Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 06:54 PM JST

PDB ID	:	5XS0
Title	:	Structure of a ssDNA bound to the outer DNA binding site of RAD52
Authors	:	Saotome, M.; Saito, K.; Yasuda, T.; Sugiyama, S.; Kurumizaka, H.; Kagawa, W.
Deposited on	:	2017-06-11
Resolution	:	3.00 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:

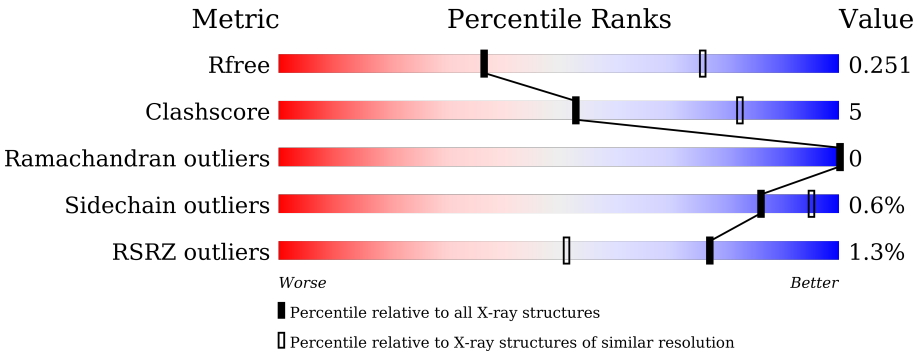
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	73% 12% 14%
1	B	215	70% 13% 17%
1	C	215	71% 14% 14%
1	D	215	76% 9% 14%
1	E	215	75% 11% 14%
1	F	215	74% 11% 14%

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Mol	Chain	Length	Quality of chain
1	G	215	2% 70% 15% 14%
1	H	215	1% 73% 12% 14%
1	I	215	73% 13% 14%
1	J	215	1% 70% 16% 14%
1	K	215	73% 12% 14%
1	L	215	2% 77% 8% 14%
1	M	215	2% 73% 10% 17%
1	N	215	72% 13% 14%
1	O	215	1% 75% 10% 14%
1	P	215	72% 14% 14%
1	Q	215	74% 12% 14%
1	R	215	72% 13% 14%
1	S	215	1% 73% 13% 14%
1	T	215	1% 73% 13% 14%
1	U	215	1% 73% 13% 14%
1	V	215	1% 77% 8% 14%
2	W	6	83% 17%
3	X	8	62% 38%
4	Y	10	40% 60%
5	Z	9	67% 33%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 32445 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
			1450	907	261	274	8			
1	B	178	Total	C	N	O	S	0	0	0
			1415	887	253	267	8			
1	C	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	D	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	E	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	F	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	G	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	H	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	I	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	J	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	K	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	L	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	M	178	Total	C	N	O	S	0	0	0
			1415	887	253	267	8			
1	N	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	O	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	P	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	R	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	S	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	T	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	U	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			
1	V	184	Total	C	N	O	S	0	0	0
			1450	907	261	274	8			

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
B	-2	GLY	-	expression tag	UNP P43351
B	-1	SER	-	expression tag	UNP P43351
B	0	HIS	-	expression tag	UNP P43351
C	-2	GLY	-	expression tag	UNP P43351
C	-1	SER	-	expression tag	UNP P43351
C	0	HIS	-	expression tag	UNP P43351
D	-2	GLY	-	expression tag	UNP P43351
D	-1	SER	-	expression tag	UNP P43351
D	0	HIS	-	expression tag	UNP P43351
E	-2	GLY	-	expression tag	UNP P43351
E	-1	SER	-	expression tag	UNP P43351
E	0	HIS	-	expression tag	UNP P43351
F	-2	GLY	-	expression tag	UNP P43351
F	-1	SER	-	expression tag	UNP P43351
F	0	HIS	-	expression tag	UNP P43351
G	-2	GLY	-	expression tag	UNP P43351
G	-1	SER	-	expression tag	UNP P43351
G	0	HIS	-	expression tag	UNP P43351
H	-2	GLY	-	expression tag	UNP P43351
H	-1	SER	-	expression tag	UNP P43351
H	0	HIS	-	expression tag	UNP P43351
I	-2	GLY	-	expression tag	UNP P43351
I	-1	SER	-	expression tag	UNP P43351
I	0	HIS	-	expression tag	UNP P43351

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-2	GLY	-	expression tag	UNP P43351
J	-1	SER	-	expression tag	UNP P43351
J	0	HIS	-	expression tag	UNP P43351
K	-2	GLY	-	expression tag	UNP P43351
K	-1	SER	-	expression tag	UNP P43351
K	0	HIS	-	expression tag	UNP P43351
L	-2	GLY	-	expression tag	UNP P43351
L	-1	SER	-	expression tag	UNP P43351
L	0	HIS	-	expression tag	UNP P43351
M	-2	GLY	-	expression tag	UNP P43351
M	-1	SER	-	expression tag	UNP P43351
M	0	HIS	-	expression tag	UNP P43351
N	-2	GLY	-	expression tag	UNP P43351
N	-1	SER	-	expression tag	UNP P43351
N	0	HIS	-	expression tag	UNP P43351
O	-2	GLY	-	expression tag	UNP P43351
O	-1	SER	-	expression tag	UNP P43351
O	0	HIS	-	expression tag	UNP P43351
P	-2	GLY	-	expression tag	UNP P43351
P	-1	SER	-	expression tag	UNP P43351
P	0	HIS	-	expression tag	UNP P43351
Q	-2	GLY	-	expression tag	UNP P43351
Q	-1	SER	-	expression tag	UNP P43351
Q	0	HIS	-	expression tag	UNP P43351
R	-2	GLY	-	expression tag	UNP P43351
R	-1	SER	-	expression tag	UNP P43351
R	0	HIS	-	expression tag	UNP P43351
S	-2	GLY	-	expression tag	UNP P43351
S	-1	SER	-	expression tag	UNP P43351
S	0	HIS	-	expression tag	UNP P43351
T	-2	GLY	-	expression tag	UNP P43351
T	-1	SER	-	expression tag	UNP P43351
T	0	HIS	-	expression tag	UNP P43351
U	-2	GLY	-	expression tag	UNP P43351
U	-1	SER	-	expression tag	UNP P43351
U	0	HIS	-	expression tag	UNP P43351
V	-2	GLY	-	expression tag	UNP P43351
V	-1	SER	-	expression tag	UNP P43351
V	0	HIS	-	expression tag	UNP P43351

- Molecule 2 is a DNA chain called ssDNA (5'-D(*CP*CP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	6	Total	C	N	O	P	0	0	0
			111	54	18	34	5			

- Molecule 3 is a DNA chain called ssDNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	8	Total	C	N	O	P	0	0	0
			149	72	24	46	7			

- Molecule 4 is a DNA chain called ssDNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Y	10	Total	C	N	O	P	0	0	0
			187	90	30	58	9			

- Molecule 5 is a DNA chain called ssDNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*C)-3').

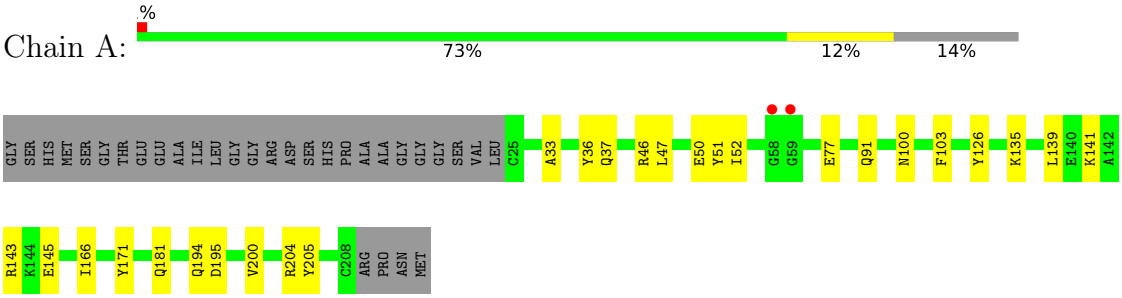
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Z	9	Total	C	N	O	P	0	0	0
			168	81	27	52	8			

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.

