



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2019 – 02:21 PM EDT

PDB ID : 6NQR
Title : Crystal structure of fast switching M159T mutant of fluorescent protein Dronpa (Dronpa2)- Y63(3-NO₂Y)
Authors : Lin, C.-Y.; Romei, M.G.; Mathews, I.I.; Boxer, S.G.
Deposited on : 2019-01-21
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

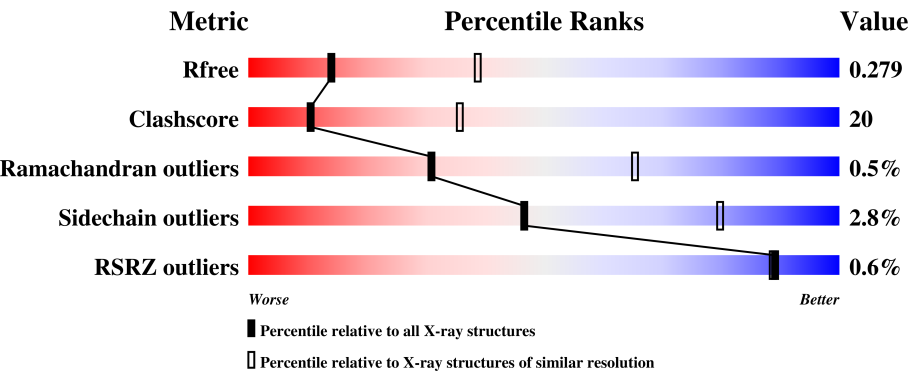
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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}	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	255	<div><div></div><div>58%26%15%</div></div>
1	B	255	<div><div></div><div>62%22%15%</div></div>
1	C	255	<div><div></div><div>53%31%15%</div></div>
1	D	255	<div><div>%</div><div>55%27%16%</div></div>
1	E	255	<div><div>%</div><div>55%29%15%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	255	
1	G	255	
1	H	255	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	KY7	F	63	-	-	X	-
1	KY7	G	63	X	-	-	-

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13844 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 Fluorescent protein Dronpa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1725	1102	289	325	9			
1	B	217	Total	C	N	O	S	0	0	0
			1740	1108	295	328	9			
1	C	218	Total	C	N	O	S	0	0	0
			1744	1113	293	329	9			
1	D	215	Total	C	N	O	S	0	0	0
			1725	1100	290	326	9			
1	E	216	Total	C	N	O	S	0	0	0
			1711	1092	285	325	9			
1	F	217	Total	C	N	O	S	0	0	0
			1717	1095	285	328	9			
1	G	222	Total	C	N	O	S	0	0	0
			1758	1122	294	333	9			
1	H	217	Total	C	N	O	S	0	0	0
			1724	1100	287	328	9			

There are 328 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	GLY	-	expression tag	UNP Q5TLG6
A	-26	SER	-	expression tag	UNP Q5TLG6
A	-25	SER	-	expression tag	UNP Q5TLG6
A	-24	HIS	-	expression tag	UNP Q5TLG6
A	-23	HIS	-	expression tag	UNP Q5TLG6
A	-22	HIS	-	expression tag	UNP Q5TLG6
A	-21	HIS	-	expression tag	UNP Q5TLG6
A	-20	HIS	-	expression tag	UNP Q5TLG6
A	-19	HIS	-	expression tag	UNP Q5TLG6
A	-18	SER	-	expression tag	UNP Q5TLG6
A	-17	SER	-	expression tag	UNP Q5TLG6
A	-16	GLY	-	expression tag	UNP Q5TLG6
A	-15	LEU	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	VAL	-	expression tag	UNP Q5TLG6
A	-13	PRO	-	expression tag	UNP Q5TLG6
A	-12	GLY	-	expression tag	UNP Q5TLG6
A	-11	GLY	-	expression tag	UNP Q5TLG6
A	-10	SER	-	expression tag	UNP Q5TLG6
A	-9	HIS	-	expression tag	UNP Q5TLG6
A	-8	MET	-	expression tag	UNP Q5TLG6
A	-7	VAL	-	expression tag	UNP Q5TLG6
A	-6	SER	-	expression tag	UNP Q5TLG6
A	-5	LYS	-	expression tag	UNP Q5TLG6
A	-4	GLY	-	expression tag	UNP Q5TLG6
A	-3	GLU	-	expression tag	UNP Q5TLG6
A	-2	GLU	-	expression tag	UNP Q5TLG6
A	-1	ASN	-	expression tag	UNP Q5TLG6
A	0	ASN	-	expression tag	UNP Q5TLG6
A	1	MET	-	expression tag	UNP Q5TLG6
A	2	ALA	-	expression tag	UNP Q5TLG6
A	63	KY7	CYS	chromophore	UNP Q5TLG6
A	63	KY7	TYR	chromophore	UNP Q5TLG6
A	63	KY7	GLY	chromophore	UNP Q5TLG6
A	159	THR	MET	engineered mutation	UNP Q5TLG6
A	218	GLY	GLU	engineered mutation	UNP Q5TLG6
A	224	MET	-	expression tag	UNP Q5TLG6
A	225	ASP	-	expression tag	UNP Q5TLG6
A	226	GLU	-	expression tag	UNP Q5TLG6
A	227	LEU	-	expression tag	UNP Q5TLG6
A	228	TYR	-	expression tag	UNP Q5TLG6
A	229	LYS	-	expression tag	UNP Q5TLG6
B	-27	GLY	-	expression tag	UNP Q5TLG6
B	-26	SER	-	expression tag	UNP Q5TLG6
B	-25	SER	-	expression tag	UNP Q5TLG6
B	-24	HIS	-	expression tag	UNP Q5TLG6
B	-23	HIS	-	expression tag	UNP Q5TLG6
B	-22	HIS	-	expression tag	UNP Q5TLG6
B	-21	HIS	-	expression tag	UNP Q5TLG6
B	-20	HIS	-	expression tag	UNP Q5TLG6
B	-19	HIS	-	expression tag	UNP Q5TLG6
B	-18	SER	-	expression tag	UNP Q5TLG6
B	-17	SER	-	expression tag	UNP Q5TLG6
B	-16	GLY	-	expression tag	UNP Q5TLG6
B	-15	LEU	-	expression tag	UNP Q5TLG6
B	-14	VAL	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	PRO	-	expression tag	UNP Q5TLG6
B	-12	GLY	-	expression tag	UNP Q5TLG6
B	-11	GLY	-	expression tag	UNP Q5TLG6
B	-10	SER	-	expression tag	UNP Q5TLG6
B	-9	HIS	-	expression tag	UNP Q5TLG6
B	-8	MET	-	expression tag	UNP Q5TLG6
B	-7	VAL	-	expression tag	UNP Q5TLG6
B	-6	SER	-	expression tag	UNP Q5TLG6
B	-5	LYS	-	expression tag	UNP Q5TLG6
B	-4	GLY	-	expression tag	UNP Q5TLG6
B	-3	GLU	-	expression tag	UNP Q5TLG6
B	-2	GLU	-	expression tag	UNP Q5TLG6
B	-1	ASN	-	expression tag	UNP Q5TLG6
B	0	ASN	-	expression tag	UNP Q5TLG6
B	1	MET	-	expression tag	UNP Q5TLG6
B	2	ALA	-	expression tag	UNP Q5TLG6
B	63	KY7	CYS	chromophore	UNP Q5TLG6
B	63	KY7	TYR	chromophore	UNP Q5TLG6
B	63	KY7	GLY	chromophore	UNP Q5TLG6
B	159	THR	MET	engineered mutation	UNP Q5TLG6
B	218	GLY	GLU	engineered mutation	UNP Q5TLG6
B	224	MET	-	expression tag	UNP Q5TLG6
B	225	ASP	-	expression tag	UNP Q5TLG6
B	226	GLU	-	expression tag	UNP Q5TLG6
B	227	LEU	-	expression tag	UNP Q5TLG6
B	228	TYR	-	expression tag	UNP Q5TLG6
B	229	LYS	-	expression tag	UNP Q5TLG6
C	-27	GLY	-	expression tag	UNP Q5TLG6
C	-26	SER	-	expression tag	UNP Q5TLG6
C	-25	SER	-	expression tag	UNP Q5TLG6
C	-24	HIS	-	expression tag	UNP Q5TLG6
C	-23	HIS	-	expression tag	UNP Q5TLG6
C	-22	HIS	-	expression tag	UNP Q5TLG6
C	-21	HIS	-	expression tag	UNP Q5TLG6
C	-20	HIS	-	expression tag	UNP Q5TLG6
C	-19	HIS	-	expression tag	UNP Q5TLG6
C	-18	SER	-	expression tag	UNP Q5TLG6
C	-17	SER	-	expression tag	UNP Q5TLG6
C	-16	GLY	-	expression tag	UNP Q5TLG6
C	-15	LEU	-	expression tag	UNP Q5TLG6
C	-14	VAL	-	expression tag	UNP Q5TLG6
C	-13	PRO	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	GLY	-	expression tag	UNP Q5TLG6
C	-11	GLY	-	expression tag	UNP Q5TLG6
C	-10	SER	-	expression tag	UNP Q5TLG6
C	-9	HIS	-	expression tag	UNP Q5TLG6
C	-8	MET	-	expression tag	UNP Q5TLG6
C	-7	VAL	-	expression tag	UNP Q5TLG6
C	-6	SER	-	expression tag	UNP Q5TLG6
C	-5	LYS	-	expression tag	UNP Q5TLG6
C	-4	GLY	-	expression tag	UNP Q5TLG6
C	-3	GLU	-	expression tag	UNP Q5TLG6
C	-2	GLU	-	expression tag	UNP Q5TLG6
C	-1	ASN	-	expression tag	UNP Q5TLG6
C	0	ASN	-	expression tag	UNP Q5TLG6
C	1	MET	-	expression tag	UNP Q5TLG6
C	2	ALA	-	expression tag	UNP Q5TLG6
C	63	KY7	CYS	chromophore	UNP Q5TLG6
C	63	KY7	TYR	chromophore	UNP Q5TLG6
C	63	KY7	GLY	chromophore	UNP Q5TLG6
C	159	THR	MET	engineered mutation	UNP Q5TLG6
C	218	GLY	GLU	engineered mutation	UNP Q5TLG6
C	224	MET	-	expression tag	UNP Q5TLG6
C	225	ASP	-	expression tag	UNP Q5TLG6
C	226	GLU	-	expression tag	UNP Q5TLG6
C	227	LEU	-	expression tag	UNP Q5TLG6
C	228	TYR	-	expression tag	UNP Q5TLG6
C	229	LYS	-	expression tag	UNP Q5TLG6
D	-27	GLY	-	expression tag	UNP Q5TLG6
D	-26	SER	-	expression tag	UNP Q5TLG6
D	-25	SER	-	expression tag	UNP Q5TLG6
D	-24	HIS	-	expression tag	UNP Q5TLG6
D	-23	HIS	-	expression tag	UNP Q5TLG6
D	-22	HIS	-	expression tag	UNP Q5TLG6
D	-21	HIS	-	expression tag	UNP Q5TLG6
D	-20	HIS	-	expression tag	UNP Q5TLG6
D	-19	HIS	-	expression tag	UNP Q5TLG6
D	-18	SER	-	expression tag	UNP Q5TLG6
D	-17	SER	-	expression tag	UNP Q5TLG6
D	-16	GLY	-	expression tag	UNP Q5TLG6
D	-15	LEU	-	expression tag	UNP Q5TLG6
D	-14	VAL	-	expression tag	UNP Q5TLG6
D	-13	PRO	-	expression tag	UNP Q5TLG6
D	-12	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	GLY	-	expression tag	UNP Q5TLG6
D	-10	SER	-	expression tag	UNP Q5TLG6
D	-9	HIS	-	expression tag	UNP Q5TLG6
D	-8	MET	-	expression tag	UNP Q5TLG6
D	-7	VAL	-	expression tag	UNP Q5TLG6
D	-6	SER	-	expression tag	UNP Q5TLG6
D	-5	LYS	-	expression tag	UNP Q5TLG6
D	-4	GLY	-	expression tag	UNP Q5TLG6
D	-3	GLU	-	expression tag	UNP Q5TLG6
D	-2	GLU	-	expression tag	UNP Q5TLG6
D	-1	ASN	-	expression tag	UNP Q5TLG6
D	0	ASN	-	expression tag	UNP Q5TLG6
D	1	MET	-	expression tag	UNP Q5TLG6
D	2	ALA	-	expression tag	UNP Q5TLG6
D	63	KY7	CYS	chromophore	UNP Q5TLG6
D	63	KY7	TYR	chromophore	UNP Q5TLG6
D	63	KY7	GLY	chromophore	UNP Q5TLG6
D	159	THR	MET	engineered mutation	UNP Q5TLG6
D	218	GLY	GLU	engineered mutation	UNP Q5TLG6
D	224	MET	-	expression tag	UNP Q5TLG6
D	225	ASP	-	expression tag	UNP Q5TLG6
D	226	GLU	-	expression tag	UNP Q5TLG6
D	227	LEU	-	expression tag	UNP Q5TLG6
D	228	TYR	-	expression tag	UNP Q5TLG6
D	229	LYS	-	expression tag	UNP Q5TLG6
E	-27	GLY	-	expression tag	UNP Q5TLG6
E	-26	SER	-	expression tag	UNP Q5TLG6
E	-25	SER	-	expression tag	UNP Q5TLG6
E	-24	HIS	-	expression tag	UNP Q5TLG6
E	-23	HIS	-	expression tag	UNP Q5TLG6
E	-22	HIS	-	expression tag	UNP Q5TLG6
E	-21	HIS	-	expression tag	UNP Q5TLG6
E	-20	HIS	-	expression tag	UNP Q5TLG6
E	-19	HIS	-	expression tag	UNP Q5TLG6
E	-18	SER	-	expression tag	UNP Q5TLG6
E	-17	SER	-	expression tag	UNP Q5TLG6
E	-16	GLY	-	expression tag	UNP Q5TLG6
E	-15	LEU	-	expression tag	UNP Q5TLG6
E	-14	VAL	-	expression tag	UNP Q5TLG6
E	-13	PRO	-	expression tag	UNP Q5TLG6
E	-12	GLY	-	expression tag	UNP Q5TLG6
E	-11	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	SER	-	expression tag	UNP Q5TLG6
E	-9	HIS	-	expression tag	UNP Q5TLG6
E	-8	MET	-	expression tag	UNP Q5TLG6
E	-7	VAL	-	expression tag	UNP Q5TLG6
E	-6	SER	-	expression tag	UNP Q5TLG6
E	-5	LYS	-	expression tag	UNP Q5TLG6
E	-4	GLY	-	expression tag	UNP Q5TLG6
E	-3	GLU	-	expression tag	UNP Q5TLG6
E	-2	GLU	-	expression tag	UNP Q5TLG6
E	-1	ASN	-	expression tag	UNP Q5TLG6
E	0	ASN	-	expression tag	UNP Q5TLG6
E	1	MET	-	expression tag	UNP Q5TLG6
E	2	ALA	-	expression tag	UNP Q5TLG6
E	63	KY7	CYS	chromophore	UNP Q5TLG6
E	63	KY7	TYR	chromophore	UNP Q5TLG6
E	63	KY7	GLY	chromophore	UNP Q5TLG6
E	159	THR	MET	engineered mutation	UNP Q5TLG6
E	218	GLY	GLU	engineered mutation	UNP Q5TLG6
E	224	MET	-	expression tag	UNP Q5TLG6
E	225	ASP	-	expression tag	UNP Q5TLG6
E	226	GLU	-	expression tag	UNP Q5TLG6
E	227	LEU	-	expression tag	UNP Q5TLG6
E	228	TYR	-	expression tag	UNP Q5TLG6
E	229	LYS	-	expression tag	UNP Q5TLG6
F	-27	GLY	-	expression tag	UNP Q5TLG6
F	-26	SER	-	expression tag	UNP Q5TLG6
F	-25	SER	-	expression tag	UNP Q5TLG6
F	-24	HIS	-	expression tag	UNP Q5TLG6
F	-23	HIS	-	expression tag	UNP Q5TLG6
F	-22	HIS	-	expression tag	UNP Q5TLG6
F	-21	HIS	-	expression tag	UNP Q5TLG6
F	-20	HIS	-	expression tag	UNP Q5TLG6
F	-19	HIS	-	expression tag	UNP Q5TLG6
F	-18	SER	-	expression tag	UNP Q5TLG6
F	-17	SER	-	expression tag	UNP Q5TLG6
F	-16	GLY	-	expression tag	UNP Q5TLG6
F	-15	LEU	-	expression tag	UNP Q5TLG6
F	-14	VAL	-	expression tag	UNP Q5TLG6
F	-13	PRO	-	expression tag	UNP Q5TLG6
F	-12	GLY	-	expression tag	UNP Q5TLG6
F	-11	GLY	-	expression tag	UNP Q5TLG6
F	-10	SER	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	HIS	-	expression tag	UNP Q5TLG6
F	-8	MET	-	expression tag	UNP Q5TLG6
F	-7	VAL	-	expression tag	UNP Q5TLG6
F	-6	SER	-	expression tag	UNP Q5TLG6
F	-5	LYS	-	expression tag	UNP Q5TLG6
F	-4	GLY	-	expression tag	UNP Q5TLG6
F	-3	GLU	-	expression tag	UNP Q5TLG6
F	-2	GLU	-	expression tag	UNP Q5TLG6
F	-1	ASN	-	expression tag	UNP Q5TLG6
F	0	ASN	-	expression tag	UNP Q5TLG6
F	1	MET	-	expression tag	UNP Q5TLG6
F	2	ALA	-	expression tag	UNP Q5TLG6
F	63	KY7	CYS	chromophore	UNP Q5TLG6
F	63	KY7	TYR	chromophore	UNP Q5TLG6
F	63	KY7	GLY	chromophore	UNP Q5TLG6
F	159	THR	MET	engineered mutation	UNP Q5TLG6
F	218	GLY	GLU	engineered mutation	UNP Q5TLG6
F	224	MET	-	expression tag	UNP Q5TLG6
F	225	ASP	-	expression tag	UNP Q5TLG6
F	226	GLU	-	expression tag	UNP Q5TLG6
F	227	LEU	-	expression tag	UNP Q5TLG6
F	228	TYR	-	expression tag	UNP Q5TLG6
F	229	LYS	-	expression tag	UNP Q5TLG6
G	-27	GLY	-	expression tag	UNP Q5TLG6
G	-26	SER	-	expression tag	UNP Q5TLG6
G	-25	SER	-	expression tag	UNP Q5TLG6
G	-24	HIS	-	expression tag	UNP Q5TLG6
G	-23	HIS	-	expression tag	UNP Q5TLG6
G	-22	HIS	-	expression tag	UNP Q5TLG6
G	-21	HIS	-	expression tag	UNP Q5TLG6
G	-20	HIS	-	expression tag	UNP Q5TLG6
G	-19	HIS	-	expression tag	UNP Q5TLG6
G	-18	SER	-	expression tag	UNP Q5TLG6
G	-17	SER	-	expression tag	UNP Q5TLG6
G	-16	GLY	-	expression tag	UNP Q5TLG6
G	-15	LEU	-	expression tag	UNP Q5TLG6
G	-14	VAL	-	expression tag	UNP Q5TLG6
G	-13	PRO	-	expression tag	UNP Q5TLG6
G	-12	GLY	-	expression tag	UNP Q5TLG6
G	-11	GLY	-	expression tag	UNP Q5TLG6
G	-10	SER	-	expression tag	UNP Q5TLG6
G	-9	HIS	-	expression tag	UNP Q5TLG6

