	2.32	0.55
1:G:152:LYS:O	1:G:156:ARG:HG3	2.05	0.55
1:C:204:ARG:NH2	1:D:78:MET:O	2.37	0.55
1:E:37:GLN:HG2	1:E:41:LYS:HE2	1.88	0.55
1:F:192:LYS:NZ	1:F:197:GLU:OE1	2.39	0.55
1:I:39:ILE:HA	1:I:78:MET:HE1	1.88	0.55
1:C:168:ASP:HB3	1:C:171:TYR:HB3	1.87	0.54
1:G:186:VAL:HG21	1:H:171:TYR:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:163:GLY:O	1:J:166:ILE:HG22	2.07	0.54
1:J:186:VAL:HG21	1:K:171:TYR:HA	1.89	0.54
1:F:91:GLN:OE1	1:F:143:ARG:NH1	2.33	0.54
1:K:153:ARG:HE	1:K:156:ARG:HH21	1.56	0.54
1:K:37:GLN:HG2	1:K:41:LYS:HE2	1.90	0.53
1:H:208:CYS:HB2	1:J:33:ALA:HB2	1.88	0.53
1:A:71:VAL:HG21	1:A:152:LYS:HG2	1.89	0.53
1:G:52:ILE:HD11	1:G:171:TYR:OH	2.09	0.53
1:F:200:VAL:HG22	1:G:38:ALA:HB1	1.91	0.53
1:B:70:ARG:NH2	2:B:309:HOH:O	2.40	0.53
1:G:46:ARG:HB3	2:G:302:HOH:O	2.08	0.53
1:D:197:GLU:OE2	1:E:45:GLN:NE2	2.35	0.53
1:H:140:GLU:OE2	1:H:144:LYS:NZ	2.27	0.53
1:F:77:GLU:CD	1:G:44:ARG:HH12	2.11	0.53
1:F:189:THR:HG23	1:F:190:LYS:HG2	1.89	0.53
1:B:96:VAL:HG13	1:B:105:VAL:HG22	1.90	0.52
1:J:43:LEU:HA	1:J:161:ALA:HB3	1.92	0.52
1:C:77:GLU:OE1	1:D:44:ARG:NH1	2.42	0.52
1:G:105:VAL:HG11	1:G:139:LEU:HD23	1.92	0.52
1:J:129:SER:OG	2:J:303:HOH:O	2.19	0.52
1:I:83:GLY:HA2	1:I:116:LYS:CG	2.40	0.51
1:E:52:ILE:HG13	1:E:175:LEU:HD11	1.92	0.51
1:B:195:ASP:HB3	1:C:77:GLU:HG3	1.91	0.51
1:J:140:GLU:HG3	1:J:144:LYS:HD2	1.93	0.51
1:H:83:GLY:HA2	1:H:116:LYS:HG2	1.91	0.51
1:I:102:ALA:HB1	1:I:131:GLY:HA2	1.93	0.51
1:F:66:ILE:CG1	1:F:166:ILE:HD11	2.38	0.51
1:E:192:LYS:HB2	1:F:45:GLN:OE1	2.10	0.51
1:G:204:ARG:HH21	1:H:39:ILE:HD11	1.76	0.51
1:J:46:ARG:HB3	1:J:171:TYR:CE2	2.45	0.51
1:E:79:PHE:O	1:E:83:GLY:HA3	2.11	0.51
1:G:47:LEU:HB3	1:G:51:TYR:CD2	2.43	0.51
1:G:80:GLY:HA2	1:H:40:GLN:OE1	2.10	0.50
1:I:152:LYS:O	1:I:156:ARG:HG3	2.11	0.50
1:G:143:ARG:NH2	2:G:306:HOH:O	2.42	0.50
1:H:93:VAL:HG12	1:H:107:VAL:HG22	1.93	0.50
1:I:46:ARG:NH1	2:I:317:HOH:O	2.44	0.50
1:K:71:VAL:HG21	1:K:152:LYS:HG2	1.94	0.50
1:C:192:LYS:NZ	1:C:197:GLU:OE1	2.35	0.49
1:C:61:GLN:N	1:C:61:GLN:OE1	2.45	0.49
