WORLDWIDE wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 1, 2023 – 04:09 PM JST

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)

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

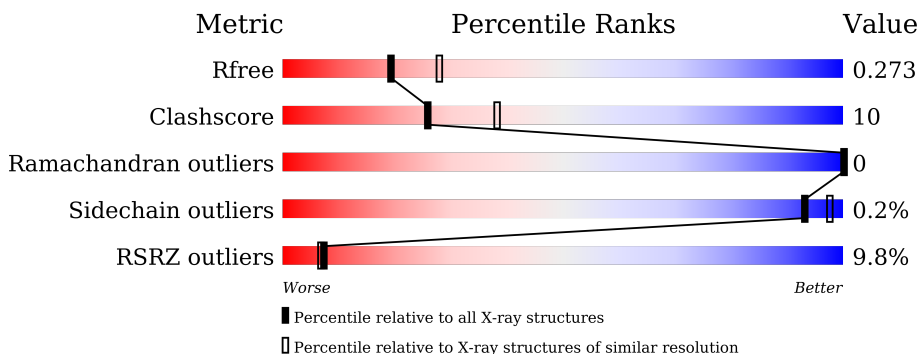|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.40 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.
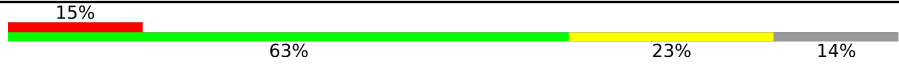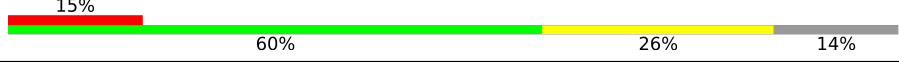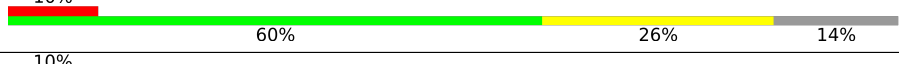
Metric	Percentile Ranks	Value
Rfree		0.273
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		0.2%
RSRZ outliers		9.8%

Worse   Better

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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	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	10% / 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.

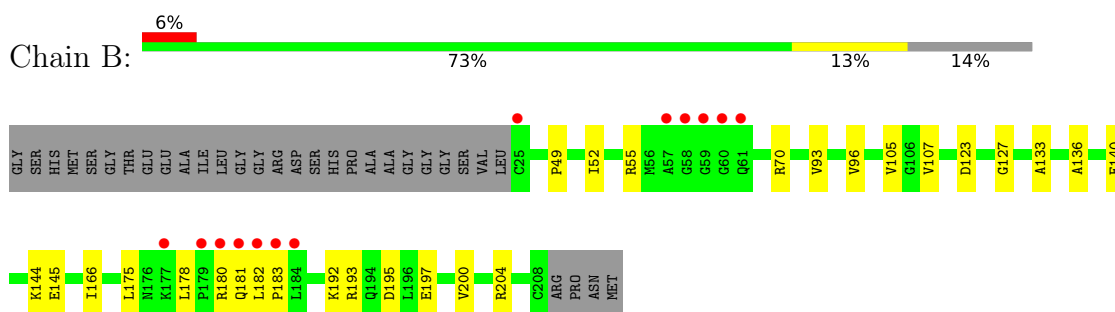| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total 55	O 55	0	0
2	B	50	Total 50	O 50	0	0
2	C	54	Total 54	O 54	0	0
2	D	56	Total 56	O 56	0	0
2	E	48	Total 48	O 48	0	0
2	F	20	Total 20	O 20	0	0
2	G	15	Total 15	O 15	0	0
2	H	22	Total 22	O 22	0	0
2	I	26	Total 26	O 26	0	0
2	J	15	Total 15	O 15	0	0
2	K	39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