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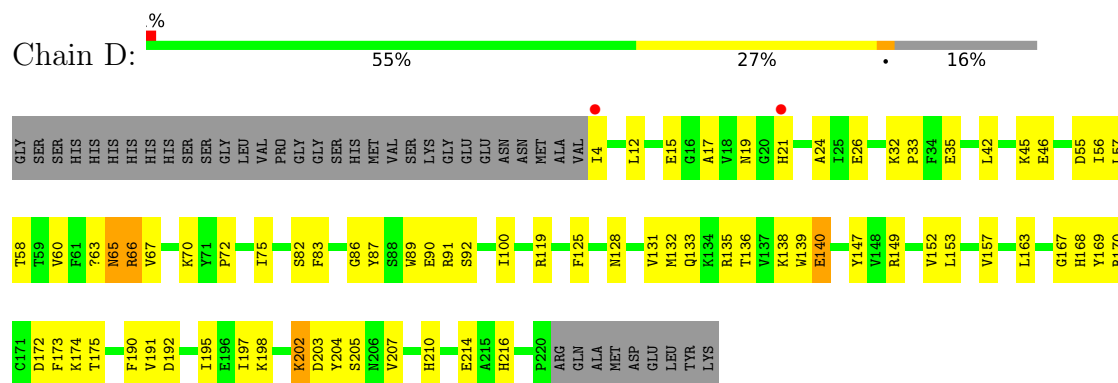
Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	MET	-	expression tag	UNP Q5TLG6
G	-7	VAL	-	expression tag	UNP Q5TLG6
G	-6	SER	-	expression tag	UNP Q5TLG6
G	-5	LYS	-	expression tag	UNP Q5TLG6
G	-4	GLY	-	expression tag	UNP Q5TLG6
G	-3	GLU	-	expression tag	UNP Q5TLG6
G	-2	GLU	-	expression tag	UNP Q5TLG6
G	-1	ASN	-	expression tag	UNP Q5TLG6
G	0	ASN	-	expression tag	UNP Q5TLG6
G	1	MET	-	expression tag	UNP Q5TLG6
G	2	ALA	-	expression tag	UNP Q5TLG6
G	63	KY7	CYS	chromophore	UNP Q5TLG6
G	63	KY7	TYR	chromophore	UNP Q5TLG6
G	63	KY7	GLY	chromophore	UNP Q5TLG6
G	159	THR	MET	engineered mutation	UNP Q5TLG6
G	218	GLY	GLU	engineered mutation	UNP Q5TLG6
G	224	MET	-	expression tag	UNP Q5TLG6
G	225	ASP	-	expression tag	UNP Q5TLG6
G	226	GLU	-	expression tag	UNP Q5TLG6
G	227	LEU	-	expression tag	UNP Q5TLG6
G	228	TYR	-	expression tag	UNP Q5TLG6
G	229	LYS	-	expression tag	UNP Q5TLG6
H	-27	GLY	-	expression tag	UNP Q5TLG6
H	-26	SER	-	expression tag	UNP Q5TLG6
H	-25	SER	-	expression tag	UNP Q5TLG6
H	-24	HIS	-	expression tag	UNP Q5TLG6
H	-23	HIS	-	expression tag	UNP Q5TLG6
H	-22	HIS	-	expression tag	UNP Q5TLG6
H	-21	HIS	-	expression tag	UNP Q5TLG6
H	-20	HIS	-	expression tag	UNP Q5TLG6
H	-19	HIS	-	expression tag	UNP Q5TLG6
H	-18	SER	-	expression tag	UNP Q5TLG6
H	-17	SER	-	expression tag	UNP Q5TLG6
H	-16	GLY	-	expression tag	UNP Q5TLG6
H	-15	LEU	-	expression tag	UNP Q5TLG6
H	-14	VAL	-	expression tag	UNP Q5TLG6
H	-13	PRO	-	expression tag	UNP Q5TLG6
H	-12	GLY	-	expression tag	UNP Q5TLG6
H	-11	GLY	-	expression tag	UNP Q5TLG6
H	-10	SER	-	expression tag	UNP Q5TLG6
H	-9	HIS	-	expression tag	UNP Q5TLG6
H	-8	MET	-	expression tag	UNP Q5TLG6

