Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 06:26 PM EDT

PDB ID	:	2GFB
Title	:	CRYSTAL STRUCTURE OF A CATALYTIC FAB HAVING ESTERASE-LIKE ACTIVITY
Authors	:	Golinelli-Pimpaneau, B.; Knossow, M.
Deposited on	:	1994-07-07
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 (i) 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 (i)) were used in the production of this report:

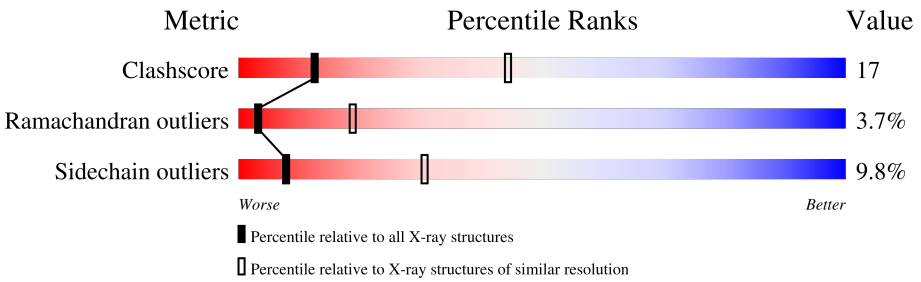
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	62% 34% 5%
1	C	214	61% 34% 5%
1	E	214	64% 31% 6%
1	G	214	71% 25% •
1	I	214	69% 25% 7%
1	K	214	66% 30% •
1	M	214	63% 31% 6%
1	O	214	64% 30% 6%

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Mol	Chain	Length	Quality of chain
2	B	219	59% 31% 10% •
2	D	219	63% 28% 7% •
2	F	219	68% 24% 6% •
2	H	219	62% 31% 6% •
2	J	219	60% 32% 6% •
2	L	219	62% 32% 5% •
2	N	219	59% 34% 6% •
2	P	219	58% 35% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 26336 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 IGG2A CNJ206 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1650	1023	277	343	7	0	0	0
1	C	214	1650	1023	277	343	7	0	0	0
1	E	214	1650	1023	277	343	7	0	0	0
1	G	214	1650	1023	277	343	7	0	0	0
1	I	214	1650	1023	277	343	7	0	0	0
1	K	214	1650	1023	277	343	7	0	0	0
1	M	214	1650	1023	277	343	7	0	0	0
1	O	214	1650	1023	277	343	7	0	0	0

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLU	ASP	conflict	GB 12002892
A	30	SER	GLY	conflict	GB 12002892
A	31	GLY	VAL	conflict	GB 12002892
A	32	TYR	SER	conflict	GB 12002892
A	34	SER	ASN	conflict	GB 12002892
A	39	LYS	GLU	conflict	GB 12002892
A	50	ALA	GLY	conflict	GB 12002892
A	51	ALA	THR	conflict	GB 12002892
A	53	THR	ARG	conflict	GB 12002892
A	84	ALA	VAL	conflict	GB 12002892
A	96	TYR	PRO	conflict	GB 12002892
A	99	GLY	-	insertion	GB 12002892
A	102	THR	SER	conflict	GB 12002892

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Chain	Residue	Modelled	Actual	Comment	Reference
A	103	LYS	ALA	conflict	GB 12002892
A	104	LEU	PRO	conflict	GB 12002892
A	105	GLU	SER	conflict	GB 12002892
A	106	ILE	CYS	conflict	GB 12002892
A	107	LEU	LYS	conflict	GB 12002892
A	109	GLY	ALA	conflict	GB 12002892
A	110	GLY	ASP	conflict	GB 12002892
A	?	-	VAL	deletion	GB 12002892
C	28	GLU	ASP	conflict	GB 12002892
C	30	SER	GLY	conflict	GB 12002892
C	31	GLY	VAL	conflict	GB 12002892
C	32	TYR	SER	conflict	GB 12002892
C	34	SER	ASN	conflict	GB 12002892
C	39	LYS	GLU	conflict	GB 12002892
C	50	ALA	GLY	conflict	GB 12002892
C	51	ALA	THR	conflict	GB 12002892
C	53	THR	ARG	conflict	GB 12002892
C	84	ALA	VAL	conflict	GB 12002892
C	96	TYR	PRO	conflict	GB 12002892
C	99	GLY	-	insertion	GB 12002892
C	102	THR	SER	conflict	GB 12002892
C	103	LYS	ALA	conflict	GB 12002892
C	104	LEU	PRO	conflict	GB 12002892
C	105	GLU	SER	conflict	GB 12002892
C	106	ILE	CYS	conflict	GB 12002892
C	107	LEU	LYS	conflict	GB 12002892
C	109	GLY	ALA	conflict	GB 12002892
C	110	GLY	ASP	conflict	GB 12002892
C	?	-	VAL	deletion	GB 12002892
E	28	GLU	ASP	conflict	GB 12002892
E	30	SER	GLY	conflict	GB 12002892
E	31	GLY	VAL	conflict	GB 12002892
E	32	TYR	SER	conflict	GB 12002892
E	34	SER	ASN	conflict	GB 12002892
E	39	LYS	GLU	conflict	GB 12002892
E	50	ALA	GLY	conflict	GB 12002892
E	51	ALA	THR	conflict	GB 12002892
E	53	THR	ARG	conflict	GB 12002892
E	84	ALA	VAL	conflict	GB 12002892
E	96	TYR	PRO	conflict	GB 12002892
E	99	GLY	-	insertion	GB 12002892
E	102	THR	SER	conflict	GB 12002892

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Chain	Residue	Modelled	Actual	Comment	Reference
E	103	LYS	ALA	conflict	GB 12002892
E	104	LEU	PRO	conflict	GB 12002892
E	105	GLU	SER	conflict	GB 12002892
E	106	ILE	CYS	conflict	GB 12002892
E	107	LEU	LYS	conflict	GB 12002892
E	109	GLY	ALA	conflict	GB 12002892
E	110	GLY	ASP	conflict	GB 12002892
E	?	-	VAL	deletion	GB 12002892
G	28	GLU	ASP	conflict	GB 12002892
G	30	SER	GLY	conflict	GB 12002892
G	31	GLY	VAL	conflict	GB 12002892
G	32	TYR	SER	conflict	GB 12002892
G	34	SER	ASN	conflict	GB 12002892
G	39	LYS	GLU	conflict	GB 12002892
G	50	ALA	GLY	conflict	GB 12002892
G	51	ALA	THR	conflict	GB 12002892
G	53	THR	ARG	conflict	GB 12002892
G	84	ALA	VAL	conflict	GB 12002892
G	96	TYR	PRO	conflict	GB 12002892
G	99	GLY	-	insertion	GB 12002892
G	102	THR	SER	conflict	GB 12002892
G	103	LYS	ALA	conflict	GB 12002892
G	104	LEU	PRO	conflict	GB 12002892
G	105	GLU	SER	conflict	GB 12002892
G	106	ILE	CYS	conflict	GB 12002892
G	107	LEU	LYS	conflict	GB 12002892
G	109	GLY	ALA	conflict	GB 12002892
G	110	GLY	ASP	conflict	GB 12002892
G	?	-	VAL	deletion	GB 12002892
I	28	GLU	ASP	conflict	GB 12002892
I	30	SER	GLY	conflict	GB 12002892
I	31	GLY	VAL	conflict	GB 12002892
I	32	TYR	SER	conflict	GB 12002892
I	34	SER	ASN	conflict	GB 12002892
I	39	LYS	GLU	conflict	GB 12002892
I	50	ALA	GLY	conflict	GB 12002892
I	51	ALA	THR	conflict	GB 12002892
I	53	THR	ARG	conflict	GB 12002892
I	84	ALA	VAL	conflict	GB 12002892
I	96	TYR	PRO	conflict	GB 12002892
I	99	GLY	-	insertion	GB 12002892
I	102	THR	SER	conflict	GB 12002892

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Chain	Residue	Modelled	Actual	Comment	Reference
I	103	LYS	ALA	conflict	GB 12002892
I	104	LEU	PRO	conflict	GB 12002892
I	105	GLU	SER	conflict	GB 12002892
I	106	ILE	CYS	conflict	GB 12002892
I	107	LEU	LYS	conflict	GB 12002892
I	109	GLY	ALA	conflict	GB 12002892
I	110	GLY	ASP	conflict	GB 12002892
I	?	-	VAL	deletion	GB 12002892
K	28	GLU	ASP	conflict	GB 12002892
K	30	SER	GLY	conflict	GB 12002892
K	31	GLY	VAL	conflict	GB 12002892
K	32	TYR	SER	conflict	GB 12002892
K	34	SER	ASN	conflict	GB 12002892
K	39	LYS	GLU	conflict	GB 12002892
K	50	ALA	GLY	conflict	GB 12002892
K	51	ALA	THR	conflict	GB 12002892
K	53	THR	ARG	conflict	GB 12002892
K	84	ALA	VAL	conflict	GB 12002892
K	96	TYR	PRO	conflict	GB 12002892
K	99	GLY	-	insertion	GB 12002892
K	102	THR	SER	conflict	GB 12002892
K	103	LYS	ALA	conflict	GB 12002892
K	104	LEU	PRO	conflict	GB 12002892
K	105	GLU	SER	conflict	GB 12002892
K	106	ILE	CYS	conflict	GB 12002892
K	107	LEU	LYS	conflict	GB 12002892
K	109	GLY	ALA	conflict	GB 12002892
K	110	GLY	ASP	conflict	GB 12002892
K	?	-	VAL	deletion	GB 12002892
M	28	GLU	ASP	conflict	GB 12002892
M	30	SER	GLY	conflict	GB 12002892
M	31	GLY	VAL	conflict	GB 12002892
M	32	TYR	SER	conflict	GB 12002892
M	34	SER	ASN	conflict	GB 12002892
M	39	LYS	GLU	conflict	GB 12002892
M	50	ALA	GLY	conflict	GB 12002892
M	51	ALA	THR	conflict	GB 12002892
M	53	THR	ARG	conflict	GB 12002892
M	84	ALA	VAL	conflict	GB 12002892
M	96	TYR	PRO	conflict	GB 12002892
M	99	GLY	-	insertion	GB 12002892
M	102	THR	SER	conflict	GB 12002892

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Chain	Residue	Modelled	Actual	Comment	Reference
M	103	LYS	ALA	conflict	GB 12002892
M	104	LEU	PRO	conflict	GB 12002892
M	105	GLU	SER	conflict	GB 12002892
M	106	ILE	CYS	conflict	GB 12002892
M	107	LEU	LYS	conflict	GB 12002892
M	109	GLY	ALA	conflict	GB 12002892
M	110	GLY	ASP	conflict	GB 12002892
M	?	-	VAL	deletion	GB 12002892
O	28	GLU	ASP	conflict	GB 12002892
O	30	SER	GLY	conflict	GB 12002892
O	31	GLY	VAL	conflict	GB 12002892
O	32	TYR	SER	conflict	GB 12002892
O	34	SER	ASN	conflict	GB 12002892
O	39	LYS	GLU	conflict	GB 12002892
O	50	ALA	GLY	conflict	GB 12002892
O	51	ALA	THR	conflict	GB 12002892
O	53	THR	ARG	conflict	GB 12002892
O	84	ALA	VAL	conflict	GB 12002892
O	96	TYR	PRO	conflict	GB 12002892
O	99	GLY	-	insertion	GB 12002892
O	102	THR	SER	conflict	GB 12002892
O	103	LYS	ALA	conflict	GB 12002892
O	104	LEU	PRO	conflict	GB 12002892
O	105	GLU	SER	conflict	GB 12002892
O	106	ILE	CYS	conflict	GB 12002892
O	107	LEU	LYS	conflict	GB 12002892
O	109	GLY	ALA	conflict	GB 12002892
O	110	GLY	ASP	conflict	GB 12002892
O	?	-	VAL	deletion	GB 12002892

- Molecule 2 is a protein called IGG2A CNJ206 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	219	1642	1036	274	324	8	0	0	0
			Total	C	N	O	S			
2	D	219	1642	1036	274	324	8	0	0	0
			Total	C	N	O	S			
2	F	219	1642	1036	274	324	8	0	0	0
			Total	C	N	O	S			
2	H	219	1642	1036	274	324	8	0	0	0
			Total	C	N	O	S			
2	J	219	1642	1036	274	324	8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	219	1642	1036	274	324	8	0	0	0
			Total	C	N	O	S			
2	N	219	1642	1036	274	324	8	0	0	0
			Total	C	N	O	S			
2	P	219	1642	1036	274	324	8	0	0	0

There are 232 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	GLN	LYS	conflict	GB 4091056
B	18	ARG	LEU	conflict	GB 4091056
B	30	SER	ARG	conflict	GB 4091056
B	32	PHE	HIS	conflict	GB 4091056
B	33	GLY	ALA	conflict	GB 4091056
B	35	HIS	SER	conflict	GB 4091056
B	40	ALA	SER	conflict	GB 4091056
B	44	GLY	ARG	conflict	GB 4091056
B	50	TYR	GLU	conflict	GB 4091056
B	?	-	ASN	deletion	GB 4091056
B	52	SER	THR	conflict	GB 4091056
B	54	SER	THR	conflict	GB 4091056
B	55	SER	TYR	conflict	GB 4091056
B	57	ILE	-	insertion	GB 4091056
B	58	TYR	PHE	conflict	GB 4091056
B	60	ALA	SER	conflict	GB 4091056
B	64	LYS	THR	conflict	GB 4091056
B	74	PRO	ALA	conflict	GB 4091056
B	79	PHE	TYR	conflict	GB 4091056
B	81	GLN	GLU	conflict	GB 4091056
B	82A	THR	SER	conflict	GB 4091056
B	95	GLY	-	insertion	GB 4091056
B	97	TYR	GLY	conflict	GB 4091056
B	98	TYR	SER	conflict	GB 4091056
B	99	GLY	SER	conflict	GB 4091056
B	100A	ARG	SER	conflict	GB 4091056
B	100B	GLY	PHE	conflict	GB 4091056
B	101	ALA	VAL	conflict	GB 4091056
B	?	-	ALA	deletion	GB 4091056
D	13	GLN	LYS	conflict	GB 4091056
D	18	ARG	LEU	conflict	GB 4091056
D	30	SER	ARG	conflict	GB 4091056

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Chain	Residue	Modelled	Actual	Comment	Reference
D	32	PHE	HIS	conflict	GB 4091056
D	33	GLY	ALA	conflict	GB 4091056
D	35	HIS	SER	conflict	GB 4091056
D	40	ALA	SER	conflict	GB 4091056
D	44	GLY	ARG	conflict	GB 4091056
D	50	TYR	GLU	conflict	GB 4091056
D	?	-	ASN	deletion	GB 4091056
D	52	SER	THR	conflict	GB 4091056
D	54	SER	THR	conflict	GB 4091056
D	55	SER	TYR	conflict	GB 4091056
D	57	ILE	-	insertion	GB 4091056
D	58	TYR	PHE	conflict	GB 4091056
D	60	ALA	SER	conflict	GB 4091056
D	64	LYS	THR	conflict	GB 4091056
D	74	PRO	ALA	conflict	GB 4091056
D	79	PHE	TYR	conflict	GB 4091056
D	81	GLN	GLU	conflict	GB 4091056
D	82A	THR	SER	conflict	GB 4091056
D	95	GLY	-	insertion	GB 4091056
D	97	TYR	GLY	conflict	GB 4091056
D	98	TYR	SER	conflict	GB 4091056
D	99	GLY	SER	conflict	GB 4091056
D	100A	ARG	SER	conflict	GB 4091056
D	100B	GLY	PHE	conflict	GB 4091056
D	101	ALA	VAL	conflict	GB 4091056
D	?	-	ALA	deletion	GB 4091056
F	13	GLN	LYS	conflict	GB 4091056
F	18	ARG	LEU	conflict	GB 4091056
F	30	SER	ARG	conflict	GB 4091056
F	32	PHE	HIS	conflict	GB 4091056
F	33	GLY	ALA	conflict	GB 4091056
F	35	HIS	SER	conflict	GB 4091056
F	40	ALA	SER	conflict	GB 4091056
F	44	GLY	ARG	conflict	GB 4091056
F	50	TYR	GLU	conflict	GB 4091056
F	?	-	ASN	deletion	GB 4091056
F	52	SER	THR	conflict	GB 4091056
F	54	SER	THR	conflict	GB 4091056
F	55	SER	TYR	conflict	GB 4091056
F	57	ILE	-	insertion	GB 4091056
F	58	TYR	PHE	conflict	GB 4091056
F	60	ALA	SER	conflict	GB 4091056

