



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:39 PM UTC

PDB ID : 5JRB / pdb_00005jrb
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

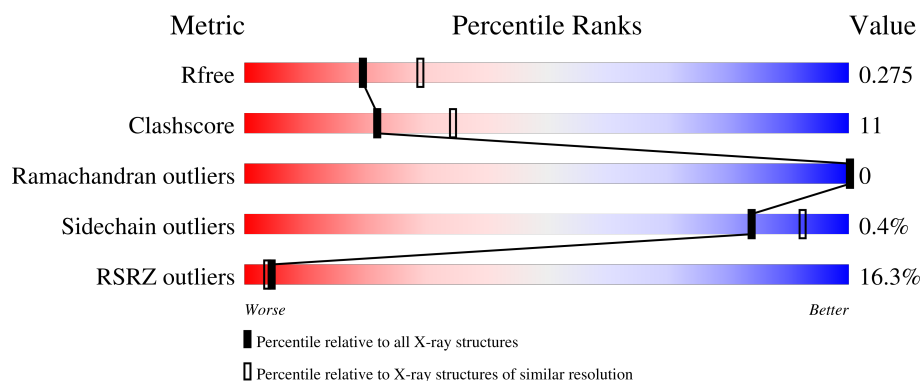
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	4% 75% 10% 14%
1	B	215	4% 73% 13% 14%
1	C	215	6% 73% 13% 14%
1	D	215	6% 72% 14% 14%
1	E	215	6% 67% 19% 14%

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Mol	Chain	Length	Quality of chain
1	F	215	
1	G	215	
1	H	215	
1	I	215	
1	J	215	
1	K	215	

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

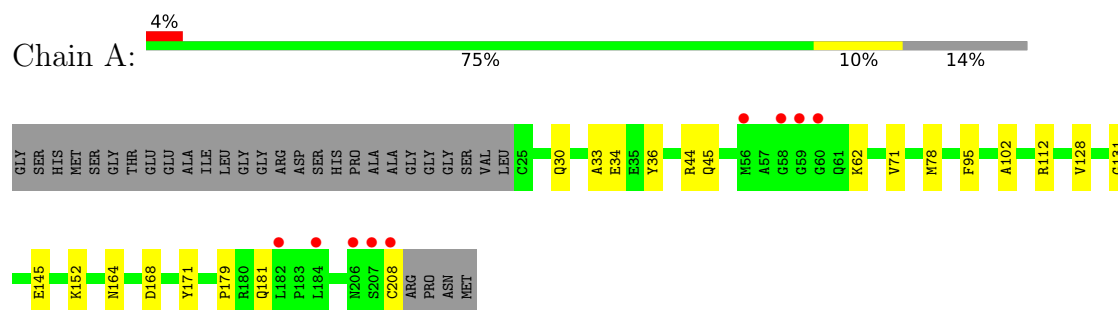
- Molecule 2 is water.

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

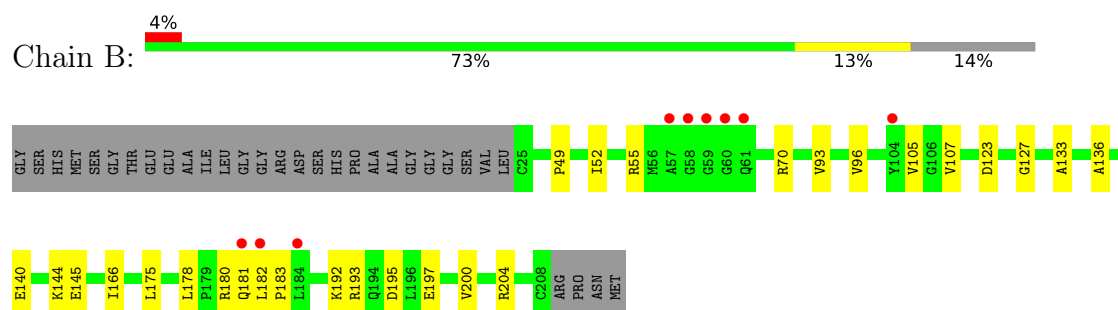
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