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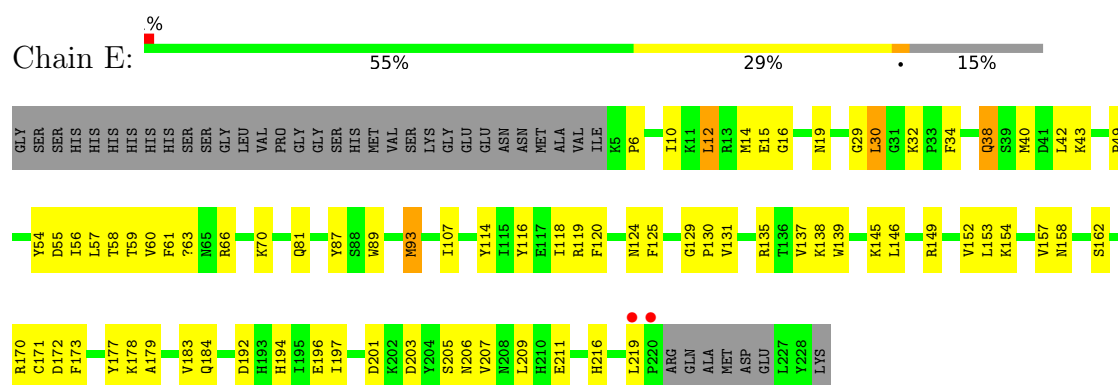
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	VAL	-	expression tag	UNP Q5TLG6
H	-6	SER	-	expression tag	UNP Q5TLG6
H	-5	LYS	-	expression tag	UNP Q5TLG6
H	-4	GLY	-	expression tag	UNP Q5TLG6
H	-3	GLU	-	expression tag	UNP Q5TLG6
H	-2	GLU	-	expression tag	UNP Q5TLG6
H	-1	ASN	-	expression tag	UNP Q5TLG6
H	0	ASN	-	expression tag	UNP Q5TLG6
H	1	MET	-	expression tag	UNP Q5TLG6
H	2	ALA	-	expression tag	UNP Q5TLG6
H	63	KY7	CYS	chromophore	UNP Q5TLG6
H	63	KY7	TYR	chromophore	UNP Q5TLG6
H	63	KY7	GLY	chromophore	UNP Q5TLG6
H	159	THR	MET	engineered mutation	UNP Q5TLG6
H	218	GLY	GLU	engineered mutation	UNP Q5TLG6
H	224	MET	-	expression tag	UNP Q5TLG6
H	225	ASP	-	expression tag	UNP Q5TLG6
H	226	GLU	-	expression tag	UNP Q5TLG6
H	227	LEU	-	expression tag	UNP Q5TLG6
H	228	TYR	-	expression tag	UNP Q5TLG6
H	229	LYS	-	expression tag	UNP Q5TLG6

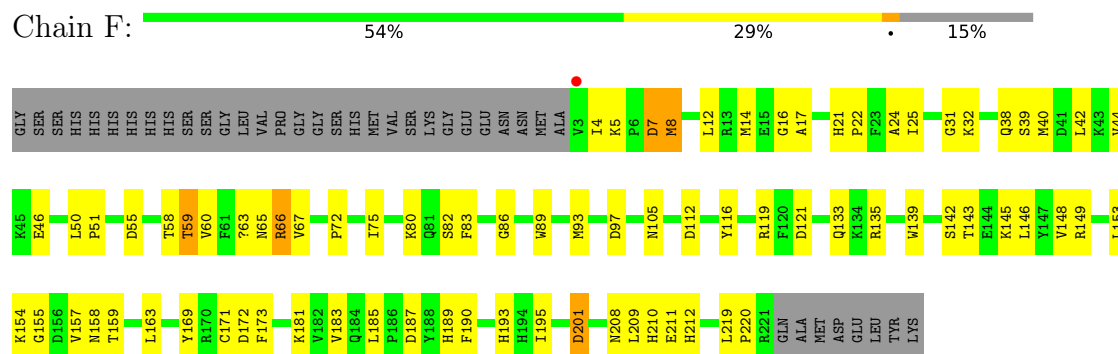
- Molecule 1: Fluorescent protein Dronpa



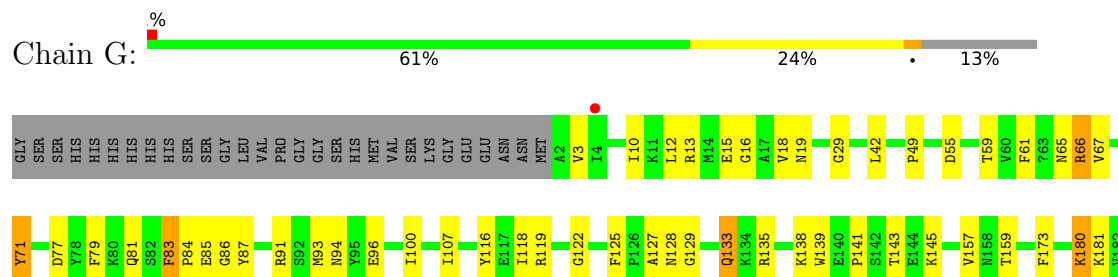
- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa

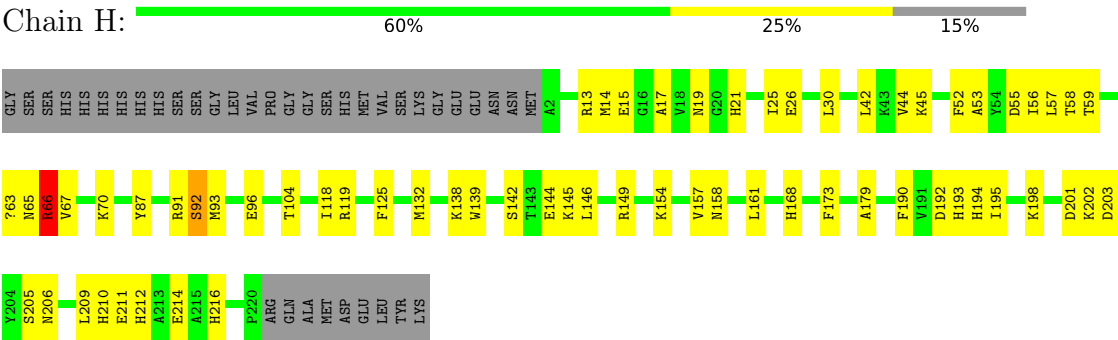


- Molecule 1: Fluorescent protein Dronpa





● Molecule 1: Fluorescent protein Dronpa



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.61Å 79.43Å 85.93Å 89.96° 92.53° 94.76°	Depositor
Resolution (Å)	37.51 – 2.90 37.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	87.5 (37.51-2.90) 87.6 (37.51-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.13RC2_2986: ???)	Depositor
R, R_{free}	0.216 , 0.283 0.219 , 0.279	Depositor DCC
R_{free} test set	1831 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 10.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.096 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13844	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KY7

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	0.54	0/1747	0.66	0/2365
1	B	0.46	0/1762	0.54	0/2382
1	C	0.46	0/1765	0.62	0/2385
1	D	0.47	0/1747	0.60	1/2363 (0.0%)
1	E	0.56	0/1732	0.68	0/2345
1	F	0.48	0/1739	0.68	0/2359
1	G	0.43	0/1779	0.62	0/2405
1	H	0.55	0/1746	0.65	0/2364
All	All	0.50	0/14017	0.63	1/18968 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	1	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	65	ASN	N-CA-C	-5.29	96.72	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	63	KY7	CA1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	83	PHE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1725	0	1611	58	0
1	B	1740	0	1634	52	0
1	C	1744	0	1632	86	0
1	D	1725	0	1620	55	0
1	E	1711	0	1574	94	0
1	F	1717	0	1577	84	0
1	G	1758	0	1636	81	0
1	H	1724	0	1603	60	0
All	All	13844	0	12887	530	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 20.