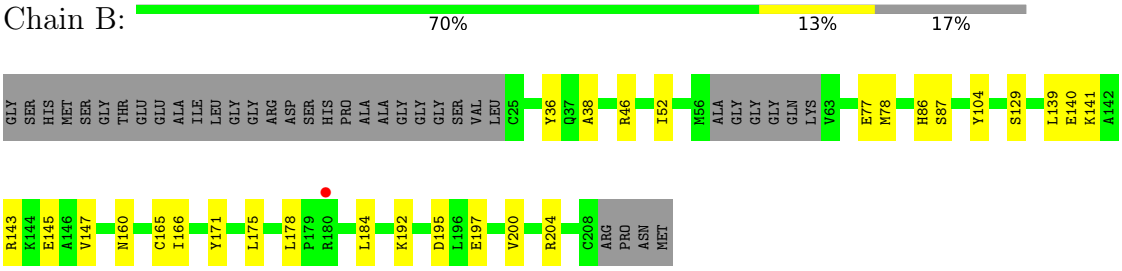
• Molecule 1: DNA repair protein RAD52 homolog

Chain A:



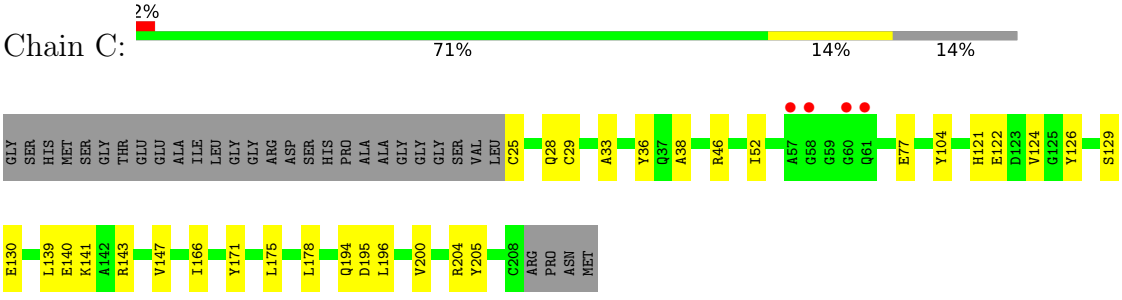
• Molecule 1: DNA repair protein RAD52 homolog

Chain B:



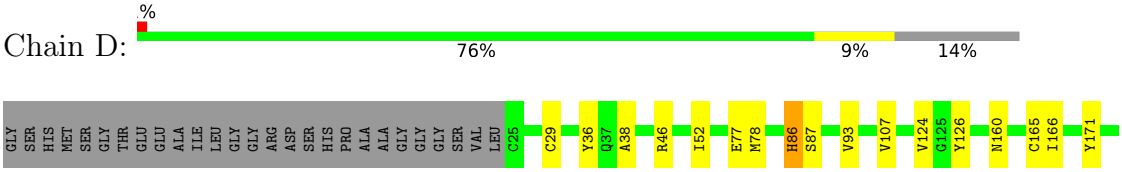
• Molecule 1: DNA repair protein RAD52 homolog

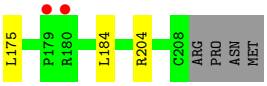
Chain C:



• Molecule 1: DNA repair protein RAD52 homolog

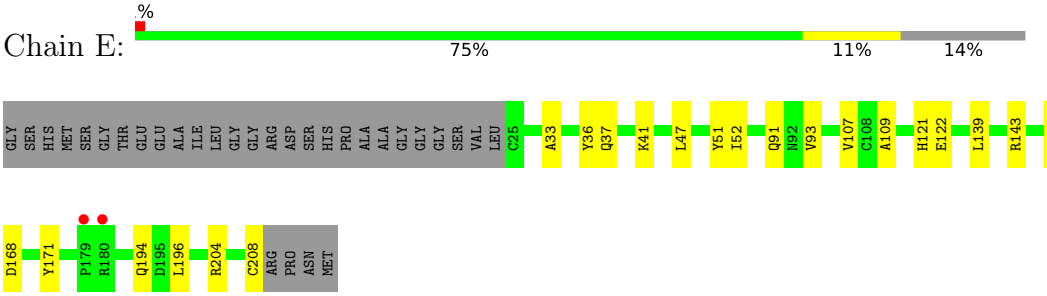
Chain D:





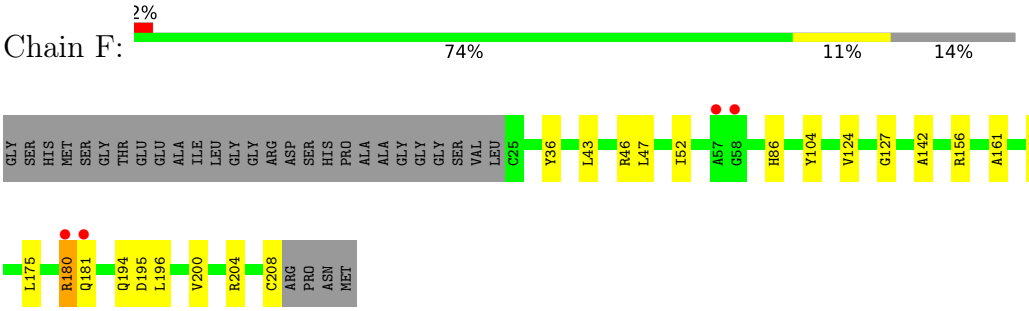
• Molecule 1: DNA repair protein RAD52 homolog

Chain E:



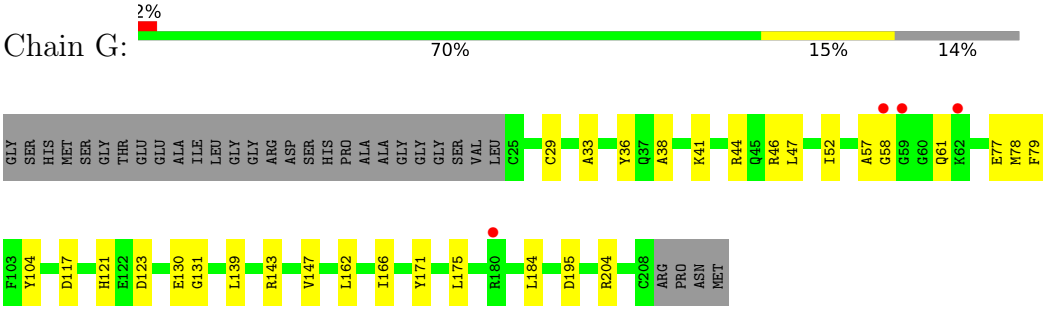
• Molecule 1: DNA repair protein RAD52 homolog

Chain F:



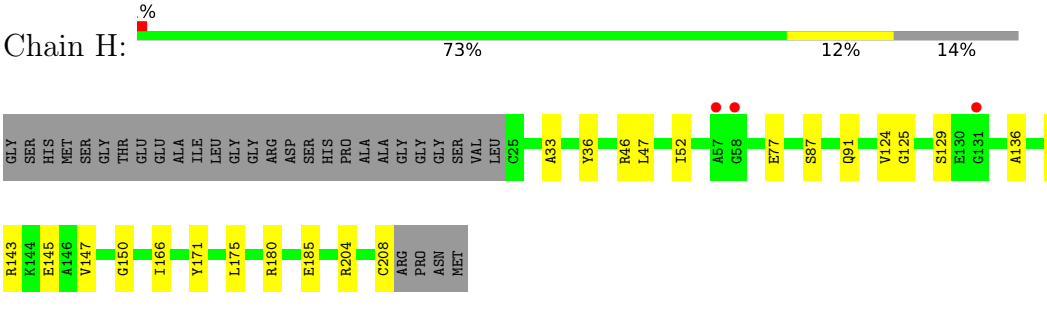
• Molecule 1: DNA repair protein RAD52 homolog

Chain G:



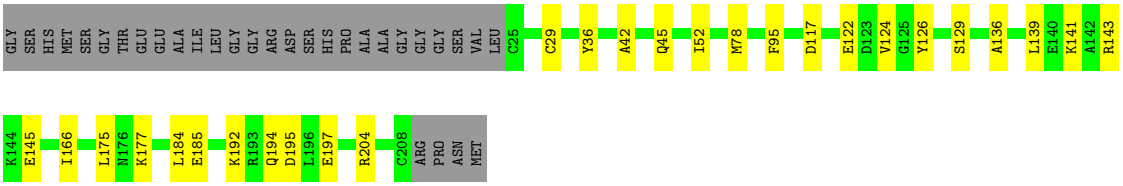
• Molecule 1: DNA repair protein RAD52 homolog

Chain H:



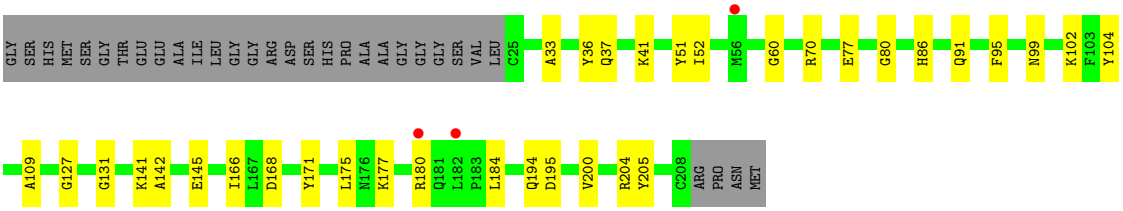
• Molecule 1: DNA repair protein RAD52 homolog

Chain I:



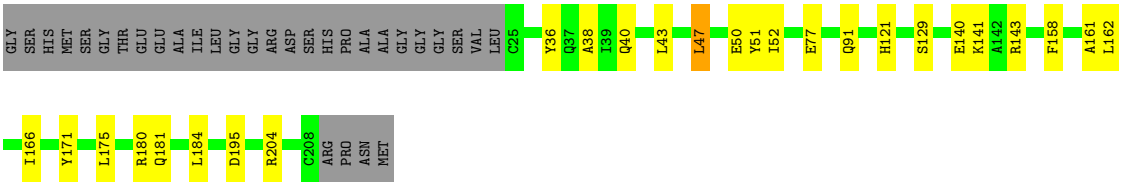
• Molecule 1: DNA repair protein RAD52 homolog