3 Residue-property plots ⓘ

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.
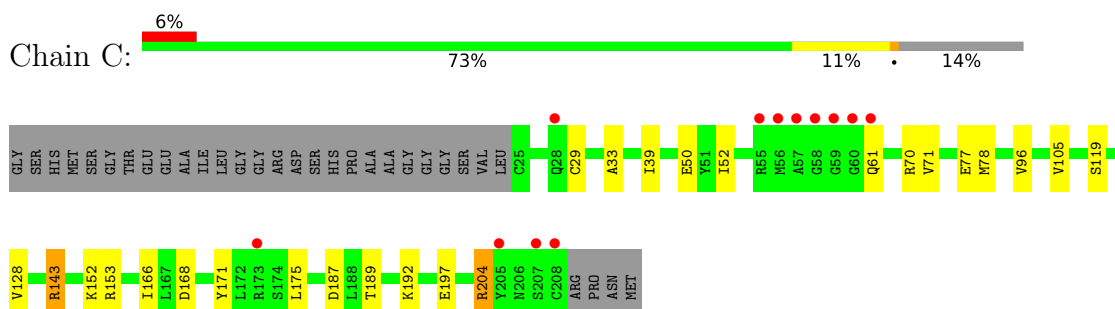
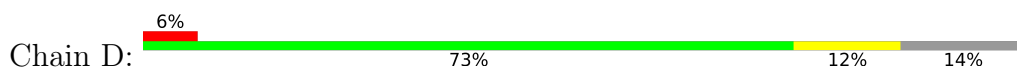• Molecule 1: DNA repair protein RAD52 homolog
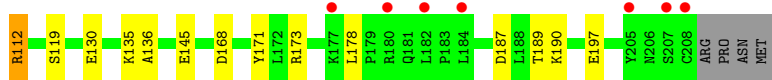
Chain A:

• 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:

GLY SER HIS MET SER GLY THR GLU GLU ALA ILE LEU GLY GLY ARG ASP SER HIS PRO ALA ALA GLY GLY GLY SER VAL LEU C25 Q28 Y36 R44 Q45 R46 R55 M56 A57 G58 G59 E67 E77 M78 F79 G83 V93 N100 F103 Y104 V107

R112 S119 E130 K135 A136 E145 D168 Y171 L172 R173 K177 L178 P179 R180 Q181 L182 P183 L184 D187 L188 T189 K190 E197 Y205 N206 S207 C208 ARG PRO ASN MET

• Molecule 1: DNA repair protein RAD52 homolog

Chain E:
5%
68% | 17% | 14%

GLY SER HIS MET SER GLY THR GLU GLU ALA ILE LEU GLY GLY ARG ASP SER HIS PRO ALA ALA GLY GLY GLY SER VAL LEU C25 Y36 Q37 K41 Q45 I52 A57 G58 G59 G60 Q61 V71 F79 G83 V96 F103 Y104 V105 Q114 G118

V128 S129 E130 K135 A136 D149 K152 N160 I166 L167 D168 K169 D170 Y171 L172 R173 S174 L175 R180 Q181 L184 E185 V186 T189 K190 A191 K192 R193 Q194 D195 L196 E197 P198 S199 V200 R204 Y205 N206 S207 C208 ARG PRO ASN MET

• Molecule 1: DNA repair protein RAD52 homolog

Chain F:
10%
69% | 16% | 14%

GLY SER HIS MET SER GLY THR GLU GLU ALA ILE LEU GLY GLY ARG ASP SER HIS PRO ALA ALA GLY GLY GLY SER VAL LEU C25 Q28 Q29 Q45 E50 Y51 I52 M56 A57 G58 G59 I66 R70 V71 E77 M78 F79 G83 Q91 N99 Y104

V128 G131 E140 R143 K144 K152 R156 N164 C165 I166 L167 D168 Y171 L175 L178 P179 R180 Q181 L182 P183 L184 E185 V186 D187 L188 T189 K190 A191 K192 L196 E197 P198 S199 V200 A203 R204 Y205 N206 S207 C208 ARG PRO ASN MET