All (530) 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:F:5:LYS:N	1:F:8:MET:HE1	1.25	1.43
1:F:63:KY7:OB	1:F:142:SER:OG	1.54	1.24
1:G:85:GLU:OE1	1:G:181:LYS:HD3	1.37	1.23
1:F:5:LYS:CA	1:F:8:MET:HE1	1.69	1.21
1:E:81:GLN:HG2	1:E:183:VAL:CG2	1.69	1.20
1:D:55:ASP:OD2	1:D:136:THR:OG1	1.57	1.19
1:F:5:LYS:H	1:F:8:MET:CE	1.56	1.18
1:G:10:ILE:HD11	1:G:116:TYR:CE1	1.79	1.16
1:F:5:LYS:HB3	1:F:8:MET:HE3	1.17	1.16
1:F:5:LYS:HB3	1:F:8:MET:CE	1.75	1.14
1:F:158:ASN:OD1	1:F:172:ASP:OD1	1.65	1.13
1:F:5:LYS:CB	1:F:8:MET:CE	2.26	1.12
1:H:63:KY7:OB	1:H:142:SER:OG	1.65	1.12
1:A:143:THR:HG23	1:A:192:ASP:OD2	1.48	1.12
1:E:81:GLN:HG2	1:E:183:VAL:HG23	1.20	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:138:LYS:NZ	1:H:194:HIS:NE2	2.02	1.08
1:F:5:LYS:N	1:F:8:MET:CE	2.13	1.06
1:G:127:ALA:O	1:G:133:GLN:NE2	1.87	1.05
1:B:65:ASN:OD1	1:B:87:TYR:OH	1.72	1.03
1:C:128:ASN:HA	1:C:133:GLN:NE2	1.73	1.02
1:E:201:ASP:OD1	1:E:206:ASN:HB2	1.61	1.01
1:C:63:KY7:CB1	1:C:211:GLU:OE1	2.09	1.00
1:F:5:LYS:CA	1:F:8:MET:CE	2.39	0.99
1:E:63:KY7:CB2	1:E:66:ARG:NH2	2.26	0.98
1:G:10:ILE:HD11	1:G:116:TYR:CZ	2.01	0.95
1:E:10:ILE:HG22	1:E:29:GLY:O	1.66	0.94
1:E:81:GLN:CG	1:E:183:VAL:CG2	2.48	0.91
1:A:172:ASP:OD1	1:A:174:LYS:NZ	2.03	0.90
1:C:200:HIS:ND1	1:C:204:TYR:CZ	2.41	0.89
1:G:85:GLU:OE1	1:G:181:LYS:CD	2.19	0.89
1:H:66:ARG:HH11	1:H:66:ARG:HG3	1.37	0.88
1:D:65:ASN:OD1	1:D:87:TYR:OH	1.92	0.88
1:F:63:KY7:C2	1:F:66:ARG:HH12	1.86	0.87
1:C:200:HIS:CE1	1:C:204:TYR:CZ	2.63	0.86
1:C:50:LEU:O	1:C:134:LYS:NZ	2.09	0.86
1:F:97:ASP:OD1	1:F:169:TYR:OH	1.95	0.85
1:F:5:LYS:CB	1:F:8:MET:HE3	1.99	0.84
1:E:10:ILE:HG22	1:E:29:GLY:C	1.99	0.83
1:E:81:GLN:CG	1:E:183:VAL:HG23	2.07	0.82
1:G:86:GLY:C	1:G:180:LYS:HD2	1.99	0.82
1:C:195:ILE:HD13	1:C:211:GLU:HB2	1.60	0.82
1:F:201:ASP:N	1:F:201:ASP:OD1	2.11	0.81
1:G:133:GLN:HG2	1:G:135:ARG:HH12	1.43	0.81
1:C:107:ILE:HD13	1:C:116:TYR:CD1	2.14	0.81
1:D:19:ASN:HD21	1:D:125:PHE:H	1.28	0.81
1:B:146:LEU:HB3	1:B:153:LEU:HD11	1.62	0.81
1:H:201:ASP:OD2	1:H:206:ASN:N	2.14	0.80
1:F:5:LYS:H	1:F:8:MET:HE1	0.97	0.80
1:E:10:ILE:CG2	1:E:29:GLY:N	2.45	0.79
1:E:158:ASN:ND2	1:E:172:ASP:OD1	2.15	0.79
1:C:157:VAL:HG12	1:C:173:PHE:HB2	1.63	0.78
1:D:203:ASP:OD2	1:D:205:SER:OG	2.02	0.78
1:A:201:ASP:OD2	1:A:206:ASN:ND2	2.14	0.78
1:F:63:KY7:O2	1:F:66:ARG:NH1	2.12	0.78
1:G:10:ILE:CD1	1:G:116:TYR:CZ	2.67	0.77
1:A:52:PHE:HE1	1:A:57:LEU:HD11	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:KY7:OB	1:F:142:SER:CB	2.34	0.75
1:F:148:VAL:HG21	1:F:185:LEU:HD13	1.67	0.75
1:C:8:MET:HE3	1:C:114:TYR:CZ	2.22	0.74
1:C:201:ASP:OD2	1:C:201:ASP:N	2.19	0.74
1:E:157:VAL:HG12	1:E:173:PHE:HB2	1.69	0.74
1:H:13:ARG:NH1	1:H:26:GLU:OE2	2.21	0.73
1:C:55:ASP:O	1:C:139:TRP:NE1	2.21	0.72
1:A:127:ALA:O	1:A:133:GLN:NE2	2.23	0.72
1:C:200:HIS:ND1	1:C:204:TYR:CE2	2.57	0.72
1:A:63:KY7:CB1	1:A:211:GLU:OE2	2.38	0.72
1:C:170:ARG:NH1	1:C:172:ASP:OD1	2.22	0.72
1:E:10:ILE:HG22	1:E:29:GLY:CA	2.19	0.72
1:G:83:PHE:CE1	1:G:86:GLY:HA2	2.25	0.71
1:A:145:LYS:O	1:A:145:LYS:HG2	1.89	0.71
1:C:138:LYS:HG2	1:C:139:TRP:N	2.04	0.71
1:G:81:GLN:O	1:G:181:LYS:NZ	2.17	0.71
1:H:52:PHE:HE1	1:H:57:LEU:HD11	1.55	0.70
1:H:65:ASN:OD1	1:H:67:VAL:HB	1.92	0.70
1:E:135:ARG:HH22	1:H:198:LYS:NZ	1.89	0.70
1:B:19:ASN:HD21	1:B:125:PHE:H	1.39	0.69
1:C:13:ARG:HD2	1:C:26:GLU:HG2	1.74	0.69
1:E:157:VAL:CG1	1:E:173:PHE:HB2	2.22	0.69
1:G:86:GLY:O	1:G:180:LYS:HD2	1.93	0.69
1:F:40:MET:O	1:F:208:ASN:ND2	2.26	0.69
1:G:65:ASN:O	1:G:66:ARG:NH1	2.27	0.68
1:A:11:LYS:HD2	1:A:113:CYS:SG	2.34	0.68
1:B:147:TYR:OH	1:E:170:ARG:NE	2.25	0.68
1:A:125:PHE:CD1	1:A:131:VAL:HG11	2.29	0.68
1:G:12:LEU:HD13	1:G:116:TYR:CD1	2.29	0.68
1:A:196:GLU:HG3	1:A:198:LYS:HE2	1.76	0.67
1:F:44:VAL:HG21	1:F:50:LEU:HD11	1.74	0.67
1:E:81:GLN:HG2	1:E:183:VAL:HG21	1.72	0.67
1:A:106:ASP:OD2	1:A:180:LYS:NZ	2.27	0.67
1:D:133:GLN:OE1	1:D:135:ARG:NH2	2.28	0.67
1:E:152:VAL:HG12	1:E:153:LEU:N	2.10	0.67
1:C:10:ILE:N	1:C:29:GLY:O	2.28	0.67
1:A:65:ASN:ND2	1:A:107:ILE:HD13	2.10	0.67
1:D:55:ASP:OD2	1:D:136:THR:CB	2.41	0.66
1:G:94:ASN:OD1	1:G:100:ILE:HD11	1.95	0.66
1:G:128:ASN:HA	1:G:133:GLN:NE2	2.11	0.66
1:C:227:LEU:HB3	1:D:167:GLY:HA3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:LEU:HD22	1:E:61:PHE:CE1	2.31	0.65
1:F:55:ASP:O	1:F:139:TRP:NE1	2.27	0.65
1:C:125:PHE:CD1	1:C:131:VAL:HG11	2.31	0.65
1:C:52:PHE:HE1	1:C:57:LEU:HD11	1.61	0.65
1:E:10:ILE:HD11	1:E:116:TYR:CZ	2.31	0.65
1:G:67:VAL:HG12	1:G:79:PHE:HB3	1.78	0.65
1:C:63:KY7:C2	1:C:66:ARG:HH12	2.10	0.65
1:D:26:GLU:HB2	1:D:45:LYS:HE3	1.79	0.65
1:F:5:LYS:C	1:F:8:MET:HE1	2.15	0.64
1:G:157:VAL:HG12	1:G:173:PHE:HB2	1.79	0.64
1:F:148:VAL:CG2	1:F:185:LEU:HD13	2.27	0.64
1:E:10:ILE:CG2	1:E:29:GLY:CA	2.74	0.64
1:E:10:ILE:CG2	1:E:29:GLY:H	2.11	0.64
1:G:49:PRO:HB3	1:G:203:ASP:OD1	1.98	0.64
1:E:55:ASP:O	1:E:139:TRP:NE1	2.24	0.64
1:G:94:ASN:OD1	1:G:100:ILE:CD1	2.46	0.64
1:C:18:VAL:O	1:C:21:HIS:HB2	1.98	0.63
1:E:10:ILE:HG23	1:E:29:GLY:N	2.14	0.63
1:G:12:LEU:HD13	1:G:116:TYR:HD1	1.63	0.63
1:E:152:VAL:HG12	1:E:177:TYR:O	1.98	0.63
1:C:128:ASN:HA	1:C:133:GLN:CD	2.19	0.63
1:G:66:ARG:HB3	1:G:79:PHE:CE1	2.34	0.62
1:C:128:ASN:CA	1:C:133:GLN:NE2	2.56	0.62
1:C:200:HIS:CE1	1:C:204:TYR:OH	2.52	0.62
1:D:63:KY7:OA	1:D:157:VAL:HG11	1.99	0.62
1:H:201:ASP:O	1:H:203:ASP:N	2.31	0.62
1:H:17:ALA:HA	1:H:21:HIS:O	2.00	0.62
1:E:10:ILE:HG22	1:E:29:GLY:N	2.13	0.62
1:F:149:ARG:NH1	1:G:96:GLU:OE2	2.30	0.62
1:A:170:ARG:NH2	1:D:174:LYS:HE3	2.16	0.61
1:E:81:GLN:CD	1:E:183:VAL:HG22	2.20	0.61
1:H:58:THR:HG23	1:H:209:LEU:HD11	1.82	0.61
1:E:60:VAL:HG13	1:E:89:TRP:HH2	1.66	0.60
1:H:138:LYS:NZ	1:H:194:HIS:CD2	2.70	0.60
1:G:129:GLY:O	1:G:133:GLN:HB2	2.02	0.60
1:A:170:ARG:NH1	1:D:147:TYR:OH	2.34	0.60
1:B:65:ASN:OD1	1:B:87:TYR:CZ	2.52	0.60
1:D:17:ALA:HA	1:D:21:HIS:O	2.01	0.60
1:G:197:ILE:HG13	1:G:209:LEU:HD13	1.83	0.60
1:F:5:LYS:CB	1:F:8:MET:HE2	2.28	0.60
1:F:195:ILE:HD12	1:F:210:HIS:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PRO:O	1:D:190:PHE:HZ	1.84	0.59
1:C:4:ILE:HD13	1:C:80:LYS:HG2	1.83	0.59
1:E:125:PHE:CD1	1:E:131:VAL:HG11	2.37	0.59
1:E:40:MET:SD	1:E:42:LEU:HD11	2.40	0.59
1:B:145:LYS:HD2	1:E:158:ASN:O	2.02	0.59
1:C:8:MET:HE3	1:C:114:TYR:CE2	2.37	0.59
1:E:138:LYS:NZ	1:E:139:TRP:O	2.35	0.59
1:A:15:GLU:O	1:A:119:ARG:HD2	2.03	0.59
1:F:39:SER:HB2	1:F:209:LEU:O	2.02	0.59
1:C:195:ILE:HG13	1:C:209:LEU:HD11	1.84	0.59
1:F:24:ALA:HB3	1:F:46:GLU:HB2	1.84	0.59
1:B:182:VAL:HG22	1:C:184:GLN:HG3	1.85	0.59
1:D:55:ASP:O	1:D:139:TRP:NE1	2.32	0.59
1:G:133:GLN:HG2	1:G:135:ARG:NH1	2.15	0.59
1:E:107:ILE:HD12	1:E:116:TYR:HE1	1.68	0.58
1:H:66:ARG:NH1	1:H:66:ARG:HG3	2.12	0.58
1:C:107:ILE:HD13	1:C:116:TYR:CE1	2.38	0.58
1:C:129:GLY:O	1:C:133:GLN:CG	2.51	0.58
1:C:163:LEU:HD21	1:C:169:TYR:HB2	1.85	0.58
1:D:203:ASP:OD2	1:D:205:SER:CB	2.50	0.58
1:A:200:HIS:CD2	1:A:204:TYR:CZ	2.91	0.58
1:E:81:GLN:CD	1:E:183:VAL:CG2	2.72	0.58
1:F:5:LYS:H	1:F:8:MET:HE2	1.62	0.58
1:A:66:ARG:CZ	1:A:66:ARG:HA	2.33	0.58
1:F:50:LEU:HD12	1:F:50:LEU:H	1.68	0.58
1:F:143:THR:HG21	1:G:143:THR:HG21	1.85	0.58
1:D:91:ARG:HD3	1:D:175:THR:OG1	2.04	0.57
1:C:199:SER:OG	1:C:208:ASN:CB	2.52	0.57
1:A:55:ASP:O	1:A:139:TRP:NE1	2.34	0.57
1:B:37:LYS:HG3	1:B:212:HIS:ND1	2.19	0.57
1:C:138:LYS:CG	1:C:139:TRP:N	2.67	0.57
1:B:38:GLN:OE1	1:B:211:GLU:HB3	2.04	0.57
1:A:173:PHE:HD2	1:A:173:PHE:N	2.03	0.57
1:B:60:VAL:HG13	1:B:89:TRP:HH2	1.70	0.57
1:E:59:THR:HG22	1:E:63:KY7:CD2	2.35	0.57
1:B:65:ASN:C	1:B:67:VAL:H	2.07	0.56
1:H:14:MET:SD	1:H:57:LEU:HD22	2.45	0.56
1:A:31:GLY:HA3	1:A:68:PHE:HE2	1.70	0.56
1:C:41:ASP:OD2	1:C:208:ASN:ND2	2.38	0.56
1:E:152:VAL:CG1	1:E:177:TYR:O	2.53	0.56
1:F:12:LEU:HD21	1:F:40:MET:SD	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ASN:HA	1:C:87:TYR:HH	1.71	0.56
1:E:38:GLN:NE2	1:E:211:GLU:HB3	2.21	0.56
1:G:13:ARG:NH2	1:G:15:GLU:OE2	2.38	0.56
1:G:55:ASP:O	1:G:139:TRP:NE1	2.36	0.56
1:B:181:LYS:HG2	1:B:182:VAL:N	2.20	0.56
1:D:33:PRO:HB3	1:D:67:VAL:HG12	1.88	0.56
1:E:201:ASP:OD1	1:E:206:ASN:CB	2.45	0.56
1:C:65:ASN:HA	1:C:87:TYR:OH	2.06	0.55
1:A:174:LYS:O	1:E:124:ASN:ND2	2.39	0.55
1:E:119:ARG:HD3	1:E:120:PHE:N	2.22	0.55
1:A:173:PHE:CD2	1:A:173:PHE:N	2.74	0.55
1:B:85:GLU:N	1:B:85:GLU:OE1	2.39	0.55
1:D:32:LYS:HD3	1:D:35:GLU:OE2	2.06	0.55
1:G:86:GLY:C	1:G:180:LYS:CD	2.73	0.55
1:E:158:ASN:CG	1:E:172:ASP:OD1	2.45	0.55
1:F:158:ASN:CG	1:F:172:ASP:OD1	2.40	0.55
1:G:192:ASP:OD1	1:G:216:HIS:NE2	2.33	0.55
1:A:65:ASN:O	1:A:66:ARG:NH1	2.39	0.55
1:C:158:ASN:OD1	1:C:170:ARG:NH1	2.39	0.55
1:H:195:ILE:HD12	1:H:210:HIS:O	2.07	0.55
1:F:5:LYS:O	1:F:8:MET:CE	2.55	0.55
1:A:31:GLY:HA3	1:A:68:PHE:CE2	2.41	0.55
1:C:107:ILE:CD1	1:C:116:TYR:CE1	2.91	0.54
1:E:15:GLU:O	1:E:119:ARG:HA	2.07	0.54
1:F:149:ARG:HH12	1:G:96:GLU:CD	2.08	0.54
1:E:196:GLU:O	1:E:209:LEU:HD12	2.07	0.54
1:B:195:ILE:HD11	1:B:209:LEU:HD21	1.89	0.54
1:G:66:ARG:HB3	1:G:79:PHE:CD1	2.42	0.54
1:C:159:THR:O	1:C:170:ARG:HD2	2.08	0.54
1:C:195:ILE:HD12	1:C:210:HIS:O	2.08	0.54
1:E:66:ARG:HG2	1:E:66:ARG:NH1	2.21	0.54
1:H:15:GLU:O	1:H:119:ARG:HD2	2.07	0.54
1:B:104:THR:HG22	1:B:119:ARG:HB3	1.90	0.53
1:B:55:ASP:O	1:B:139:TRP:NE1	2.34	0.53
1:A:14:MET:SD	1:A:57:LEU:HD23	2.49	0.53
1:A:60:VAL:HG13	1:A:89:TRP:HH2	1.74	0.53
1:B:182:VAL:HG11	1:C:81:GLN:OE1	2.09	0.53
1:G:195:ILE:HD11	1:G:209:LEU:HD21	1.90	0.53
1:F:7:ASP:OD2	1:F:32:LYS:HE2	2.09	0.53
1:C:65:ASN:HD22	1:C:68:PHE:HE2	1.56	0.53
1:E:107:ILE:HD12	1:E:116:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:MET:N	1:F:25:ILE:O	2.29	0.53
1:C:112:ASP:N	1:C:112:ASP:OD1	2.37	0.53
1:C:129:GLY:O	1:C:133:GLN:HG3	2.08	0.53
1:E:152:VAL:HG12	1:E:153:LEU:H	1.73	0.53
1:G:16:GLY:HA2	1:G:119:ARG:CZ	2.39	0.53
1:B:65:ASN:ND2	1:B:67:VAL:HB	2.24	0.52
1:C:199:SER:OG	1:C:208:ASN:HB2	2.09	0.52
1:G:66:ARG:HA	1:G:66:ARG:HH11	1.74	0.52
1:H:65:ASN:C	1:H:67:VAL:H	2.12	0.52
1:C:200:HIS:HA	1:C:206:ASN:O	2.10	0.52
1:F:63:KY7:CD2	1:F:63:KY7:N2	2.73	0.52
1:C:168:HIS:O	1:H:149:ARG:NH2	2.42	0.52
1:A:34:PHE:O	1:A:70:LYS:HG3	2.09	0.52
1:F:12:LEU:HB3	1:F:116:TYR:HB2	1.91	0.52
1:F:5:LYS:C	1:F:8:MET:CE	2.74	0.52
1:D:198:LYS:HE2	1:D:210:HIS:CG	2.44	0.52
1:E:12:LEU:CB	1:E:116:TYR:HB2	2.40	0.52
1:H:144:GLU:HA	1:H:157:VAL:HG22	1.91	0.52
1:E:63:KY7:CA3	1:E:63:KY7:N	2.73	0.51
1:G:86:GLY:O	1:G:180:LYS:CD	2.56	0.51
1:H:63:KY7:CD2	1:H:63:KY7:N2	2.73	0.51
1:C:72:PRO:HD2	1:C:75:ILE:HD12	1.92	0.51
1:A:63:KY7:CA3	1:A:63:KY7:N	2.73	0.51
1:A:90:GLU:OE1	1:E:19:ASN:HA	2.09	0.51
1:B:219:LEU:HG	1:E:192:ASP:HB3	1.91	0.51
1:F:157:VAL:HG12	1:F:173:PHE:HB2	1.93	0.51
1:F:60:VAL:O	1:F:60:VAL:HG12	2.10	0.51
1:A:85:GLU:CD	1:A:181:LYS:HD3	2.31	0.51
1:D:63:KY7:OH	1:D:63:KY7:OB	2.28	0.51
1:C:120:PHE:CD1	1:C:120:PHE:C	2.84	0.51
1:E:192:ASP:OD2	1:E:216:HIS:NE2	2.39	0.51
1:G:66:ARG:CG	1:G:79:PHE:CE1	2.94	0.51
1:C:199:SER:OG	1:C:208:ASN:HB3	2.11	0.51
1:F:59:THR:O	1:F:63:KY7:N2	2.44	0.51
1:B:63:KY7:CD2	1:B:63:KY7:N2	2.73	0.51
1:F:75:ILE:HG21	1:F:189:HIS:CD2	2.45	0.51
1:G:12:LEU:HD23	1:G:42:LEU:HD21	1.92	0.51
1:H:63:KY7:OA	1:H:173:PHE:CD1	2.63	0.51
1:D:66:ARG:HD2	1:D:191:VAL:HG11	1.92	0.50
1:C:63:KY7:N2	1:C:63:KY7:CD2	2.73	0.50
1:F:5:LYS:O	1:F:8:MET:HE1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:KY7:OA	1:H:173:PHE:CE1	2.64	0.50
1:A:90:GLU:O	1:A:175:THR:HA	2.10	0.50
1:E:135:ARG:HH22	1:H:198:LYS:HZ3	1.57	0.50
1:F:82:SER:O	1:F:86:GLY:N	2.30	0.50
1:E:10:ILE:HG22	1:E:29:GLY:H	1.73	0.50
1:H:65:ASN:C	1:H:67:VAL:N	2.64	0.50
1:A:148:VAL:HG21	1:A:185:LEU:HB3	1.94	0.50
1:G:138:LYS:HE2	1:G:139:TRP:O	2.11	0.50
1:C:160:ALA:HB2	1:C:170:ARG:HD2	1.93	0.49
1:H:138:LYS:HZ1	1:H:194:HIS:CD2	2.24	0.49
1:A:77:ASP:O	1:A:81:GLN:HG2	2.12	0.49
1:B:55:ASP:OD2	1:B:136:THR:OG1	2.26	0.49