Chain J:



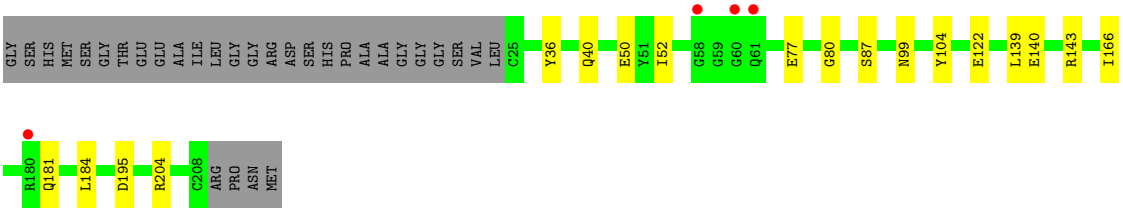
• Molecule 1: DNA repair protein RAD52 homolog

Chain K:



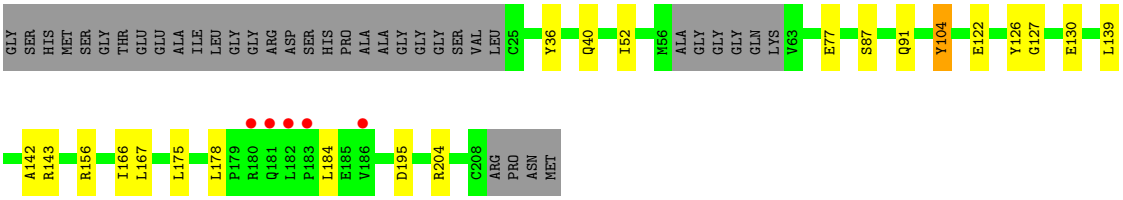
• Molecule 1: DNA repair protein RAD52 homolog

Chain L:



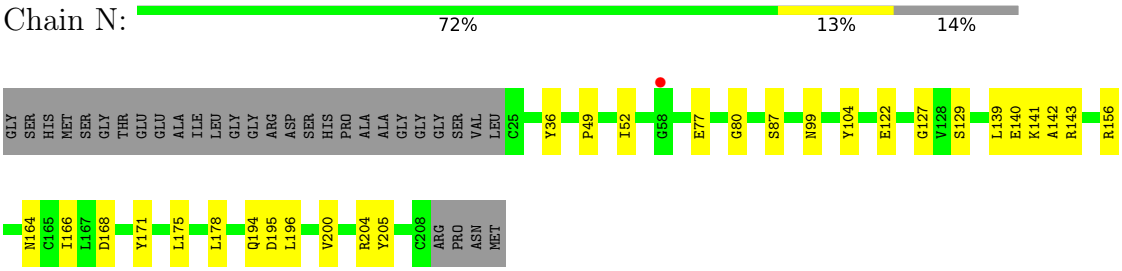
• Molecule 1: DNA repair protein RAD52 homolog

Chain M:



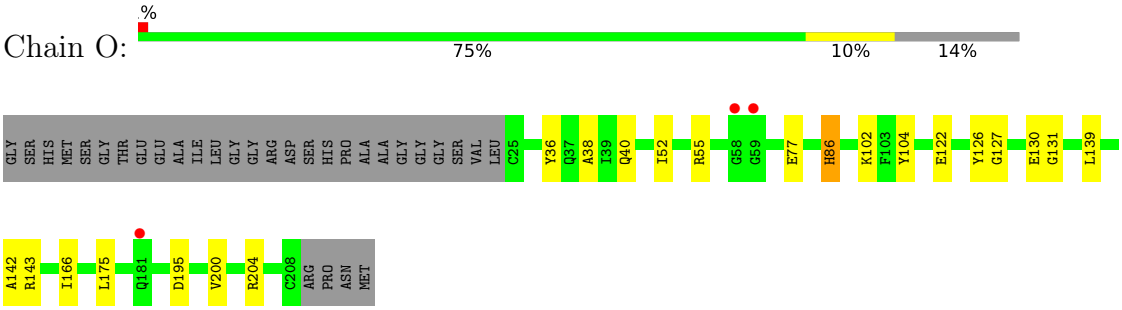
• Molecule 1: DNA repair protein RAD52 homolog

Chain N:



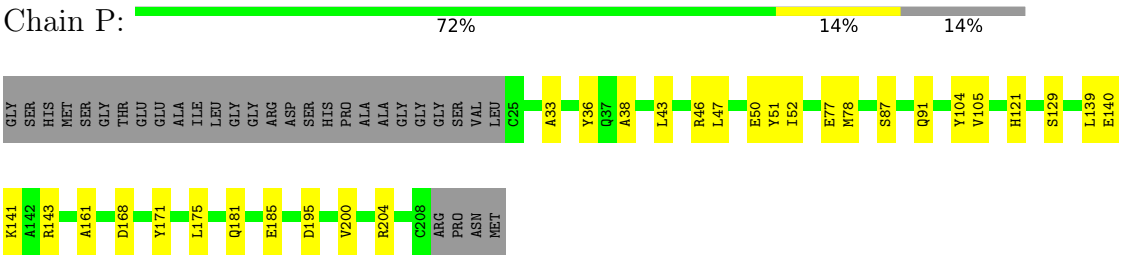
• Molecule 1: DNA repair protein RAD52 homolog

Chain O:



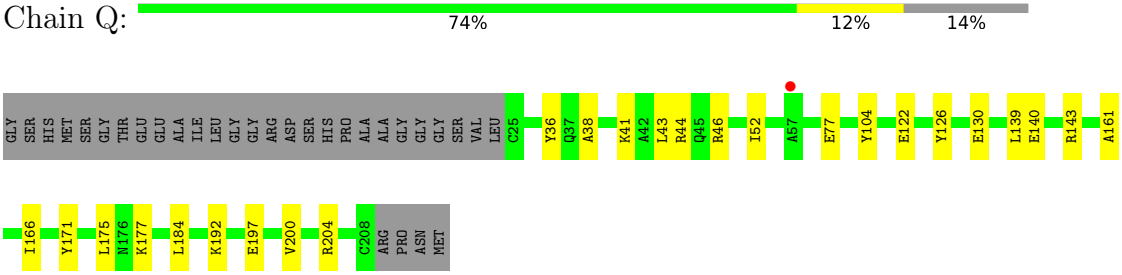
• Molecule 1: DNA repair protein RAD52 homolog

Chain P:



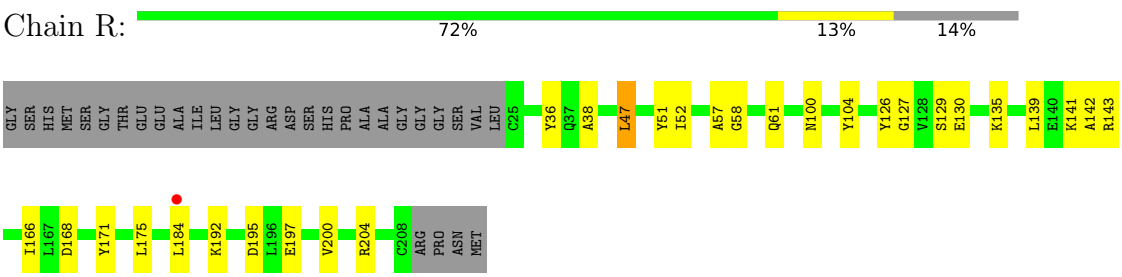
• Molecule 1: DNA repair protein RAD52 homolog

Chain Q:



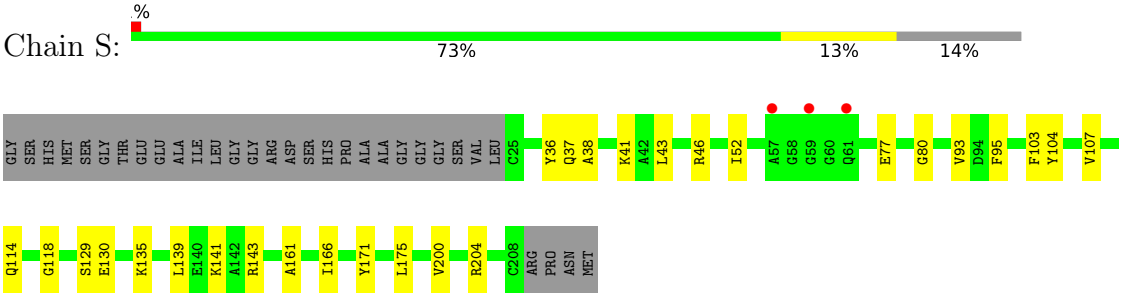
• Molecule 1: DNA repair protein RAD52 homolog

Chain R:



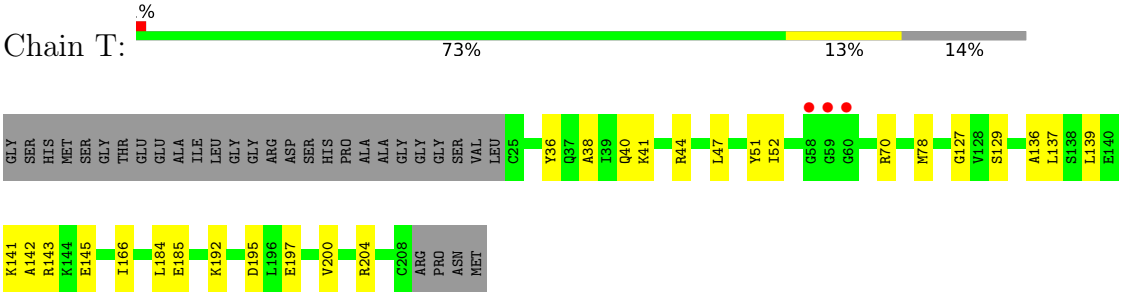
• Molecule 1: DNA repair protein RAD52 homolog

Chain S:



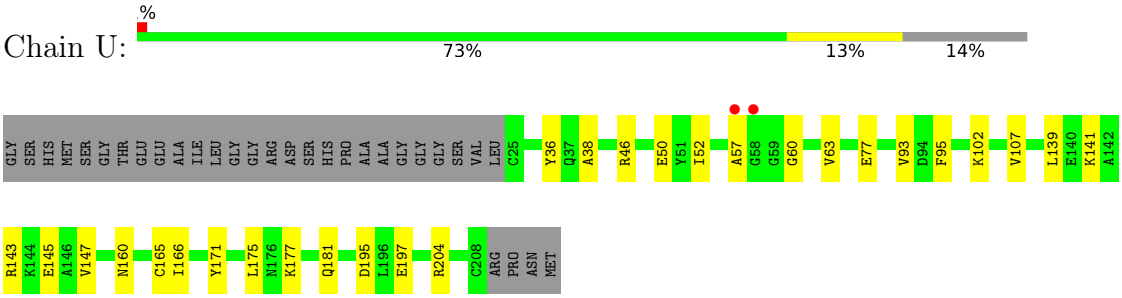
• Molecule 1: DNA repair protein RAD52 homolog

Chain T:



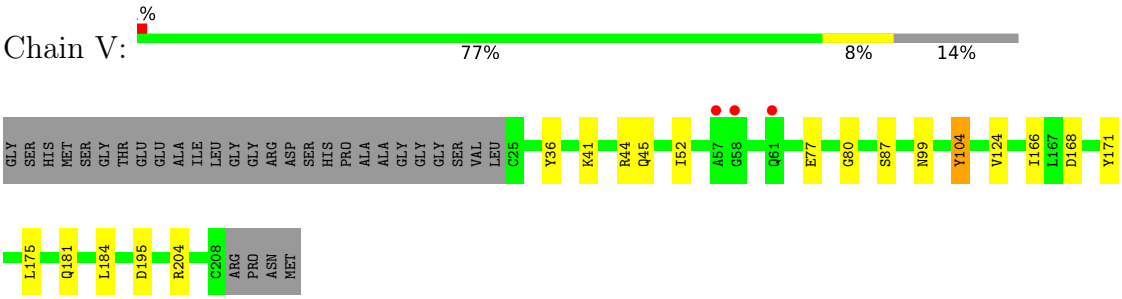
• Molecule 1: DNA repair protein RAD52 homolog

Chain U:



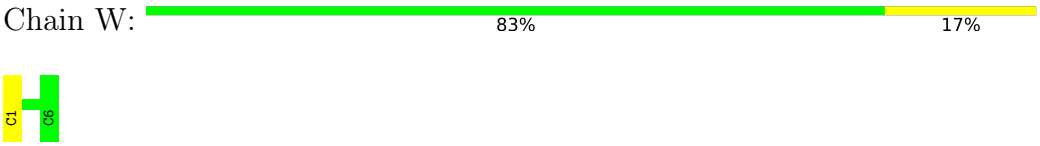
• Molecule 1: DNA repair protein RAD52 homolog

Chain V:



• Molecule 2: ssDNA (5'-D(*CP*CP*CP*CP*CP*C)-3')

Chain W:

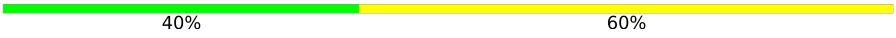


• Molecule 3: ssDNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*C)-3')

Chain X:

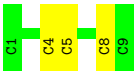
• Molecule 4: ssDNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')

Chain Y:



• Molecule 5: ssDNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.22Å 164.41Å 166.09Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	48.53 – 3.00 48.53 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.53-3.00) 99.9 (48.53-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.221 , 0.251 0.222 , 0.251	Depositor DCC
R_{free} test set	5188 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	70.8	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k 0.022 for -h,-l,-k 0.042 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32445	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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	0.27	0/1474	0.44	0/1981
1	B	0.26	0/1438	0.43	0/1933
1	C	0.27	0/1474	0.44	0/1981
1	D	0.26	0/1474	0.44	0/1981
1	E	0.27	0/1474	0.44	0/1981
1	F	0.26	0/1474	0.44	0/1981
1	G	0.27	0/1474	0.44	0/1981
1	H	0.27	0/1474	0.44	0/1981
1	I	0.27	0/1474	0.44	0/1981
1	J	0.26	0/1474	0.45	0/1981
1	K	0.25	0/1474	0.44	0/1981
1	L	0.27	0/1474	0.44	0/1981
1	M	0.26	0/1438	0.44	0/1933
1	N	0.26	0/1474	0.44	0/1981
1	O	0.27	0/1474	0.45	0/1981
1	P	0.26	0/1474	0.44	0/1981
1	Q	0.26	0/1474	0.44	0/1981
1	R	0.28	0/1474	0.45	0/1981
1	S	0.26	0/1474	0.44	0/1981
1	T	0.26	0/1474	0.44	0/1981
1	U	0.26	0/1474	0.44	0/1981
1	V	0.27	0/1474	0.45	0/1981
2	W	0.71	0/122	0.79	0/184
3	X	0.60	0/164	0.90	0/248
4	Y	0.70	0/206	0.77	0/312
5	Z	0.61	0/185	0.84	0/280
All	All	0.28	0/33033	0.45	0/44510

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	1450	0	1433	19	1
1	B	1415	0	1397	23	0
1	C	1450	0	1433	25	0
1	D	1450	0	1433	16	0
1	E	1450	0	1433	17	0
1	F	1450	0	1433	20	0
1	G	1450	0	1433	25	0
1	H	1450	0	1433	21	0
1	I	1450	0	1433	22	0
1	J	1450	0	1433	25	0
1	K	1450	0	1433	21	0
1	L	1450	0	1433	18	0
1	M	1415	0	1397	18	0
1	N	1450	0	1433	25	0
1	O	1450	0	1433	18	0
1	P	1450	0	1433	22	0
1	Q	1450	0	1433	19	0
1	R	1450	0	1433	21	0
1	S	1450	0	1433	20	0
1	T	1450	0	1433	26	0
1	U	1450	0	1433	21	1
1	V	1450	0	1433	19	0
2	W	111	0	68	1	0
3	X	149	0	90	3	0
4	Y	187	0	112	9	0
5	Z	168	0	101	3	0
All	All	32445	0	31825	348	1

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 5.