1:G:39:ILE:HA	1:G:78:MET:HE2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:VAL:HG21	1:C:152:LYS:HG2	1.95	0.49
1:I:163:GLY:O	1:I:166:ILE:HG22	2.13	0.49
1:E:170:ASP:OD2	2:E:303:HOH:O	2.19	0.49
1:I:160:ASN:HA	1:I:164:ASN:HB3	1.95	0.48
1:A:145:GLU:HB2	2:A:307:HOH:O	2.14	0.48
1:F:165:CYS:HA	2:F:302:HOH:O	2.13	0.48
1:G:81:TYR:HE1	1:H:36:TYR:CD1	2.31	0.48
1:H:204:ARG:HD2	1:J:36:TYR:OH	2.14	0.48
1:E:180:ARG:HD2	1:E:181:GLN:N	2.26	0.48
1:G:47:LEU:HD22	1:G:51:TYR:CE2	2.48	0.48
1:K:112:ARG:NE	2:K:306:HOH:O	2.17	0.48
1:F:156:ARG:NE	2:F:305:HOH:O	2.46	0.48
1:I:144:LYS:HG2	1:J:153:ARG:NH1	2.29	0.48
1:F:156:ARG:CZ	2:F:305:HOH:O	2.62	0.48
1:G:208:CYS:HB2	1:I:33:ALA:HB2	1.96	0.48
1:E:96:VAL:HG13	1:E:105:VAL:HG22	1.96	0.48
1:J:35:GLU:OE2	1:J:116:LYS:NZ	2.34	0.48
1:G:25:CYS:HB2	1:H:117:ASP:O	2.14	0.48
2:J:301:HOH:O	1:K:48:GLY:N	2.16	0.48
1:D:93:VAL:HG13	1:D:107:VAL:HG22	1.95	0.47
1:E:104:TYR:HD1	1:E:130:GLU:HG2	1.79	0.47
1:F:99:ASN:HB2	1:F:104:TYR:CE1	2.49	0.47
1:I:184:LEU:H	1:I:184:LEU:HD12	1.78	0.47
1:F:156:ARG:O	1:F:164:ASN:HB2	2.14	0.47
1:F:186:VAL:HG21	1:G:46:ARG:NE	2.29	0.47
1:A:45:GLN:NE2	1:K:197:GLU:OE2	2.42	0.47
1:F:71:VAL:HG21	1:F:152:LYS:HG2	1.95	0.47
1:G:103:PHE:O	2:G:303:HOH:O	2.20	0.47
1:G:46:ARG:NH1	1:G:171:TYR:HB2	2.29	0.47
1:A:78:MET:C	1:K:204:ARG:HH22	2.17	0.47
1:G:73:ASN:HD21	1:H:160:ASN:HD21	1.60	0.47
1:A:33:ALA:HB2	1:J:208:CYS:HB2	1.95	0.47
1:C:143:ARG:NH2	2:C:305:HOH:O	2.46	0.47
1:F:192:LYS:HB2	1:G:45:GLN:OE1	2.15	0.47
1:D:168:ASP:HB3	1:D:171:TYR:HB3	1.96	0.47
1:H:83:GLY:HA2	1:H:116:LYS:HD3	1.95	0.47
1:B:182:LEU:CG	1:B:183:PRO:HD2	2.45	0.47
1:D:104:TYR:HD2	1:D:130:GLU:HG2	1.80	0.47
1:E:197:GLU:HB3	1:E:200:VAL:HG12	1.96	0.47
1:B:93:VAL:HG22	1:B:107:VAL:HG22	1.96	0.47
1:F:144:LYS:HG2	1:G:153:ARG:HH12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ARG:HD3	1:D:171:TYR:CD1	2.51	0.46
1:G:135:LYS:HE3	1:H:95:PHE:CD2	2.51	0.46
1:H:96:VAL:HG13	1:H:105:VAL:HG22	1.97	0.46
1:F:79:PHE:O	1:F:83:GLY:HA3	2.15	0.46
1:C:96:VAL:HG13	1:C:105:VAL:HG22	1.97	0.46
1:E:198:PRO:N	2:E:311:HOH:O	2.49	0.46
1:E:166:ILE:HD13	1:E:166:ILE:HA	1.74	0.46
