



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 01:01 am GMT

PDB ID : 3C6L  
Title : Crystal structure of mouse MHC class II I-Ab/3K peptide complexed with mouse TCR 2W20  
Authors : Dai, S.  
Deposited on : 2008-02-04  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
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) : trunk30967

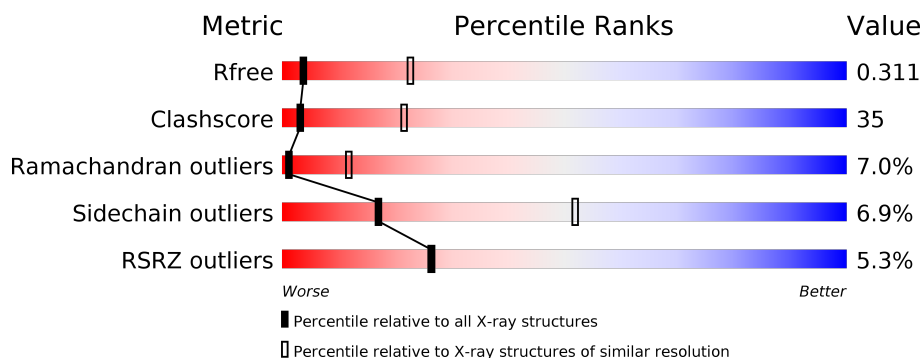
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1928 (3.50-3.30)
Clashscore	122126	2051 (3.50-3.30)
Ramachandran outliers	120053	2006 (3.50-3.30)
Sidechain outliers	120020	2006 (3.50-3.30)
RSRZ outliers	108989	1827 (3.50-3.30)

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  $\geq 3$ , 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	185	<div> <div>11%</div> <div>49%</div> <div>41%</div> <div>8%</div> <div>•</div> </div>
1	E	185	<div> <div>13%</div> <div>47%</div> <div>43%</div> <div>9%</div> <div>••</div> </div>
2	B	236	<div> <div>5%</div> <div>50%</div> <div>39%</div> <div>7%</div> <div>••</div> </div>
2	F	236	<div> <div>3%</div> <div>52%</div> <div>39%</div> <div>8%</div> <div></div> </div>
3	C	182	<div> <div>2%</div> <div>46%</div> <div>48%</div> <div>5%</div> <div>•</div> </div>
3	G	182	<div> <div>3%</div> <div>51%</div> <div>46%</div> <div></div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	217	<div><div></div><div>33%45%8%12%</div></div>
4	H	217	<div><div>4%</div><div>35%46%7%12%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12716 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 TCR 2W20 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1476	935	243	291	7			
1	E	184	Total	C	N	O	S	0	0	0
			1464	926	242	289	7			

- Molecule 2 is a protein called TCR 2W20 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1797	1129	319	343	6			
2	F	236	Total	C	N	O	S	0	0	0
			1870	1175	330	359	6			

- Molecule 3 is a protein called H-2 class II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	182	Total	C	N	O	S	0	0	0
			1459	944	230	282	3			
3	G	182	Total	C	N	O	S	0	0	0
			1459	944	230	282	3			

- Molecule 4 is a protein called 3K peptide, Linker, and H-2 class II histocompatibility antigen (A beta chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	192	Total	C	N	O	S	0	0	0
			1594	1002	288	297	7			
4	H	192	Total	C	N	O	S	0	0	0
			1594	1002	288	297	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	14	GLY	-	LINKER	UNP P14483
D	15	GLY	-	LINKER	UNP P14483
D	16	GLY	-	LINKER	UNP P14483
D	17	GLY	-	LINKER	UNP P14483
D	18	SER	-	LINKER	UNP P14483
D	19	LEU	-	LINKER	UNP P14483
D	20	VAL	-	LINKER	UNP P14483
D	21	PRO	-	LINKER	UNP P14483
D	22	ARG	-	LINKER	UNP P14483
D	23	GLY	-	LINKER	UNP P14483
D	24	SER	-	LINKER	UNP P14483
D	25	GLY	-	LINKER	UNP P14483
D	26	GLY	-	LINKER	UNP P14483
D	27	GLY	-	LINKER	UNP P14483
D	28	GLY	-	LINKER	UNP P14483
D	216	LYS	ARG	ENGINEERED	UNP P14483
H	14	GLY	-	LINKER	UNP P14483
H	15	GLY	-	LINKER	UNP P14483
H	16	GLY	-	LINKER	UNP P14483
H	17	GLY	-	LINKER	UNP P14483
H	18	SER	-	LINKER	UNP P14483
H	19	LEU	-	LINKER	UNP P14483
H	20	VAL	-	LINKER	UNP P14483
H	21	PRO	-	LINKER	UNP P14483
H	22	ARG	-	LINKER	UNP P14483
H	23	GLY	-	LINKER	UNP P14483
H	24	SER	-	LINKER	UNP P14483
H	25	GLY	-	LINKER	UNP P14483
H	26	GLY	-	LINKER	UNP P14483
H	27	GLY	-	LINKER	UNP P14483
H	28	GLY	-	LINKER	UNP P14483
H	216	LYS	ARG	ENGINEERED	UNP P14483