All (348) 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:T:185:GLU:OE2	1:U:177:LYS:NZ	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:ALA:HB3	1:G:61:GLN:HG3	1.71	0.70
1:N:99:ASN:HB2	1:N:104:TYR:HE1	1.57	0.69
1:R:57:ALA:HB3	1:R:61:GLN:HG3	1.75	0.69
1:J:37:GLN:HG2	1:J:41:LYS:HE2	1.76	0.68
1:M:195:ASP:HB3	1:N:77:GLU:HG3	1.76	0.67
1:R:52:ILE:HG13	1:R:175:LEU:HD11	1.79	0.64
1:H:185:GLU:OE2	1:I:177:LYS:NZ	2.31	0.64
1:L:204:ARG:NH1	1:N:36:TYR:OH	2.25	0.64
1:E:204:ARG:HD2	1:G:36:TYR:OH	1.98	0.63
1:I:42:ALA:HA	1:I:45:GLN:HE21	1.63	0.63
1:T:52:ILE:HD12	1:T:166:ILE:HD13	1.82	0.62
1:C:52:ILE:HD12	1:C:166:ILE:HD13	1.82	0.61
1:M:36:TYR:OH	1:V:204:ARG:NH1	2.31	0.60
5:Z:4:DC:H2"	5:Z:5:DC:OP1	2.00	0.60
1:G:195:ASP:HB3	1:H:77:GLU:HG3	1.83	0.60
1:O:102:LYS:NZ	4:Y:4:DC:OP2	2.26	0.60
1:C:204:ARG:HD2	1:E:36:TYR:OH	2.02	0.59
1:I:52:ILE:HD12	1:I:166:ILE:HD13	1.83	0.59
1:I:204:ARG:HD2	1:K:36:TYR:OH	2.03	0.59
1:P:168:ASP:HB3	1:P:171:TYR:HB3	1.85	0.59
1:H:52:ILE:HG13	1:H:175:LEU:HD11	1.85	0.58
1:O:204:ARG:HD2	1:Q:36:TYR:OH	2.03	0.58
1:F:204:ARG:NH2	1:G:78:MET:O	2.36	0.58
1:L:36:TYR:OH	1:U:204:ARG:NH1	2.32	0.58
1:S:204:ARG:NH2	1:T:78:MET:O	2.36	0.58
1:U:52:ILE:HD12	1:U:166:ILE:HD13	1.85	0.58
1:V:52:ILE:HG13	1:V:175:LEU:HD11	1.85	0.58
1:K:47:LEU:O	1:K:171:TYR:OH	2.17	0.58
1:S:80:GLY:HA2	1:T:40:GLN:HE22	1.68	0.58
1:D:204:ARG:HD2	1:F:36:TYR:OH	2.04	0.57
1:L:77:GLU:HG3	1:V:195:ASP:HB3	1.85	0.57
1:O:52:ILE:HG13	1:O:175:LEU:HD11	1.87	0.57
1:U:195:ASP:HB3	1:V:77:GLU:HG3	1.87	0.57
1:S:52:ILE:HG13	1:S:175:LEU:HD11	1.87	0.57
1:G:52:ILE:HG13	1:G:175:LEU:HD11	1.87	0.56
1:I:192:LYS:NZ	1:I:197:GLU:OE2	2.31	0.56
1:U:50:GLU:HG3	1:U:181:GLN:HE22	1.70	0.56
1:M:36:TYR:OH	1:V:204:ARG:HD2	2.06	0.56
1:T:195:ASP:HB3	1:U:77:GLU:HG3	1.87	0.56
1:K:52:ILE:HD12	1:K:166:ILE:HD13	1.86	0.56
1:J:200:VAL:HG22	1:K:38:ALA:HB1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:140:GLU:HB2	1:O:126:TYR:CD2	2.41	0.56
1:G:204:ARG:HD2	1:I:36:TYR:OH	2.05	0.56
1:R:195:ASP:HB3	1:S:77:GLU:HG3	1.87	0.56
1:G:58:GLY:HA3	4:Y:3:DC:H4'	1.88	0.55
1:T:200:VAL:HG22	1:U:38:ALA:HB1	1.89	0.55
1:R:204:ARG:HD2	1:T:36:TYR:OH	2.06	0.55
1:L:52:ILE:HD12	1:L:166:ILE:HD13	1.88	0.55
1:P:195:ASP:HB3	1:Q:77:GLU:HG3	1.89	0.55
1:J:195:ASP:HB3	1:K:77:GLU:HG3	1.89	0.55
4:Y:1:DC:H3'	4:Y:2:DC:C6	2.41	0.55
1:A:204:ARG:HD2	1:C:36:TYR:OH	2.07	0.55
1:P:204:ARG:HD2	1:R:36:TYR:OH	2.06	0.55
1:U:160:ASN:HB3	1:U:165:CYS:HB3	1.89	0.55
1:C:129:SER:HB2	1:C:141:LYS:HD2	1.89	0.54
1:B:175:LEU:HD23	1:B:178:LEU:HD12	1.89	0.54
1:F:195:ASP:HB3	1:G:77:GLU:HG3	1.90	0.54
1:I:195:ASP:HB3	1:J:77:GLU:HG3	1.90	0.54
1:O:200:VAL:HG22	1:P:38:ALA:HB1	1.90	0.54
1:N:204:ARG:HD2	1:P:36:TYR:OH	2.07	0.54
1:P:50:GLU:HG3	1:P:181:GLN:OE1	2.07	0.54
1:D:52:ILE:HD12	1:D:166:ILE:HD13	1.88	0.54
1:L:140:GLU:HB2	1:M:126:TYR:CD2	2.43	0.54
1:F:204:ARG:HD2	1:H:36:TYR:OH	2.07	0.54
1:R:52:ILE:HD12	1:R:166:ILE:HD13	1.89	0.54
1:N:195:ASP:HB3	1:O:77:GLU:HG3	1.91	0.53
1:C:204:ARG:NH2	1:D:78:MET:O	2.41	0.53
1:Q:204:ARG:HD2	1:S:36:TYR:OH	2.08	0.53
3:X:4:DC:H2"	3:X:5:DC:OP1	2.07	0.53
1:B:52:ILE:HD12	1:B:166:ILE:HD13	1.90	0.53
1:A:195:ASP:HB3	1:B:77:GLU:HG3	1.91	0.53
1:Q:140:GLU:HB2	1:R:126:TYR:CD2	2.43	0.53
1:S:80:GLY:HA2	1:T:40:GLN:NE2	2.24	0.53
1:U:102:LYS:NZ	3:X:5:DC:OP2	2.34	0.53
1:M:156:ARG:HD3	1:M:167:LEU:HD11	1.91	0.53
1:V:52:ILE:HD12	1:V:166:ILE:HD13	1.91	0.53
1:B:204:ARG:HD2	1:D:36:TYR:OH	2.08	0.53
1:L:99:ASN:HB2	1:L:104:TYR:CE1	2.44	0.52
1:I:185:GLU:OE2	1:J:177:LYS:NZ	2.32	0.52
1:U:57:ALA:HB3	1:U:63:VAL:HG21	1.90	0.52
4:Y:1:DC:H3'	4:Y:2:DC:H6	1.73	0.52
1:G:104:TYR:CD2	1:G:130:GLU:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:204:ARG:NH2	1:P:78:MET:O	2.41	0.52
1:C:52:ILE:HG13	1:C:175:LEU:HD11	1.91	0.52
1:G:52:ILE:HD12	1:G:166:ILE:HD13	1.90	0.52
1:U:147:VAL:HG21	1:V:124:VAL:HG23	1.91	0.52
1:U:197:GLU:OE2	1:V:45:GLN:NE2	2.37	0.52
1:T:41:LYS:HG2	1:T:44:ARG:HH21	1.74	0.52
1:J:52:ILE:HG13	1:J:175:LEU:HD11	1.92	0.52
1:Q:192:LYS:NZ	1:Q:197:GLU:OE2	2.35	0.52
1:T:137:LEU:HD22	3:X:2:DC:H2"	1.92	0.52
1:B:36:TYR:OH	1:K:204:ARG:HD2	2.09	0.52
1:L:204:ARG:HD2	1:N:36:TYR:OH	2.10	0.51
1:R:204:ARG:NH1	1:T:36:TYR:OH	2.34	0.51
1:A:77:GLU:HG3	1:K:195:ASP:HB3	1.93	0.51
1:S:129:SER:HB2	1:S:141:LYS:HD2	1.93	0.51
1:J:102:LYS:HD3	1:J:131:GLY:HA2	1.92	0.51
1:F:52:ILE:HD12	1:F:166:ILE:HD13	1.92	0.51
1:N:99:ASN:HB2	1:N:104:TYR:CE1	2.42	0.50
1:S:104:TYR:CD2	1:S:130:GLU:HB3	2.45	0.50
1:F:168:ASP:HB3	1:F:171:TYR:HB3	1.93	0.50
1:J:91:GLN:HE21	1:J:109:ALA:HB2	1.76	0.50
1:L:36:TYR:OH	1:U:204:ARG:HD2	2.12	0.50
1:T:204:ARG:HD2	1:V:36:TYR:OH	2.11	0.50
1:U:141:LYS:HE2	1:U:145:GLU:OE2	2.11	0.50
1:C:200:VAL:HG22	1:D:38:ALA:HB1	1.93	0.50
1:H:204:ARG:HD2	1:J:36:TYR:OH	2.12	0.50
1:Q:200:VAL:HG22	1:R:38:ALA:HB1	1.94	0.50
1:T:47:LEU:HB3	1:T:51:TYR:HD2	1.76	0.50
1:U:46:ARG:HD3	1:U:171:TYR:CD2	2.47	0.50
1:A:36:TYR:OH	1:J:204:ARG:HD2	2.12	0.49
1:S:52:ILE:HD12	1:S:166:ILE:HD13	1.94	0.49
1:F:208:CYS:HB2	1:H:33:ALA:HB2	1.93	0.49
1:I:141:LYS:HE2	1:I:145:GLU:OE2	2.12	0.49
1:L:139:LEU:O	1:L:143:ARG:HG3	2.12	0.49
1:B:195:ASP:HB3	1:C:77:GLU:HG3	1.94	0.49
1:M:52:ILE:HD12	1:M:166:ILE:HD13	1.93	0.49
1:G:91:GLN:OE1	1:G:143:ARG:NE	2.41	0.49
1:U:50:GLU:HG3	1:U:181:GLN:NE2	2.27	0.49
1:V:41:LYS:HG2	1:V:44:ARG:HH21	1.77	0.49
1:B:86:HIS:ND1	1:C:121:HIS:HD2	2.11	0.49
1:N:49:PRO:HG3	1:N:178:LEU:HD13	1.94	0.49
1:N:52:ILE:HD12	1:N:166:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:47:LEU:HD22	1:P:51:TYR:CD2	2.48	0.49
1:B:160:ASN:HB3	1:B:165:CYS:HB3	1.95	0.49
1:R:58:GLY:HA3	2:W:1:DC:O3'	2.13	0.49
1:F:194:GLN:NE2	1:F:196:LEU:O	2.44	0.48
1:J:141:LYS:HE2	1:J:145:GLU:OE2	2.12	0.48
1:S:200:VAL:HG22	1:T:38:ALA:HB1	1.94	0.48
1:U:52:ILE:HG13	1:U:175:LEU:HD11	1.95	0.48
1:L:40:GLN:HE22	1:V:80:GLY:HA2	1.78	0.48