1:K:124:VAL:O	1:K:153:ARG:HD3	2.16	0.46
1:K:192:LYS:NZ	1:K:197:GLU:OE2	2.37	0.46
1:H:128:VAL:HG12	2:H:314:HOH:O	2.15	0.45
1:K:112:ARG:NH2	2:K:306:HOH:O	2.41	0.45
1:B:200:VAL:HG23	2:B:328:HOH:O	2.16	0.45
1:B:144:LYS:HE3	1:C:153:ARG:HD2	1.98	0.45
1:E:168:ASP:HB3	1:E:171:TYR:HB3	1.98	0.45
1:H:143:ARG:NH2	2:H:313:HOH:O	2.46	0.45
1:K:93:VAL:HA	1:K:107:VAL:HG22	1.98	0.45
1:E:204:ARG:NE	1:G:36:TYR:OH	2.44	0.45
1:H:107:VAL:HG11	1:H:143:ARG:HA	1.97	0.45
1:A:179:PRO:O	1:A:181:GLN:NE2	2.50	0.45
1:C:52:ILE:HG13	1:C:175:LEU:HD11	1.98	0.45
1:A:34:GLU:CD	1:A:34:GLU:H	2.20	0.45
1:K:52:ILE:HG13	1:K:175:LEU:HD11	1.98	0.45
1:G:99:ASN:HB2	1:G:104:TYR:CE1	2.48	0.45
1:I:96:VAL:HG13	1:I:105:VAL:HG12	1.99	0.44
1:A:102:ALA:HB1	1:A:131:GLY:HA2	1.99	0.44
1:A:30:GLN:HG3	2:A:305:HOH:O	2.17	0.44
1:A:168:ASP:HB3	1:A:171:TYR:HB3	1.99	0.44
1:D:136:ALA:HB1	1:E:128:VAL:HG22	1.99	0.44
1:I:105:VAL:HG22	1:I:129:SER:HB3	1.99	0.44
1:I:190:LYS:H	1:I:190:LYS:HG2	1.50	0.44
1:B:166:ILE:HA	1:B:166:ILE:HD12	1.80	0.44
1:F:168:ASP:HB3	1:F:171:TYR:HB3	1.99	0.44
1:I:132:LEU:HG	2:I:311:HOH:O	2.17	0.44
1:I:166:ILE:HG23	1:I:167:LEU:HG	1.99	0.44
1:K:97:ASP:HB2	1:K:104:TYR:HB2	2.00	0.44
1:J:49:PRO:HG2	1:J:181:GLN:NE2	2.33	0.44
1:D:178:LEU:HD12	2:D:312:HOH:O	2.17	0.44
1:H:103:PHE:O	2:H:306:HOH:O	2.20	0.44
1:H:71:VAL:HG21	1:H:152:LYS:HG2	1.99	0.44
1:D:104:TYR:CD2	1:D:130:GLU:HG2	2.53	0.43
1:G:81:TYR:HE1	1:H:36:TYR:HD1	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:GLY:HA2	1:I:116:LYS:CD	2.47	0.43
1:A:95:PHE:CE2	1:K:135:LYS:HG2	2.53	0.43
1:F:140:GLU:O	1:F:144:LYS:HG3	2.17	0.43
1:H:93:VAL:O	1:H:93:VAL:HG23	2.18	0.43
2:C:306:HOH:O	1:D:119:SER:HB2	2.17	0.43
1:G:149:ASP:O	1:G:153:ARG:HG3	2.18	0.43
1:H:123:ASP:OD2	2:H:307:HOH:O	2.21	0.43
1:H:143:ARG:O	1:H:147:VAL:HG23	2.18	0.43
1:C:166:ILE:HA	1:C:166:ILE:HD13	1.72	0.43
1:C:77:GLU:OE2	1:D:44:ARG:HD3	2.17	0.43
1:B:55:ARG:HD2	1:B:55:ARG:HA	1.87	0.43
1:E:173:ARG:NE	2:E:317:HOH:O	2.50	0.43
1:G:103:PHE:CE2	1:G:135:LYS:HB2	2.54	0.43
1:G:186:VAL:HG23	1:H:174:SER:HB2	2.00	0.43
1:F:140:GLU:HG3	1:F:144:LYS:HE3	2.00	0.43