1:C:16:GLY:HA2	1:C:119:ARG:CZ	2.43	0.49
1:A:141:PRO:O	1:D:190:PHE:CZ	2.64	0.49
1:H:212:HIS:NE2	1:H:214:GLU:OE2	2.43	0.49
1:B:129:GLY:O	1:B:133:GLN:HG3	2.12	0.49
1:F:59:THR:O	1:F:63:KY7:C1	2.61	0.49
1:D:82:SER:O	1:D:86:GLY:N	2.33	0.49
1:G:42:LEU:HD22	1:G:61:PHE:CE1	2.46	0.49
1:E:10:ILE:HG23	1:E:29:GLY:H	1.76	0.49
1:E:34:PHE:O	1:E:70:LYS:HG3	2.12	0.49
1:G:65:ASN:OD1	1:G:107:ILE:HD13	2.12	0.49
1:F:133:GLN:HB2	1:F:135:ARG:HD2	1.95	0.49
1:G:133:GLN:CG	1:G:135:ARG:NH1	2.75	0.49
1:G:87:TYR:N	1:G:180:LYS:HD2	2.27	0.49
1:H:63:KY7:OB	1:H:142:SER:CB	2.58	0.49
1:B:192:ASP:HB2	1:E:219:LEU:HD13	1.95	0.48
1:B:60:VAL:HG21	1:B:120:PHE:CD1	2.47	0.48
1:E:152:VAL:HG11	1:E:178:LYS:HB3	1.95	0.48
1:C:24:ALA:HB3	1:C:46:GLU:HG3	1.93	0.48
1:D:72:PRO:HD2	1:D:75:ILE:HD12	1.95	0.48
1:E:54:TYR:CE2	1:E:207:VAL:HG21	2.48	0.48
1:G:94:ASN:HA	1:G:100:ILE:HD13	1.96	0.48
1:H:65:ASN:HA	1:H:87:TYR:OH	2.13	0.48
1:B:147:TYR:HB3	1:B:188:TYR:CD2	2.48	0.48
1:B:50:LEU:O	1:B:134:LYS:NZ	2.30	0.48
1:F:21:HIS:NE2	1:F:51:PRO:HG3	2.28	0.48
1:G:77:ASP:O	1:G:81:GLN:HG2	2.14	0.48
1:H:138:LYS:HG2	1:H:139:TRP:N	2.28	0.48
1:H:19:ASN:OD1	1:H:125:PHE:HB2	2.13	0.48
1:E:66:ARG:HG2	1:E:66:ARG:HH11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:ILE:HD12	1:G:116:TYR:OH	2.13	0.48
1:C:99:GLY:HA3	1:C:125:PHE:CE1	2.48	0.48
1:E:59:THR:HG22	1:E:63:KY7:CE2	2.43	0.48
1:H:52:PHE:CE1	1:H:57:LEU:HD11	2.44	0.48
1:A:99:GLY:HA3	1:A:125:PHE:CE1	2.49	0.48
1:C:158:ASN:O	1:H:145:LYS:HD3	2.13	0.48
1:F:163:LEU:HD21	1:F:169:TYR:HB2	1.96	0.48
1:F:142:SER:OG	1:F:193:HIS:HB2	2.14	0.48
1:D:170:ARG:HE	1:D:170:ARG:HB2	1.48	0.47
1:F:16:GLY:HA2	1:F:119:ARG:CZ	2.44	0.47
1:D:192:ASP:OD2	1:D:216:HIS:NE2	2.39	0.47
1:D:202:LYS:C	1:D:204:TYR:H	2.16	0.47
1:D:15:GLU:O	1:D:119:ARG:HD2	2.14	0.47
1:D:131:VAL:HG12	1:D:132:MET:HE2	1.96	0.47
1:G:133:GLN:HB3	1:G:135:ARG:NH1	2.30	0.47
1:C:63:KY7:N	1:C:63:KY7:CA3	2.77	0.47
1:A:112:ASP:OD1	1:A:112:ASP:N	2.43	0.47
1:B:65:ASN:C	1:B:67:VAL:N	2.68	0.47
1:F:63:KY7:CA3	1:F:63:KY7:N	2.77	0.47
1:C:129:GLY:O	1:C:133:GLN:HG2	2.15	0.47
1:D:58:THR:HB	1:D:195:ILE:HD11	1.97	0.47
1:F:219:LEU:HD23	1:F:220:PRO:HD2	1.97	0.47
1:B:19:ASN:OD1	1:B:125:PHE:HB2	2.15	0.47
1:E:38:GLN:NE2	1:E:211:GLU:OE2	2.48	0.47
1:H:15:GLU:O	1:H:119:ARG:HA	2.15	0.47
1:F:145:LYS:O	1:F:155:GLY:HA2	2.15	0.47
1:A:54:TYR:CZ	1:A:207:VAL:HG21	2.49	0.46
1:B:92:SER:CB	1:D:100:ILE:HG21	2.44	0.46
1:D:147:TYR:O	1:D:153:LEU:HD12	2.15	0.46
1:E:43:LYS:HA	1:E:205:SER:O	2.14	0.46
1:H:192:ASP:OD2	1:H:216:HIS:NE2	2.44	0.46
1:H:26:GLU:HB3	1:H:45:LYS:HE3	1.97	0.46
1:H:55:ASP:O	1:H:139:TRP:NE1	2.44	0.46
1:A:172:ASP:CG	1:A:174:LYS:HZ3	2.19	0.46
1:C:39:SER:HB2	1:C:210:HIS:CE1	2.49	0.46
1:C:91:ARG:HE	1:C:175:THR:HB	1.80	0.46
1:B:200:HIS:HA	1:B:206:ASN:O	2.16	0.46
1:C:8:MET:CE	1:C:114:TYR:CZ	2.96	0.46
1:E:14:MET:HB2	1:E:118:ILE:HB	1.97	0.46
1:G:12:LEU:CD1	1:G:116:TYR:HB2	2.45	0.46
1:G:19:ASN:HD21	1:G:125:PHE:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:LYS:HB3	1:H:214:GLU:HG2	1.98	0.46
1:H:138:LYS:HG2	1:H:139:TRP:O	2.16	0.46
1:E:149:ARG:HD3	1:G:227:LEU:HB2	1.97	0.46
1:C:17:ALA:HA	1:C:21:HIS:O	2.15	0.46
1:C:149:ARG:NH2	1:H:168:HIS:O	2.48	0.46
1:D:133:GLN:HB2	1:D:135:ARG:HG3	1.98	0.46
1:D:157:VAL:HG12	1:D:173:PHE:HB2	1.97	0.46
1:H:104:THR:O	1:H:118:ILE:HA	2.16	0.46
1:C:63:KY7:O2	1:C:66:ARG:NH2	2.42	0.45
1:A:158:ASN:ND2	1:D:172:ASP:OD2	2.49	0.45
1:H:93:MET:HG2	1:H:173:PHE:CD2	2.50	0.45
1:F:219:LEU:CD2	1:F:220:PRO:HD2	2.46	0.45
1:F:159:THR:HG22	1:G:145:LYS:HZ1	1.81	0.45
1:C:10:ILE:HD11	1:C:68:PHE:CZ	2.51	0.45
1:C:60:VAL:HG13	1:C:89:TRP:HH2	1.80	0.45
1:D:24:ALA:HB3	1:D:46:GLU:HG3	1.99	0.45
1:G:128:ASN:HA	1:G:133:GLN:HE21	1.78	0.45
1:A:65:ASN:ND2	1:A:107:ILE:HG21	2.31	0.45
1:F:8:MET:HG2	1:F:112:ASP:O	2.16	0.45
1:G:18:VAL:HA	1:G:122:GLY:O	2.17	0.45
1:H:63:KY7:CB1	1:H:211:GLU:OE1	2.64	0.45
1:F:146:LEU:HB2	1:F:189:HIS:CE1	2.50	0.45
1:F:63:KY7:C2	1:F:66:ARG:NH1	2.66	0.45
1:F:72:PRO:HG2	1:F:75:ILE:HG13	1.98	0.45
1:A:219:LEU:HG	1:D:192:ASP:CB	2.46	0.45
1:G:10:ILE:HG22	1:G:29:GLY:C	2.37	0.45
1:G:81:GLN:OE1	1:G:183:VAL:HB	2.17	0.45
1:H:144:GLU:HG2	1:H:146:LEU:HD11	1.98	0.45
1:B:12:LEU:HD11	1:B:42:LEU:HD23	1.98	0.45
1:B:86:GLY:O	1:B:180:LYS:HB2	2.17	0.45
1:B:43:LYS:HA	1:B:205:SER:O	2.17	0.45
1:F:97:ASP:CG	1:F:169:TYR:OH	2.55	0.45
1:F:8:MET:CG	1:F:112:ASP:O	2.65	0.45
1:C:200:HIS:CE1	1:C:204:TYR:CE1	3.05	0.45
1:D:92:SER:OG	1:D:100:ILE:HD11	2.16	0.45
1:F:17:ALA:O	1:F:121:ASP:HA	2.17	0.45
1:B:92:SER:HB2	1:D:100:ILE:HG21	1.99	0.44
1:E:58:THR:HG21	1:E:197:ILE:HD11	1.99	0.44
1:F:12:LEU:HD21	1:F:40:MET:CE	2.47	0.44
1:B:76:VAL:HB	1:B:186:PRO:HB3	1.99	0.44
1:E:38:GLN:HE21	1:E:211:GLU:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ARG:HD3	1:C:119:ARG:HA	1.75	0.44
1:C:195:ILE:CD1	1:C:211:GLU:HB2	2.41	0.44
1:G:139:TRP:CZ3	1:G:159:THR:HG23	2.53	0.44
1:D:140:GLU:OE1	1:D:168:HIS:CD2	2.71	0.44
1:E:183:VAL:HG22	1:E:184:GLN:H	1.82	0.44
1:G:196:GLU:O	1:G:209:LEU:HD12	2.17	0.44
1:D:63:KY7:N2	1:D:63:KY7:CD2	2.79	0.44
1:F:146:LEU:HA	1:F:154:LYS:O	2.18	0.44
1:G:133:GLN:O	1:G:135:ARG:HG3	2.16	0.44
1:G:67:VAL:HG11	1:G:83:PHE:HE2	1.83	0.44
1:C:149:ARG:NH1	1:H:96:GLU:OE2	2.42	0.44
1:B:60:VAL:HG21	1:B:120:PHE:HD1	1.83	0.44
1:F:21:HIS:CD2	1:F:51:PRO:HG3	2.53	0.44
1:B:191:VAL:HG12	1:B:193:HIS:CD2	2.52	0.44
1:G:93:MET:HG2	1:G:173:PHE:CE1	2.52	0.44
1:C:200:HIS:ND1	1:C:204:TYR:CE1	2.84	0.43
1:C:4:ILE:HG23	1:C:8:MET:HE1	2.00	0.43
1:D:4:ILE:HD11	1:D:83:PHE:HB2	1.98	0.43
1:E:30:LEU:HA	1:E:30:LEU:HD13	1.66	0.43
1:A:99:GLY:HA3	1:A:125:PHE:CD1	2.54	0.43
1:C:8:MET:CE	1:C:114:TYR:CE2	3.00	0.43
1:C:8:MET:CE	1:C:114:TYR:OH	2.66	0.43
1:B:221:ARG:HB3	1:E:194:HIS:CE1	2.53	0.43
1:E:66:ARG:HH11	1:E:66:ARG:CG	2.32	0.43
1:F:181:LYS:HE2	1:F:183:VAL:HG12	2.00	0.43
1:G:10:ILE:CD1	1:G:116:TYR:OH	2.67	0.43
1:G:19:ASN:OD1	1:G:125:PHE:HB2	2.18	0.43
1:B:41:ASP:HA	1:B:207:VAL:O	2.18	0.43
1:E:135:ARG:HH22	1:H:198:LYS:HZ1	1.60	0.43
1:E:152:VAL:CG1	1:E:153:LEU:N	2.80	0.43
1:F:4:ILE:HD12	1:F:80:LYS:HG2	2.01	0.43
1:A:25:ILE:HD11	1:A:42:LEU:HB3	2.01	0.43
1:D:65:ASN:ND2	1:D:67:VAL:HB	2.32	0.43
1:E:81:GLN:O	1:E:81:GLN:HG2	2.19	0.43
1:H:91:ARG:HG3	1:H:92:SER:N	2.33	0.43
1:C:67:VAL:HG11	1:C:83:PHE:CE2	2.54	0.43
1:B:221:ARG:HB3	1:E:194:HIS:HE1	1.84	0.43
1:C:141:PRO:O	1:H:190:PHE:HZ	2.01	0.43
1:A:81:GLN:O	1:A:181:LYS:HE3	2.19	0.43
1:D:197:ILE:HG23	1:D:207:VAL:HG13	2.01	0.43
1:E:6:PRO:CB	1:E:32:LYS:HZ1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:PHE:HZ	1:G:141:PRO:O	2.01	0.43
1:A:139:TRP:CD2	1:A:161:LEU:HG	2.53	0.43
1:E:93:MET:HB2	1:E:171:CYS:SG	2.59	0.43
1:H:201:ASP:OD1	1:H:205:SER:HB2	2.19	0.43
1:D:163:LEU:HD21	1:D:169:TYR:HB2	1.99	0.43
1:E:10:ILE:HD12	1:E:114:TYR:HB2	2.01	0.43
1:E:16:GLY:HA2	1:E:119:ARG:CZ	2.49	0.43
1:E:146:LEU:HA	1:E:154:LYS:O	2.19	0.43
1:E:49:PRO:HB3	1:E:203:ASP:HB2	1.99	0.43
1:C:52:PHE:CE1	1:C:57:LEU:HD11	2.49	0.42
1:D:12:LEU:HD21	1:D:42:LEU:HD21	2.01	0.42
1:A:78:TYR:HA	1:A:81:GLN:HE21	1.84	0.42
1:E:152:VAL:CG1	1:E:178:LYS:HB3	2.48	0.42
1:H:87:TYR:HB2	1:H:179:ALA:HA	2.01	0.42
1:G:16:GLY:HA2	1:G:119:ARG:NH2	2.35	0.42
1:G:145:LYS:NZ	1:G:188:TYR:OH	2.39	0.42
1:E:56:ILE:HG13	1:E:57:LEU:HD23	2.02	0.42
1:E:63:KY7:CD2	1:E:63:KY7:N2	2.82	0.42
1:F:21:HIS:HA	1:F:22:PRO:HD3	1.70	0.42
1:G:145:LYS:HG3	1:G:190:PHE:CD1	2.54	0.42
1:A:63:KY7:OB	1:A:193:HIS:CD2	2.72	0.42
1:G:59:THR:O	1:G:91:ARG:NH1	2.48	0.42
1:H:139:TRP:CZ3	1:H:161:LEU:HG	2.55	0.42
1:A:157:VAL:HG12	1:A:173:PHE:HB2	2.01	0.42
1:D:56:ILE:HG13	1:D:57:LEU:HD23	2.01	0.42
1:F:12:LEU:CB	1:F:116:TYR:HB2	2.50	0.42
1:F:185:LEU:HA	1:F:185:LEU:HD23	1.81	0.42
1:F:31:GLY:HA2	1:F:38:GLN:HA	2.01	0.42
1:F:63:KY7:CB1	1:F:211:GLU:OE2	2.68	0.42
1:F:157:VAL:HG22	1:F:159:THR:HG23	2.01	0.42
1:G:133:GLN:CG	1:G:135:ARG:HH12	2.21	0.42
1:H:201:ASP:OD2	1:H:206:ASN:O	2.38	0.42
1:H:66:ARG:NH1	1:H:66:ARG:CG	2.72	0.42
1:D:149:ARG:O	1:D:152:VAL:HG12	2.19	0.42
1:E:93:MET:H	1:E:93:MET:HG2	1.69	0.42
1:G:107:ILE:HG12	1:G:116:TYR:CD2	2.55	0.42
1:A:219:LEU:HG	1:D:192:ASP:HB3	2.01	0.42
1:D:60:VAL:HG13	1:D:89:TRP:HH2	1.85	0.42
1:E:145:LYS:HB2	1:E:145:LYS:HE2	1.73	0.42
1:G:12:LEU:HD11	1:G:118:ILE:CD1	2.50	0.42
1:G:143:THR:HA	1:G:192:ASP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:VAL:HG22	1:E:162:SER:O	2.19	0.42
1:G:85:GLU:OE1	1:G:181:LYS:CG	2.67	0.42
1:H:146:LEU:HA	1:H:154:LYS:O	2.20	0.42
1:B:65:ASN:OD1	1:B:87:TYR:CE1	2.73	0.41
1:C:104:THR:O	1:C:118:ILE:HA	2.20	0.41
1:C:12:LEU:HB2	1:C:116:TYR:HB2	2.02	0.41
1:C:145:LYS:HD2	1:H:158:ASN:O	2.19	0.41
1:B:60:VAL:HG13	1:B:89:TRP:CH2	2.53	0.41
1:D:70:LYS:HB3	1:D:214:GLU:HG2	2.01	0.41
1:G:181:LYS:HE2	1:G:183:VAL:CG1	2.50	0.41
1:A:139:TRP:CE3	1:A:161:LEU:HG	2.55	0.41
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.92	0.41
1:C:170:ARG:HE	1:C:171:CYS:H	1.68	0.41
1:G:66:ARG:HG2	1:G:79:PHE:CE1	2.56	0.41
1:H:144:GLU:HB3	1:H:193:HIS:HE1	1.85	0.41
1:B:91:ARG:HH11	1:B:91:ARG:HD2	1.71	0.41
1:E:12:LEU:HB2	1:E:116:TYR:HB2	2.03	0.41
1:C:142:SER:HB2	1:H:145:LYS:NZ	2.35	0.41
1:H:25:ILE:HG12	1:H:44:VAL:HA	2.02	0.41
1:H:53:ALA:O	1:H:56:ILE:HG12	2.21	0.41
1:A:148:VAL:HG11	1:A:185:LEU:HD13	2.02	0.41
1:B:163:LEU:HD11	1:B:169:TYR:HB2	2.03	0.41
1:B:25:ILE:HD11	1:B:50:LEU:HD11	2.01	0.41
1:F:146:LEU:HD12	1:F:153:LEU:HG	2.02	0.41
1:A:40:MET:SD	1:A:42:LEU:HD11	2.61	0.41
1:A:52:PHE:CE1	1:A:57:LEU:HD11	2.41	0.41
1:F:93:MET:HB3	1:F:171:CYS:SG	2.60	0.41
1:G:3:VAL:O	1:G:3:VAL:HG12	2.21	0.41
1:C:200:HIS:HE1	1:C:204:TYR:OH	2.00	0.41
1:C:77:ASP:C	1:C:81:GLN:HE21	2.19	0.41
1:B:192:ASP:OD1	1:B:216:HIS:NE2	2.50	0.41
1:E:61:PHE:O	1:E:116:TYR:HE2	2.03	0.41
1:F:63:KY7:CD1	1:F:193:HIS:ND1	2.84	0.41
1:F:67:VAL:HG21	1:F:83:PHE:CE2	2.56	0.41
1:F:212:HIS:CD2	1:G:219:LEU:HD13	2.55	0.41
1:H:87:TYR:CB	1:H:179:ALA:HA	2.51	0.41
1:A:138:LYS:C	1:A:161:LEU:HD23	2.41	0.41
1:C:34:PHE:O	1:C:70:LYS:HG3	2.21	0.41
1:F:154:LYS:HB3	1:F:154:LYS:HE2	1.68	0.41
1:G:66:ARG:CB	1:G:79:PHE:CE1	3.02	0.41
1:A:8:MET:HE3	1:A:8:MET:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ASN:O	1:E:145:LYS:HE3	2.20	0.40
1:B:53:ALA:O	1:B:56:ILE:HG12	2.20	0.40
1:B:87:TYR:CB	1:B:179:ALA:HA	2.51	0.40
1:G:15:GLU:O	1:G:119:ARG:HA	2.21	0.40
1:B:66:ARG:HH11	1:B:66:ARG:HA	1.85	0.40
1:D:15:GLU:O	1:D:119:ARG:HA	2.21	0.40
1:D:203:ASP:N	1:D:203:ASP:OD1	2.52	0.40
1:E:129:GLY:HA2	1:E:130:PRO:HD3	1.78	0.40
1:F:89:TRP:CE2	1:F:105:ASN:HB3	2.56	0.40
1:G:71:TYR:OH	1:G:189:HIS:NE2	2.39	0.40
1:E:14:MET:HA	1:E:118:ILE:O	2.21	0.40
1:E:63:KY7:O2	1:E:63:KY7:C	2.69	0.40
1:F:219:LEU:HD23	1:F:219:LEU:HA	1.82	0.40
1:G:181:LYS:HE2	1:G:183:VAL:HG12	2.03	0.40
1:E:135:ARG:NH2	1:H:198:LYS:NZ	2.64	0.40
1:A:200:HIS:CD2	1:A:204:TYR:CE1	3.09	0.40
1:B:87:TYR:HB2	1:B:179:ALA:HA	2.04	0.40
1:C:53:ALA:O	1:C:56:ILE:HG12	2.22	0.40
1:E:81:GLN:O	1:E:81:GLN:CG	2.70	0.40
1:D:138:LYS:HG2	1:D:139:TRP:N	2.36	0.40
1:B:19:ASN:ND2	1:D:90:GLU:OE2	2.42	0.40
1:E:87:TYR:CB	1:E:179:ALA:HA	2.51	0.40
1:G:12:LEU:HD11	1:G:118:ILE:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	214/255 (84%)	208 (97%)	5 (2%)	1 (0%)	31 65
1	B	214/255 (84%)	207 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	213/255 (84%)	207 (97%)	5 (2%)	1 (0%)	31	65
1	D	212/255 (83%)	204 (96%)	6 (3%)	2 (1%)	19	52
1	E	211/255 (83%)	203 (96%)	8 (4%)	0	100	100
1	F	214/255 (84%)	209 (98%)	4 (2%)	1 (0%)	31	65
1	G	217/255 (85%)	209 (96%)	7 (3%)	1 (0%)	31	65
1	H	214/255 (84%)	204 (95%)	8 (4%)	2 (1%)	19	52
All	All	1709/2040 (84%)	1651 (97%)	50 (3%)	8 (0%)	31	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	65	ASN
1	F	65	ASN
1	A	201	ASP
1	H	202	LYS
1	D	202	LYS
1	D	66	ARG
1	H	66	ARG
1	G	84	PRO