1:M:204:ARG:HD2	1:O:36:TYR:OH	2.13	0.48
1:C:139:LEU:O	1:C:143:ARG:HG3	2.13	0.48
1:N:129:SER:HB2	1:N:141:LYS:HD2	1.95	0.48
1:A:204:ARG:NH2	1:B:78:MET:O	2.46	0.48
1:F:46:ARG:HD3	1:F:171:TYR:HD1	1.79	0.48
1:L:50:GLU:HG3	1:L:181:GLN:OE1	2.14	0.48
1:M:127:GLY:HA3	1:M:142:ALA:O	2.13	0.48
1:H:208:CYS:HB2	1:J:33:ALA:HB2	1.95	0.48
1:J:80:GLY:HA2	1:K:40:GLN:HE22	1.78	0.48
1:F:180:ARG:NH1	1:F:181:GLN:O	2.47	0.48
1:I:29:CYS:O	1:I:117:ASP:HA	2.13	0.48
1:N:80:GLY:HA2	1:O:40:GLN:HE22	1.79	0.48
1:O:195:ASP:HB3	1:P:77:GLU:HG3	1.95	0.48
1:A:46:ARG:HD3	1:A:171:TYR:CD1	2.48	0.47
1:C:194:GLN:NE2	1:C:196:LEU:O	2.42	0.47
1:C:195:ASP:HB3	1:D:77:GLU:HG3	1.96	0.47
1:E:47:LEU:HB3	1:E:51:TYR:HD2	1.79	0.47
1:N:87:SER:HA	1:O:122:GLU:HB3	1.96	0.47
1:H:147:VAL:HG21	1:I:124:VAL:HG23	1.96	0.47
1:S:46:ARG:HD3	1:S:171:TYR:CD2	2.49	0.47
1:B:192:LYS:NZ	1:B:197:GLU:OE2	2.33	0.47
1:A:50:GLU:HG3	1:A:181:GLN:OE1	2.13	0.47
1:K:158:PHE:HB2	1:K:162:LEU:HD12	1.96	0.47
1:N:194:GLN:NE2	1:N:196:LEU:O	2.40	0.47
1:Q:139:LEU:O	1:Q:143:ARG:HG3	2.14	0.47
1:T:51:TYR:HD1	1:T:70:ARG:HD2	1.79	0.47
1:J:168:ASP:HB3	1:J:171:TYR:HB3	1.97	0.47
1:S:204:ARG:HD2	1:U:36:TYR:OH	2.15	0.47
1:J:102:LYS:NZ	5:Z:8:DC:OP2	2.48	0.47
1:M:175:LEU:HD23	1:M:178:LEU:HD12	1.95	0.47
1:L:122:GLU:HB3	1:V:87:SER:HA	1.95	0.47
1:N:175:LEU:HD23	1:N:178:LEU:HD12	1.96	0.47
1:A:141:LYS:HE2	1:A:145:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:ILE:HD12	1:E:166:ILE:HD13	1.96	0.47
1:V:99:ASN:HB2	1:V:104:TYR:CE1	2.49	0.47
1:M:104:TYR:CD2	1:M:130:GLU:HB3	2.51	0.46
1:M:139:LEU:O	1:M:143:ARG:HG3	2.15	0.46
1:B:52:ILE:HG13	1:B:175:LEU:HD11	1.98	0.46
1:A:200:VAL:HG22	1:B:38:ALA:HB1	1.96	0.46
1:P:43:LEU:HD23	1:P:161:ALA:HB3	1.98	0.46
1:J:52:ILE:HD12	1:J:166:ILE:HD13	1.96	0.46
1:T:141:LYS:HE2	1:T:145:GLU:OE2	2.16	0.46
1:G:102:LYS:HE2	1:G:131:GLY:O	2.16	0.46
1:J:60:GLY:HA3	5:Z:5:DC:OP1	2.16	0.46
1:V:184:LEU:HD22	1:V:184:LEU:H	1.80	0.46
1:H:140:GLU:HB2	1:I:126:TYR:CD2	2.51	0.46
1:K:43:LEU:HD23	1:K:161:ALA:HB3	1.97	0.46
1:N:168:ASP:HB3	1:N:171:TYR:HB3	1.97	0.46
1:Q:41:LYS:HG2	1:Q:44:ARG:HH21	1.81	0.46
1:H:204:ARG:NH2	1:I:78:MET:O	2.49	0.46
1:K:129:SER:HB2	1:K:141:LYS:HD3	1.98	0.46
1:R:127:GLY:HA3	1:R:142:ALA:O	2.15	0.46
1:E:139:LEU:O	1:E:143:ARG:HG3	2.16	0.45
1:L:40:GLN:NE2	1:V:80:GLY:HA2	2.31	0.45
1:A:194:GLN:OE1	1:A:194:GLN:N	2.49	0.45
1:H:46:ARG:HD3	1:H:171:TYR:CD2	2.52	0.45
1:N:139:LEU:O	1:N:143:ARG:HG3	2.17	0.45
1:T:127:GLY:HA3	1:T:142:ALA:O	2.16	0.45
1:E:93:VAL:HG22	1:E:107:VAL:HG22	1.98	0.45
1:Q:184:LEU:HD22	1:Q:184:LEU:H	1.81	0.45
1:R:204:ARG:HD2	1:T:36:TYR:CZ	2.52	0.45
1:Q:46:ARG:HD3	1:Q:171:TYR:HD1	1.82	0.45
1:E:147:VAL:HG21	1:F:124:VAL:CG2	2.46	0.45
1:F:46:ARG:HD3	1:F:171:TYR:CD1	2.52	0.45
1:J:184:LEU:HD22	1:J:184:LEU:H	1.82	0.45
1:R:129:SER:HB2	1:R:141:LYS:HD3	1.99	0.45
1:E:37:GLN:HG2	1:E:41:LYS:HE2	1.98	0.45
1:J:127:GLY:HA3	1:J:142:ALA:O	2.17	0.45
1:K:52:ILE:HG13	1:K:175:LEU:HD11	1.98	0.45
1:M:87:SER:HA	1:N:122:GLU:HB3	1.98	0.45
1:P:200:VAL:HG22	1:Q:38:ALA:HB1	1.98	0.45
1:R:47:LEU:HB3	1:R:51:TYR:HD2	1.82	0.45
1:R:135:LYS:HE3	1:S:95:PHE:CG	2.52	0.45
1:A:47:LEU:HD22	1:A:51:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:ARG:HD3	1:F:167:LEU:HD11	1.99	0.45
1:G:46:ARG:HD3	1:G:171:TYR:CD1	2.51	0.45
1:N:52:ILE:HG13	1:N:175:LEU:HD11	1.98	0.45
1:P:52:ILE:HG13	1:P:175:LEU:HD11	1.99	0.45
1:S:139:LEU:O	1:S:143:ARG:HG3	2.17	0.45
4:Y:2:DC:H2'	4:Y:3:DC:C6	2.52	0.45
1:A:205:TYR:CE1	1:C:33:ALA:HB1	2.52	0.45
1:C:205:TYR:CE1	1:E:33:ALA:HB1	2.52	0.45
1:D:93:VAL:HG22	1:D:107:VAL:HG22	1.97	0.45
1:C:147:VAL:HG21	1:D:124:VAL:HG23	1.98	0.44
1:H:52:ILE:HD12	1:H:166:ILE:HD13	1.99	0.44
1:H:141:LYS:HE2	1:H:145:GLU:OE2	2.17	0.44
1:I:52:ILE:HG13	1:I:175:LEU:HD11	1.97	0.44
1:Q:52:ILE:HG13	1:Q:175:LEU:HD11	1.98	0.44
1:H:91:GLN:OE1	1:H:143:ARG:NE	2.43	0.44
1:K:184:LEU:H	1:K:184:LEU:HD22	1.82	0.44
1:N:200:VAL:HG22	1:O:38:ALA:HB1	1.98	0.44
1:F:43:LEU:HD23	1:F:161:ALA:HB3	2.00	0.44
1:G:147:VAL:HG21	1:H:124:VAL:HG23	1.99	0.44
1:L:87:SER:HA	1:M:122:GLU:HB3	1.99	0.44
1:T:192:LYS:NZ	1:T:197:GLU:OE2	2.40	0.44
1:E:91:GLN:HE21	1:E:109:ALA:HB2	1.82	0.44
1:E:147:VAL:HG21	1:F:124:VAL:HG23	2.00	0.44
1:F:47:LEU:O	1:F:171:TYR:OH	2.28	0.44
1:I:129:SER:HB2	1:I:141:LYS:HD3	1.99	0.44
1:P:46:ARG:HD3	1:P:171:TYR:CD1	2.53	0.44
1:S:37:GLN:HG2	1:S:41:LYS:HE2	2.00	0.44
1:A:103:PHE:CE1	1:A:135:LYS:HD3	2.53	0.44
1:L:195:ASP:HB3	1:M:77:GLU:HG3	2.00	0.44
1:P:139:LEU:O	1:P:143:ARG:HG3	2.18	0.44
1:K:180:ARG:HD2	1:K:180:ARG:HA	1.89	0.44
1:O:139:LEU:O	1:O:143:ARG:HG3	2.18	0.44
1:E:168:ASP:HB3	1:E:171:TYR:HB3	1.99	0.43
1:K:50:GLU:HG3	1:K:181:GLN:HE22	1.83	0.43
1:D:86:HIS:CD2	1:E:121:HIS:HD2	2.36	0.43
1:O:131:GLY:HA3	4:Y:6:DC:N4	2.33	0.43
1:S:43:LEU:HD23	1:S:161:ALA:HB3	2.00	0.43
1:A:52:ILE:HD12	1:A:166:ILE:HD13	2.00	0.43
1:B:200:VAL:HG22	1:C:38:ALA:HB1	2.00	0.43
1:G:79:PHE:HE2	1:G:162:LEU:HD11	1.83	0.43
1:Q:52:ILE:HD12	1:Q:166:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:139:LEU:O	1:R:143:ARG:HG3	2.19	0.43
1:S:103:PHE:CE1	1:S:135:LYS:HD3	2.53	0.43
1:B:46:ARG:HD3	1:B:171:TYR:CD1	2.53	0.43
1:C:175:LEU:HD23	1:C:178:LEU:HD12	1.99	0.43
1:V:168:ASP:HB3	1:V:171:TYR:HB3	1.99	0.43
1:R:184:LEU:H	1:R:184:LEU:HD22	1.83	0.43
1:T:129:SER:HB2	1:T:141:LYS:HD3	2.01	0.43
1:G:41:LYS:HG2	1:G:44:ARG:HH21	1.83	0.43
1:I:136:ALA:HB2	1:J:95:PHE:HZ	1.84	0.43
1:B:87:SER:HA	1:C:122:GLU:HB3	2.00	0.43
1:E:194:GLN:NE2	1:E:196:LEU:O	2.47	0.43
1:L:80:GLY:HA2	1:M:40:GLN:NE2	2.33	0.43
1:R:192:LYS:NZ	1:R:197:GLU:OE2	2.38	0.43
1:G:79:PHE:CE2	1:G:162:LEU:HD11	2.54	0.43
1:I:194:GLN:N	1:I:194:GLN:OE1	2.51	0.43
1:A:126:TYR:CD2	1:K:140:GLU:HB2	2.54	0.42
1:H:147:VAL:HG21	1:I:124:VAL:CG2	2.48	0.42
1:U:139:LEU:O	1:U:143:ARG:HG3	2.19	0.42
1:C:104:TYR:CD2	1:C:130:GLU:HB3	2.54	0.42
1:C:147:VAL:HG21	1:D:124:VAL:CG2	2.49	0.42