• Molecule 1: DNA repair protein RAD52 homolog

Chain G:
15%
63% | 23% | 14%

GLY SER HIS MET SER GLY THR GLU GLU ALA ILE LEU GLY GLY ARG ASP SER HIS PRO ALA ALA GLY GLY GLY SER VAL LEU C25 Q28 A33 Y36 Q37 A38 I39 Q40 R44 Q45 R46 L47 Y51 I52 M56 A57 G58 G59 G60 Q61 C64 V71 I72 N73

E77 M78 F79 G80 Y81 V93 N99 F103 Y104 V105 G106 V107 V124 E130 G131 K135 L139 E140 K141 A142 R143 D149 K152 R153 R156 N160 M164 C165 Y171 L172 R173 S174 L175 N176 K177 L178 P179 R180 Q181 L182 P183 L184 E185 V186 D187 L188 T189
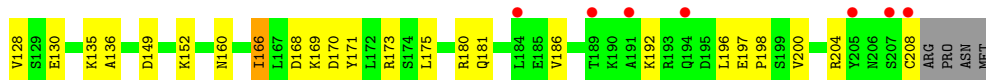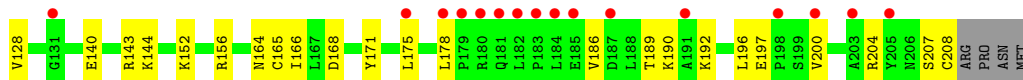
K192 R193 Q194 E197 V200 A203 R204 Y205 N206 S207 C208 ARG PRO ASN MET

• Molecule 1: DNA repair protein RAD52 homolog

Chain H:
15%
60% | 26% | 14%

GLY SER HIS MET SER GLY THR GLU GLU ALA ILE LEU GLY GLY ARG ASP SER HIS PRO ALA ALA GLY GLY GLY SER VAL LEU C25 A33 E34 E35 Y36 I39 Q40 R44 L47 G48 P49 E50 Y51 R55 M56 A57 G58 G59 G60 Q61 K62 V63 C64 R70 V71 M78

F79 G83 V93 D94 F95 V96 N99 N100 F103 Y104 V105 G106 V107 R112 K116 D117 D123 Y126 G127 V128 S129 E130 G131 S134 K135 A136 L137 E140 R143 K144 V147 K152 R156 N160 A161 L162 G163 N164 C165 I166 Y171 S174 L175

N176 K177 L178 P179 R180 Q181 L182 P183 L184 E185 V186 D187 L188 T189 K190 A191 K192 R193 Q194 D195 L196 E197 R204 Y205 N206 S207 C208 ARG PRO ASN MET

• Molecule 1: DNA repair protein RAD52 homolog

Chain I:
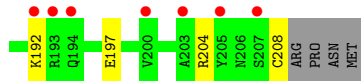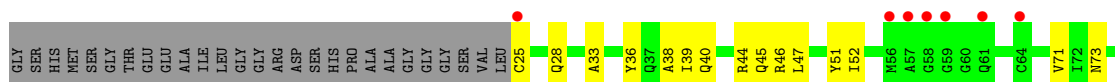
10%

60% 26% 14%

GLY SER HIS MET SER GLY THR GLU GLU ALA ILE LEU GLY GLY ARG ASP SER HIS PRO ALA ALA GLY GLY SER VAL LEU C25 A33 E34 E35 Y36 I39 R44 Q45 R46 L47 Y51 R55 M56 A57 G58 G59 G60 Q61 K62 V63 C64 Y65 R70 V71 E77 M78

Y81 N82 G83 D94 F95 V96 A102 V105 G106 V107 C108 R112 K116 V124 V128 S129 E130 G131 L132 A136 K141 A142 R143 K144 T148 K152 R153 R156 G159 N160 A161 L162 G163 N164 C165 I166 L167 Y171 S174 L175 N176 R180 Q181