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	179/217 (82%)	174 (97%)	5 (3%)	47	80
1	B	182/217 (84%)	179 (98%)	3 (2%)	65	88
1	C	182/217 (84%)	176 (97%)	6 (3%)	41	75
1	D	181/217 (83%)	179 (99%)	2 (1%)	76	93
1	E	175/217 (81%)	171 (98%)	4 (2%)	53	83
1	F	177/217 (82%)	169 (96%)	8 (4%)	30	64
1	G	182/217 (84%)	176 (97%)	6 (3%)	41	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	179/217 (82%)	173 (97%)	6 (3%)	40 74
All	All	1437/1736 (83%)	1397 (97%)	40 (3%)	47 80

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	71	TYR
1	A	74	ASN
1	A	92	SER
1	A	121	ASP
1	B	38	GLN
1	B	43	LYS
1	B	92	SER
1	C	7	ASP
1	C	119	ARG
1	C	133	GLN
1	C	175	THR
1	C	200	HIS
1	C	201	ASP
1	D	128	ASN
1	D	140	GLU
1	E	12	LEU
1	E	30	LEU
1	E	38	GLN
1	E	93	MET
1	F	7	ASP
1	F	8	MET
1	F	42	LEU
1	F	58	THR
1	F	59	THR
1	F	66	ARG
1	F	187	ASP
1	F	201	ASP
1	G	66	ARG
1	G	71	TYR
1	G	133	GLN
1	G	180	LYS
1	G	184	GLN
1	G	199	SER
1	H	30	LEU
1	H	42	LEU