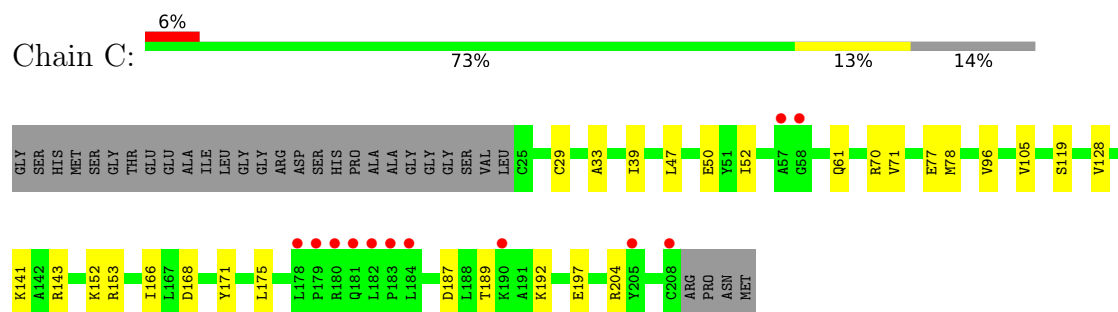
- Molecule 1: DNA repair protein RAD52 homolog



- Molecule 1: DNA repair protein RAD52 homolog

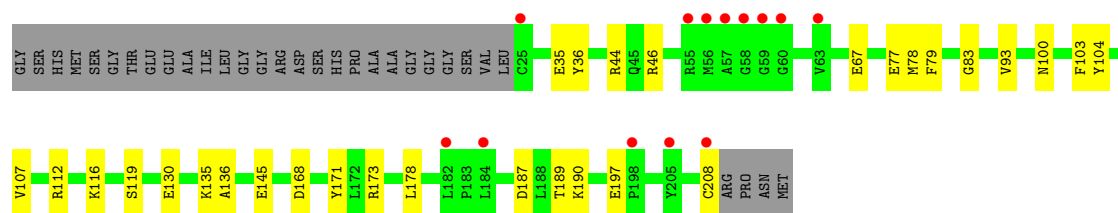


- Molecule 1: DNA repair protein RAD52 homolog

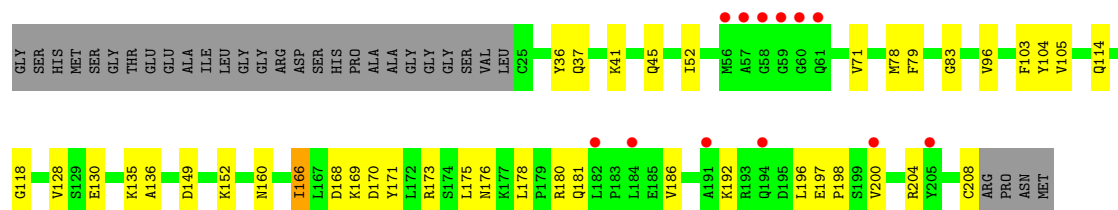


- Molecule 1: DNA repair protein RAD52 homolog

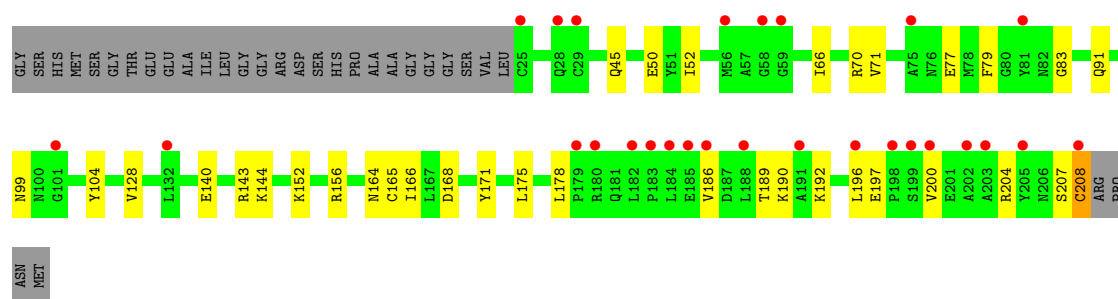




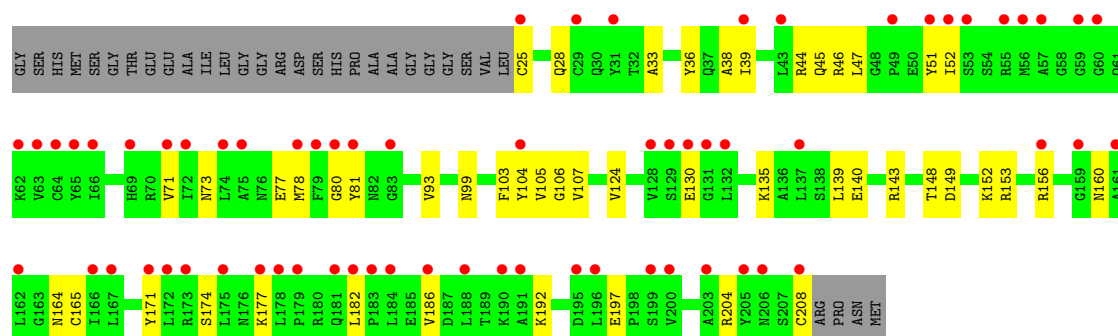
• Molecule 1: DNA repair protein RAD52 homolog