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Chain	Residue	Modelled	Actual	Comment	Reference
F	64	LYS	THR	conflict	GB 4091056
F	74	PRO	ALA	conflict	GB 4091056
F	79	PHE	TYR	conflict	GB 4091056
F	81	GLN	GLU	conflict	GB 4091056
F	82A	THR	SER	conflict	GB 4091056
F	95	GLY	-	insertion	GB 4091056
F	97	TYR	GLY	conflict	GB 4091056
F	98	TYR	SER	conflict	GB 4091056
F	99	GLY	SER	conflict	GB 4091056
F	100A	ARG	SER	conflict	GB 4091056
F	100B	GLY	PHE	conflict	GB 4091056
F	101	ALA	VAL	conflict	GB 4091056
F	?	-	ALA	deletion	GB 4091056
H	13	GLN	LYS	conflict	GB 4091056
H	18	ARG	LEU	conflict	GB 4091056
H	30	SER	ARG	conflict	GB 4091056
H	32	PHE	HIS	conflict	GB 4091056
H	33	GLY	ALA	conflict	GB 4091056
H	35	HIS	SER	conflict	GB 4091056
H	40	ALA	SER	conflict	GB 4091056
H	44	GLY	ARG	conflict	GB 4091056
H	50	TYR	GLU	conflict	GB 4091056
H	?	-	ASN	deletion	GB 4091056
H	52	SER	THR	conflict	GB 4091056
H	54	SER	THR	conflict	GB 4091056
H	55	SER	TYR	conflict	GB 4091056
H	57	ILE	-	insertion	GB 4091056
H	58	TYR	PHE	conflict	GB 4091056
H	60	ALA	SER	conflict	GB 4091056
H	64	LYS	THR	conflict	GB 4091056
H	74	PRO	ALA	conflict	GB 4091056
H	79	PHE	TYR	conflict	GB 4091056
H	81	GLN	GLU	conflict	GB 4091056
H	82A	THR	SER	conflict	GB 4091056
H	95	GLY	-	insertion	GB 4091056
H	97	TYR	GLY	conflict	GB 4091056
H	98	TYR	SER	conflict	GB 4091056
H	99	GLY	SER	conflict	GB 4091056
H	100A	ARG	SER	conflict	GB 4091056
H	100B	GLY	PHE	conflict	GB 4091056
H	101	ALA	VAL	conflict	GB 4091056
H	?	-	ALA	deletion	GB 4091056

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Chain	Residue	Modelled	Actual	Comment	Reference
J	13	GLN	LYS	conflict	GB 4091056
J	18	ARG	LEU	conflict	GB 4091056
J	30	SER	ARG	conflict	GB 4091056
J	32	PHE	HIS	conflict	GB 4091056
J	33	GLY	ALA	conflict	GB 4091056
J	35	HIS	SER	conflict	GB 4091056
J	40	ALA	SER	conflict	GB 4091056
J	44	GLY	ARG	conflict	GB 4091056
J	50	TYR	GLU	conflict	GB 4091056
J	?	-	ASN	deletion	GB 4091056
J	52	SER	THR	conflict	GB 4091056
J	54	SER	THR	conflict	GB 4091056
J	55	SER	TYR	conflict	GB 4091056
J	57	ILE	-	insertion	GB 4091056
J	58	TYR	PHE	conflict	GB 4091056
J	60	ALA	SER	conflict	GB 4091056
J	64	LYS	THR	conflict	GB 4091056
J	74	PRO	ALA	conflict	GB 4091056
J	79	PHE	TYR	conflict	GB 4091056
J	81	GLN	GLU	conflict	GB 4091056
J	82A	THR	SER	conflict	GB 4091056
J	95	GLY	-	insertion	GB 4091056
J	97	TYR	GLY	conflict	GB 4091056
J	98	TYR	SER	conflict	GB 4091056
J	99	GLY	SER	conflict	GB 4091056
J	100A	ARG	SER	conflict	GB 4091056
J	100B	GLY	PHE	conflict	GB 4091056
J	101	ALA	VAL	conflict	GB 4091056
J	?	-	ALA	deletion	GB 4091056
L	13	GLN	LYS	conflict	GB 4091056
L	18	ARG	LEU	conflict	GB 4091056
L	30	SER	ARG	conflict	GB 4091056
L	32	PHE	HIS	conflict	GB 4091056
L	33	GLY	ALA	conflict	GB 4091056
L	35	HIS	SER	conflict	GB 4091056
L	40	ALA	SER	conflict	GB 4091056
L	44	GLY	ARG	conflict	GB 4091056
L	50	TYR	GLU	conflict	GB 4091056
L	?	-	ASN	deletion	GB 4091056
L	52	SER	THR	conflict	GB 4091056
L	54	SER	THR	conflict	GB 4091056
L	55	SER	TYR	conflict	GB 4091056

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Chain	Residue	Modelled	Actual	Comment	Reference
L	57	ILE	-	insertion	GB 4091056
L	58	TYR	PHE	conflict	GB 4091056
L	60	ALA	SER	conflict	GB 4091056
L	64	LYS	THR	conflict	GB 4091056
L	74	PRO	ALA	conflict	GB 4091056
L	79	PHE	TYR	conflict	GB 4091056
L	81	GLN	GLU	conflict	GB 4091056
L	82A	THR	SER	conflict	GB 4091056
L	95	GLY	-	insertion	GB 4091056
L	97	TYR	GLY	conflict	GB 4091056
L	98	TYR	SER	conflict	GB 4091056
L	99	GLY	SER	conflict	GB 4091056
L	100A	ARG	SER	conflict	GB 4091056
L	100B	GLY	PHE	conflict	GB 4091056
L	101	ALA	VAL	conflict	GB 4091056
L	?	-	ALA	deletion	GB 4091056
N	13	GLN	LYS	conflict	GB 4091056
N	18	ARG	LEU	conflict	GB 4091056
N	30	SER	ARG	conflict	GB 4091056
N	32	PHE	HIS	conflict	GB 4091056
N	33	GLY	ALA	conflict	GB 4091056
N	35	HIS	SER	conflict	GB 4091056
N	40	ALA	SER	conflict	GB 4091056
N	44	GLY	ARG	conflict	GB 4091056
N	50	TYR	GLU	conflict	GB 4091056
N	?	-	ASN	deletion	GB 4091056
N	52	SER	THR	conflict	GB 4091056
N	54	SER	THR	conflict	GB 4091056
N	55	SER	TYR	conflict	GB 4091056
N	57	ILE	-	insertion	GB 4091056
N	58	TYR	PHE	conflict	GB 4091056
N	60	ALA	SER	conflict	GB 4091056
N	64	LYS	THR	conflict	GB 4091056
N	74	PRO	ALA	conflict	GB 4091056
N	79	PHE	TYR	conflict	GB 4091056
N	81	GLN	GLU	conflict	GB 4091056
N	82A	THR	SER	conflict	GB 4091056
N	95	GLY	-	insertion	GB 4091056
N	97	TYR	GLY	conflict	GB 4091056
N	98	TYR	SER	conflict	GB 4091056
N	99	GLY	SER	conflict	GB 4091056
N	100A	ARG	SER	conflict	GB 4091056

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Chain	Residue	Modelled	Actual	Comment	Reference
N	100B	GLY	PHE	conflict	GB 4091056
N	101	ALA	VAL	conflict	GB 4091056
N	?	-	ALA	deletion	GB 4091056
P	13	GLN	LYS	conflict	GB 4091056
P	18	ARG	LEU	conflict	GB 4091056
P	30	SER	ARG	conflict	GB 4091056
P	32	PHE	HIS	conflict	GB 4091056
P	33	GLY	ALA	conflict	GB 4091056
P	35	HIS	SER	conflict	GB 4091056
P	40	ALA	SER	conflict	GB 4091056
P	44	GLY	ARG	conflict	GB 4091056
P	50	TYR	GLU	conflict	GB 4091056
P	?	-	ASN	deletion	GB 4091056
P	52	SER	THR	conflict	GB 4091056
P	54	SER	THR	conflict	GB 4091056
P	55	SER	TYR	conflict	GB 4091056
P	57	ILE	-	insertion	GB 4091056
P	58	TYR	PHE	conflict	GB 4091056
P	60	ALA	SER	conflict	GB 4091056
P	64	LYS	THR	conflict	GB 4091056
P	74	PRO	ALA	conflict	GB 4091056
P	79	PHE	TYR	conflict	GB 4091056
P	81	GLN	GLU	conflict	GB 4091056
P	82A	THR	SER	conflict	GB 4091056
P	95	GLY	-	insertion	GB 4091056
P	97	TYR	GLY	conflict	GB 4091056
P	98	TYR	SER	conflict	GB 4091056
P	99	GLY	SER	conflict	GB 4091056
P	100A	ARG	SER	conflict	GB 4091056
P	100B	GLY	PHE	conflict	GB 4091056
P	101	ALA	VAL	conflict	GB 4091056
P	?	-	ALA	deletion	GB 4091056

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: IGG2A CNJ206 FAB (LIGHT CHAIN)

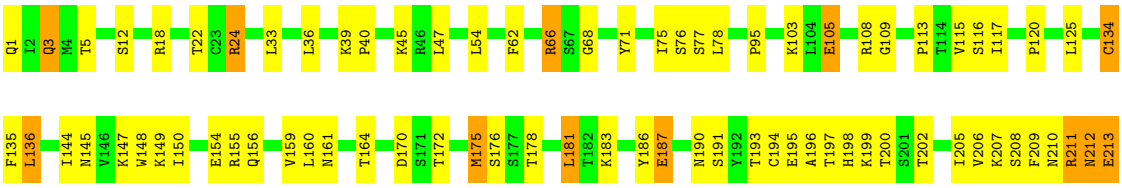
Chain A: 62% 34% 5%

• Molecule 1: IGG2A CNJ206 FAB (LIGHT CHAIN)

Chain C: 61% 34% 5%

• Molecule 1: IGG2A CNJ206 FAB (LIGHT CHAIN)

Chain E: 64% 31% 6%



C214

- Molecule 1: IGG2A CNJ206 FAB (LIGHT CHAIN)

Chain G:

Q1 I2 Q3 S12 T22 C23 L33 L36 K39 P40 K45 R46 L47 V58 P59 S65 R66 S67 G68 Y71 S76 S77 L78 L89 P95 K103 L104 E105 R108 G109 V115 S116 I117 F118 P119 S122 L125 T126 G129 L136 N137

D143 K147 W148 K149 I150 S153 Q156 L160 T164 D165 Q166 D170 S171 T172 Y173 S174 M175 L181 Y186 E187 N190 S191 Y192 T193 C194 E195 A196 T197 H198 V206 K207 S208 F209 N210 R211 N212 E213 C214

- Molecule 1: IGG2A CNJ206 FAB (LIGHT CHAIN)

Chain I:

Q1 I2 Q3 S12 A13 S14 L15 L33 L36 Q37 Q38 K39 P40 L47 L54 F62 S65 R66 S67 G68 Y71 S76 S77 L78 L89 Q90 Y91 S94 P95 Y96 E105 I106 L107 R108 G109 V115 S116 I117 F118 P119 L125 L136 K147 W148

K149 I150 R155 Q156 L160 N161 T164 D170 S171 T172 Y173 S174 M175 S176 S177 L181 T182 K183 Y186 E187 N190 S191 Y192 T193 C194 E195 A196 T197 H198 K199 T200 S201 T202 V206 K207 S208 R211 N212 E213 C214

- Molecule 1: IGG2A CNJ206 FAB (LIGHT CHAIN)

Chain K:

Q1 I2 Q3 S12 C23 L33 L36 K39 P40 K45 R46 L47 A51 V58 P59 S65 R66 S67 G68 Y71 S76 S77 L78 E79 S80 L89 Q90 Y91 S94 P95 Y96 E105 R108 G109 V115 S116 I117 F118 P119 S122 E123 Q124 L125

T126 S127 G128 G129 V132 V133 C134 F135 L136 D143 I144 N145 W148 K149 I150 Q156 L160 T164 Y173 S174 M175 S176 L181 T182 K183 Y186 E187 N190 S191 Y192 T193 C194 E195 A196 T197 H198 K199 T200 I205 V206 K207 S208 R211 N212 E213 C214

- Molecule 1: IGG2A CNJ206 FAB (LIGHT CHAIN)

Chain M:

Q1 I2 Q3 S12 L15 L21 T22 C23 R24 L33 S34 W35 L36 K39 P40 K45 R46 L47 I48 L54 F62 R66 S67 G68 S69 D70 Y71 S72 L73 S76 S77 L78 E79 S80 D85 L89 S94 P95 Y96 T97 K103 L104 E105 I106 L107 R108

G109 V115 S116 I117 F118 P119 S122 L125 T126 L136 N137 K147 W148 K149 I150 S153 E154 R46 R155 Q156 L160 N161 T164 D165 Q166 D170 S171 T172 Y173 S174 M175 S176 S177 T178 L179 T180 L181 T182 K183 D184 E187 T193 C194 E195 A196 T197 H198 K199 T200 S201

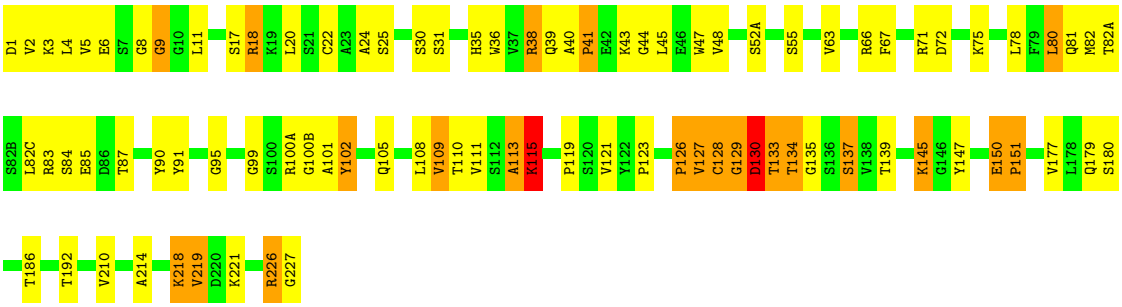
T202 I205 V206 K207 S208 R211 N212 E213 C214

- Molecule 1: IGG2A CNJ206 FAB (LIGHT CHAIN)

Chain O:

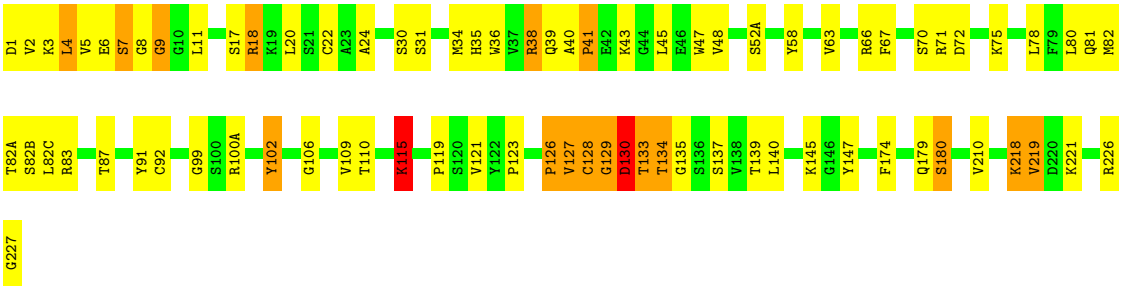
• Molecule 2: IGG2A CNJ206 FAB (HEAVY CHAIN)

Chain B: 59% 31% 10%



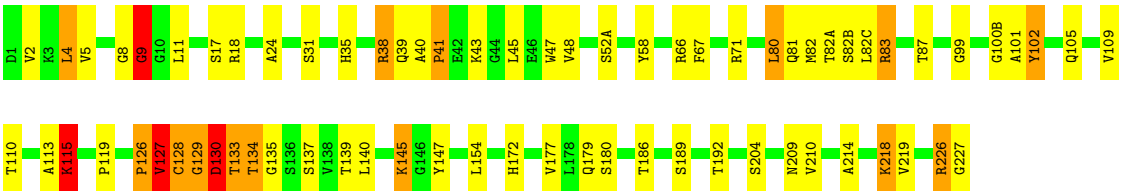
• Molecule 2: IGG2A CNJ206 FAB (HEAVY CHAIN)