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Mol	Chain	Res	Type
1	H	59	THR
1	H	66	ARG
1	H	92	SER
1	H	132	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	H	193	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KY7	A	63	1	24,25,26	4.10	12 (50%)	30,35,37	3.77	13 (43%)
1	KY7	B	63	1	24,25,26	4.09	11 (45%)	30,35,37	3.79	14 (46%)
1	KY7	C	63	1	24,25,26	3.98	9 (37%)	30,35,37	3.81	15 (50%)
1	KY7	D	63	1	24,25,26	3.79	10 (41%)	30,35,37	3.78	15 (50%)
1	KY7	E	63	1	24,25,26	4.10	10 (41%)	30,35,37	4.37	12 (40%)
1	KY7	F	63	1	24,25,26	3.89	10 (41%)	30,35,37	4.03	16 (53%)
1	KY7	G	63	1	24,25,26	3.82	8 (33%)	30,35,37	3.48	15 (50%)
1	KY7	H	63	1	24,25,26	3.52	7 (29%)	30,35,37	3.86	13 (43%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KY7	A	63	1	-	0/11/33/34	0/2/2/2
1	KY7	B	63	1	-	0/11/33/34	0/2/2/2
1	KY7	C	63	1	-	0/11/33/34	0/2/2/2
1	KY7	D	63	1	-	0/11/33/34	0/2/2/2
1	KY7	E	63	1	-	1/11/33/34	0/2/2/2
1	KY7	F	63	1	-	1/11/33/34	0/2/2/2
1	KY7	G	63	1	1/1/6/8	0/11/33/34	0/2/2/2
1	KY7	H	63	1	-	0/11/33/34	0/2/2/2

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	KY7	CB1-CA1	-12.64	1.38	1.52
1	E	63	KY7	CB1-CA1	-12.57	1.38	1.52
1	C	63	KY7	CB1-CA1	-12.41	1.38	1.52
1	A	63	KY7	CB1-CA1	-12.09	1.39	1.52
1	G	63	KY7	CB1-CA1	-11.49	1.40	1.52
1	E	63	KY7	CA1-C1	-11.46	1.35	1.51
1	F	63	KY7	CA1-C1	-11.00	1.36	1.51
1	B	63	KY7	CA1-C1	-11.00	1.36	1.51
1	F	63	KY7	CB1-CA1	-10.84	1.40	1.52
1	D	63	KY7	CB1-CA1	-10.70	1.40	1.52
1	C	63	KY7	CA1-C1	-10.60	1.36	1.51
1	D	63	KY7	CA1-C1	-10.43	1.37	1.51
1	H	63	KY7	CB1-CA1	-9.95	1.41	1.52
1	G	63	KY7	CA1-C1	-9.83	1.37	1.51
1	A	63	KY7	CA1-C1	-9.59	1.38	1.51
1	H	63	KY7	CA1-C1	-9.34	1.38	1.51
1	D	63	KY7	CA2-C2	-4.74	1.43	1.48
1	G	63	KY7	C2-N3	-4.50	1.29	1.39
1	D	63	KY7	C2-N3	-4.50	1.29	1.39
1	A	63	KY7	C2-N3	-4.17	1.30	1.39
1	H	63	KY7	C2-N3	-4.05	1.30	1.39
1	B	63	KY7	C2-N3	-3.97	1.30	1.39
1	B	63	KY7	CA2-C2	-3.94	1.44	1.48
1	H	63	KY7	CA2-C2	-3.84	1.44	1.48
1	F	63	KY7	CA2-C2	-3.78	1.44	1.48
1	C	63	KY7	C2-N3	-3.68	1.31	1.39
1	G	63	KY7	CA2-C2	-3.30	1.45	1.48
1	E	63	KY7	CA2-C2	-2.98	1.45	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	KY7	CA2-N2	-2.97	1.32	1.38
1	F	63	KY7	C2-N3	-2.87	1.33	1.39
1	A	63	KY7	C1-N3	-2.79	1.32	1.37
1	F	63	KY7	C1-N2	-2.76	1.28	1.32
1	C	63	KY7	CA2-N2	-2.75	1.32	1.38
1	E	63	KY7	C1-N2	-2.63	1.28	1.32
1	E	63	KY7	CA1-N	-2.58	1.35	1.49
1	F	63	KY7	CA2-N2	-2.52	1.33	1.38
1	E	63	KY7	C2-N3	-2.51	1.33	1.39
1	C	63	KY7	C1-N2	-2.50	1.28	1.32
1	G	63	KY7	CA1-N	-2.49	1.35	1.49
1	B	63	KY7	O2-C2	-2.45	1.18	1.23
1	B	63	KY7	C1-N2	-2.42	1.28	1.32
1	D	63	KY7	O2-C2	-2.42	1.18	1.23
1	B	63	KY7	OB-NA	-2.35	1.18	1.22
1	A	63	KY7	CA2-C2	-2.33	1.46	1.48
1	E	63	KY7	CA2-N2	-2.29	1.33	1.38
1	D	63	KY7	C1-N2	-2.27	1.28	1.32
1	B	63	KY7	CA2-N2	-2.27	1.33	1.38
1	E	63	KY7	CB1-SG1	-2.26	1.76	1.81
1	G	63	KY7	O2-C2	-2.22	1.18	1.23
1	A	63	KY7	CA1-N	-2.17	1.37	1.49
1	A	63	KY7	C1-N2	-2.12	1.29	1.32
1	F	63	KY7	C1-N3	-2.02	1.33	1.37
1	A	63	KY7	CB1-SG1	-2.01	1.77	1.81
1	C	63	KY7	CA3-N3	-2.01	1.43	1.47
1	A	63	KY7	CA2-N2	-2.00	1.34	1.38
1	A	63	KY7	CG2-CB2	2.11	1.51	1.46
1	D	63	KY7	CB2-CA2	2.29	1.37	1.35
1	D	63	KY7	CA1-N	2.53	1.62	1.49
1	C	63	KY7	CA1-N	2.58	1.62	1.49
1	B	63	KY7	CA1-N	2.61	1.63	1.49
1	H	63	KY7	CA1-N	2.66	1.63	1.49
1	F	63	KY7	CA1-N	2.68	1.63	1.49
1	H	63	KY7	CB2-CA2	4.05	1.38	1.35
1	B	63	KY7	CB2-CA2	4.20	1.38	1.35
1	F	63	KY7	CB2-CA2	4.93	1.39	1.35
1	C	63	KY7	CB2-CA2	5.15	1.39	1.35
1	G	63	KY7	CB2-CA2	5.20	1.39	1.35
1	B	63	KY7	CA3-C	5.44	1.68	1.49
1	C	63	KY7	CA3-C	5.46	1.68	1.49
1	G	63	KY7	CA3-C	5.62	1.68	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	KY7	CB2-CA2	5.65	1.39	1.35
1	A	63	KY7	CA3-C	5.67	1.68	1.49
1	D	63	KY7	CA3-C	5.76	1.69	1.49
1	E	63	KY7	CA3-C	5.78	1.69	1.49
1	H	63	KY7	CA3-C	5.89	1.69	1.49
1	F	63	KY7	CA3-C	6.21	1.70	1.49
1	A	63	KY7	CB2-CA2	8.13	1.42	1.35