• Molecule 1: DNA repair protein RAD52 homolog

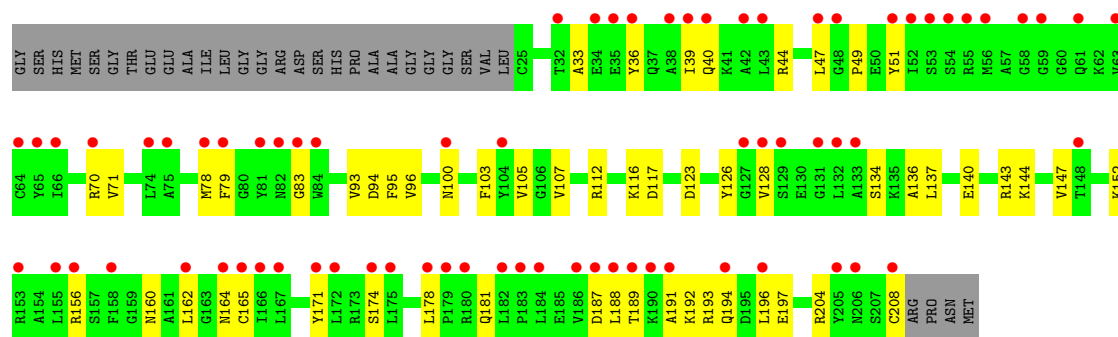


• Molecule 1: DNA repair protein RAD52 homolog

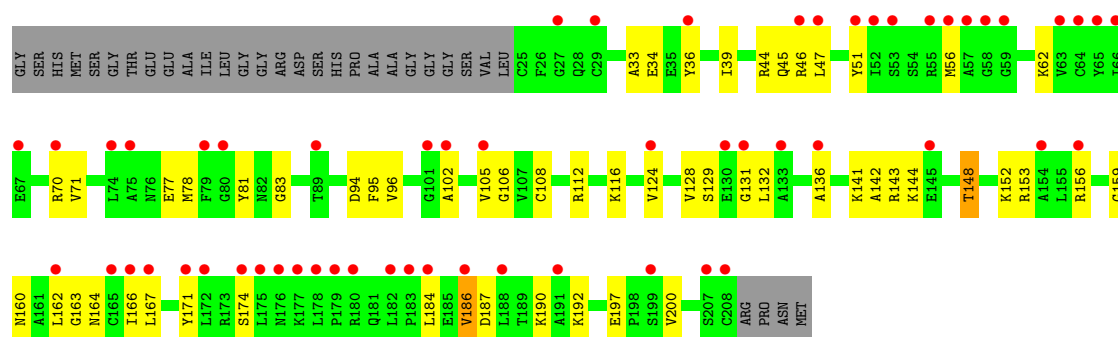


• Molecule 1: DNA repair protein RAD52 homolog

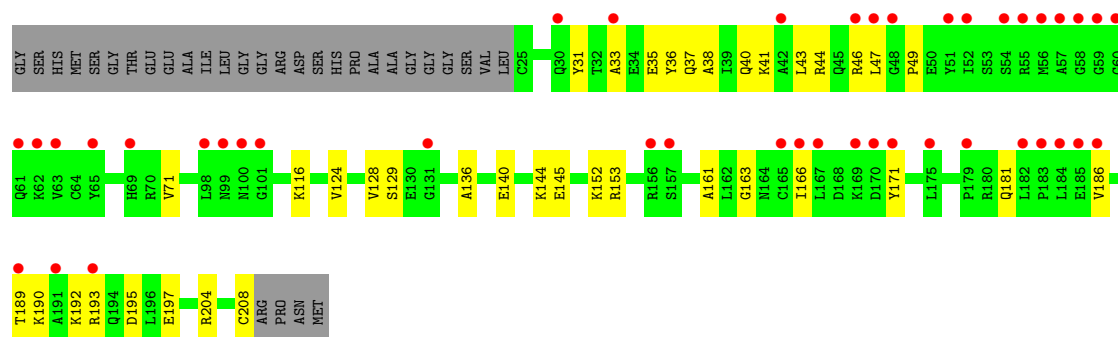




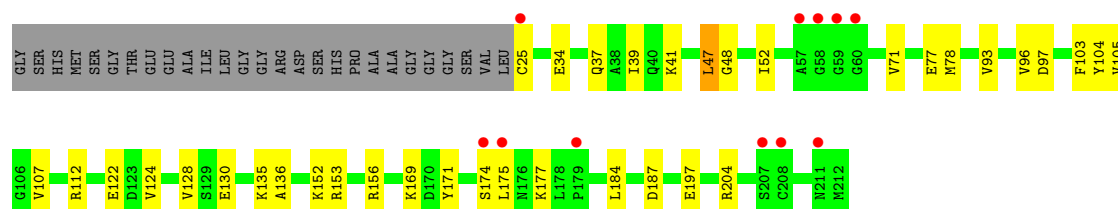
• Molecule 1: DNA repair protein RAD52 homolog



• Molecule 1: DNA repair protein RAD52 homolog



• Molecule 1: DNA repair protein RAD52 homolog



4 Data and refinement statistics

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 49.26 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.26-2.40) 99.5 (49.26-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.224 , 0.273 0.225 , 0.275	Depositor DCC
R_{free} test set	4865 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)	0.32 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.42	0/1462	0.63	0/1968
1	B	0.41	0/1462	0.64	0/1968
1	C	0.39	0/1462	0.61	0/1968
1	D	0.40	0/1462	0.61	0/1968
1	E	0.39	0/1462	0.62	0/1968
1	F	0.35	0/1462	0.57	0/1968
1	G	0.29	0/1462	0.54	0/1968
1	H	0.31	0/1462	0.56	0/1968
1	I	0.31	0/1462	0.58	0/1968
1	J	0.33	0/1462	0.58	0/1968
1	K	0.37	0/1497	0.61	0/2015
All	All	0.36	0/16117	0.59	0/21695

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1438	0	1416	20	0
1	B	1438	0	1416	24	0
1	C	1438	0	1416	27	0
1	D	1438	0	1416	26	0
1	E	1438	0	1416	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1438	0	1416	36	0
1	G	1438	0	1416	55	0
1	H	1438	0	1416	59	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	9	0
2	F	20	0	0	6	0
2	G	15	0	0	6	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	336	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 11.

All (336) 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:A:62:LYS:NZ	2:A:301:HOH:O	1.98	0.95
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:ILE:HG23	1:I:78:MET:HE2	1.66	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:K:39:ILE:HG23	1:K:78:MET:HE2	1.72	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:B:192:LYS:NZ	1:B:197:GLU:OE2	2.25	0.69