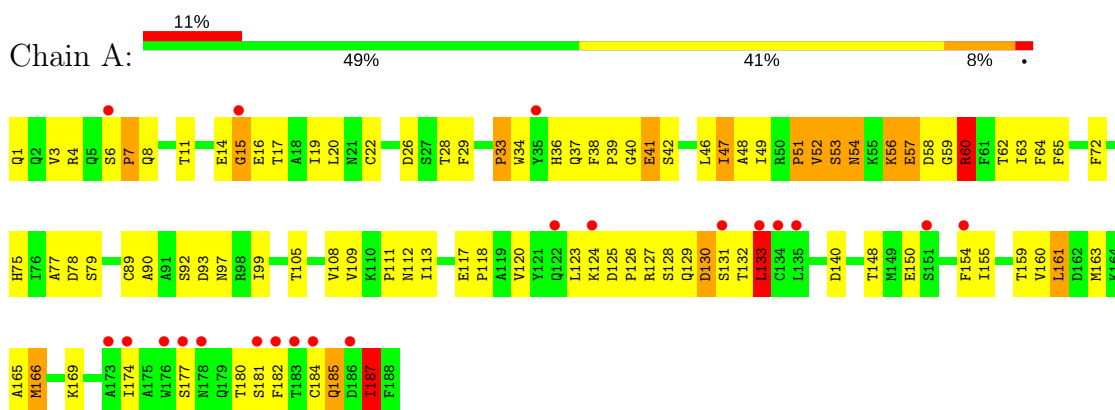
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	E	2	Total Ca 2 2	0	0

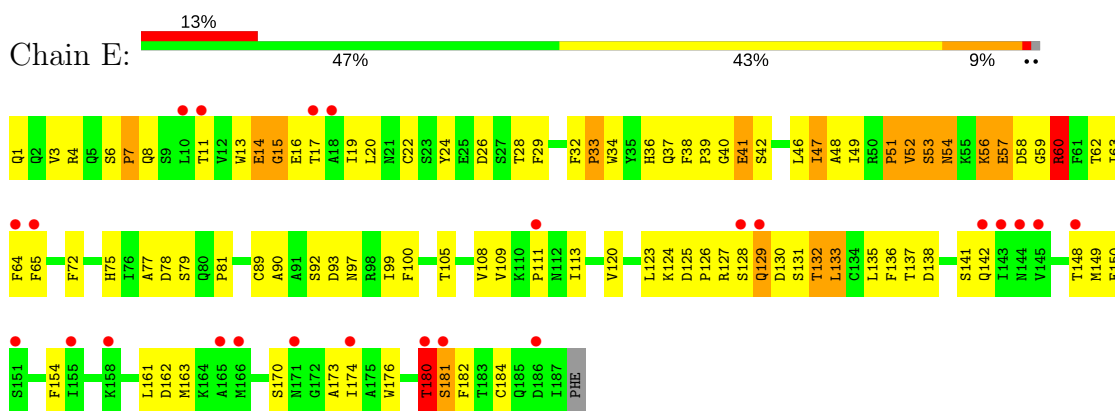
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