Chain D: 63% 28% 7%



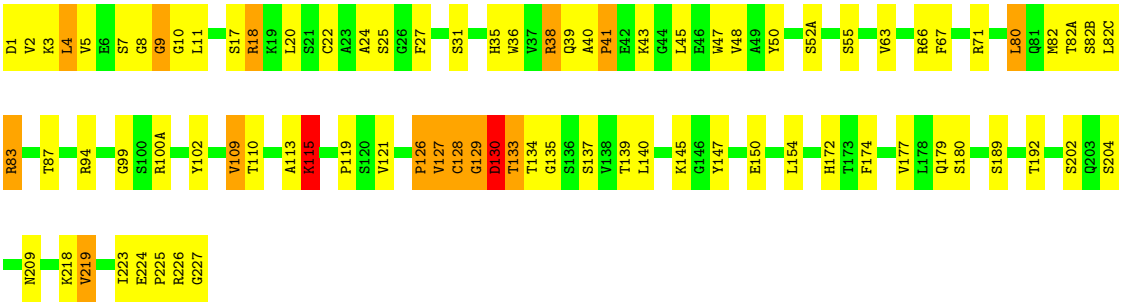
• Molecule 2: IGG2A CNJ206 FAB (HEAVY CHAIN)

Chain F: 68% 24% 6%



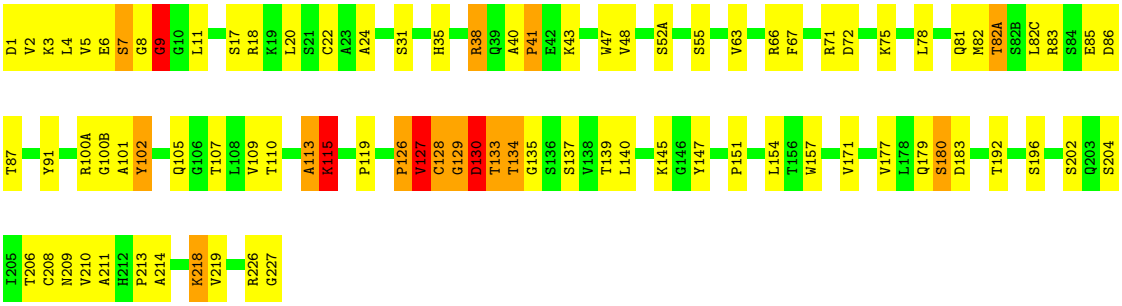
• Molecule 2: IGG2A CNJ206 FAB (HEAVY CHAIN)

Chain H: 62% 31% 6%



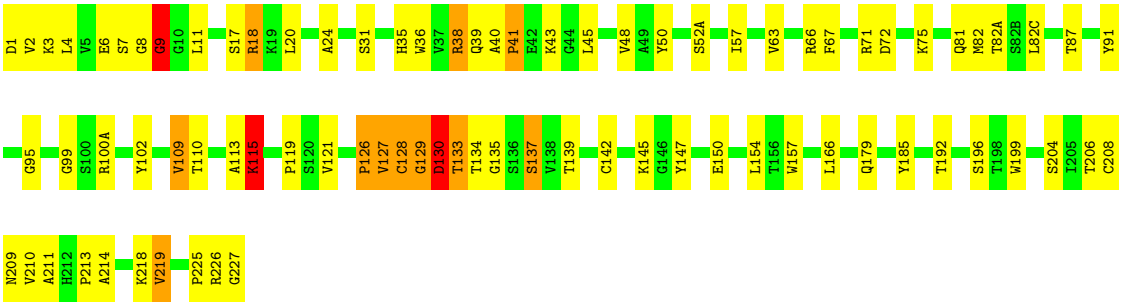
• Molecule 2: IGG2A CNJ206 FAB (HEAVY CHAIN)

Chain J:



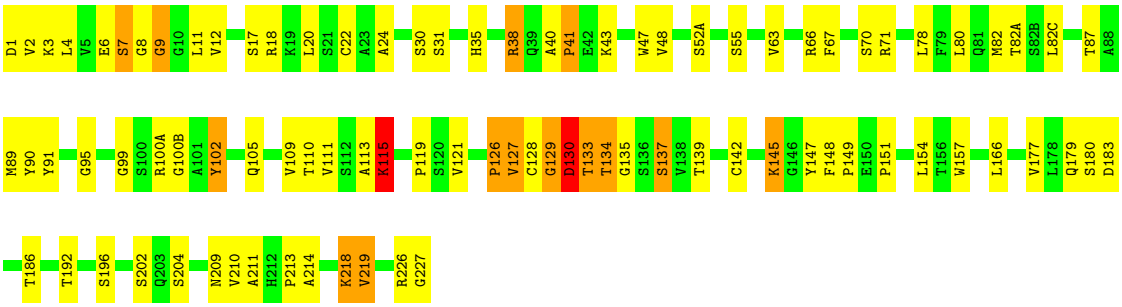
• Molecule 2: IGG2A CNJ206 FAB (HEAVY CHAIN)

Chain L:



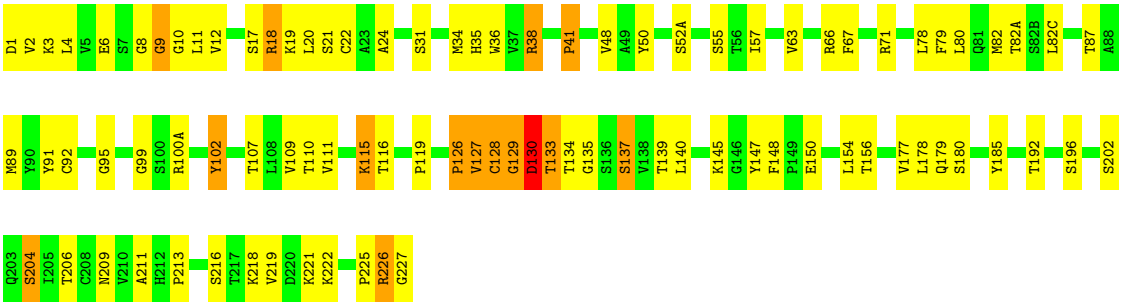
• Molecule 2: IGG2A CNJ206 FAB (HEAVY CHAIN)

Chain N:



• Molecule 2: IGG2A CNJ206 FAB (HEAVY CHAIN)

Chain P: 58% 35% 6%



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	198.70Å 68.06Å 83.66Å 71.90° 112.20° 119.60°	Depositor
Resolution (Å)	7.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.213 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26336	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.66	0/1684	0.89	1/2280 (0.0%)
1	C	0.67	0/1684	0.89	2/2280 (0.1%)
1	E	0.64	0/1684	0.90	1/2280 (0.0%)
1	G	0.67	0/1684	0.88	1/2280 (0.0%)
1	I	0.66	0/1684	0.89	1/2280 (0.0%)
1	K	0.66	0/1684	0.88	1/2280 (0.0%)
1	M	0.65	0/1684	0.92	2/2280 (0.1%)
1	O	0.71	0/1684	0.88	1/2280 (0.0%)
2	B	0.63	0/1684	0.90	4/2294 (0.2%)
2	D	0.66	0/1684	0.91	3/2294 (0.1%)
2	F	0.64	0/1684	0.90	4/2294 (0.2%)
2	H	0.61	0/1684	0.90	4/2294 (0.2%)
2	J	0.64	0/1684	0.90	4/2294 (0.2%)
2	L	0.63	0/1684	0.91	3/2294 (0.1%)
2	N	0.66	0/1684	0.93	3/2294 (0.1%)
2	P	0.64	0/1684	0.89	2/2294 (0.1%)
All	All	0.65	0/26944	0.90	37/36592 (0.1%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	130	ASP	N-CA-C	6.67	129.00	111.00
2	B	130	ASP	N-CA-C	6.49	128.52	111.00
1	K	33	LEU	CA-CB-CG	6.43	130.09	115.30
2	J	130	ASP	N-CA-C	6.37	128.19	111.00
2	F	115	LYS	N-CA-C	6.33	128.08	111.00
2	J	9	GLY	N-CA-C	6.28	128.79	113.10
1	E	33	LEU	CA-CB-CG	6.25	129.68	115.30
1	I	33	LEU	CA-CB-CG	6.21	129.58	115.30
2	P	130	ASP	N-CA-C	6.13	127.54	111.00
1	M	33	LEU	CA-CB-CG	6.12	129.37	115.30
2	F	130	ASP	N-CA-C	6.07	127.39	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	33	LEU	CA-CB-CG	6.04	129.19	115.30
2	L	9	GLY	N-CA-C	6.00	128.10	113.10
1	G	33	LEU	CA-CB-CG	5.95	128.99	115.30
2	D	130	ASP	N-CA-C	5.92	127.00	111.00
2	N	115	LYS	N-CA-C	5.92	126.99	111.00
2	D	9	GLY	N-CA-C	5.88	127.79	113.10
2	D	115	LYS	N-CA-C	5.87	126.86	111.00
1	A	33	LEU	CA-CB-CG	5.86	128.77	115.30
2	H	113	ALA	N-CA-C	5.78	126.60	111.00
2	H	9	GLY	N-CA-C	5.74	127.45	113.10
2	L	130	ASP	N-CA-C	5.69	126.35	111.00
2	B	115	LYS	N-CA-C	5.68	126.33	111.00
2	H	130	ASP	N-CA-C	5.59	126.10	111.00
1	M	184	ASP	CB-CG-OD1	5.58	123.33	118.30
2	B	9	GLY	N-CA-C	5.57	127.02	113.10
2	P	9	GLY	N-CA-C	5.53	126.91	113.10
2	L	115	LYS	N-CA-C	5.49	125.81	111.00
2	H	115	LYS	N-CA-C	5.42	125.64	111.00
2	B	113	ALA	N-CA-C	5.38	125.53	111.00
2	F	9	GLY	N-CA-C	5.32	126.39	113.10
1	C	33	LEU	CA-CB-CG	5.28	127.44	115.30
2	J	113	ALA	N-CA-C	5.27	125.23	111.00
2	F	113	ALA	N-CA-C	5.19	125.02	111.00
2	J	115	LYS	N-CA-C	5.13	124.84	111.00
1	C	160	LEU	CA-CB-CG	5.06	126.94	115.30
2	N	9	GLY	N-CA-C	5.01	125.62	113.10

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	1650	0	1583	59	0
1	C	1650	0	1583	61	0
1	E	1650	0	1583	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1650	0	1583	38	0
1	I	1650	0	1583	46	0
1	K	1650	0	1583	44	0
1	M	1650	0	1583	56	0
1	O	1650	0	1583	49	0
2	B	1642	0	1600	77	0
2	D	1642	0	1600	69	0
2	F	1642	0	1600	58	0
2	H	1642	0	1600	68	0
2	J	1642	0	1600	63	0
2	L	1642	0	1600	64	0
2	N	1642	0	1600	68	0
2	P	1642	0	1600	67	0
All	All	26336	0	25464	872	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 17.