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
1:H:188:LEU:HD11	1:I:174:SER:HB3	1.76	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:K:47:LEU:O	1:K:171:TYR:OH	2.12	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:C:39:ILE:HG23	1:C:78:MET:HE2	1.81	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:G:39:ILE:HG23	1:G:78:MET:HE2	1.83	0.60
1:I:144:LYS:HE3	1:J:153:ARG:NH1	2.16	0.60
1:D:100:ASN:O	1:D:100:ASN:ND2	2.35	0.59
1:J:31:TYR:CE1	1:J:116:LYS:HE3	2.37	0.59
1:H:147:VAL:HG21	1:I:124:VAL:HG23	1.82	0.59
1:H:160:ASN:HA	1:H:164:ASN:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:GLY:HA2	1:I:116:LYS:HD3	1.84	0.59
1:I:136:ALA:HB1	1:J:128:VAL:HG22	1.83	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: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:F:77:GLU:CD	1:G:44:ARG:HH12	2.11	0.57
1:D:67:GLU:OE2	1:E:169:LYS:NZ	2.37	0.57
1:H:100:ASN:ND2	1:H:100:ASN:O	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:77:GLU:OE1	1:J:44:ARG:NE	2.32	0.56
1:I:129:SER:HB2	1:I:141:LYS:HD3	1.87	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:136:ALA:HB1	1:I:128:VAL:HG22	1.88	0.56
1:H:187:ASP:OD2	1:H:189:THR:OG1	2.24	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:204:ARG:O	1:F:207:SER:OG	2.27	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: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:A:78:MET:C	1:K:204:ARG:HH22	2.17	0.52
1:G:105:VAL:HG11	1:G:139:LEU:HD23	1.92	0.52
1:H:47:LEU:O	1:H:171:TYR:OH	2.26	0.52
1:H:39:ILE:HG23	1:H:78:MET:HE2	1.90	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:E:192:LYS:HB2	1:F:45:GLN:OE1	2.10	0.51
1:F:66:ILE:CG1	1:F:166:ILE:HD11	2.38	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:A:34:GLU:H	1:A:34:GLU:CD	2.20	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:47:LEU:O	1:C:171:TYR:OH	2.28	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