1:H:191:ALA:O	1:H:193:ARG:HG3	2.18	0.43
1:G:143:ARG:NH1	1:H:94:ASP:OD1	2.52	0.43
1:I:171:TYR:O	1:I:174:SER:HB2	2.19	0.43
1:H:112:ARG:NE	2:H:310:HOH:O	2.43	0.43
1:H:79:PHE:HE2	1:H:162:LEU:HD21	1.84	0.42
1:I:200:VAL:HG12	1:J:38:ALA:HB1	2.00	0.42
1:I:105:VAL:HG23	1:I:142:ALA:HB2	2.00	0.42
1:G:103:PHE:CZ	1:G:135:LYS:HB2	2.54	0.42
1:H:112:ARG:NH2	2:H:310:HOH:O	2.35	0.42
1:J:136:ALA:HB1	1:K:128:VAL:HG22	2.01	0.42
1:C:29:CYS:SG	2:D:352:HOH:O	2.62	0.42
1:H:152:LYS:O	1:H:156:ARG:HG3	2.19	0.42
1:E:71:VAL:HG21	1:E:152:LYS:HG2	2.01	0.42
1:K:153:ARG:HH21	1:K:156:ARG:NH2	2.18	0.42
1:B:52:ILE:HG13	1:B:175:LEU:HD11	2.02	0.42
1:K:96:VAL:HG13	1:K:105:VAL:HG22	2.02	0.42
1:B:49:PRO:HG2	1:B:181:GLN:NE2	2.35	0.42
1:I:44:ARG:N	2:I:306:HOH:O	2.52	0.42
1:G:204:ARG:HD2	1:I:36:TYR:OH	2.20	0.41
1:F:204:ARG:HH12	1:G:80:GLY:N	2.18	0.41
1:K:174:SER:O	1:K:177:LYS:HB3	2.20	0.41
1:K:184:LEU:H	1:K:184:LEU:HD12	1.84	0.41
1:F:186:VAL:HG11	1:G:171:TYR:HA	2.03	0.41
1:G:182:LEU:HD23	1:G:182:LEU:HA	1.85	0.41
1:H:83:GLY:HA2	1:H:116:LYS:CG	2.50	0.41
1:I:132:LEU:N	2:I:311:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:CYS:HB2	1:G:33:ALA:HB2	2.03	0.41
1:H:47:LEU:HD12	1:H:51:TYR:CE2	2.55	0.41
1:J:193:ARG:HD3	1:J:193:ARG:HA	1.71	0.41
1:D:145:GLU:OE1	2:D:303:HOH:O	2.22	0.41
1:E:160:ASN:ND2	2:E:305:HOH:O	2.26	0.41
1:F:204:ARG:O	1:F:207:SER:OG	2.27	0.41
1:G:160:ASN:HA	1:G:164:ASN:HB3	2.02	0.41
1:D:173:ARG:NH1	2:D:311:HOH:O	2.53	0.41
1:F:144:LYS:CG	1:G:153:ARG:NH1	2.83	0.41
1:I:124:VAL:O	1:I:153:ARG:HD3	2.20	0.41
1:I:162:LEU:O	2:I:310:HOH:O	2.22	0.41
1:I:167:LEU:HA	1:I:167:LEU:HD23	1.89	0.41
1:I:34:GLU:H	1:I:34:GLU:CD	2.24	0.41
1:G:124:VAL:O	1:G:153:ARG:HD3	2.20	0.41
2:J:301:HOH:O	1:K:47:LEU:HA	2.19	0.41
1:B:127:GLY:HA2	1:B:145:GLU:HG2	2.03	0.41
1:C:39:ILE:HG23	1:C:78:MET:CE	2.51	0.41
1:D:187:ASP:CG	1:D:189:THR:HG22	2.41	0.41
1:D:79:PHE:O	1:D:83:GLY:HA3	2.21	0.41
1:E:136:ALA:HB1	1:F:128:VAL:HG22	2.03	0.41
1:G:104:TYR:HD2	1:G:130:GLU:HG2	1.85	0.41
1:G:140:GLU:HB2	1:H:126:TYR:CD2	2.56	0.41
1:D:103:PHE:CE2	1:D:135:LYS:HB2	2.55	0.41