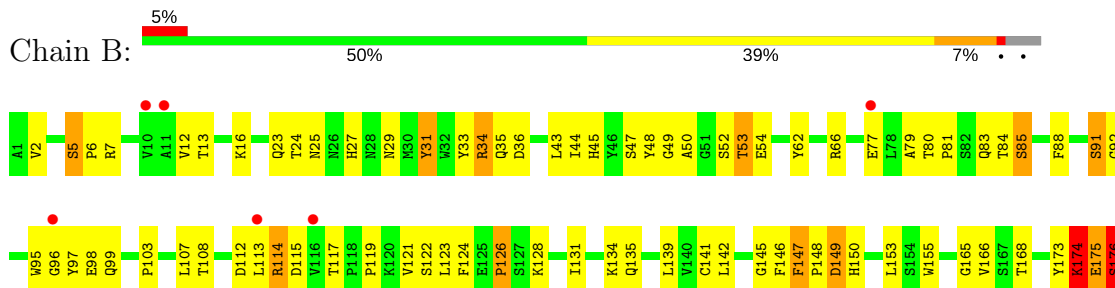
#### • Molecule 1: TCR 2W20 alpha chain



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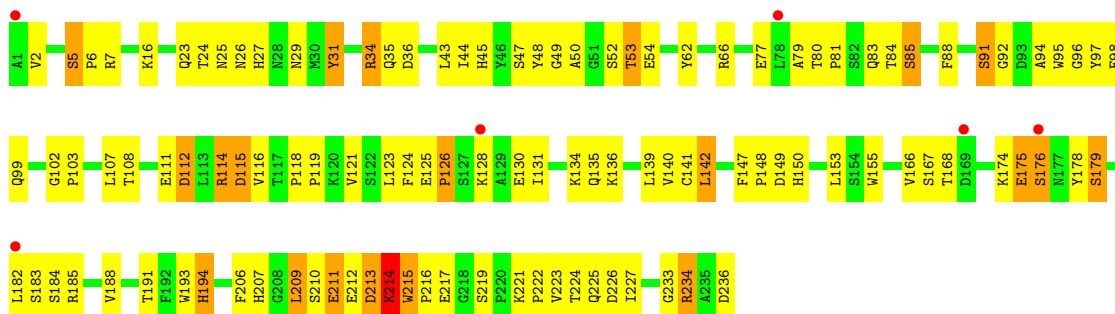


#### • Molecule 2: TCR 2W20 beta chain

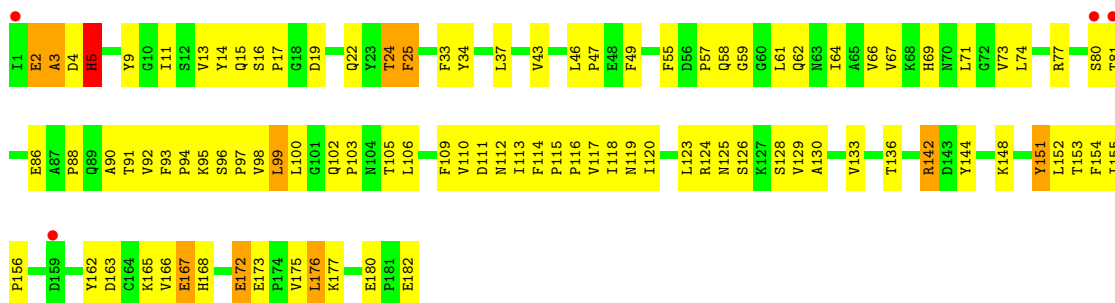




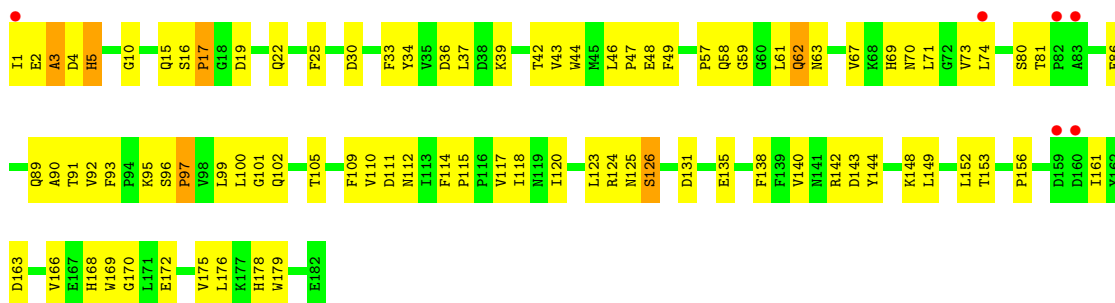
• Molecule 2: TCR 2W20 beta chain



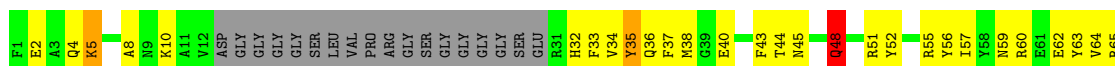
• Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain