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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:HD12	1:I:184:LEU:H	1.78	0.47
1:A:45:GLN:NE2	1:K:197:GLU:OE2	2.42	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:F:71:VAL:HG21	1:F:152:LYS:HG2	1.95	0.47
1:G:46:ARG:NH1	1:G:171:TYR:HB2	2.29	0.47
1:G:103:PHE:O	2:G:303:HOH:O	2.20	0.47
1:A:33:ALA:HB2	1:J:208:CYS:HB2	1.95	0.47
1:G:73:ASN:HD21	1:H:160:ASN:HD21	1.60	0.47
1:C:143:ARG:NH2	2:C:305:HOH:O	2.46	0.47
1:D:168:ASP:HB3	1:D:171:TYR:HB3	1.96	0.47
1:F:192:LYS:HB2	1:G:45:GLN:OE1	2.15	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
1:D:46:ARG:HD3	1:D:171:TYR:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:34:GLU:H	1:I:34:GLU:CD	2.24	0.46
1:E:198:PRO:N	2:E:311:HOH:O	2.49	0.46
1:D:187:ASP:CG	1:D:189:THR:HG22	2.41	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: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: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:E:196:LEU:C	2:E:311:HOH:O	2.60	0.44
1:A:30:GLN:HG3	2:A:305:HOH:O	2.17	0.44
1:A:102:ALA:HB1	1:A:131:GLY:HA2	1.99	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:HD12	1:B:166:ILE:HA	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:71:VAL:HG21	1:H:152:LYS:HG2	1.99	0.44
1:H:103:PHE:O	2:H:306:HOH:O	2.20	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:77:GLU:OE2	1:D:44:ARG:HD3	2.17	0.43
1:C:166:ILE:HD13	1:C:166:ILE:HA	1.72	0.43
1:B:55:ARG:HA	1:B:55:ARG:HD2	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:G:143:ARG:NH1	1:H:94:ASP:OD1	2.52	0.43
1:H:191:ALA:O	1:H:193:ARG:HG3	2.18	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:C:128:VAL:O	1:C:141:LYS:NZ	2.52	0.42
1:D:35:GLU:OE1	1:D:116:LYS:NZ	2.52	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:F:204:ARG:HH12	1:G:80:GLY:N	2.18	0.41
1:G:204:ARG:HD2	1:I:36:TYR:OH	2.20	0.41
1:K:174:SER:O	1:K:177:LYS:HB3	2.20	0.41
1:K:184:LEU:HD12	1:K:184:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:176:ASN:C	1:E:178:LEU:H	2.28	0.41
1:G:160:ASN:HA	1:G:164:ASN:HB3	2.02	0.41
1:C:77:GLU:CD	1:D:44:ARG:HH11	2.28	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:HD23	1:I:167:LEU:HA	1.89	0.41
1:E:78:MET:HE2	1:E:78:MET:HB2	1.92	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: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: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

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%)	149 (99%)	1 (1%)	76	88
1	E	150/171 (88%)	149 (99%)	1 (1%)	76	88
1	F	150/171 (88%)	149 (99%)	1 (1%)	76	88
1	G	150/171 (88%)	149 (99%)	1 (1%)	76	88
1	H	150/171 (88%)	150 (100%)	0	100	100
1	I	150/171 (88%)	148 (99%)	2 (1%)	61	80
1	J	150/171 (88%)	150 (100%)	0	100	100
1	K	154/171 (90%)	153 (99%)	1 (1%)	78	89
All	All	1654/1881 (88%)	1647 (100%)	7 (0%)	84	92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	208	CYS
1	E	166	ILE
1	F	208	CYS
1	G	148	THR
1	I	148	THR
1	I	186	VAL
1	K	47	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	HIS
1	D	100	ASN
1	E	37	GLN
1	E	114	GLN
1	F	69	HIS
1	G	28	GLN
1	G	69	HIS
1	G	114	GLN
1	G	164	ASN
1	G	181	GLN
1	H	37	GLN
1	H	160	ASN
1	H	164	ASN
1	H	194	GLN