1:J:194:GLN:N	1:J:194:GLN:OE1	2.52	0.42
4:Y:1:DC:C2'	4:Y:2:DC:H5'	2.50	0.42
1:D:46:ARG:HD3	1:D:171:TYR:HD1	1.84	0.42
1:F:86:HIS:ND1	1:G:121:HIS:HD2	2.17	0.42
1:G:139:LEU:O	1:G:143:ARG:HG3	2.18	0.42
1:J:51:TYR:HD1	1:J:70:ARG:HD2	1.85	0.42
1:L:204:ARG:HD2	1:N:36:TYR:CZ	2.55	0.42
1:S:93:VAL:HG22	1:S:107:VAL:HG22	2.02	0.42
1:C:25:CYS:SG	1:C:28:GLN:HG3	2.60	0.42
1:H:125:GLY:HA3	1:H:150:GLY:N	2.34	0.42
1:B:139:LEU:O	1:B:143:ARG:HG3	2.19	0.42
1:B:147:VAL:HG21	1:C:124:VAL:HG23	2.02	0.42
1:B:184:LEU:HD22	1:B:184:LEU:H	1.84	0.42
1:G:184:LEU:HD22	1:G:184:LEU:H	1.85	0.42
1:N:175:LEU:HD23	1:N:175:LEU:HA	1.87	0.42
1:G:46:ARG:HD3	1:G:171:TYR:HD1	1.85	0.42
4:Y:1:DC:H2'	4:Y:2:DC:H5'	2.02	0.42
1:D:87:SER:HA	1:E:122:GLU:HB3	2.02	0.42
1:T:204:ARG:NH1	1:V:36:TYR:OH	2.37	0.42
1:K:91:GLN:OE1	1:K:143:ARG:NE	2.47	0.42
1:B:141:LYS:O	1:B:145:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:29:CYS:O	1:G:117:ASP:HA	2.20	0.42
1:P:91:GLN:OE1	1:P:143:ARG:NE	2.45	0.42
1:R:104:TYR:CD2	1:R:130:GLU:HB3	2.54	0.42
1:T:204:ARG:HD2	1:V:36:TYR:CZ	2.55	0.42
1:V:181:GLN:NE2	1:V:184:LEU:HD11	2.35	0.42
1:D:160:ASN:HB3	1:D:165:CYS:HB3	2.02	0.41
1:J:180:ARG:HD2	1:J:180:ARG:HA	1.89	0.41
1:L:184:LEU:HD22	1:L:184:LEU:H	1.85	0.41
1:M:91:GLN:OE1	1:M:143:ARG:NE	2.47	0.41
1:N:127:GLY:HA3	1:N:142:ALA:O	2.19	0.41
1:C:46:ARG:HD3	1:C:171:TYR:CD1	2.55	0.41
1:E:47:LEU:HD12	1:E:51:TYR:CE2	2.56	0.41
1:N:205:TYR:CE1	1:P:33:ALA:HB1	2.55	0.41
1:O:52:ILE:HD12	1:O:166:ILE:HD13	2.01	0.41
1:P:185:GLU:OE2	1:Q:177:LYS:NZ	2.52	0.41
1:T:47:LEU:HD12	1:T:51:TYR:CE2	2.55	0.41
1:F:175:LEU:HD23	1:F:175:LEU:HA	1.90	0.41
1:K:47:LEU:HB3	1:K:51:TYR:HD2	1.85	0.41
1:R:200:VAL:HG22	1:S:38:ALA:HB1	2.01	0.41
1:O:86:HIS:CD2	1:P:121:HIS:HD2	2.38	0.41
1:P:129:SER:HB2	1:P:141:LYS:HD2	2.02	0.41
1:Q:46:ARG:HD3	1:Q:171:TYR:CD1	2.56	0.41
1:R:168:ASP:HB3	1:R:171:TYR:HB3	2.01	0.41
1:B:36:TYR:CZ	1:K:204:ARG:HD2	2.55	0.41
1:O:127:GLY:HA3	1:O:142:ALA:O	2.21	0.41
1:D:184:LEU:HD22	1:D:184:LEU:H	1.86	0.41
1:S:114:GLN:HE21	1:S:118:GLY:HA2	1.85	0.41
1:B:129:SER:HB2	1:B:141:LYS:HD2	2.02	0.41
1:B:140:GLU:HB2	1:C:126:TYR:CD1	2.56	0.41
1:H:139:LEU:O	1:H:143:ARG:HG3	2.20	0.41
1:A:139:LEU:O	1:A:143:ARG:HG3	2.20	0.41
1:D:52:ILE:HG13	1:D:175:LEU:HD11	2.02	0.41
1:G:131:GLY:HA3	4:Y:9:DC:N4	2.36	0.41
1:H:136:ALA:HB2	1:I:95:PHE:HZ	1.86	0.41
1:I:139:LEU:O	1:I:143:ARG:HG3	2.20	0.41
1:I:184:LEU:HD22	1:I:184:LEU:H	1.86	0.41
1:J:86:HIS:ND1	1:K:121:HIS:HD2	2.18	0.41
1:N:156:ARG:HG3	1:N:164:ASN:HA	2.03	0.41
1:O:104:TYR:CD2	1:O:130:GLU:HB3	2.56	0.41
1:P:105:VAL:HG11	1:P:139:LEU:HD23	2.03	0.41
1:E:208:CYS:HB2	1:G:33:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:VAL:HG22	1:G:38:ALA:HB1	2.02	0.41
1:M:175:LEU:HD23	1:M:175:LEU:HA	1.88	0.41
1:P:140:GLU:HB2	1:Q:126:TYR:CD2	2.56	0.41
1:A:33:ALA:HB1	1:J:205:TYR:CE1	2.55	0.40
1:P:87:SER:HA	1:Q:122:GLU:HB3	2.02	0.40
1:T:136:ALA:HB2	1:U:95:PHE:HZ	1.85	0.40
1:F:127:GLY:HA3	1:F:142:ALA:O	2.20	0.40
1:Q:43:LEU:HD23	1:Q:161:ALA:HB3	2.03	0.40
1:C:140:GLU:HB2	1:D:126:TYR:CD2	2.56	0.40
1:H:87:SER:HA	1:I:122:GLU:HB3	2.02	0.40
1:Q:104:TYR:CD2	1:Q:130:GLU:HB3	2.57	0.40
1:T:139:LEU:O	1:T:143:ARG:HG3	2.22	0.40
1:T:184:LEU:HD22	1:T:184:LEU:H	1.86	0.40
1:U:93:VAL:HG22	1:U:107:VAL:HG22	2.03	0.40
1:B:36:TYR:OH	1:K:204:ARG:NH1	2.40	0.40
1:A:47:LEU:HD22	1:A:51:TYR:CE2	2.57	0.40
1:A:91:GLN:OE1	1:A:143:ARG:NE	2.49	0.40
1:H:129:SER:HB2	1:H:141:LYS:HD3	2.04	0.40
1:M:184:LEU:HD22	1:M:184:LEU:H	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASN:ND2	1:U:60:GLY:O[1_554]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	182/215 (85%)	180 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	174/215 (81%)	172 (99%)	2 (1%)	0	100	100
1	C	182/215 (85%)	180 (99%)	2 (1%)	0	100	100
1	D	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
1	E	182/215 (85%)	178 (98%)	4 (2%)	0	100	100
1	F	182/215 (85%)	180 (99%)	2 (1%)	0	100	100
1	G	182/215 (85%)	181 (100%)	1 (0%)	0	100	100
1	H	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
1	I	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
1	J	182/215 (85%)	178 (98%)	4 (2%)	0	100	100
1	K	182/215 (85%)	181 (100%)	1 (0%)	0	100	100
1	L	182/215 (85%)	180 (99%)	2 (1%)	0	100	100
1	M	174/215 (81%)	172 (99%)	2 (1%)	0	100	100
1	N	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
1	O	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
1	P	182/215 (85%)	178 (98%)	4 (2%)	0	100	100
1	Q	182/215 (85%)	180 (99%)	2 (1%)	0	100	100
1	R	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
1	S	182/215 (85%)	180 (99%)	2 (1%)	0	100	100
1	T	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
1	U	182/215 (85%)	179 (98%)	3 (2%)	0	100	100
1	V	182/215 (85%)	180 (99%)	2 (1%)	0	100	100
All	All	3988/4730 (84%)	3932 (99%)	56 (1%)	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	153/174 (88%)	152 (99%)	1 (1%)	84 94
1	B	151/174 (87%)	150 (99%)	1 (1%)	84 94
1	C	153/174 (88%)	152 (99%)	1 (1%)	84 94
1	D	153/174 (88%)	151 (99%)	2 (1%)	69 89
1	E	153/174 (88%)	153 (100%)	0	100 100
1	F	153/174 (88%)	151 (99%)	2 (1%)	69 89
1	G	153/174 (88%)	151 (99%)	2 (1%)	69 89
1	H	153/174 (88%)	151 (99%)	2 (1%)	69 89
1	I	153/174 (88%)	153 (100%)	0	100 100
1	J	153/174 (88%)	151 (99%)	2 (1%)	69 89
1	K	153/174 (88%)	152 (99%)	1 (1%)	84 94
1	L	153/174 (88%)	153 (100%)	0	100 100
1	M	151/174 (87%)	150 (99%)	1 (1%)	84 94
1	N	153/174 (88%)	153 (100%)	0	100 100
1	O	153/174 (88%)	151 (99%)	2 (1%)	69 89
1	P	153/174 (88%)	152 (99%)	1 (1%)	84 94
1	Q	153/174 (88%)	153 (100%)	0	100 100
1	R	153/174 (88%)	151 (99%)	2 (1%)	69 89
1	S	153/174 (88%)	153 (100%)	0	100 100
1	T	153/174 (88%)	153 (100%)	0	100 100
1	U	153/174 (88%)	153 (100%)	0	100 100
1	V	153/174 (88%)	152 (99%)	1 (1%)	84 94
All	All	3362/3828 (88%)	3341 (99%)	21 (1%)	86 95