1:G:93:VAL:HG12	1:G:107:VAL:HG22	2.02	0.41
1:J:189:THR:HG23	1:J:190:LYS:N	2.36	0.41
1:B:180:ARG:NH1	1:B:181:GLN:O	2.53	0.41
1:B:140:GLU:HG3	1:B:144:LYS:HD2	2.03	0.40
1:K:97:ASP:O	1:K:103:PHE:HA	2.21	0.40
1:F:50:GLU:OE1	1:F:50:GLU:N	2.32	0.40
1:H:47:LEU:O	1:H:171:TYR:OH	2.26	0.40
1:B:193:ARG:CZ	1:C:50:GLU:OE1	2.69	0.40
1:G:174:SER:O	1:G:177:LYS:HG2	2.22	0.40
1:I:129:SER:CB	1:I:141:LYS:HD3	2.51	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	182/215 (85%)	180 (99%)	2 (1%)	0	100	100
1	B	182/215 (85%)	181 (100%)	1 (0%)	0	100	100
1	C	182/215 (85%)	178 (98%)	4 (2%)	0	100	100
1	D	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
1	E	182/215 (85%)	177 (97%)	5 (3%)	0	100	100
1	F	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
1	G	182/215 (85%)	178 (98%)	4 (2%)	0	100	100
1	H	182/215 (85%)	176 (97%)	6 (3%)	0	100	100
1	I	182/215 (85%)	176 (97%)	6 (3%)	0	100	100
1	J	182/215 (85%)	173 (95%)	9 (5%)	0	100	100
1	K	186/215 (86%)	184 (99%)	2 (1%)	0	100	100
All	All	2006/2365 (85%)	1961 (98%)	45 (2%)	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	150/171 (88%)	150 (100%)	0	100	100
1	B	150/171 (88%)	150 (100%)	0	100	100
1	C	150/171 (88%)	150 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	150/171 (88%)	150 (100%)	0	100 100
1	E	150/171 (88%)	149 (99%)	1 (1%)	88 95
1	F	150/171 (88%)	150 (100%)	0	100 100
1	G	150/171 (88%)	149 (99%)	1 (1%)	88 95
1	H	150/171 (88%)	150 (100%)	0	100 100
1	I	150/171 (88%)	150 (100%)	0	100 100
1	J	150/171 (88%)	149 (99%)	1 (1%)	88 95
1	K	154/171 (90%)	154 (100%)	0	100 100
All	All	1654/1881 (88%)	1651 (100%)	3 (0%)	95 99

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	166	ILE
1	G	40	GLN
1	J	170	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	114	GLN
1	E	114	GLN
1	G	28	GLN
1	G	114	GLN
1	H	160	ASN
1	H	194	GLN
1	I	164	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no 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, 95^{th} 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	184/215 (85%)	0.09	7 (3%) 44 45	23, 37, 86, 140	0