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Mol	Chain	Res	Type
1	I	164	ASN
1	J	164	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	184/215 (85%)	0.07	9 (4%)	35 31	23, 37, 86, 140	0
1	B	184/215 (85%)	0.20	9 (4%)	35 31	20, 36, 85, 102	0
1	C	184/215 (85%)	0.26	12 (6%)	25 21	20, 40, 101, 133	0
1	D	184/215 (85%)	0.27	13 (7%)	22 18	19, 40, 88, 119	0
1	E	184/215 (85%)	0.32	12 (6%)	25 21	23, 43, 86, 104	0
1	F	184/215 (85%)	0.84	27 (14%)	6 4	28, 56, 107, 130	0
1	G	184/215 (85%)	1.68	65 (35%)	1 1	37, 71, 133, 153	0
1	H	184/215 (85%)	1.80	72 (39%)	1 0	44, 74, 151, 170	0
1	I	184/215 (85%)	1.68	57 (30%)	1 1	42, 70, 140, 168	0
1	J	184/215 (85%)	1.34	43 (23%)	2 1	35, 58, 119, 159	0
1	K	188/215 (87%)	0.53	11 (5%)	28 24	28, 48, 94, 127	0
All	All	2028/2365 (85%)	0.82	330 (16%)	4 4	19, 53, 117, 170	0