All (872) 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)
2:D:133:THR:HB	2:D:137:SER:O	1.71	0.91
2:H:126:PRO:HA	2:H:129:GLY:HA3	1.54	0.89
2:F:126:PRO:HA	2:F:129:GLY:HA3	1.54	0.87
2:F:133:THR:HB	2:F:137:SER:O	1.75	0.87
2:B:126:PRO:HA	2:B:129:GLY:HA3	1.55	0.87
2:B:133:THR:HB	2:B:137:SER:O	1.76	0.86
1:A:3:GLN:HA	1:A:3:GLN:HE21	1.38	0.86
1:E:116:SER:HA	2:F:130:ASP:HB2	1.58	0.86
1:E:3:GLN:HE21	1:E:3:GLN:HA	1.39	0.85
1:I:3:GLN:HA	1:I:3:GLN:HE21	1.41	0.84
1:I:116:SER:HA	2:J:130:ASP:HB2	1.59	0.84
2:L:133:THR:HB	2:L:137:SER:O	1.75	0.84
2:H:133:THR:HB	2:H:137:SER:O	1.77	0.84
2:N:87:THR:HG23	2:N:110:THR:HA	1.60	0.84
1:K:3:GLN:HE21	1:K:3:GLN:HA	1.43	0.84
1:A:116:SER:HA	2:B:130:ASP:HB2	1.60	0.83
2:J:127:VAL:HB	2:J:227:GLY:HA3	1.62	0.81
1:M:116:SER:HA	2:N:130:ASP:HB2	1.63	0.81
2:L:127:VAL:HB	2:L:227:GLY:HA3	1.63	0.81
1:A:105:GLU:HG2	1:A:166:GLN:OE1	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:133:THR:HB	2:J:137:SER:O	1.82	0.80
2:J:126:PRO:HA	2:J:129:GLY:HA3	1.63	0.79
2:N:133:THR:HB	2:N:137:SER:O	1.83	0.79
2:P:127:VAL:HB	2:P:227:GLY:HA3	1.65	0.79
1:E:66:ARG:HD3	1:E:68:GLY:O	1.81	0.79
1:C:3:GLN:HE21	1:C:3:GLN:HA	1.48	0.78
2:N:127:VAL:HB	2:N:227:GLY:HA3	1.65	0.78
2:D:126:PRO:HA	2:D:129:GLY:HA3	1.66	0.78
1:M:3:GLN:HE21	1:M:3:GLN:HA	1.50	0.77
1:O:66:ARG:HG3	1:O:71:TYR:CE2	2.19	0.77
1:K:116:SER:HA	2:L:130:ASP:HB2	1.67	0.77
1:G:108:ARG:HG2	1:G:109:GLY:N	1.98	0.77
2:P:133:THR:HB	2:P:137:SER:O	1.85	0.77
2:D:38:ARG:HG2	2:D:48:VAL:CG2	2.15	0.77
1:E:115:VAL:HG22	1:E:136:LEU:HD13	1.66	0.77
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.67	0.76
1:A:12:SER:HA	1:A:105:GLU:O	1.84	0.76
1:K:108:ARG:HG2	1:K:109:GLY:N	2.01	0.76
2:H:127:VAL:HB	2:H:227:GLY:HA3	1.68	0.76
2:N:126:PRO:HA	2:N:129:GLY:HA3	1.67	0.76
1:A:108:ARG:HG2	1:A:109:GLY:N	2.00	0.75
1:M:12:SER:HA	1:M:105:GLU:O	1.87	0.75
1:G:116:SER:HA	2:H:130:ASP:HB2	1.68	0.75
2:L:38:ARG:HG2	2:L:48:VAL:CG2	2.16	0.75
1:E:108:ARG:HG2	1:E:109:GLY:N	2.02	0.75
2:P:126:PRO:HA	2:P:129:GLY:HA3	1.68	0.75
1:G:3:GLN:HE21	1:G:3:GLN:HA	1.50	0.74
1:M:66:ARG:HD3	1:M:68:GLY:O	1.87	0.74
2:J:1:ASP:HB2	2:J:100(A):ARG:NH2	2.03	0.74
1:I:66:ARG:HD3	1:I:68:GLY:O	1.87	0.73
2:L:126:PRO:HA	2:L:129:GLY:HA3	1.69	0.73
1:C:108:ARG:HG2	1:C:109:GLY:N	2.04	0.73
1:E:195:GLU:HB3	1:E:206:VAL:HG22	1.68	0.73
2:B:127:VAL:HB	2:B:227:GLY:HA3	1.70	0.73
1:C:39:LYS:HG3	1:C:40:PRO:HD2	1.71	0.72
1:O:160:LEU:HD23	2:P:179:GLN:NE2	2.04	0.72
1:I:108:ARG:HG2	1:I:109:GLY:N	2.03	0.72
1:A:66:ARG:HD3	1:A:68:GLY:O	1.88	0.72
2:D:115:LYS:H	2:D:115:LYS:HD3	1.55	0.72
2:H:82:MET:HE2	2:H:82(C):LEU:HD21	1.70	0.72
2:D:127:VAL:HB	2:D:227:GLY:HA3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:119:PRO:HD3	2:N:128:CYS:SG	2.30	0.71
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.73	0.71
1:C:12:SER:HA	1:C:105:GLU:O	1.91	0.71
2:H:4:LEU:HD12	2:H:24:ALA:HA	1.72	0.71
1:O:3:GLN:HE21	1:O:3:GLN:HA	1.56	0.71
2:L:127:VAL:HG12	2:L:128:CYS:SG	2.31	0.71
2:P:1:ASP:OD2	2:P:100(A):ARG:HG3	1.91	0.70
1:C:195:GLU:HB3	1:C:206:VAL:HG22	1.74	0.70
2:N:38:ARG:HG2	2:N:48:VAL:CG2	2.22	0.70
2:D:4:LEU:HD12	2:D:24:ALA:HA	1.70	0.70
2:H:38:ARG:HG2	2:H:48:VAL:CG2	2.21	0.70
1:E:12:SER:HA	1:E:105:GLU:O	1.92	0.70
2:H:127:VAL:HG12	2:H:128:CYS:SG	2.32	0.70
2:F:40:ALA:HB3	2:F:43:LYS:HB2	1.73	0.70
2:B:4:LEU:HD12	2:B:24:ALA:HA	1.74	0.69
2:B:38:ARG:HG2	2:B:48:VAL:CG2	2.22	0.69
2:D:1:ASP:N	2:D:100(A):ARG:HH21	1.90	0.69
2:F:38:ARG:HG2	2:F:48:VAL:CG2	2.22	0.69
2:F:127:VAL:HB	2:F:227:GLY:HA3	1.74	0.69
2:N:3:LYS:NZ	2:P:216:SER:HB3	2.08	0.69
1:O:119:PRO:HD3	2:P:128:CYS:SG	2.34	0.68
2:P:17:SER:HB2	2:P:82:MET:O	1.93	0.68
1:C:161:ASN:HB3	1:C:175:MET:HE3	1.76	0.68
2:P:38:ARG:HG2	2:P:48:VAL:CG2	2.23	0.68
1:M:39:LYS:HG3	1:M:40:PRO:HD2	1.75	0.68
1:A:39:LYS:HG3	1:A:40:PRO:HD2	1.76	0.67
2:B:115:LYS:H	2:B:115:LYS:HD3	1.59	0.67
2:F:115:LYS:H	2:F:115:LYS:HD3	1.57	0.67
1:A:195:GLU:HB3	1:A:206:VAL:HG22	1.75	0.67
1:M:66:ARG:HG3	1:M:71:TYR:CE2	2.30	0.67
2:P:87:THR:HG23	2:P:110:THR:HA	1.75	0.67
1:I:66:ARG:HG3	1:I:71:TYR:CE2	2.30	0.67
1:A:119:PRO:HD3	2:B:128:CYS:SG	2.34	0.67
2:F:127:VAL:CG1	2:F:128:CYS:SG	2.82	0.67
1:M:115:VAL:HG22	1:M:136:LEU:HD13	1.76	0.67
2:P:115:LYS:H	2:P:115:LYS:HD3	1.60	0.67
2:D:40:ALA:HB3	2:D:43:LYS:HB2	1.76	0.67
1:O:108:ARG:HG2	1:O:109:GLY:N	2.09	0.67
1:C:116:SER:HA	2:D:130:ASP:HB2	1.76	0.67
2:H:87:THR:HG23	2:H:110:THR:HA	1.77	0.66
2:D:1:ASP:H1	2:D:100(A):ARG:NH2	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:145:LYS:HB3	2:N:186:THR:HG23	1.76	0.66
2:J:115:LYS:HD3	2:J:115:LYS:H	1.61	0.65
1:A:115:VAL:HG22	1:A:136:LEU:HD13	1.77	0.65
2:D:1:ASP:N	2:D:100(A):ARG:NH2	2.44	0.65
2:N:127:VAL:HB	2:N:227:GLY:CA	2.27	0.65
2:B:127:VAL:HB	2:B:227:GLY:CA	2.26	0.65
1:M:108:ARG:HG2	1:M:109:GLY:N	2.12	0.65
2:F:127:VAL:HG12	2:F:128:CYS:SG	2.36	0.65
2:J:127:VAL:HB	2:J:227:GLY:CA	2.27	0.65
1:K:195:GLU:HB3	1:K:206:VAL:HG22	1.79	0.64
1:O:116:SER:HA	2:P:130:ASP:HB2	1.80	0.64
1:G:115:VAL:HG22	1:G:136:LEU:HD13	1.79	0.64
1:A:193:THR:HG23	1:A:208:SER:OG	1.97	0.64
2:F:126:PRO:C	2:F:128:CYS:H	2.00	0.64
2:L:115:LYS:H	2:L:115:LYS:HD3	1.62	0.64
2:L:4:LEU:HD12	2:L:24:ALA:HA	1.79	0.64
2:F:4:LEU:HD12	2:F:24:ALA:HA	1.80	0.64
1:G:195:GLU:HB3	1:G:206:VAL:HG22	1.80	0.64
1:E:108:ARG:HG2	1:E:109:GLY:H	1.62	0.64
1:E:39:LYS:HG3	1:E:40:PRO:HD2	1.80	0.64
1:M:195:GLU:HB3	1:M:206:VAL:HG22	1.79	0.64
2:H:115:LYS:H	2:H:115:LYS:HD3	1.63	0.63
1:K:122:SER:O	1:K:126:THR:HG23	1.97	0.63
2:L:87:THR:HG23	2:L:110:THR:HA	1.80	0.63
1:M:24:ARG:HD2	1:M:70:ASP:OD1	1.99	0.63
1:G:66:ARG:HD3	1:G:68:GLY:O	1.98	0.63
2:B:126:PRO:C	2:B:128:CYS:H	2.02	0.63
2:H:126:PRO:C	2:H:128:CYS:H	2.00	0.63
2:N:40:ALA:HB3	2:N:43:LYS:HB2	1.81	0.62
2:P:126:PRO:C	2:P:128:CYS:H	2.02	0.62
1:E:195:GLU:CB	1:E:206:VAL:HG22	2.29	0.62
2:N:4:LEU:HD12	2:N:24:ALA:HA	1.81	0.62
2:D:17:SER:HB2	2:D:82:MET:O	2.00	0.62
2:J:83:ARG:HG3	2:J:83:ARG:HH11	1.64	0.62
1:I:115:VAL:HG22	1:I:136:LEU:HD13	1.81	0.62
2:P:4:LEU:HD12	2:P:24:ALA:HA	1.82	0.62
1:C:5:THR:HB	1:C:24:ARG:CG	2.30	0.61
2:J:126:PRO:C	2:J:128:CYS:H	2.03	0.61
2:J:38:ARG:HG2	2:J:48:VAL:CG2	2.29	0.61
1:C:117:ILE:O	2:D:129:GLY:HA2	2.00	0.61
1:C:119:PRO:HD3	2:D:128:CYS:SG	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.82	0.61
2:F:35:HIS:HD2	2:F:47:TRP:HE1	1.48	0.61
1:G:150:ILE:HD11	1:G:181:LEU:HD21	1.81	0.61
1:O:150:ILE:HD11	1:O:181:LEU:HD21	1.80	0.61
1:O:76:SER:O	1:O:77:SER:HB3	2.01	0.61
2:D:126:PRO:C	2:D:128:CYS:H	2.02	0.61
1:E:193:THR:HG23	1:E:208:SER:OG	2.01	0.60
1:M:115:VAL:HG22	1:M:136:LEU:CD1	2.31	0.60
1:E:161:ASN:HB3	1:E:175:MET:HE3	1.82	0.60
1:G:39:LYS:HG3	1:G:40:PRO:HD2	1.83	0.60
1:M:160:LEU:HD23	2:N:179:GLN:NE2	2.16	0.60
1:O:122:SER:O	1:O:126:THR:HG23	2.01	0.60
2:L:126:PRO:C	2:L:128:CYS:H	2.03	0.60
1:I:195:GLU:HB3	1:I:206:VAL:HG22	1.83	0.60
2:N:126:PRO:C	2:N:128:CYS:H	2.05	0.60
2:D:127:VAL:HG12	2:D:128:CYS:SG	2.42	0.60
1:E:183:LYS:O	1:E:187:GLU:HG2	2.02	0.60
1:G:122:SER:O	1:G:126:THR:HG23	2.01	0.60
1:I:12:SER:HA	1:I:105:GLU:O	2.02	0.60
2:L:126:PRO:O	2:L:127:VAL:HG12	2.01	0.60
1:O:66:ARG:HD3	1:O:68:GLY:O	2.02	0.60
2:F:126:PRO:O	2:F:127:VAL:HG12	2.02	0.60
1:G:12:SER:HA	1:G:105:GLU:O	2.01	0.60
1:M:105:GLU:HG2	1:M:166:GLN:OE1	2.01	0.59
2:D:126:PRO:O	2:D:127:VAL:HG12	2.02	0.59
1:I:160:LEU:HD23	2:J:179:GLN:NE2	2.18	0.59
2:L:139:THR:HG22	2:L:192:THR:HG23	1.82	0.59
2:N:148:PHE:CE1	2:N:149:PRO:HB3	2.37	0.59
2:P:128:CYS:O	2:P:130:ASP:N	2.35	0.59
2:H:127:VAL:CG1	2:H:128:CYS:SG	2.90	0.59
1:I:108:ARG:NH1	1:I:109:GLY:O	2.36	0.59
1:K:119:PRO:HD3	2:L:128:CYS:SG	2.43	0.59
2:D:36:TRP:O	2:D:48:VAL:HB	2.02	0.59
2:N:115:LYS:H	2:N:115:LYS:HD3	1.68	0.59
2:J:83:ARG:HB3	2:J:85:GLU:OE1	2.03	0.59
1:A:66:ARG:HG3	1:A:71:TYR:CE2	2.38	0.58
1:E:66:ARG:HG3	1:E:71:TYR:CE2	2.37	0.58
2:H:17:SER:HB2	2:H:82:MET:O	2.03	0.58
1:I:193:THR:HG23	1:I:208:SER:OG	2.03	0.58
2:P:127:VAL:HB	2:P:227:GLY:CA	2.32	0.58
1:M:147:LYS:HD3	1:M:149:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:ARG:NH1	1:E:109:GLY:O	2.36	0.58
2:L:127:VAL:HB	2:L:227:GLY:CA	2.31	0.58
2:L:127:VAL:CG1	2:L:128:CYS:SG	2.91	0.58
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.85	0.58
2:L:35:HIS:CE1	2:L:95:GLY:HA2	2.39	0.58
2:L:40:ALA:HB3	2:L:43:LYS:HB2	1.86	0.58
1:A:160:LEU:HD11	2:B:177:VAL:HB	1.85	0.58
2:F:17:SER:HB2	2:F:82:MET:O	2.03	0.58
1:C:21:LEU:HD22	1:C:102:THR:HG21	1.86	0.58
2:H:133:THR:O	2:H:139:THR:HG23	2.04	0.58
1:I:54:LEU:HD11	1:I:62:PHE:O	2.04	0.58
1:K:117:ILE:O	2:L:129:GLY:HA2	2.04	0.58
1:M:76:SER:O	1:M:77:SER:HB3	2.03	0.58
2:N:6:GLU:O	2:N:7:SER:HB3	2.03	0.58
2:D:82:MET:HE2	2:D:82(C):LEU:HD21	1.86	0.58
2:J:100(B):GLY:CA	2:J:105:GLN:HE22	2.16	0.58
1:K:39:LYS:HG3	1:K:40:PRO:HD2	1.86	0.58
2:B:145:LYS:HB3	2:B:186:THR:HG23	1.86	0.57
2:N:139:THR:HG22	2:N:192:THR:HG23	1.86	0.57
1:C:54:LEU:HD11	1:C:62:PHE:O	2.03	0.57
2:F:126:PRO:HA	2:F:129:GLY:CA	2.31	0.57
2:D:22:CYS:HB3	2:D:78:LEU:HB3	1.86	0.57
2:L:128:CYS:O	2:L:130:ASP:N	2.37	0.57
2:H:126:PRO:O	2:H:127:VAL:HG12	2.04	0.57
2:J:40:ALA:HB3	2:J:43:LYS:HB2	1.87	0.57
2:N:119:PRO:HB3	2:N:147:TYR:HB3	1.85	0.57
2:P:52(A):SER:HA	2:P:71:ARG:CZ	2.34	0.57
1:K:66:ARG:HD3	1:K:68:GLY:O	2.04	0.57
1:O:117:ILE:O	2:P:129:GLY:HA2	2.04	0.57
2:P:139:THR:HG22	2:P:192:THR:HG23	1.85	0.57
2:D:52(A):SER:HA	2:D:71:ARG:CZ	2.34	0.57
1:K:12:SER:HA	1:K:105:GLU:O	2.04	0.57
2:N:128:CYS:O	2:N:130:ASP:N	2.38	0.57
1:C:195:GLU:CB	1:C:206:VAL:HG22	2.34	0.56
2:H:3:LYS:HA	2:H:100(A):ARG:O	2.04	0.56
2:N:145:LYS:CB	2:N:186:THR:HG23	2.35	0.56
2:B:35:HIS:HD2	2:B:47:TRP:HE1	1.52	0.56
1:C:115:VAL:HG22	1:C:136:LEU:HD13	1.87	0.56
1:A:76:SER:O	1:A:77:SER:HB3	2.05	0.56
1:K:160:LEU:HD23	2:L:179:GLN:NE2	2.19	0.56
1:O:187:GLU:HA	1:O:211:ARG:CZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:35:HIS:CD2	2:L:50:TYR:HD1	2.23	0.56
1:C:193:THR:HG23	1:C:208:SER:OG	2.05	0.56
2:H:35:HIS:CD2	2:H:50:TYR:HD1	2.24	0.56
1:A:147:LYS:HD3	1:A:149:LYS:NZ	2.19	0.56
1:G:187:GLU:O	1:G:211:ARG:NH1	2.37	0.56
1:M:117:ILE:HG22	2:N:130:ASP:OD2	2.06	0.56
2:N:126:PRO:O	2:N:127:VAL:HG12	2.05	0.56
1:I:117:ILE:O	2:J:129:GLY:HA2	2.05	0.56
2:P:154:LEU:HA	2:P:209:ASN:O	2.05	0.56
2:F:87:THR:HG23	2:F:110:THR:HA	1.88	0.56
1:C:108:ARG:HD2	1:C:171:SER:O	2.06	0.55
1:E:117:ILE:O	2:F:129:GLY:HA2	2.06	0.55
1:G:45:LYS:HG3	2:H:99:GLY:HA3	1.88	0.55
2:J:100(B):GLY:HA3	2:J:105:GLN:HE22	1.72	0.55
2:D:82(B):SER:HB3	2:D:83:ARG:NH1	2.21	0.55
1:I:211:ARG:O	1:I:212:ASN:HB2	2.06	0.55
2:J:4:LEU:HD12	2:J:24:ALA:HA	1.89	0.55
1:G:193:THR:HG23	1:G:208:SER:OG	2.06	0.55
1:I:39:LYS:HG3	1:I:40:PRO:HD2	1.89	0.55
2:L:82:MET:HE2	2:L:82(C):LEU:HD21	1.88	0.55
1:C:122:SER:O	1:C:126:THR:HG23	2.06	0.55
1:A:105:GLU:HG3	1:A:173:TYR:OH	2.07	0.55
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.88	0.55
2:H:128:CYS:O	2:H:130:ASP:N	2.39	0.55
1:I:108:ARG:HG2	1:I:109:GLY:H	1.72	0.55
2:B:1:ASP:N	2:B:100(A):ARG:NH2	2.55	0.55
1:E:160:LEU:HD11	2:F:177:VAL:HB	1.88	0.55
2:L:36:TRP:O	2:L:48:VAL:HB	2.06	0.55
2:F:134:THR:HB	2:F:137:SER:OG	2.06	0.55
1:G:117:ILE:O	2:H:129:GLY:HA2	2.07	0.55
2:H:127:VAL:HB	2:H:227:GLY:CA	2.35	0.55
1:K:66:ARG:HG3	1:K:71:TYR:CE2	2.42	0.55
2:L:17:SER:HB2	2:L:82:MET:O	2.07	0.55
1:G:108:ARG:HG2	1:G:109:GLY:H	1.72	0.54
1:A:195:GLU:CB	1:A:206:VAL:HG22	2.37	0.54
1:C:5:THR:HB	1:C:24:ARG:HG2	1.90	0.54
1:C:113:PRO:HG3	1:C:144:ILE:HD11	1.88	0.54
1:I:117:ILE:HG22	2:J:130:ASP:OD2	2.07	0.54
1:A:21:LEU:HD12	1:A:73:LEU:HD23	1.88	0.54
1:O:12:SER:HA	1:O:105:GLU:O	2.07	0.54
1:A:117:ILE:O	2:B:129:GLY:HA2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:150:ILE:HD11	1:K:181:LEU:HD21	1.89	0.54
1:O:150:ILE:CD1	1:O:181:LEU:HD21	2.38	0.54
2:P:35:HIS:HE1	2:P:95:GLY:O	1.90	0.54
1:A:211:ARG:O	1:A:212:ASN:HB2	2.08	0.54
1:C:24:ARG:HG2	1:C:24:ARG:HH11	1.73	0.54
2:D:127:VAL:HB	2:D:227:GLY:CA	2.38	0.54
1:K:115:VAL:HG22	1:K:136:LEU:CD1	2.38	0.54
2:N:210:VAL:O	2:N:218:LYS:HD3	2.08	0.54
1:O:39:LYS:HG3	1:O:40:PRO:HD2	1.90	0.54
1:A:45:LYS:HG3	2:B:99:GLY:HA3	1.89	0.54
2:J:8:GLY:HA3	2:J:20:LEU:HA	1.89	0.54
1:M:183:LYS:O	1:M:187:GLU:HB2	2.07	0.54
2:P:35:HIS:CE1	2:P:95:GLY:HA2	2.43	0.54
1:A:198:HIS:CE1	1:A:200:THR:HG23	2.43	0.54
1:O:147:LYS:HD3	1:O:149:LYS:NZ	2.23	0.54
1:M:193:THR:HG23	1:M:208:SER:OG	2.08	0.53
1:C:189:HIS:O	1:C:211:ARG:HD3	2.07	0.53
1:G:76:SER:O	1:G:77:SER:HB3	2.07	0.53
1:I:150:ILE:HD11	1:I:181:LEU:HD21	1.90	0.53
1:O:134:CYS:HB2	1:O:148:TRP:CZ2	2.44	0.53
2:P:211:ALA:O	2:P:213:PRO:HD3	2.09	0.53
2:B:1:ASP:H3	2:B:100(A):ARG:HH21	1.56	0.53
1:C:108:ARG:HG2	1:C:109:GLY:H	1.73	0.53
1:O:117:ILE:HG22	2:P:130:ASP:OD2	2.07	0.53
2:F:127:VAL:HG13	2:F:128:CYS:SG	2.48	0.53
2:N:3:LYS:HE2	2:P:216:SER:HB3	1.90	0.53
2:D:18:ARG:HG2	2:D:18:ARG:HH11	1.74	0.53
1:A:136:LEU:N	1:A:136:LEU:HD22	2.24	0.53
2:B:3:LYS:HE3	2:B:25:SER:OG	2.09	0.53
2:N:3:LYS:CE	2:P:216:SER:HB3	2.39	0.53