1	B	184/215 (85%)	0.25	13 (7%) 19 19	20, 36, 85, 102	0
1	C	184/215 (85%)	0.06	12 (6%) 22 22	20, 40, 101, 133	0
1	D	184/215 (85%)	0.22	13 (7%) 19 19	19, 40, 88, 119	0
1	E	184/215 (85%)	0.26	11 (5%) 25 25	23, 43, 86, 104	0
1	F	184/215 (85%)	0.53	20 (10%) 7 7	28, 56, 107, 130	0
1	G	184/215 (85%)	1.08	33 (17%) 2 2	37, 71, 133, 153	0
1	H	184/215 (85%)	1.13	32 (17%) 2 2	44, 74, 151, 170	0
1	I	184/215 (85%)	0.85	22 (11%) 6 5	42, 70, 140, 168	0
1	J	184/215 (85%)	0.88	21 (11%) 7 7	35, 58, 119, 159	0
1	K	188/215 (87%)	0.19	11 (5%) 26 26	28, 48, 94, 127	0
All	All	2028/2365 (85%)	0.50	195 (9%) 10 10	19, 53, 117, 170	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	58	GLY	15.8
1	J	60	GLY	14.5
1	J	59	GLY	12.8
1	A	59	GLY	11.0
1	H	59	GLY	10.7
1	J	61	GLN	9.8
1	J	57	ALA	9.3
1	J	58	GLY	8.8
1	K	58	GLY	8.6
1	K	59	GLY	8.6
1	A	182	LEU	7.7
1	D	57	ALA	7.7

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Mol	Chain	Res	Type	RSRZ
1	B	60	GLY	7.6
1	H	58	GLY	7.6
1	I	56	MET	7.6
1	C	58	GLY	7.4
1	F	58	GLY	7.2
1	F	182	LEU	7.0
1	D	59	GLY	7.0
1	J	179	PRO	6.7
1	C	59	GLY	6.7
1	G	181	GLN	6.7
1	D	182	LEU	6.3
1	F	57	ALA	6.1
1	I	184	LEU	6.1
1	G	182	LEU	6.1
1	I	57	ALA	6.0
1	H	57	ALA	5.9
1	A	58	GLY	5.7
1	F	181	GLN	5.7
1	H	56	MET	5.6
1	B	181	GLN	5.5
1	F	56	MET	5.4
1	B	182	LEU	5.3
1	H	55	ARG	5.2
1	B	61	GLN	5.1
1	K	57	ALA	5.1
1	I	207	SER	5.1
1	J	62	LYS	5.1
1	C	57	ALA	5.0
1	C	61	GLN	5.0
1	I	59	GLY	5.0
1	B	59	GLY	5.0
1	G	57	ALA	4.9
1	H	190	LYS	4.6
1	F	184	LEU	4.6
1	H	104	TYR	4.6
1	B	58	GLY	4.5
1	I	58	GLY	4.5
1	H	207	SER	4.5
1	F	59	GLY	4.3
1	J	56	MET	4.3
1	A	61	GLN	4.2
1	I	182	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	184	LEU	4.0
1	G	61	GLN	4.0
1	G	184	LEU	4.0
1	J	182	LEU	3.9
1	K	179	PRO	3.9
1	F	205	TYR	3.9
1	H	180	ARG	3.9
1	I	65	TYR	3.9
1	H	206	ASN	3.8
1	F	183	PRO	3.8
1	G	59	GLY	3.8
1	C	60	GLY	3.7
1	G	200	VAL	3.7
1	I	180	ARG	3.7
1	C	208	CYS	3.7
1	E	58	GLY	3.7
1	F	180	ARG	3.7
1	E	208	CYS	3.6
1	G	58	GLY	3.5
1	B	180	ARG	3.5
1	J	193	ARG	3.5
1	K	56	MET	3.5
1	H	34	GLU	3.5
1	I	63	VAL	3.5
1	A	56	MET	3.4
1	J	55	ARG	3.4
1	D	208	CYS	3.4