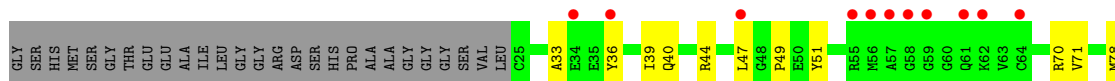L182 P183 L184 E185 V186 D187 K190 A191 K192 E197 V200 S207 C208 ARG PRO ASN MET

• Molecule 1: DNA repair protein RAD52 homolog

Chain J:

10%

67% 18% 14%

GLY SER HIS MET SER GLY THR GLU GLU ALA ILE LEU GLY GLY ARG ASP SER HIS PRO ALA ALA GLY GLY SER VAL LEU C25 Q28 C29 Q30 Y31 T32 A33 E34 E35 Y36 Q37 A38 I39 Q40 K41 A42 L43 R44 Q45 R46 L47 G48 P49 R55 M56 A57 G58 G59 G60 Q61 K62

V71 N100 K116 V124 V128 S129 A136 E140 K144 E145 K152 R153 A161 L162 G163 I166 L167 D170 Y171 L172 R173 S174 L175 N176 K177 L178 P179 R180 Q181 L182 V186 T189 K190 A191 K192 R193 Q194 D195 L196 E197 R204 C208 ARG PRO

ASN MET

• Molecule 1: DNA repair protein RAD52 homolog

Chain K:

5%

70% 16% 13%

GLY SER HIS MET SER GLY THR GLU GLU ALA ILE LEU GLY GLY ARG ASP SER HIS PRO ALA ALA GLY GLY SER VAL LEU C25 Q30 E34 Q37 K41 L47 G48 I52 M56 A57 G58 G59 K62 V71 E77 M78 V93 V96 D97 F103

Y104 V105 G106 V107 R112 E122 D123 V124 V128 S129 E130 K135 A136 K152 R153 R156 K169 D170 Y171 L172 R173 S174 L175 N176 K177 L178 P179 L182 P183 L184 D187 K192 E197 R204 M212

4 Data and refinement statistics ⓘ

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 0.224 , 0.273	Depositor DCC
R_{free} test set	4841 reflections (4.99%)	wwPDB-VP
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.*

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[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	0.49	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.

The worst 5 of 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

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	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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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%)	84	92
1	F	150/171 (88%)	150 (100%)	0	100	100
1	G	150/171 (88%)	149 (99%)	1 (1%)	84	92
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%)	84	92
1	K	154/171 (90%)	154 (100%)	0	100	100
All	All	1654/1881 (88%)	1651 (100%)	3 (0%)	93	97

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

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

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	184/215 (85%)	0.09	7 (3%)	40	39	23, 37, 86, 140	0
1	B	184/215 (85%)	0.25	13 (7%)	16	14	20, 36, 85, 102	0
1	C	184/215 (85%)	0.06	12 (6%)	18	17	20, 40, 101, 133	0
1	D	184/215 (85%)	0.22	13 (7%)	16	14	19, 40, 88, 119	0
1	E	184/215 (85%)	0.26	11 (5%)	21	20	23, 43, 86, 104	0
1	F	184/215 (85%)	0.53	22 (11%)	4	3	28, 56, 107, 130	0
1	G	184/215 (85%)	1.07	33 (17%)	1	1	37, 71, 133, 153	0
1	H	184/215 (85%)	1.13	33 (17%)	1	1	44, 74, 151, 170	0
1	I	184/215 (85%)	0.85	22 (11%)	4	3	42, 70, 140, 168	0
1	J	184/215 (85%)	0.88	21 (11%)	5	4	35, 58, 119, 159	0
1	K	188/215 (87%)	0.19	11 (5%)	22	21	28, 48, 94, 127	0
All	All	2028/2365 (85%)	0.50	198 (9%)	7	7	19, 53, 117, 170	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	58	GLY	15.7
1	J	60	GLY	14.7
1	J	59	GLY	12.6
1	A	59	GLY	11.0
1	H	59	GLY	10.8

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.