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	B	104	TYR
1	C	29	CYS
1	D	29	CYS
1	D	86	HIS
1	F	104	TYR
1	F	180	ARG
1	G	47	LEU

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Mol	Chain	Res	Type
1	G	123	ASP
1	H	47	LEU
1	H	180	ARG
1	J	99	ASN
1	J	104	TYR
1	K	47	LEU
1	M	104	TYR
1	O	55	ARG
1	O	86	HIS
1	P	104	TYR
1	R	47	LEU
1	R	100	ASN
1	V	104	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	37	GLN
1	C	121	HIS
1	D	86	HIS
1	E	114	GLN
1	I	45	GLN
1	M	69	HIS
1	O	86	HIS
1	Q	69	HIS
1	Q	114	GLN
1	S	69	HIS
1	T	40	GLN
1	T	45	GLN
1	U	181	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.11	2 (1%) 80 56	38, 67, 124, 154	0
1	B	178/215 (82%)	-0.14	1 (0%) 89 72	40, 68, 112, 138	0
1	C	184/215 (85%)	-0.13	4 (2%) 62 33	41, 68, 121, 156	0
1	D	184/215 (85%)	-0.07	2 (1%) 80 56	43, 69, 128, 145	0
1	E	184/215 (85%)	-0.08	2 (1%) 80 56	42, 75, 129, 142	0
1	F	184/215 (85%)	-0.06	4 (2%) 62 33	40, 73, 124, 156	0
1	G	184/215 (85%)	-0.03	4 (2%) 62 33	43, 72, 124, 137	0
1	H	184/215 (85%)	-0.11	3 (1%) 72 44	42, 77, 129, 146	0
1	I	184/215 (85%)	-0.09	0 100 100	42, 77, 132, 149	0
1	J	184/215 (85%)	-0.06	3 (1%) 72 44	39, 76, 129, 150	0
1	K	184/215 (85%)	-0.10	0 100 100	41, 72, 119, 152	0
1	L	184/215 (85%)	-0.05	4 (2%) 62 33	42, 75, 128, 155	0
1	M	178/215 (82%)	-0.05	5 (2%) 53 25	41, 80, 123, 153	0
1	N	184/215 (85%)	-0.10	1 (0%) 91 75	43, 78, 123, 152	0
1	O	184/215 (85%)	-0.04	3 (1%) 72 44	39, 75, 128, 149	0
1	P	184/215 (85%)	-0.13	0 100 100	37, 72, 114, 133	0
1	Q	184/215 (85%)	-0.13	1 (0%) 91 75	38, 70, 118, 144	0
1	R	184/215 (85%)	-0.08	1 (0%) 91 75	38, 73, 121, 133	0
1	S	184/215 (85%)	-0.05	3 (1%) 72 44	41, 77, 121, 157	0
1	T	184/215 (85%)	-0.03	3 (1%) 72 44	45, 81, 132, 147	0
1	U	184/215 (85%)	-0.04	2 (1%) 80 56	45, 78, 129, 140	0
1	V	184/215 (85%)	-0.07	3 (1%) 72 44	42, 77, 128, 150	0
2	W	6/6 (100%)	-0.21	0 100 100	71, 81, 106, 113	0
3	X	8/8 (100%)	-0.41	0 100 100	78, 95, 103, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
4	Y	10/10 (100%)	0.06	0 100 100	67, 79, 104, 108	0
5	Z	9/9 (100%)	-0.12	0 100 100	81, 91, 113, 120	0
All	All	4069/4763 (85%)	-0.08	51 (1%) 77 51	37, 74, 127, 157	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	58	GLY	7.1
1	A	59	GLY	5.2
1	F	181	GLN	5.1
1	G	58	GLY	5.0
1	O	59	GLY	4.6
1	F	58	GLY	4.4
1	C	58	GLY	4.3
1	S	57	ALA	3.8
1	O	181	GLN	3.8
1	V	61	GLN	3.5
1	C	61	GLN	3.3
1	V	57	ALA	3.3
1	F	180	ARG	3.2
1	H	57	ALA	3.2
1	G	59	GLY	3.2
1	M	180	ARG	3.0
1	T	58	GLY	3.0
1	V	58	GLY	2.8
1	H	131	GLY	2.8
1	U	58	GLY	2.8
1	J	56	MET	2.7
1	A	58	GLY	2.7
1	H	58	GLY	2.7
1	S	61	GLN	2.5
1	J	182	LEU	2.5
1	T	60	GLY	2.5
1	J	180	ARG	2.5
1	F	57	ALA	2.4
1	T	59	GLY	2.4
1	M	186	VAL	2.4
1	U	57	ALA	2.3
1	M	181	GLN	2.3
1	B	180	ARG	2.3
1	M	183	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	57	ALA	2.2
1	E	180	ARG	2.2
1	L	61	GLN	2.2
1	M	182	LEU	2.2
1	E	179	PRO	2.2
1	L	60	GLY	2.1
1	S	59	GLY	2.1
1	R	184	LEU	2.1
1	G	62	LYS	2.1
1	G	180	ARG	2.1
1	Q	57	ALA	2.1
1	C	60	GLY	2.1
1	N	58	GLY	2.1
1	L	180	ARG	2.0
1	L	58	GLY	2.0
1	D	180	ARG	2.0
1	D	179	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.