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	63	KY7	O2-C2-CA2	-13.22	123.55	130.96
1	C	63	KY7	O-C-CA3	-13.09	86.86	126.39
1	H	63	KY7	O-C-CA3	-12.81	87.72	126.39
1	E	63	KY7	O-C-CA3	-12.70	88.05	126.39
1	B	63	KY7	O-C-CA3	-11.86	90.58	126.39
1	G	63	KY7	O-C-CA3	-11.70	91.08	126.39
1	D	63	KY7	O-C-CA3	-11.62	91.32	126.39
1	F	63	KY7	O-C-CA3	-11.22	92.51	126.39
1	F	63	KY7	O2-C2-CA2	-11.06	124.75	130.96
1	A	63	KY7	O-C-CA3	-10.93	93.40	126.39
1	B	63	KY7	CG2-CB2-CA2	-9.03	118.97	130.01
1	A	63	KY7	C2-CA2-N2	-8.27	103.13	108.92
1	F	63	KY7	CG2-CB2-CA2	-7.89	120.36	130.01
1	D	63	KY7	CG2-CB2-CA2	-7.63	120.68	130.01
1	H	63	KY7	CG2-CB2-CA2	-7.46	120.88	130.01
1	C	63	KY7	CG2-CB2-CA2	-6.84	121.65	130.01
1	E	63	KY7	CG2-CB2-CA2	-6.54	122.01	130.01
1	G	63	KY7	C2-CA2-N2	-5.90	104.78	108.92
1	E	63	KY7	C2-CA2-N2	-5.72	104.91	108.92
1	C	63	KY7	C2-CA2-N2	-5.07	105.37	108.92
1	B	63	KY7	CA1-CB1-SG1	-5.02	103.12	114.42
1	H	63	KY7	N3-C1-N2	-4.78	108.15	111.45
1	B	63	KY7	C2-CA2-N2	-4.76	105.58	108.92
1	C	63	KY7	CA1-CB1-SG1	-4.67	103.91	114.42
1	C	63	KY7	O2-C2-CA2	-4.57	128.39	130.96
1	H	63	KY7	C2-CA2-N2	-4.54	105.74	108.92
1	F	63	KY7	C2-CA2-N2	-4.50	105.77	108.92
1	A	63	KY7	CG2-CB2-CA2	-4.49	124.52	130.01
1	F	63	KY7	CA3-N3-C1	-4.43	122.01	127.20
1	D	63	KY7	O2-C2-CA2	-4.21	128.59	130.96
1	G	63	KY7	CG2-CB2-CA2	-4.16	124.93	130.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63	KY7	C2-CA2-N2	-4.10	106.05	108.92
1	E	63	KY7	CA1-CB1-SG1	-3.95	105.53	114.42
1	G	63	KY7	N3-C1-N2	-3.95	108.72	111.45
1	A	63	KY7	CA1-CB1-SG1	-3.68	106.13	114.42
1	B	63	KY7	O2-C2-CA2	-3.68	128.89	130.96
1	A	63	KY7	N3-C1-N2	-3.67	108.91	111.45
1	C	63	KY7	CA3-N3-C1	-3.60	122.98	127.20
1	G	63	KY7	CA1-CB1-SG1	-3.47	106.61	114.42
1	F	63	KY7	CB1-CA1-C1	-3.46	103.30	110.54
1	D	63	KY7	CA1-CB1-SG1	-3.32	106.94	114.42
1	H	63	KY7	O2-C2-CA2	-3.26	129.13	130.96
1	D	63	KY7	N3-C1-N2	-2.98	109.39	111.45
1	B	63	KY7	N3-C1-N2	-2.85	109.48	111.45
1	C	63	KY7	CB2-CA2-N2	-2.78	124.88	128.83
1	D	63	KY7	CA3-N3-C2	-2.77	117.49	123.83
1	A	63	KY7	CD1-CE1-CZ	-2.73	117.72	121.43
1	E	63	KY7	CB1-CA1-C1	-2.73	104.84	110.54
1	G	63	KY7	CD1-CE1-CZ	-2.72	117.75	121.43
1	H	63	KY7	CA3-N3-C2	-2.65	117.75	123.83
1	D	63	KY7	CG2-CD1-CE1	-2.44	118.14	120.20
1	G	63	KY7	CE2-CD2-CG2	-2.19	118.38	121.26
1	B	63	KY7	CA3-N3-C2	-2.14	118.92	123.83
1	F	63	KY7	CG2-CD1-CE1	-2.12	118.41	120.20
1	G	63	KY7	CA3-N3-C2	-2.04	119.16	123.83
1	B	63	KY7	CE2-CD2-CG2	-2.00	118.63	121.26
1	G	63	KY7	CD1-CE1-NA	2.00	118.68	116.06
1	F	63	KY7	C1-CA1-N	2.04	116.72	109.01
1	C	63	KY7	OB-NA-CE1	2.07	122.69	119.00
1	B	63	KY7	C2-N3-C1	2.11	109.06	107.97
1	F	63	KY7	CA3-N3-C2	2.14	128.73	123.83
1	C	63	KY7	CD1-CE1-NA	2.15	118.87	116.06
1	G	63	KY7	C1-CA1-N	2.36	117.93	109.01
1	F	63	KY7	CA1-C1-N3	2.46	128.05	124.85
1	H	63	KY7	CB2-CA2-C2	2.46	125.25	122.28
1	F	63	KY7	C2-N3-C1	2.48	109.26	107.97
1	C	63	KY7	CA1-C1-N3	2.56	128.19	124.85
1	C	63	KY7	C2-N3-C1	2.61	109.32	107.97
1	F	63	KY7	CA2-C2-N3	2.66	104.62	103.35
1	G	63	KY7	CA3-N3-C1	2.84	130.52	127.20
1	E	63	KY7	CA1-C1-N3	2.91	128.65	124.85
1	D	63	KY7	CB1-CA1-C1	2.95	116.71	110.54
1	C	63	KY7	CB1-CA1-C1	3.00	116.81	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	63	KY7	O2-C2-N3	3.03	130.48	124.31
1	G	63	KY7	OB-NA-CE1	3.04	124.42	119.00
1	F	63	KY7	O2-C2-N3	3.10	130.62	124.31
1	A	63	KY7	C1-CA1-N	3.20	121.08	109.01
1	C	63	KY7	CA2-C2-N3	3.21	104.89	103.35
1	E	63	KY7	CB2-CA2-C2	3.29	126.26	122.28
1	A	63	KY7	OB-NA-CE1	3.35	124.97	119.00
1	D	63	KY7	CD1-CE1-NA	3.36	120.45	116.06
1	F	63	KY7	CD1-CE1-NA	3.44	120.56	116.06
1	D	63	KY7	CB2-CA2-C2	3.77	126.83	122.28
1	H	63	KY7	CA1-C1-N3	3.90	129.94	124.85
1	A	63	KY7	CB2-CA2-C2	4.04	127.16	122.28
1	A	63	KY7	CD1-CE1-NA	4.06	121.38	116.06
1	B	63	KY7	CA3-N3-C1	4.10	132.00	127.20
1	H	63	KY7	C2-N3-C1	4.13	110.11	107.97
1	B	63	KY7	CB2-CA2-C2	4.16	127.30	122.28
1	H	63	KY7	CA3-N3-C1	4.18	132.09	127.20
1	B	63	KY7	CA1-C1-N3	4.22	130.36	124.85
1	E	63	KY7	CD1-CE1-NA	4.24	121.61	116.06
1	G	63	KY7	C2-N3-C1	4.41	110.26	107.97
1	F	63	KY7	CB2-CA2-C2	4.47	127.68	122.28
1	D	63	KY7	CA1-C1-N3	4.59	130.84	124.85
1	H	63	KY7	CA2-C2-N3	4.61	105.56	103.35
1	A	63	KY7	C2-N3-C1	4.92	110.52	107.97
1	D	63	KY7	CA2-N2-C1	5.24	109.64	105.77
1	B	63	KY7	CA2-C2-N3	5.28	105.88	103.35
1	D	63	KY7	CA3-N3-C1	5.48	133.62	127.20
1	E	63	KY7	CA2-C2-N3	5.49	105.98	103.35
1	A	63	KY7	CA2-C2-N3	5.59	106.02	103.35
1	G	63	KY7	CA2-N2-C1	5.68	109.96	105.77
1	B	63	KY7	CA2-N2-C1	5.73	110.00	105.77
1	H	63	KY7	CB1-CA1-C1	5.79	122.65	110.54
1	D	63	KY7	CA2-C2-N3	5.80	106.12	103.35
1	C	63	KY7	CA2-N2-C1	5.81	110.06	105.77
1	F	63	KY7	CA2-N2-C1	6.01	110.20	105.77
1	G	63	KY7	CA2-C2-N3	6.06	106.25	103.35
1	H	63	KY7	CA2-N2-C1	6.18	110.33	105.77
1	C	63	KY7	CB2-CA2-C2	6.18	129.75	122.28
1	E	63	KY7	CA2-N2-C1	6.92	110.87	105.77
1	A	63	KY7	CA2-N2-C1	7.63	111.40	105.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	G	63	KY7	CA1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	63	KY7	C-CA3-N3-C2
1	E	63	KY7	C-CA3-N3-C2

There are no ring outliers.

7 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	KY7	3	0
1	B	63	KY7	1	0
1	C	63	KY7	5	0
1	D	63	KY7	3	0
1	E	63	KY7	6	0
1	F	63	KY7	11	0
1	H	63	KY7	6	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	216/255 (84%)	-0.30	0 100 100	31, 54, 82, 102	0
1	B	216/255 (84%)	-0.35	1 (0%) 90 90	31, 50, 75, 98	0
1	C	217/255 (85%)	-0.23	1 (0%) 90 90	31, 53, 80, 98	0
1	D	214/255 (83%)	-0.36	2 (0%) 84 83	28, 51, 76, 120	0
1	E	215/255 (84%)	-0.25	2 (0%) 84 83	32, 54, 76, 90	0
1	F	216/255 (84%)	-0.25	1 (0%) 90 90	34, 56, 87, 115	0
1	G	221/255 (86%)	-0.17	3 (1%) 75 75	30, 57, 86, 120	0
1	H	216/255 (84%)	-0.37	0 100 100	31, 51, 81, 100	0
All	All	1731/2040 (84%)	-0.28	10 (0%) 89 89	28, 53, 81, 120	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	220	PRO	3.7
1	F	3	VAL	3.4
1	B	165	GLY	2.8
1	G	220	PRO	2.7
1	D	4	ILE	2.6
1	E	220	PRO	2.5
1	G	224	MET	2.4
1	E	219	LEU	2.2
1	D	21	HIS	2.2
1	G	4	ILE	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KY7	A	63	24/25	0.87	0.25	54,75,85,90	0
1	KY7	H	63	24/25	0.87	0.25	54,75,85,90	0
1	KY7	E	63	24/25	0.89	0.26	54,75,85,90	0
1	KY7	G	63	24/25	0.91	0.25	54,75,85,90	0
1	KY7	C	63	24/25	0.91	0.27	54,75,85,90	0
1	KY7	D	63	24/25	0.92	0.23	54,75,85,90	0
1	KY7	B	63	24/25	0.93	0.20	54,75,85,90	0
1	KY7	F	63	24/25	0.94	0.21	54,75,85,90	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.