1	A	184	LEU	3.4
1	D	184	LEU	3.4
1	G	64	CYS	3.4
1	E	184	LEU	3.3
1	H	184	LEU	3.3
1	B	179	PRO	3.3
1	G	179	PRO	3.3
1	J	30	GLN	3.3
1	G	25	CYS	3.3
1	H	61	GLN	3.2
1	G	56	MET	3.2
1	I	55	ARG	3.1
1	H	185	GLU	3.1
1	G	180	ARG	3.0
1	C	205	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	62	LYS	3.0
1	K	25	CYS	3.0
1	C	56	MET	3.0
1	F	178	LEU	3.0
1	I	186	VAL	3.0
1	H	103	PHE	3.0
1	G	178	LEU	3.0
1	F	185	GLU	2.9
1	G	205	TYR	2.9
1	G	185	GLU	2.9
1	J	178	LEU	2.9
1	G	183	PRO	2.8
1	G	177	LYS	2.8
1	H	177	LYS	2.8
1	E	189	THR	2.8
1	A	181	GLN	2.8
1	H	171	TYR	2.8
1	F	175	LEU	2.8
1	E	61	GLN	2.7
1	G	203	ALA	2.7
1	K	178	LEU	2.7
1	G	175	LEU	2.7
1	I	61	GLN	2.7
1	J	181	GLN	2.7
1	D	205	TYR	2.7
1	G	171	TYR	2.7
1	B	183	PRO	2.7
1	I	208	CYS	2.7
1	H	130	GLU	2.6
1	J	180	ARG	2.6
1	K	62	LYS	2.6
1	H	131	GLY	2.6
1	I	60	GLY	2.6
1	D	177	LYS	2.6
1	E	194	GLN	2.6
1	K	173	ARG	2.6
1	F	28	GLN	2.5
1	D	180	ARG	2.5
1	C	55	ARG	2.5
1	G	104	TYR	2.5
1	D	55	ARG	2.5
1	B	57	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	194	GLN	2.4
1	E	60	GLY	2.4
1	H	175	LEU	2.4
1	I	181	GLN	2.4
1	J	173	ARG	2.4
1	C	207	SER	2.4
1	I	64	CYS	2.4
1	D	56	MET	2.4
1	E	191	ALA	2.4
1	F	179	PRO	2.4
1	E	207	SER	2.4
1	C	173	ARG	2.3
1	E	205	TYR	2.3
1	I	102	ALA	2.3
1	F	200	VAL	2.3
1	C	28	GLN	2.3
1	I	171	TYR	2.3
1	K	182	LEU	2.3
1	E	57	ALA	2.3
1	F	191	ALA	2.3
1	G	187	ASP	2.3
1	F	187	ASP	2.3
1	G	156	ARG	2.2
1	H	99	ASN	2.2
1	H	47	LEU	2.2
1	B	25	CYS	2.2
1	H	189	THR	2.2
1	I	167	LEU	2.2
1	H	36	TYR	2.2
1	F	203	ALA	2.2
1	J	28	GLN	2.2
1	I	176	ASN	2.2
1	I	175	LEU	2.2
1	H	156	ARG	2.2
1	H	166	ILE	2.2
1	H	179	PRO	2.2
1	G	172	LEU	2.2
1	F	29	CYS	2.2
1	B	177	LYS	2.1
1	G	131	GLY	2.1
1	H	64	CYS	2.1
1	G	186	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	130	GLU	2.1
1	H	208	CYS	2.1
1	K	30	GLN	2.1
1	J	167	LEU	2.1
1	J	177	LYS	2.1
1	J	175	LEU	2.1
1	G	189	THR	2.1
1	J	100	ASN	2.1
1	H	194	GLN	2.1
1	D	207	SER	2.0
1	G	193	ARG	2.0
1	D	28	GLN	2.0
1	G	192	LYS	2.0
1	G	207	SER	2.0
1	H	182	LEU	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 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.