2:B:80:LEU:HD13	2:B:82:MET:HG3	1.91	0.53
2:D:35:HIS:HD2	2:D:47:TRP:HE1	1.56	0.53
2:D:128:CYS:O	2:D:130:ASP:N	2.41	0.53
2:L:119:PRO:HB3	2:L:147:TYR:HB3	1.90	0.53
2:D:135:GLY:C	2:D:137:SER:H	2.11	0.53
1:C:105:GLU:HG2	1:C:166:GLN:OE1	2.10	0.52
2:H:126:PRO:HA	2:H:129:GLY:CA	2.32	0.52
2:J:154:LEU:HA	2:J:209:ASN:O	2.09	0.52
1:O:45:LYS:HG3	2:P:99:GLY:HA3	1.91	0.52
1:C:45:LYS:HG3	2:D:99:GLY:HA3	1.91	0.52
2:P:127:VAL:HG12	2:P:128:CYS:SG	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:GLN:NE2	1:K:96:TYR:HA	2.25	0.52
1:C:198:HIS:CE1	1:C:200:THR:HG23	2.44	0.52
1:K:136:LEU:N	1:K:136:LEU:HD22	2.24	0.52
2:L:1:ASP:N	2:L:100(A):ARG:HH21	2.08	0.52
2:P:10:GLY:HA3	2:P:18:ARG:NH2	2.23	0.52
1:E:45:LYS:HG3	2:F:99:GLY:HA3	1.90	0.52
2:F:210:VAL:O	2:F:218:LYS:HD3	2.08	0.52
2:H:66:ARG:HB3	2:H:82(A):THR:O	2.08	0.52
1:O:115:VAL:HG22	1:O:136:LEU:CD1	2.40	0.52
2:P:34:MET:HB3	2:P:78:LEU:HD22	1.91	0.52
2:P:35:HIS:CD2	2:P:50:TYR:HD1	2.27	0.52
2:P:63:VAL:HB	2:P:67:PHE:CG	2.45	0.52
2:B:66:ARG:O	2:B:82(A):THR:HB	2.09	0.52
2:L:39:GLN:HB2	2:L:45:LEU:HD23	1.91	0.52
2:L:121:VAL:HB	2:L:219:VAL:HG21	1.92	0.52
2:B:126:PRO:O	2:B:127:VAL:HG12	2.10	0.52
2:D:133:THR:O	2:D:139:THR:HG23	2.10	0.52
2:J:22:CYS:HB3	2:J:78:LEU:HB3	1.92	0.52
2:B:22:CYS:HB3	2:B:78:LEU:HB3	1.92	0.52
2:B:63:VAL:HB	2:B:67:PHE:CG	2.44	0.52
1:C:115:VAL:HG22	1:C:136:LEU:CD1	2.39	0.52
2:P:8:GLY:HA3	2:P:20:LEU:HA	1.91	0.52
2:D:115:LYS:HD3	2:D:115:LYS:N	2.24	0.52
2:F:127:VAL:HB	2:F:227:GLY:CA	2.39	0.52
1:G:136:LEU:N	1:G:136:LEU:HD22	2.24	0.52
2:L:63:VAL:HB	2:L:67:PHE:CG	2.45	0.52
1:M:150:ILE:HD11	1:M:181:LEU:HD21	1.92	0.52
1:A:33:LEU:HA	1:A:89:LEU:O	2.10	0.52
2:D:35:HIS:CD2	2:D:47:TRP:HE1	2.28	0.52
2:H:18:ARG:HG2	2:H:18:ARG:HH11	1.75	0.52
2:J:119:PRO:HB3	2:J:147:TYR:HB3	1.91	0.52
1:E:211:ARG:O	1:E:212:ASN:HB2	2.10	0.51
1:O:149:LYS:HA	1:O:153:SER:O	2.10	0.51
2:B:210:VAL:O	2:B:218:LYS:HD3	2.10	0.51
1:A:39:LYS:HG3	1:A:40:PRO:CD	2.39	0.51
1:A:161:ASN:HB3	1:A:175:MET:HE3	1.92	0.51
2:B:18:ARG:HG2	2:B:18:ARG:HH11	1.74	0.51
1:A:85:ASP:OD2	1:A:103:LYS:HE3	2.09	0.51
2:B:150:GLU:OE1	2:B:151:PRO:HA	2.10	0.51
1:E:117:ILE:HG22	2:F:130:ASP:OD2	2.10	0.51
2:J:6:GLU:HG2	2:J:91:TYR:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:72:ASP:HB3	2:J:75:LYS:HB3	1.90	0.51
1:K:125:LEU:HD23	1:K:129:GLY:O	2.11	0.51
2:B:30:SER:O	2:B:52(A):SER:HB2	2.09	0.51
1:O:35:TRP:C	1:O:36:LEU:HD23	2.31	0.51
1:K:143:ASP:O	1:K:198:HIS:HD2	1.94	0.51
1:O:115:VAL:HG22	1:O:136:LEU:HD13	1.92	0.51
1:C:5:THR:HB	1:C:24:ARG:HG3	1.93	0.51
2:P:147:TYR:CE1	2:P:185:TYR:HB2	2.45	0.51
1:A:160:LEU:HD23	2:B:179:GLN:NE2	2.25	0.51
2:F:35:HIS:CD2	2:F:47:TRP:HE1	2.28	0.51
2:F:38:ARG:HG2	2:F:48:VAL:HG21	1.93	0.51
1:K:76:SER:O	1:K:77:SER:HB3	2.11	0.51
1:A:115:VAL:HG22	1:A:136:LEU:CD1	2.40	0.51
1:G:160:LEU:HD23	2:H:179:GLN:NE2	2.26	0.51
2:B:17:SER:HB2	2:B:82:MET:O	2.12	0.50
2:F:100(B):GLY:CA	2:F:105:GLN:HE22	2.23	0.50
2:L:1:ASP:H3	2:L:100(A):ARG:HH21	1.57	0.50
2:N:52(A):SER:HA	2:N:71:ARG:CZ	2.42	0.50
1:C:117:ILE:HG22	2:D:130:ASP:OD2	2.11	0.50
2:F:128:CYS:O	2:F:130:ASP:N	2.44	0.50
1:G:170:ASP:O	1:G:172:THR:HG23	2.11	0.50
2:J:126:PRO:O	2:J:127:VAL:HG12	2.10	0.50
1:M:85:ASP:OD2	1:M:103:LYS:HE3	2.12	0.50
2:N:63:VAL:HB	2:N:67:PHE:CG	2.46	0.50
2:B:128:CYS:O	2:B:130:ASP:N	2.44	0.50
1:M:39:LYS:HG3	1:M:40:PRO:CD	2.40	0.50
1:M:108:ARG:HG2	1:M:109:GLY:H	1.76	0.50
2:N:82:MET:HE2	2:N:82(C):LEU:HD21	1.92	0.50
2:P:3:LYS:HA	2:P:100(A):ARG:O	2.11	0.50
2:F:52(A):SER:HA	2:F:71:ARG:NH1	2.26	0.50
2:J:17:SER:HB2	2:J:82:MET:O	2.10	0.50
1:K:136:LEU:HD23	1:K:175:MET:HB3	1.94	0.50
2:F:154:LEU:HA	2:F:209:ASN:O	2.12	0.50
2:N:135:GLY:C	2:N:137:SER:H	2.13	0.50
1:K:207:LYS:HZ1	2:L:130:ASP:HB3	1.76	0.50
1:A:122:SER:O	1:A:126:THR:HG23	2.12	0.50
2:D:8:GLY:HA3	2:D:20:LEU:HA	1.92	0.50
2:J:128:CYS:O	2:J:130:ASP:N	2.44	0.50
1:G:195:GLU:CB	1:G:206:VAL:HG22	2.41	0.50
2:B:83:ARG:O	2:B:111:VAL:HG21	2.12	0.50
2:D:119:PRO:HB3	2:D:147:TYR:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:126:PRO:C	2:H:128:CYS:N	2.65	0.50
2:B:133:THR:O	2:B:139:THR:HG23	2.13	0.49
2:H:52(A):SER:HA	2:H:71:ARG:CZ	2.42	0.49
2:J:100(B):GLY:HA3	2:J:105:GLN:NE2	2.27	0.49
1:A:108:ARG:HG2	1:A:109:GLY:H	1.72	0.49
1:E:136:LEU:N	1:E:136:LEU:HD22	2.27	0.49
2:H:52(A):SER:HA	2:H:71:ARG:NH1	2.26	0.49
1:I:76:SER:O	1:I:77:SER:HB3	2.12	0.49
2:L:135:GLY:C	2:L:137:SER:H	2.15	0.49
1:C:33:LEU:HA	1:C:89:LEU:O	2.12	0.49
1:C:174:SER:HB3	2:D:174:PHE:HE1	1.77	0.49
2:D:72:ASP:HB3	2:D:75:LYS:HB3	1.95	0.49
1:G:119:PRO:HD3	2:H:128:CYS:SG	2.53	0.49
1:G:125:LEU:HD23	1:G:129:GLY:O	2.12	0.49
2:J:35:HIS:HD2	2:J:47:TRP:HE1	1.60	0.49
2:J:211:ALA:O	2:J:213:PRO:HD3	2.11	0.49
1:A:8:PRO:CG	1:A:11:LEU:HD23	2.42	0.49
2:D:127:VAL:CG1	2:D:128:CYS:SG	3.00	0.49
2:D:67:PHE:CD1	2:D:67:PHE:N	2.80	0.49
1:I:195:GLU:CB	1:I:206:VAL:HG22	2.41	0.49
2:N:1:ASP:H3	2:N:100(A):ARG:HH21	1.61	0.49
1:C:143:ASP:O	1:C:198:HIS:HD2	1.96	0.49
1:I:147:LYS:HD3	1:I:149:LYS:NZ	2.28	0.49
1:M:160:LEU:HD11	2:N:177:VAL:HB	1.94	0.49
2:B:126:PRO:C	2:B:128:CYS:N	2.66	0.49
1:I:161:ASN:HB3	1:I:175:MET:HE3	1.95	0.49
2:B:127:VAL:CG1	2:B:227:GLY:HA3	2.43	0.49
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.94	0.49
2:F:126:PRO:C	2:F:128:CYS:N	2.65	0.49
1:M:105:GLU:HG3	1:M:173:TYR:OH	2.13	0.49
2:P:126:PRO:C	2:P:128:CYS:N	2.65	0.49
2:F:66:ARG:O	2:F:82(A):THR:HB	2.12	0.49
1:E:160:LEU:HD23	2:F:179:GLN:NE2	2.28	0.49
2:H:139:THR:HG22	2:H:192:THR:HG23	1.94	0.49
1:I:164:THR:HB	1:I:174:SER:H	1.78	0.49
1:C:1:GLN:OE1	1:C:1:GLN:HA	2.12	0.48
1:E:5:THR:HG22	1:E:24:ARG:NH2	2.28	0.48
2:H:67:PHE:N	2:H:67:PHE:HD1	2.11	0.48
2:L:8:GLY:HA3	2:L:20:LEU:HA	1.94	0.48
2:L:38:ARG:HG2	2:L:48:VAL:HG23	1.95	0.48
2:L:66:ARG:O	2:L:82(A):THR:HB	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HG22	2:B:130:ASP:OD2	2.13	0.48
2:B:67:PHE:HA	2:B:81:GLN:O	2.13	0.48
2:D:30:SER:O	2:D:52(A):SER:HB2	2.14	0.48
2:L:126:PRO:C	2:L:128:CYS:N	2.67	0.48
2:D:67:PHE:N	2:D:67:PHE:HD1	2.11	0.48
1:M:122:SER:O	1:M:126:THR:HG23	2.13	0.48
2:B:35:HIS:CD2	2:B:47:TRP:HE1	2.31	0.48
1:C:35:TRP:CZ3	1:C:88:CYS:HB3	2.49	0.48
1:K:45:LYS:HG3	2:L:99:GLY:HA3	1.94	0.48
1:M:198:HIS:CE1	1:M:200:THR:HG23	2.48	0.48
1:C:39:LYS:HG3	1:C:40:PRO:CD	2.43	0.48
1:C:108:ARG:NH1	1:C:109:GLY:O	2.45	0.48
2:D:38:ARG:HG2	2:D:48:VAL:HG23	1.94	0.48
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.96	0.48
1:E:1:GLN:OE1	1:E:1:GLN:HA	2.12	0.48
2:F:82:MET:HB3	2:F:82(C):LEU:HD21	1.95	0.48
2:H:66:ARG:O	2:H:82(A):THR:HB	2.13	0.48
2:N:126:PRO:C	2:N:128:CYS:N	2.66	0.48
2:B:126:PRO:HA	2:B:129:GLY:CA	2.34	0.48
1:E:159:VAL:HA	1:E:178:THR:O	2.13	0.48
2:J:127:VAL:CB	2:J:227:GLY:HA3	2.38	0.48
1:K:195:GLU:CB	1:K:206:VAL:HG22	2.41	0.48
2:D:121:VAL:HB	2:D:219:VAL:HG21	1.95	0.48
1:E:147:LYS:HD3	1:E:149:LYS:NZ	2.28	0.48
2:H:1:ASP:N	2:H:100(A):ARG:HH21	2.11	0.48
2:J:3:LYS:HA	2:J:100(A):ARG:O	2.14	0.48
1:M:195:GLU:CB	1:M:206:VAL:HG22	2.42	0.48
2:N:3:LYS:HZ3	2:P:216:SER:HB3	1.78	0.48
1:O:198:HIS:CE1	1:O:200:THR:HG23	2.48	0.48
2:B:127:VAL:CB	2:B:227:GLY:HA3	2.40	0.48
1:G:66:ARG:HG3	1:G:71:TYR:CE2	2.47	0.48
2:H:121:VAL:HB	2:H:219:VAL:HG21	1.96	0.48
1:M:136:LEU:N	1:M:136:LEU:HD22	2.29	0.48
1:A:54:LEU:HD11	1:A:62:PHE:O	2.14	0.48
2:B:127:VAL:HB	2:B:226:ARG:C	2.34	0.48
1:E:150:ILE:HD11	1:E:181:LEU:HD21	1.96	0.48
2:D:210:VAL:O	2:D:218:LYS:HD3	2.14	0.47
1:I:190:ASN:N	1:I:190:ASN:ND2	2.62	0.47
1:E:170:ASP:O	1:E:172:THR:HG23	2.14	0.47
2:L:6:GLU:HG2	2:L:91:TYR:HA	1.94	0.47
1:O:94:SER:HB2	1:O:95:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LYS:HD3	1:C:149:LYS:NZ	2.30	0.47
1:E:212:ASN:O	1:E:213:GLU:HB2	2.14	0.47
2:H:82(B):SER:O	2:H:83:ARG:HD3	2.14	0.47
1:I:186:TYR:HA	1:I:192:TYR:OH	2.13	0.47
2:J:87:THR:HG23	2:J:110:THR:HA	1.95	0.47
2:J:134:THR:HB	2:J:137:SER:OG	2.14	0.47
2:J:135:GLY:C	2:J:137:SER:H	2.18	0.47
2:L:199:TRP:CH2	2:L:225:PRO:HA	2.49	0.47
2:N:6:GLU:HG2	2:N:91:TYR:HA	1.96	0.47
2:D:82(B):SER:O	2:D:83:ARG:HD3	2.14	0.47
1:G:143:ASP:O	1:G:198:HIS:HD2	1.98	0.47
2:J:210:VAL:O	2:J:218:LYS:HD3	2.15	0.47
2:N:35:HIS:CE1	2:N:95:GLY:HA2	2.49	0.47
1:A:147:LYS:HD3	1:A:149:LYS:HZ2	1.80	0.47
1:C:125:LEU:HD23	1:C:129:GLY:O	2.15	0.47
2:N:35:HIS:HD2	2:N:47:TRP:HE1	1.61	0.47
2:N:126:PRO:HA	2:N:129:GLY:CA	2.42	0.47
2:D:3:LYS:HA	2:D:100(A):ARG:O	2.14	0.47
1:E:3:GLN:HE21	1:E:3:GLN:CA	2.17	0.47
2:H:67:PHE:N	2:H:67:PHE:CD1	2.81	0.47
1:K:39:LYS:HG3	1:K:40:PRO:CD	2.44	0.47
1:A:212:ASN:O	1:A:213:GLU:HB2	2.15	0.47
1:E:39:LYS:HG3	1:E:40:PRO:CD	2.43	0.47
2:H:63:VAL:HB	2:H:67:PHE:CG	2.50	0.47
2:H:66:ARG:HD3	2:H:83:ARG:NH1	2.29	0.47
2:H:135:GLY:C	2:H:137:SER:H	2.18	0.47
1:M:33:LEU:HA	1:M:89:LEU:O	2.15	0.47
1:M:155:ARG:HG2	1:M:179:LEU:HD11	1.97	0.47
2:P:4:LEU:HG	2:P:92:CYS:SG	2.55	0.47
2:B:5:VAL:HG13	2:B:101:ALA:HB2	1.97	0.47
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.97	0.47
1:E:134:CYS:HB2	1:E:148:TRP:CZ2	2.50	0.47
1:E:135:PHE:HE1	1:E:176:SER:HG	1.63	0.47
2:F:67:PHE:HA	2:F:81:GLN:O	2.15	0.47
2:J:63:VAL:HB	2:J:67:PHE:CG	2.49	0.47
2:F:52(A):SER:HA	2:F:71:ARG:CZ	2.45	0.47
2:J:52(A):SER:HA	2:J:71:ARG:CZ	2.45	0.47
2:J:127:VAL:HG12	2:J:128:CYS:SG	2.55	0.47
1:O:105:GLU:HG3	1:O:173:TYR:OH	2.14	0.47
2:D:63:VAL:HB	2:D:67:PHE:CG	2.50	0.47
2:N:4:LEU:HG	2:N:22:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:TRP:HH2	2:F:58:TYR:HB3	1.80	0.46
1:K:186:TYR:HA	1:K:192:TYR:OH	2.15	0.46
1:M:108:ARG:NH1	1:M:109:GLY:O	2.44	0.46
2:N:127:VAL:CB	2:N:227:GLY:HA3	2.40	0.46
1:A:125:LEU:O	1:A:183:LYS:HD2	2.14	0.46
2:P:1:ASP:HB3	2:P:100(A):ARG:CZ	2.45	0.46
2:B:75:LYS:HG3	2:D:119:PRO:O	2.15	0.46
2:B:82:MET:HE2	2:B:82(C):LEU:HD21	1.97	0.46
1:E:76:SER:O	1:E:77:SER:HB3	2.16	0.46
1:I:91:TYR:HA	1:I:96:TYR:CD1	2.50	0.46
1:K:115:VAL:HG22	1:K:136:LEU:HD12	1.97	0.46
1:A:1:GLN:OE1	1:A:1:GLN:HA	2.14	0.46
2:B:87:THR:HG23	2:B:110:THR:HA	1.98	0.46
2:F:145:LYS:HB3	2:F:186:THR:HG23	1.98	0.46
2:B:135:GLY:C	2:B:137:SER:H	2.17	0.46
2:J:126:PRO:C	2:J:128:CYS:N	2.68	0.46
1:K:124:GLN:O	1:K:127:SER:HB2	2.16	0.46
1:K:207:LYS:NZ	2:L:130:ASP:HB3	2.29	0.46
1:A:119:PRO:CD	2:B:128:CYS:SG	3.02	0.46
1:E:54:LEU:HD11	1:E:62:PHE:O	2.16	0.46
1:E:136:LEU:N	1:E:136:LEU:CD2	2.79	0.46
2:L:67:PHE:HA	2:L:81:GLN:O	2.16	0.46
2:N:67:PHE:CD2	2:N:80:LEU:HD11	2.51	0.46
1:C:145:ASN:O	1:C:196:ALA:HA	2.15	0.46
2:D:91:TYR:CE1	2:D:106:GLY:HA3	2.51	0.46
2:D:127:VAL:CB	2:D:227:GLY:HA3	2.44	0.46
2:N:127:VAL:HG12	2:N:128:CYS:SG	2.56	0.46
2:P:135:GLY:C	2:P:137:SER:H	2.19	0.46
1:C:136:LEU:N	1:C:136:LEU:HD22	2.31	0.46
1:O:136:LEU:N	1:O:136:LEU:HD22	2.30	0.46
2:P:204:SER:HB3	2:P:222:LYS:HE3	1.98	0.46
1:C:21:LEU:CD2	1:C:102:THR:HG21	2.45	0.46
1:C:212:ASN:O	1:C:213:GLU:HB2	2.15	0.46
1:E:145:ASN:O	1:E:196:ALA:HA	2.16	0.46
1:G:117:ILE:HG22	2:H:130:ASP:OD2	2.15	0.46
1:I:136:LEU:N	1:I:136:LEU:HD22	2.31	0.46
1:I:160:LEU:HD11	2:J:177:VAL:HB	1.98	0.46
1:K:135:PHE:HE1	1:K:176:SER:HG	1.62	0.46
2:N:1:ASP:N	2:N:100(A):ARG:HH21	2.14	0.46
1:O:170:ASP:O	1:O:172:THR:HG23	2.16	0.46
1:O:186:TYR:HA	1:O:192:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:GLY:O	2:F:9:GLY:O	2.33	0.46
2:N:100(B):GLY:CA	2:N:105:GLN:HE22	2.28	0.46
2:P:140:LEU:N	2:P:140:LEU:HD12	2.31	0.46
2:B:139:THR:HG22	2:B:192:THR:HG23	1.98	0.45
2:D:134:THR:HB	2:D:137:SER:OG	2.16	0.45
1:E:198:HIS:CE1	1:E:200:THR:HG23	2.51	0.45
1:I:119:PRO:HD3	2:J:128:CYS:SG	2.57	0.45
2:L:87:THR:HA	2:L:109:VAL:O	2.16	0.45
1:M:94:SER:HB2	1:M:95:PRO:HD3	1.98	0.45
1:O:155:ARG:NH2	1:O:181:LEU:HD23	2.32	0.45
2:F:119:PRO:HB3	2:F:147:TYR:HB3	1.98	0.45
1:I:119:PRO:HD2	2:J:227:GLY:OXT	2.16	0.45
2:P:36:TRP:O	2:P:48:VAL:HB	2.16	0.45
2:P:82:MET:HE2	2:P:82(C):LEU:HD21	1.98	0.45
1:A:3:GLN:HE21	1:A:3:GLN:CA	2.18	0.45
1:A:150:ILE:HD11	1:A:181:LEU:HD21	1.97	0.45
2:B:83:ARG:HH11	2:B:83:ARG:HG3	1.81	0.45
2:B:127:VAL:HB	2:B:227:GLY:N	2.30	0.45
1:C:136:LEU:HD23	1:C:175:MET:HB3	1.98	0.45
2:N:1:ASP:N	2:N:100(A):ARG:NH2	2.64	0.45
1:C:21:LEU:HD12	1:C:73:LEU:HD23	1.98	0.45
2:H:38:ARG:HG2	2:H:48:VAL:HG23	1.99	0.45
1:I:13:ALA:HB3	1:I:78:LEU:HD12	1.99	0.45
2:J:5:VAL:HG13	2:J:101:ALA:HB2	1.98	0.45
1:K:91:TYR:HA	1:K:96:TYR:CD1	2.52	0.45
1:K:198:HIS:CE1	1:K:200:THR:HG23	2.51	0.45
1:M:34:SER:HA	1:M:48:ILE:O	2.16	0.45
2:N:17:SER:HB2	2:N:82:MET:O	2.16	0.45
2:N:154:LEU:HA	2:N:209:ASN:O	2.17	0.45
1:O:185:GLU:O	1:O:189:HIS:HD2	2.00	0.45
2:B:72:ASP:HB3	2:B:75:LYS:HB3	1.97	0.45
2:B:100(B):GLY:CA	2:B:105:GLN:HE22	2.28	0.45
1:C:211:ARG:O	1:C:212:ASN:HB2	2.15	0.45
2:F:139:THR:HG22	2:F:192:THR:HG23	1.99	0.45
1:I:183:LYS:O	1:I:187:GLU:HG2	2.17	0.45
2:J:75:LYS:HG3	2:L:119:PRO:O	2.16	0.45
2:L:199:TRP:HH2	2:L:225:PRO:HA	1.82	0.45
1:M:119:PRO:CD	2:N:128:CYS:SG	3.02	0.45
1:O:207:LYS:NZ	2:P:130:ASP:HB3	2.31	0.45
1:A:185:GLU:O	1:A:189:HIS:HD2	1.99	0.45