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	58	GLY	7.4
1	B	59	GLY	7.1
1	B	58	GLY	5.2
1	B	60	GLY	5.2
1	D	57	ALA	5.1
1	J	57	ALA	4.7
1	D	59	GLY	4.5
1	I	166	ILE	4.5
1	J	58	GLY	4.3
1	I	184	LEU	4.3
1	H	167	LEU	4.3
1	I	65	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	J	59	GLY	4.1
1	C	184	LEU	4.1
1	I	178	LEU	4.1
1	A	58	GLY	4.1
1	H	182	LEU	4.0
1	H	156	ARG	3.9
1	G	186	VAL	3.9
1	J	182	LEU	3.8
1	J	48	GLY	3.8
1	I	171	TYR	3.7
1	I	165	CYS	3.7
1	C	182	LEU	3.7
1	H	188	LEU	3.7
1	A	56	MET	3.7
1	G	156	ARG	3.7
1	J	167	LEU	3.6
1	H	171	TYR	3.6
1	H	184	LEU	3.6
1	G	171	TYR	3.6
1	I	101	GLY	3.5
1	H	183	PRO	3.5
1	H	79	PHE	3.5
1	D	184	LEU	3.5
1	H	132	LEU	3.5
1	J	184	LEU	3.5
1	H	65	TYR	3.5
1	G	184	LEU	3.4
1	I	167	LEU	3.4
1	G	182	LEU	3.4
1	C	179	PRO	3.4
1	F	186	VAL	3.4
1	J	175	LEU	3.4
1	G	205	TYR	3.4
1	G	167	LEU	3.4
1	I	64	CYS	3.3
1	H	162	LEU	3.3
1	H	172	LEU	3.3
1	J	166	ILE	3.3
1	F	205	TYR	3.3
1	E	184	LEU	3.3
1	G	39	ILE	3.3
1	G	65	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	181	GLN	3.3
1	J	165	CYS	3.3
1	G	175	LEU	3.3
1	J	56	MET	3.3
1	I	79	PHE	3.2
1	H	70	ARG	3.2
1	K	211	ASN	3.2
1	I	47	LEU	3.2
1	I	102	ALA	3.2
1	I	208	CYS	3.2
1	I	59	GLY	3.2
1	G	191	ALA	3.2
1	F	183	PRO	3.2
1	J	131	GLY	3.2
1	K	60	GLY	3.2
1	C	181	GLN	3.2
1	F	182	LEU	3.2
1	F	184	LEU	3.1
1	G	57	ALA	3.1
1	I	179	PRO	3.1
1	G	71	VAL	3.1
1	H	205	TYR	3.1
1	A	182	LEU	3.1
1	C	178	LEU	3.1
1	G	199	SER	3.1
1	H	206	ASN	3.1
1	G	63	VAL	3.1
1	I	177	LYS	3.0
1	G	200	VAL	3.0
1	F	196	LEU	3.0
1	G	66	ILE	3.0
1	I	63	VAL	3.0
1	G	56	MET	3.0
1	G	75	ALA	3.0
1	H	186	VAL	3.0
1	A	184	LEU	3.0
1	I	182	LEU	3.0
1	C	208	CYS	3.0
1	J	60	GLY	3.0
1	I	186	VAL	2.9
1	H	189	THR	2.9
1	E	57	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	203	ALA	2.9
1	A	59	GLY	2.9
1	H	43	LEU	2.9
1	H	36	TYR	2.9
1	H	61	GLN	2.9
1	H	59	GLY	2.9
1	F	200	VAL	2.9
1	H	155	LEU	2.9
1	I	172	LEU	2.9
1	I	175	LEU	2.9
1	H	191	ALA	2.8
1	H	194	GLN	2.8
1	I	56	MET	2.8
1	H	179	PRO	2.8
1	B	182	LEU	2.8
1	F	56	MET	2.8
1	I	36	TYR	2.8
1	I	176	ASN	2.8
1	J	63	VAL	2.8
1	B	57	ALA	2.8
1	J	98	LEU	2.8
1	C	58	GLY	2.8
1	E	200	VAL	2.8
1	G	132	LEU	2.8
1	H	83	GLY	2.7
1	J	100	ASN	2.7
1	G	129	SER	2.7
1	I	174	SER	2.7
1	H	74	LEU	2.7
1	H	158	PHE	2.7
1	I	80	GLY	2.7
1	I	207	SER	2.7
1	F	188	LEU	2.7
1	H	42	ALA	2.7
1	G	64	CYS	2.7
1	H	165	CYS	2.7
1	F	198	PRO	2.7
1	G	25	CYS	2.7
1	K	59	GLY	2.7
1	B	184	LEU	2.7
1	H	175	LEU	2.7
1	H	180	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	205	TYR	2.7
1	F	81	TYR	2.7
1	H	51	TYR	2.7
1	H	148	THR	2.7
1	B	61	GLN	2.7
1	F	101	GLY	2.6
1	G	159	GLY	2.6
1	I	52	ILE	2.6
1	J	99	ASN	2.6
1	H	38	ALA	2.6
1	H	75	ALA	2.6
1	H	166	ILE	2.6
1	J	193	ARG	2.6
1	G	74	LEU	2.6
1	H	128	VAL	2.6
1	E	61	GLN	2.6
1	F	191	ALA	2.6
1	J	169	LYS	2.6
1	D	56	MET	2.6
1	J	52	ILE	2.6
1	H	178	LEU	2.6
1	H	56	MET	2.6
1	H	52	ILE	2.6
1	G	79	PHE	2.6
1	E	182	LEU	2.6
1	G	178	LEU	2.6
1	G	188	LEU	2.6
1	D	208	CYS	2.6
1	G	81	TYR	2.6
1	G	49	PRO	2.5
1	H	58	GLY	2.5
1	I	145	GLU	2.5
1	G	183	PRO	2.5
1	H	131	GLY	2.5
1	G	52	ILE	2.5
1	H	84	TRP	2.5
1	G	162	LEU	2.5
1	G	128	VAL	2.5
1	J	186	VAL	2.5
1	D	55	ARG	2.5
1	K	25	CYS	2.5
1	G	78	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	51	TYR	2.5
1	H	63	VAL	2.5
1	I	136	ALA	2.5
1	H	53	SER	2.5
1	F	25	CYS	2.5
1	F	29	CYS	2.5
1	G	172	LEU	2.5
1	I	124	VAL	2.5
1	I	180	ARG	2.5
1	H	174	SER	2.5
1	E	58	GLY	2.4
1	I	156	ARG	2.4
1	H	100	ASN	2.4
1	I	130	GLU	2.4
1	E	59	GLY	2.4
1	F	208	CYS	2.4
1	H	64	CYS	2.4
1	I	58	GLY	2.4
1	G	59	GLY	2.4
1	G	80	GLY	2.4
1	G	166	ILE	2.4
1	B	104	TYR	2.4
1	C	57	ALA	2.4
1	E	191	ALA	2.4
1	I	53	SER	2.4
1	K	207	SER	2.4
1	G	137	LEU	2.4
1	G	181	GLN	2.4
1	G	196	LEU	2.4
1	I	74	LEU	2.4
1	G	29	CYS	2.4
1	E	205	TYR	2.4
1	A	206	ASN	2.4
1	J	191	ALA	2.4
1	H	32	THR	2.3
1	G	60	GLY	2.3
1	H	34	GLU	2.3
1	J	183	PRO	2.3
1	H	55	ARG	2.3
1	J	54	SER	2.3
1	H	47	LEU	2.3
1	J	170	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	190	LYS	2.3
1	J	55	ARG	2.3
1	G	83	GLY	2.3
1	H	190	LYS	2.3
1	G	208	CYS	2.3
1	H	104	TYR	2.3
1	F	75	ALA	2.3
1	F	59	GLY	2.3
1	G	131	GLY	2.3
1	G	43	LEU	2.3
1	H	66	ILE	2.3
1	H	35	GLU	2.3
1	G	55	ARG	2.3
1	I	183	PRO	2.3
1	J	179	PRO	2.3
1	K	208	CYS	2.3
1	I	57	ALA	2.2
1	D	60	GLY	2.2
1	F	58	GLY	2.2
1	J	61	GLN	2.2
1	E	56	MET	2.2
1	I	66	ILE	2.2
1	I	188	LEU	2.2
1	I	75	ALA	2.2
1	G	104	TYR	2.2
1	J	171	TYR	2.2
1	F	28	GLN	2.2
1	J	30	GLN	2.2
1	I	27	GLY	2.2
1	I	131	GLY	2.2
1	J	47	LEU	2.2
1	I	70	ARG	2.2
1	G	31	TYR	2.2
1	C	180	ARG	2.2
1	A	60	GLY	2.2
1	A	208	CYS	2.2
1	E	60	GLY	2.2
1	H	127	GLY	2.2
1	H	54	SER	2.2
1	I	199	SER	2.2
1	F	185	GLU	2.2
1	H	153	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	55	ARG	2.2
1	C	190	LYS	2.2
1	G	62	LYS	2.2
1	I	105	VAL	2.1
1	I	154	ALA	2.1
1	J	42	ALA	2.1
1	D	182	LEU	2.1
1	H	48	GLY	2.1
1	J	65	TYR	2.1
1	H	208	CYS	2.1
1	I	46	ARG	2.1
1	J	46	ARG	2.1
1	G	177	LYS	2.1
1	H	78	MET	2.1
1	G	161	ALA	2.1
1	H	39	ILE	2.1
1	D	205	TYR	2.1
1	F	180	ARG	2.1
1	G	51	TYR	2.1
1	G	130	GLU	2.1
1	A	207	SER	2.1
1	G	53	SER	2.1
1	H	129	SER	2.1
1	K	174	SER	2.1
1	C	183	PRO	2.1
1	K	179	PRO	2.1
1	H	133	ALA	2.1
1	H	164	ASN	2.1
1	J	189	THR	2.1
1	K	58	GLY	2.1
1	I	67	GLU	2.1
1	J	185	GLU	2.1
1	J	62	LYS	2.1
1	F	199	SER	2.1
1	F	179	PRO	2.1
1	G	69	HIS	2.1
1	H	40	GLN	2.1
1	D	63	VAL	2.1
1	F	202	ALA	2.1
1	G	203	ALA	2.1
1	I	133	ALA	2.1
1	F	132	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	196	LEU	2.1
1	J	101	GLY	2.1
1	J	156	ARG	2.1
1	G	72	ILE	2.1
1	H	187	ASP	2.1
1	J	51	TYR	2.1
1	D	25	CYS	2.1
1	D	198	PRO	2.1
1	G	179	PRO	2.1
1	E	194	GLN	2.0
1	J	33	ALA	2.0
1	I	89	THR	2.0
1	J	157	SER	2.0
1	I	29	CYS	2.0
1	G	173	ARG	2.0
1	I	162	LEU	2.0
1	I	191	ALA	2.0
1	K	57	ALA	2.0
1	K	175	LEU	2.0
1	G	206	ASN	2.0
1	H	82	ASN	2.0
1	G	195	ASP	2.0
1	H	81	TYR	2.0
1	J	69	HIS	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 oligosaccharides 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.