2:B:1:ASP:H3	2:B:100(A):ARG:NH2	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:GLY:C	2:F:137:SER:H	2.18	0.45
2:H:66:ARG:HD3	2:H:83:ARG:CZ	2.47	0.45
2:J:140:LEU:HD12	2:J:140:LEU:N	2.32	0.45
2:L:154:LEU:HA	2:L:209:ASN:O	2.17	0.45
2:B:8:GLY:HA3	2:B:20:LEU:HA	1.99	0.45
1:C:2:ILE:HD12	1:C:29:ILE:HG22	1.98	0.45
2:D:67:PHE:HA	2:D:81:GLN:O	2.16	0.45
1:E:18:ARG:HA	1:E:75:ILE:O	2.17	0.45
1:G:58:VAL:HA	1:G:59:PRO:HD3	1.88	0.45
2:H:80:LEU:HD13	2:H:82:MET:HG3	1.99	0.45
2:B:83:ARG:HB3	2:B:85:GLU:OE1	2.17	0.44
1:G:105:GLU:HG3	1:G:173:TYR:OH	2.17	0.44
2:J:9:GLY:H	2:J:20:LEU:CD2	2.31	0.44
1:M:21:LEU:HD12	1:M:73:LEU:HD23	1.99	0.44
2:N:82:MET:HE3	2:N:90:TYR:CZ	2.51	0.44
1:O:120:PRO:HD2	1:O:186:TYR:CZ	2.52	0.44
1:O:212:ASN:O	1:O:213:GLU:HB2	2.17	0.44
2:D:6:GLU:O	2:D:7:SER:HB3	2.16	0.44
1:M:161:ASN:HB3	1:M:175:MET:HE3	1.99	0.44
2:N:102:TYR:HD1	2:N:102:TYR:HA	1.69	0.44
1:O:160:LEU:HD11	2:P:177:VAL:HB	1.97	0.44
2:B:108:LEU:HD12	2:B:109:VAL:N	2.32	0.44
2:B:127:VAL:HG12	2:B:128:CYS:SG	2.56	0.44
2:F:82(B):SER:O	2:F:83:ARG:NE	2.50	0.44
2:L:154:LEU:HD12	2:L:210:VAL:HG22	1.99	0.44
1:O:58:VAL:HA	1:O:59:PRO:HD3	1.85	0.44
1:C:91:TYR:HA	1:C:96:TYR:CD1	2.53	0.44
1:G:160:LEU:HD11	2:H:177:VAL:HB	1.99	0.44
2:H:172:HIS:O	2:H:189:SER:HA	2.17	0.44
2:J:179:GLN:O	2:J:180:SER:HB2	2.18	0.44
1:M:205:ILE:HD12	1:M:205:ILE:N	2.32	0.44
2:N:66:ARG:O	2:N:82(A):THR:HB	2.18	0.44
2:B:6:GLU:OE2	2:B:91:TYR:HA	2.18	0.44
1:E:136:LEU:HD11	1:E:196:ALA:HB2	1.99	0.44
2:N:134:THR:HB	2:N:137:SER:OG	2.18	0.44
2:P:12:VAL:HG11	2:P:82(C):LEU:HD12	1.99	0.44
2:P:89:MET:HG2	2:P:91:TYR:OH	2.17	0.44
1:E:205:ILE:HD12	1:E:205:ILE:N	2.33	0.44
1:E:207:LYS:NZ	2:F:130:ASP:HB3	2.33	0.44
2:H:87:THR:HA	2:H:109:VAL:O	2.18	0.44
2:L:9:GLY:H	2:L:20:LEU:CD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:175:MET:HE2	1:M:177:SER:HB2	2.00	0.44
2:D:66:ARG:O	2:D:82(A):THR:HB	2.18	0.44
1:M:207:LYS:NZ	2:N:130:ASP:HB3	2.33	0.44
2:N:89:MET:HG2	2:N:91:TYR:CZ	2.53	0.44
2:N:127:VAL:HB	2:N:227:GLY:N	2.32	0.44
2:P:19:LYS:HE2	2:P:79:PHE:CD1	2.53	0.44
1:I:33:LEU:HA	1:I:89:LEU:O	2.17	0.44
1:K:195:GLU:HA	1:K:205:ILE:O	2.17	0.44
1:M:211:ARG:O	1:M:212:ASN:HB2	2.18	0.44
2:N:211:ALA:O	2:N:213:PRO:HD3	2.17	0.44
1:A:3:GLN:HA	1:A:3:GLN:NE2	2.19	0.44
1:G:39:LYS:HG3	1:G:40:PRO:CD	2.47	0.44
1:I:207:LYS:NZ	2:J:130:ASP:HB3	2.33	0.44
1:K:105:GLU:HG3	1:K:173:TYR:OH	2.17	0.44
2:P:50:TYR:O	2:P:57:ILE:HA	2.18	0.44
2:B:39:GLN:HE21	2:B:44:GLY:HA2	1.83	0.43
2:B:84:SER:HA	2:B:111:VAL:HB	1.99	0.43
1:C:8:PRO:HG2	1:C:11:LEU:HD23	2.00	0.43
1:C:119:PRO:CD	2:D:128:CYS:SG	3.05	0.43
2:H:1:ASP:H3	2:H:100(A):ARG:HH21	1.66	0.43
2:L:66:ARG:C	2:L:67:PHE:HD1	2.20	0.43
2:D:123:PRO:HD3	2:D:221:LYS:HG2	1.99	0.43
2:D:126:PRO:C	2:D:128:CYS:N	2.69	0.43
1:G:105:GLU:HG2	1:G:166:GLN:OE1	2.18	0.43
2:L:67:PHE:N	2:L:67:PHE:CD1	2.85	0.43
1:M:89:LEU:HD12	1:M:97:THR:O	2.18	0.43
1:M:137:ASN:ND2	1:M:174:SER:HB3	2.33	0.43
1:A:113:PRO:HA	1:A:137:ASN:O	2.18	0.43
1:C:159:VAL:HA	1:C:178:THR:O	2.18	0.43
1:E:113:PRO:HG3	1:E:144:ILE:HD11	1.99	0.43
2:F:102:TYR:HD1	2:F:102:TYR:HA	1.71	0.43
1:K:115:VAL:HG22	1:K:136:LEU:HD13	2.00	0.43
2:N:8:GLY:HA3	2:N:20:LEU:HD23	1.99	0.43
2:P:126:PRO:O	2:P:127:VAL:HG12	2.18	0.43
1:E:199:LYS:HB2	1:E:199:LYS:NZ	2.33	0.43
2:F:80:LEU:HD13	2:F:82:MET:HG3	1.98	0.43
1:I:147:LYS:HD3	1:I:149:LYS:HZ2	1.82	0.43
1:K:183:LYS:O	1:K:187:GLU:HB2	2.17	0.43
2:N:22:CYS:HB3	2:N:78:LEU:HB3	2.01	0.43
2:N:82:MET:HB3	2:N:82(C):LEU:HD21	2.00	0.43
1:A:124:GLN:O	1:A:127:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HA	1:A:178:THR:O	2.19	0.43
2:F:67:PHE:N	2:F:67:PHE:CD1	2.87	0.43
1:I:212:ASN:O	1:I:213:GLU:HB2	2.18	0.43
1:K:193:THR:HG23	1:K:208:SER:OG	2.18	0.43
1:M:164:THR:HB	1:M:174:SER:H	1.84	0.43
2:N:127:VAL:CG1	2:N:128:CYS:N	2.82	0.43
1:O:145:ASN:O	1:O:196:ALA:HA	2.18	0.43
1:C:105:GLU:HG3	1:C:173:TYR:OH	2.17	0.43
1:C:207:LYS:NZ	2:D:130:ASP:HB3	2.33	0.43
2:H:8:GLY:HA3	2:H:20:LEU:HA	2.01	0.43
1:I:115:VAL:HG22	1:I:136:LEU:CD1	2.45	0.43
2:P:133:THR:O	2:P:139:THR:HG23	2.19	0.43
1:A:121:SER:O	1:A:125:LEU:HG	2.19	0.43
1:E:155:ARG:NH2	1:E:181:LEU:HD23	2.33	0.43
2:J:66:ARG:O	2:J:82(A):THR:HB	2.19	0.43
2:L:67:PHE:HD1	2:L:67:PHE:N	2.17	0.43
1:M:212:ASN:O	1:M:213:GLU:HB2	2.19	0.43
2:P:6:GLU:HA	2:P:21:SER:O	2.18	0.43
2:P:22:CYS:HB3	2:P:78:LEU:HB3	2.00	0.43
2:B:52(A):SER:HA	2:B:71:ARG:NH1	2.33	0.43
2:F:140:LEU:N	2:F:140:LEU:HD12	2.34	0.43
2:H:115:LYS:HD3	2:H:115:LYS:N	2.31	0.43
2:H:224:GLU:HA	2:H:225:PRO:HD3	1.90	0.43
2:J:6:GLU:O	2:J:7:SER:HB3	2.19	0.43
2:J:107:THR:HG23	2:J:107:THR:O	2.19	0.43
1:K:33:LEU:HA	1:K:89:LEU:O	2.18	0.43
1:O:15:LEU:HD21	1:O:106:ILE:HD13	2.01	0.43
1:A:148:TRP:O	1:A:154:GLU:HA	2.18	0.43
1:C:66:ARG:HG3	1:C:71:TYR:CE2	2.54	0.43
1:C:193:THR:CG2	1:C:206:VAL:HG13	2.49	0.43
2:D:87:THR:HG23	2:D:110:THR:HA	1.99	0.43
2:D:179:GLN:O	2:D:180:SER:HB2	2.19	0.43
2:J:35:HIS:CD2	2:J:47:TRP:HE1	2.37	0.43
2:L:127:VAL:CG1	2:L:128:CYS:N	2.81	0.43
1:C:66:ARG:HD3	1:C:68:GLY:O	2.18	0.42
1:E:193:THR:CG2	1:E:206:VAL:HG13	2.49	0.42
2:L:18:ARG:HG2	2:L:18:ARG:HH11	1.84	0.42
2:B:3:LYS:HA	2:B:100(A):ARG:O	2.19	0.42
2:B:102:TYR:HD1	2:B:102:TYR:HA	1.75	0.42
2:H:126:PRO:CA	2:H:129:GLY:HA3	2.38	0.42
2:J:82(C):LEU:HD23	2:J:86:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:72:ASP:HB3	2:L:75:LYS:HB3	2.00	0.42
2:N:12:VAL:O	2:N:111:VAL:HA	2.19	0.42
2:P:66:ARG:C	2:P:67:PHE:HD1	2.23	0.42
1:C:117:ILE:HD12	1:C:194:CYS:HB3	2.02	0.42
1:G:137:ASN:HD21	2:H:174:PHE:HZ	1.67	0.42
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.37	0.42
1:K:58:VAL:HA	1:K:59:PRO:HD3	1.93	0.42
1:M:207:LYS:HZ1	2:N:130:ASP:HB3	1.84	0.42
1:A:64:GLY:HA2	1:A:72:SER:O	2.19	0.42
2:H:128:CYS:O	2:H:129:GLY:C	2.57	0.42
1:I:155:ARG:NH2	1:I:181:LEU:HD23	2.33	0.42
1:C:150:ILE:HD11	1:C:181:LEU:HD21	2.00	0.42
2:N:35:HIS:CD2	2:N:47:TRP:HE1	2.37	0.42
2:P:119:PRO:HB3	2:P:147:TYR:HB3	2.02	0.42
2:B:134:THR:HB	2:B:137:SER:OG	2.19	0.42
2:D:139:THR:C	2:D:140:LEU:HD12	2.40	0.42
2:H:36:TRP:O	2:H:48:VAL:HB	2.19	0.42
2:L:142:CYS:HB2	2:L:157:TRP:CH2	2.54	0.42
2:P:102:TYR:HD1	2:P:102:TYR:HA	1.68	0.42
1:G:136:LEU:N	1:G:136:LEU:CD2	2.81	0.42
2:L:50:TYR:O	2:L:57:ILE:HA	2.20	0.42
1:O:36:LEU:HD23	1:O:36:LEU:N	2.34	0.42
1:O:193:THR:HG23	1:O:208:SER:OG	2.20	0.42
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.86	0.42
2:B:67:PHE:CD1	2:B:67:PHE:N	2.88	0.42
2:F:5:VAL:HG13	2:F:101:ALA:HB2	2.02	0.42
1:M:149:LYS:HA	1:M:153:SER:O	2.18	0.42
2:P:178:LEU:HD13	2:P:185:TYR:CZ	2.55	0.42
1:A:199:LYS:HB2	1:A:199:LYS:NZ	2.35	0.42
2:H:129:GLY:O	2:H:133:THR:N	2.53	0.42
2:H:140:LEU:HD23	2:H:223:ILE:HG21	2.01	0.42
1:I:175:MET:HE2	1:I:177:SER:HB2	2.02	0.42
2:J:83:ARG:HG3	2:J:83:ARG:NH1	2.32	0.42
2:N:30:SER:O	2:N:52(A):SER:HB2	2.19	0.42
1:O:193:THR:CG2	1:O:206:VAL:HG13	2.50	0.42
2:P:12:VAL:O	2:P:111:VAL:HA	2.19	0.42
1:A:8:PRO:HG3	1:A:11:LEU:HD23	2.02	0.42
1:A:175:MET:HE2	1:A:177:SER:HB2	2.02	0.42
2:B:126:PRO:CA	2:B:129:GLY:HA3	2.38	0.42
2:F:127:VAL:HB	2:F:226:ARG:C	2.40	0.42
1:G:149:LYS:HA	1:G:153:SER:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:GLN:O	1:I:37:GLN:HG3	2.20	0.42
2:J:139:THR:HG22	2:J:192:THR:OG1	2.20	0.42
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.87	0.41
1:G:190:ASN:HB3	1:G:210:ASN:OD1	2.20	0.41
2:H:10:GLY:HA3	2:H:18:ARG:NH2	2.35	0.41
1:I:170:ASP:O	1:I:172:THR:HG23	2.20	0.41
2:J:206:THR:HG22	2:J:208:CYS:N	2.35	0.41
2:L:35:HIS:HE1	2:L:95:GLY:O	2.03	0.41
2:N:121:VAL:HB	2:N:219:VAL:HG21	2.01	0.41
1:O:108:ARG:HG2	1:O:109:GLY:H	1.83	0.41
2:P:6:GLU:HG2	2:P:91:TYR:HA	2.01	0.41
2:D:6:GLU:HG3	2:D:92:CYS:SG	2.61	0.41
1:K:145:ASN:O	1:K:196:ALA:HA	2.20	0.41
2:L:206:THR:HG22	2:L:208:CYS:N	2.35	0.41
1:A:191:SER:HA	1:A:209:PHE:O	2.20	0.41
1:C:174:SER:HB3	2:D:174:PHE:CE1	2.55	0.41
2:D:5:VAL:O	2:D:22:CYS:HA	2.20	0.41
1:M:15:LEU:HD21	1:M:106:ILE:HD13	2.02	0.41
2:B:35:HIS:CE1	2:B:95:GLY:HA2	2.55	0.41
1:E:103:LYS:N	1:E:103:LYS:HD2	2.36	0.41
2:F:82:MET:HE2	2:F:82(C):LEU:HD21	2.02	0.41
2:H:27:PHE:CD2	2:H:94:ARG:HD2	2.55	0.41
1:K:3:GLN:HA	1:K:3:GLN:NE2	2.23	0.41
1:M:107:LEU:HD12	1:M:108:ARG:H	1.85	0.41
2:N:67:PHE:HD2	2:N:80:LEU:HD11	1.86	0.41
1:C:1:GLN:NE2	1:C:3:GLN:OE1	2.53	0.41
1:E:125:LEU:HD23	1:E:125:LEU:HA	1.86	0.41
1:E:190:ASN:HB3	1:E:210:ASN:OD1	2.21	0.41
2:F:100(B):GLY:HA2	2:F:105:GLN:HE22	1.85	0.41
2:H:140:LEU:HD12	2:H:140:LEU:N	2.35	0.41
1:I:125:LEU:HD23	1:I:125:LEU:HA	1.87	0.41
2:J:102:TYR:HD1	2:J:102:TYR:HA	1.72	0.41
1:M:54:LEU:HD11	1:M:62:PHE:O	2.21	0.41
1:M:155:ARG:NH2	1:M:181:LEU:HD23	2.35	0.41
1:A:103:LYS:HD2	1:A:103:LYS:N	2.35	0.41
1:C:186:TYR:HA	1:C:192:TYR:OH	2.20	0.41
2:F:67:PHE:N	2:F:67:PHE:HD1	2.19	0.41
2:F:172:HIS:O	2:F:189:SER:HA	2.21	0.41
2:H:5:VAL:O	2:H:22:CYS:HA	2.20	0.41
2:J:179:GLN:O	2:J:180:SER:CB	2.69	0.41
1:K:108:ARG:HG2	1:K:109:GLY:H	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:3:LYS:HA	2:L:100(A):ARG:O	2.20	0.41
2:B:121:VAL:HG21	2:B:219:VAL:HG22	2.03	0.41
2:D:70:SER:O	2:D:78:LEU:HD12	2.20	0.41
1:E:191:SER:HA	1:E:209:PHE:O	2.21	0.41
1:I:15:LEU:HD21	1:I:106:ILE:HD13	2.02	0.41
2:L:147:TYR:CE1	2:L:185:TYR:HB2	2.55	0.41
1:A:185:GLU:O	1:A:189:HIS:CD2	2.73	0.41
2:H:66:ARG:CD	2:H:83:ARG:CZ	2.99	0.41
2:L:128:CYS:O	2:L:129:GLY:C	2.59	0.41
1:M:193:THR:CG2	1:M:206:VAL:HG13	2.51	0.41
1:O:33:LEU:HA	1:O:89:LEU:O	2.20	0.41
2:B:82:MET:HE3	2:B:90:TYR:CZ	2.55	0.41
1:C:116:SER:O	1:C:134:CYS:HA	2.21	0.41
1:C:142:LYS:HD2	1:C:173:TYR:CE2	2.56	0.41
2:D:34:MET:HB3	2:D:78:LEU:HD22	2.01	0.41
2:F:100(B):GLY:HA3	2:F:105:GLN:NE2	2.35	0.41
1:I:155:ARG:HH22	1:I:181:LEU:HD23	1.85	0.41
1:M:155:ARG:HH22	1:M:181:LEU:HD23	1.84	0.41
1:O:107:LEU:HA	1:O:140:TYR:OH	2.20	0.41
1:O:185:GLU:O	1:O:189:HIS:CD2	2.74	0.41
2:P:107:THR:HG23	2:P:107:THR:O	2.21	0.41
2:P:115:LYS:HD3	2:P:115:LYS:N	2.27	0.41
2:P:116:THR:HG23	2:P:148:PHE:O	2.20	0.41
2:B:115:LYS:HD3	2:B:115:LYS:N	2.29	0.41
2:F:115:LYS:HD3	2:F:115:LYS:N	2.25	0.41
1:G:103:LYS:HD2	1:G:103:LYS:N	2.35	0.41
1:I:175:MET:HG2	1:I:176:SER:H	1.86	0.41
2:L:1:ASP:N	2:L:100(A):ARG:NH2	2.69	0.41
2:N:142:CYS:HB2	2:N:157:TRP:CH2	2.56	0.41
1:O:124:GLN:O	1:O:127:SER:HB2	2.21	0.41
1:O:195:GLU:HB3	1:O:206:VAL:HG22	2.03	0.41
1:A:190:ASN:ND2	1:A:190:ASN:N	2.69	0.40
2:B:66:ARG:HB3	2:B:82(A):THR:O	2.21	0.40
2:B:145:LYS:CB	2:B:186:THR:HG23	2.49	0.40
1:E:149:LYS:HB2	1:E:193:THR:HB	2.03	0.40
1:K:116:SER:O	1:K:134:CYS:HA	2.20	0.40
2:L:127:VAL:CB	2:L:227:GLY:HA3	2.41	0.40
2:L:211:ALA:O	2:L:213:PRO:HD3	2.21	0.40
1:O:155:ARG:HG2	1:O:179:LEU:HD11	2.03	0.40
2:P:206:THR:HG23	2:P:221:LYS:C	2.41	0.40
2:B:36:TRP:CE2	2:B:80:LEU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:GLU:OE2	2:D:91:TYR:HA	2.21	0.40
2:D:47:TRP:HH2	2:D:58:TYR:HB3	1.86	0.40
1:E:120:PRO:HD2	1:E:186:TYR:OH	2.20	0.40
2:J:67:PHE:HA	2:J:81:GLN:O	2.21	0.40
2:J:126:PRO:CA	2:J:129:GLY:HA3	2.43	0.40
2:J:127:VAL:HB	2:J:227:GLY:N	2.35	0.40
2:J:157:TRP:CD1	2:J:171:VAL:HG21	2.57	0.40
2:L:52(A):SER:HA	2:L:71:ARG:CZ	2.51	0.40
1:M:45:LYS:HG3	2:N:99:GLY:HA3	2.03	0.40
1:O:108:ARG:NH1	1:O:109:GLY:O	2.53	0.40
2:B:67:PHE:N	2:B:67:PHE:HD1	2.19	0.40
1:E:148:TRP:O	1:E:154:GLU:HA	2.21	0.40
1:G:147:LYS:HD3	1:G:149:LYS:NZ	2.36	0.40
2:H:3:LYS:HE3	2:H:25:SER:OG	2.22	0.40
1:K:1:GLN:OE1	1:K:1:GLN:HA	2.21	0.40
1:K:132:VAL:HG12	1:K:148:TRP:CH2	2.56	0.40
1:A:136:LEU:N	1:A:136:LEU:CD2	2.84	0.40
2:D:102:TYR:HD1	2:D:102:TYR:HA	1.75	0.40
1:E:183:LYS:O	1:E:187:GLU:CG	2.69	0.40
2:F:126:PRO:CA	2:F:129:GLY:HA3	2.38	0.40
1:I:198:HIS:CE1	1:I:200:THR:HG23	2.56	0.40
2:P:38:ARG:HG2	2:P:48:VAL:HG22	2.01	0.40
2:P:225:PRO:O	2:P:226:ARG:HB2	2.21	0.40
2:B:123:PRO:HD3	2:B:221:LYS:HG2	2.04	0.40
1:E:3:GLN:HA	1:E:3:GLN:NE2	2.20	0.40
1:G:33:LEU:HA	1:G:89:LEU:O	2.22	0.40
1:G:186:TYR:HA	1:G:192:TYR:OH	2.21	0.40
2:H:27:PHE:CE2	2:H:94:ARG:HD2	2.57	0.40
2:H:154:LEU:HA	2:H:209:ASN:O	2.22	0.40
1:M:125:LEU:HB3	1:M:183:LYS:HE3	2.02	0.40
1:M:170:ASP:O	1:M:172:THR:HG23	2.22	0.40
2:P:116:THR:HA	2:P:148:PHE:O	2.22	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	212/214 (99%)	199 (94%)	8 (4%)	5 (2%)	6	29
1	C	212/214 (99%)	196 (92%)	10 (5%)	6 (3%)	5	25
1	E	212/214 (99%)	197 (93%)	11 (5%)	4 (2%)	8	36
1	G	212/214 (99%)	199 (94%)	10 (5%)	3 (1%)	11	43
1	I	212/214 (99%)	199 (94%)	9 (4%)	4 (2%)	8	36
1	K	212/214 (99%)	199 (94%)	8 (4%)	5 (2%)	6	29
1	M	212/214 (99%)	198 (93%)	10 (5%)	4 (2%)	8	36
1	O	212/214 (99%)	199 (94%)	9 (4%)	4 (2%)	8	36
2	B	217/219 (99%)	194 (89%)	12 (6%)	11 (5%)	2	12
2	D	217/219 (99%)	193 (89%)	13 (6%)	11 (5%)	2	12
2	F	217/219 (99%)	193 (89%)	13 (6%)	11 (5%)	2	12
2	H	217/219 (99%)	195 (90%)	11 (5%)	11 (5%)	2	12
2	J	217/219 (99%)	192 (88%)	11 (5%)	14 (6%)	1	7
2	L	217/219 (99%)	191 (88%)	15 (7%)	11 (5%)	2	12
2	N	217/219 (99%)	194 (89%)	10 (5%)	13 (6%)	1	9
2	P	217/219 (99%)	191 (88%)	16 (7%)	10 (5%)	2	14
All	All	3432/3464 (99%)	3129 (91%)	176 (5%)	127 (4%)	3	19

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLY
2	B	126	PRO
2	B	129	GLY
2	B	130	ASP
2	B	226	ARG
2	D	9	GLY
2	D	126	PRO
2	D	129	GLY
2	D	130	ASP
2	D	226	ARG
2	F	9	GLY
2	F	126	PRO

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Mol	Chain	Res	Type
2	F	129	GLY
2	F	130	ASP
2	F	226	ARG
2	H	9	GLY
2	H	126	PRO
2	H	129	GLY
2	H	130	ASP
2	H	226	ARG
2	J	9	GLY
2	J	126	PRO
2	J	129	GLY
2	J	130	ASP
2	J	226	ARG
2	L	9	GLY
2	L	126	PRO
2	L	129	GLY
2	L	130	ASP
2	L	226	ARG
2	N	9	GLY
2	N	126	PRO
2	N	129	GLY
2	N	130	ASP
2	N	226	ARG
2	P	9	GLY
2	P	126	PRO
2	P	129	GLY
2	P	130	ASP
2	P	226	ARG
2	B	133	THR
2	B	134	THR
2	D	7	SER
2	D	133	THR
2	D	134	THR
2	F	133	THR
2	F	134	THR
1	G	211	ARG
2	H	133	THR
2	H	134	THR
2	J	113	ALA
2	J	134	THR
1	K	211	ARG
2	L	133	THR

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Mol	Chain	Res	Type
2	N	7	SER
2	N	134	THR
2	P	134	THR
1	A	95	PRO
1	A	213	GLU
1	C	95	PRO
1	C	211	ARG
1	C	213	GLU
1	E	95	PRO
2	F	180	SER
1	G	95	PRO
1	G	212	ASN
1	I	95	PRO
2	J	7	SER
2	J	133	THR
2	J	180	SER
1	K	94	SER
1	K	95	PRO
1	K	212	ASN
2	L	7	SER
2	L	134	THR
2	L	214	ALA
2	N	133	THR
1	O	211	ARG
2	P	41	PRO
2	P	133	THR
2	P	202	SER
1	A	212	ASN
2	B	180	SER
2	B	214	ALA
1	C	77	SER
1	E	213	GLU
2	F	214	ALA
2	J	202	SER
2	J	214	ALA
2	L	113	ALA
1	M	95	PRO
2	N	41	PRO
2	N	202	SER
1	O	95	PRO
1	A	211	ARG
2	B	41	PRO

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Mol	Chain	Res	Type
2	B	113	ALA
1	C	212	ASN
2	D	180	SER
1	E	212	ASN
2	F	41	PRO
2	H	41	PRO
2	H	180	SER
2	H	202	SER
1	I	212	ASN
1	I	213	GLU
2	J	41	PRO
2	L	41	PRO
1	M	211	ARG
1	M	212	ASN
2	N	113	ALA
2	N	214	ALA
1	O	212	ASN
1	E	211	ARG
2	H	7	SER
1	K	51	ALA
2	N	180	SER
2	P	180	SER
2	D	41	PRO
1	C	94	SER
1	I	94	SER
1	A	94	SER
2	D	127	VAL
2	F	127	VAL
2	J	127	VAL
1	O	94	SER
1	M	94	SER

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/189 (100%)	174 (92%)	15 (8%)	12	41
1	C	189/189 (100%)	174 (92%)	15 (8%)	12	41
1	E	189/189 (100%)	171 (90%)	18 (10%)	8	32
1	G	189/189 (100%)	172 (91%)	17 (9%)	9	35
1	I	189/189 (100%)	171 (90%)	18 (10%)	8	32
1	K	189/189 (100%)	171 (90%)	18 (10%)	8	32
1	M	189/189 (100%)	170 (90%)	19 (10%)	7	29
1	O	189/189 (100%)	170 (90%)	19 (10%)	7	29
2	B	183/183 (100%)	164 (90%)	19 (10%)	7	27
2	D	183/183 (100%)	168 (92%)	15 (8%)	11	39
2	F	183/183 (100%)	165 (90%)	18 (10%)	8	30
2	H	183/183 (100%)	163 (89%)	20 (11%)	6	25
2	J	183/183 (100%)	163 (89%)	20 (11%)	6	25
2	L	183/183 (100%)	164 (90%)	19 (10%)	7	27
2	N	183/183 (100%)	162 (88%)	21 (12%)	5	24
2	P	183/183 (100%)	161 (88%)	22 (12%)	5	22
All	All	2976/2976 (100%)	2683 (90%)	293 (10%)	8	30

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	22	THR
1	A	23	CYS
1	A	36	LEU
1	A	47	LEU
1	A	66	ARG
1	A	78	LEU
1	A	105	GLU
1	A	136	LEU
1	A	156	GLN
1	A	164	THR
1	A	175	MET
1	A	181	LEU
1	A	194	CYS

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Mol	Chain	Res	Type
1	A	197	THR
2	B	2	VAL
2	B	11	LEU
2	B	18	ARG
2	B	31	SER
2	B	38	ARG
2	B	41	PRO
2	B	55	SER
2	B	80	LEU
2	B	102	TYR
2	B	109	VAL
2	B	115	LYS
2	B	127	VAL
2	B	128	CYS
2	B	137	SER
2	B	145	LYS
2	B	150	GLU
2	B	151	PRO
2	B	218	LYS
2	B	219	VAL
1	C	3	GLN
1	C	22	THR
1	C	24	ARG
1	C	36	LEU
1	C	47	LEU
1	C	65	SER
1	C	66	ARG
1	C	78	LEU
1	C	105	GLU
1	C	136	LEU
1	C	156	GLN
1	C	164	THR
1	C	175	MET
1	C	181	LEU
1	C	197	THR
2	D	2	VAL
2	D	4	LEU
2	D	11	LEU
2	D	18	ARG
2	D	31	SER
2	D	38	ARG
2	D	41	PRO

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Mol	Chain	Res	Type
2	D	80	LEU
2	D	102	TYR
2	D	109	VAL
2	D	115	LYS
2	D	128	CYS
2	D	145	LYS
2	D	218	LYS
2	D	219	VAL
1	E	3	GLN
1	E	22	THR
1	E	24	ARG
1	E	36	LEU
1	E	47	LEU
1	E	66	ARG
1	E	78	LEU
1	E	105	GLU
1	E	134	CYS
1	E	136	LEU
1	E	156	GLN
1	E	164	THR
1	E	175	MET
1	E	181	LEU
1	E	187	GLU
1	E	194	CYS
1	E	197	THR
1	E	202	THR
2	F	2	VAL
2	F	4	LEU
2	F	11	LEU
2	F	18	ARG
2	F	31	SER
2	F	38	ARG
2	F	41	PRO
2	F	80	LEU
2	F	83	ARG
2	F	102	TYR
2	F	109	VAL
2	F	115	LYS
2	F	127	VAL
2	F	128	CYS
2	F	145	LYS
2	F	204	SER

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Mol	Chain	Res	Type
2	F	218	LYS
2	F	219	VAL
1	G	3	GLN
1	G	22	THR
1	G	23	CYS
1	G	36	LEU
1	G	47	LEU
1	G	65	SER
1	G	66	ARG
1	G	78	LEU
1	G	105	GLU
1	G	136	LEU
1	G	156	GLN
1	G	164	THR
1	G	175	MET
1	G	181	LEU
1	G	190	ASN
1	G	197	THR
1	G	211	ARG
2	H	2	VAL
2	H	4	LEU
2	H	11	LEU
2	H	18	ARG
2	H	31	SER
2	H	38	ARG
2	H	41	PRO
2	H	55	SER
2	H	80	LEU
2	H	83	ARG
2	H	102	TYR
2	H	109	VAL
2	H	115	LYS
2	H	127	VAL
2	H	128	CYS
2	H	145	LYS
2	H	150	GLU
2	H	204	SER
2	H	218	LYS
2	H	219	VAL
1	I	3	GLN
1	I	36	LEU
1	I	47	LEU

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Mol	Chain	Res	Type
1	I	65	SER
1	I	66	ARG
1	I	78	LEU
1	I	105	GLU
1	I	108	ARG
1	I	136	LEU
1	I	156	GLN
1	I	164	THR
1	I	181	LEU
1	I	187	GLU
1	I	190	ASN
1	I	194	CYS
1	I	197	THR
1	I	202	THR
1	I	211	ARG
2	J	2	VAL
2	J	11	LEU
2	J	18	ARG
2	J	31	SER
2	J	38	ARG
2	J	41	PRO
2	J	55	SER
2	J	82(A)	THR
2	J	102	TYR
2	J	109	VAL
2	J	115	LYS
2	J	127	VAL
2	J	128	CYS
2	J	145	LYS
2	J	151	PRO
2	J	183	ASP
2	J	196	SER
2	J	204	SER
2	J	218	LYS
2	J	219	VAL
1	K	3	GLN
1	K	23	CYS
1	K	36	LEU
1	K	47	LEU
1	K	65	SER
1	K	66	ARG
1	K	78	LEU

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Mol	Chain	Res	Type
1	K	80	SER
1	K	105	GLU
1	K	136	LEU
1	K	156	GLN
1	K	164	THR
1	K	175	MET
1	K	181	LEU
1	K	190	ASN
1	K	194	CYS
1	K	197	THR
1	K	211	ARG
2	L	2	VAL
2	L	11	LEU
2	L	18	ARG
2	L	31	SER
2	L	38	ARG
2	L	41	PRO
2	L	102	TYR
2	L	109	VAL
2	L	115	LYS
2	L	127	VAL
2	L	128	CYS
2	L	137	SER
2	L	145	LYS
2	L	150	GLU
2	L	166	LEU
2	L	196	SER
2	L	204	SER
2	L	218	LYS
2	L	219	VAL
1	M	3	GLN
1	M	23	CYS
1	M	24	ARG
1	M	36	LEU
1	M	47	LEU
1	M	66	ARG
1	M	78	LEU
1	M	80	SER
1	M	105	GLU
1	M	108	ARG
1	M	136	LEU
1	M	156	GLN

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Mol	Chain	Res	Type
1	M	164	THR
1	M	175	MET
1	M	181	LEU
1	M	194	CYS
1	M	197	THR
1	M	202	THR
1	M	211	ARG
2	N	2	VAL
2	N	11	LEU
2	N	18	ARG
2	N	31	SER
2	N	38	ARG
2	N	41	PRO
2	N	55	SER
2	N	70	SER
2	N	102	TYR
2	N	109	VAL
2	N	115	LYS
2	N	127	VAL
2	N	137	SER
2	N	145	LYS
2	N	151	PRO
2	N	166	LEU
2	N	183	ASP
2	N	196	SER
2	N	204	SER
2	N	218	LYS
2	N	219	VAL
1	O	3	GLN
1	O	24	ARG
1	O	30	SER
1	O	36	LEU
1	O	47	LEU
1	O	65	SER
1	O	66	ARG
1	O	78	LEU
1	O	80	SER
1	O	105	GLU
1	O	108	ARG
1	O	136	LEU
1	O	156	GLN
1	O	164	THR

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Mol	Chain	Res	Type
1	O	175	MET
1	O	181	LEU
1	O	190	ASN
1	O	194	CYS
1	O	197	THR
2	P	2	VAL
2	P	11	LEU
2	P	18	ARG
2	P	31	SER
2	P	38	ARG
2	P	41	PRO
2	P	55	SER
2	P	80	LEU
2	P	82(A)	THR
2	P	102	TYR
2	P	109	VAL
2	P	115	LYS
2	P	127	VAL
2	P	128	CYS
2	P	137	SER
2	P	145	LYS
2	P	150	GLU
2	P	156	THR
2	P	196	SER
2	P	204	SER
2	P	218	LYS
2	P	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	3	GLN
1	A	137	ASN
1	A	189	HIS
1	A	190	ASN
2	B	35	HIS
2	B	105	GLN
2	B	179	GLN
1	C	1	GLN
1	C	3	GLN
1	C	137	ASN

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Mol	Chain	Res	Type
1	C	189	HIS
1	C	212	ASN
2	D	35	HIS
2	D	105	GLN
2	D	172	HIS
2	D	179	GLN
1	E	1	GLN
1	E	3	GLN
1	E	137	ASN
1	E	189	HIS
1	E	190	ASN
2	F	35	HIS
2	F	105	GLN
2	F	179	GLN
1	G	1	GLN
1	G	3	GLN
1	G	137	ASN
1	G	189	HIS
1	G	190	ASN
2	H	35	HIS
2	H	179	GLN
1	I	1	GLN
1	I	3	GLN
1	I	137	ASN
1	I	190	ASN
2	J	35	HIS
2	J	105	GLN
2	J	179	GLN
1	K	1	GLN
1	K	3	GLN
1	K	137	ASN
1	K	189	HIS
1	K	190	ASN
2	L	35	HIS
2	L	105	GLN
2	L	179	GLN
1	M	1	GLN
1	M	3	GLN
1	M	137	ASN
1	M	189	HIS
1	M	190	ASN
2	N	35	HIS

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Mol	Chain	Res	Type
2	N	105	GLN
2	N	179	GLN
1	O	1	GLN
1	O	3	GLN
1	O	137	ASN
1	O	189	HIS
2	P	35	HIS
2	P	105	GLN
2	P	172	HIS
2	P	179	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.