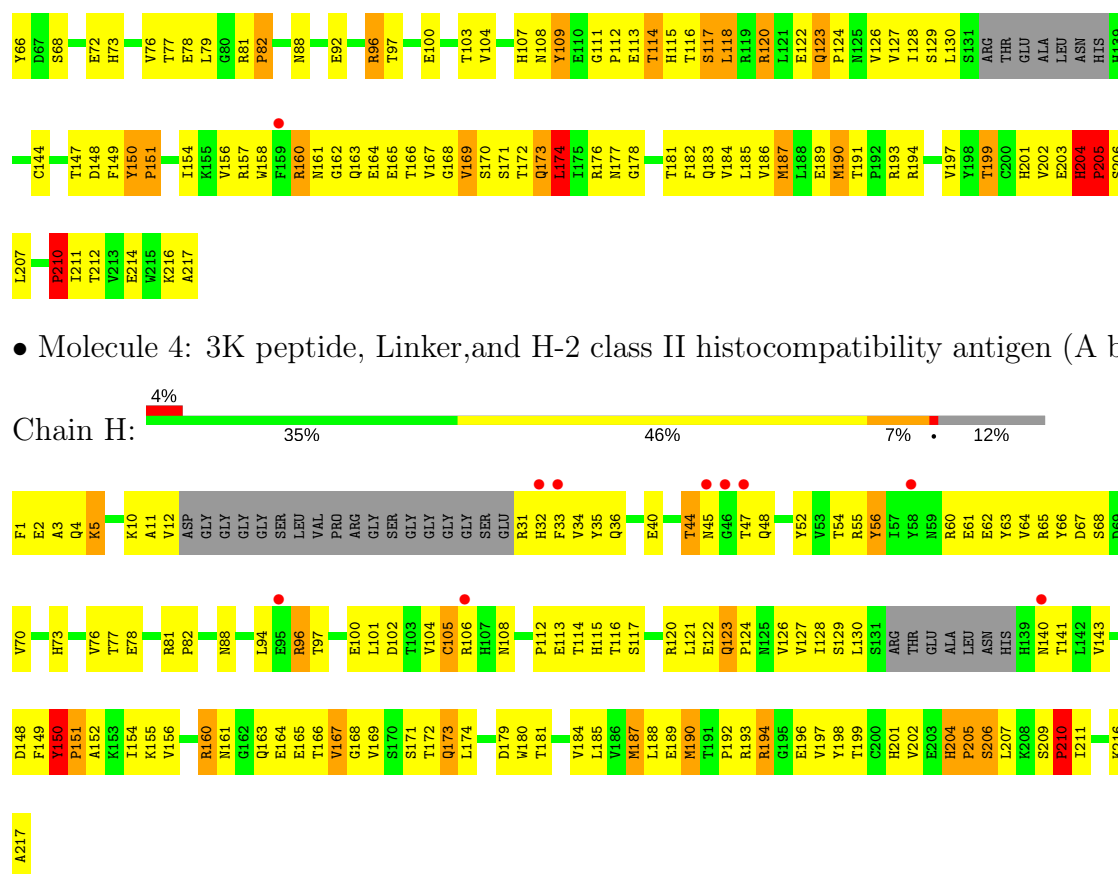


• Molecule 3: H-2 class II histocompatibility antigen, A-B alpha chain



• Molecule 4: 3K peptide, Linker, and H-2 class II histocompatibility antigen (A beta chain)





- Molecule 4: 3K peptide, Linker, and H-2 class II histocompatibility antigen (A beta chain)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.54Å 113.93Å 386.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.40 49.06 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.07-3.40) 97.2 (49.06-3.35)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.268 , 0.325 0.258 , 0.311	Depositor DCC
$R_{free}$ test set	1482 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	98.7	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 71.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12716	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA

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	0.55	0/1514	0.76	2/2053 (0.1%)
1	E	0.52	0/1501	0.73	0/2037
2	B	0.53	0/1847	0.70	1/2509 (0.0%)
2	F	0.52	0/1925	0.69	0/2618
3	C	0.67	0/1504	0.86	1/2054 (0.0%)
3	G	0.67	1/1504 (0.1%)	0.81	1/2054 (0.0%)
4	D	0.67	0/1632	0.87	2/2210 (0.1%)
4	H	0.68	0/1632	0.82	0/2210
All	All	0.60	1/13059 (0.0%)	0.78	7/17745 (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
3	C	0	2
4	D	0	1
4	H	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	44	TRP	CB-CG	-5.51	1.40	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	LEU	CA-CB-CG	6.31	129.82	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	ILE	N-CA-C	6.11	127.50	111.00
3	C	5	HIS	N-CA-C	5.67	126.29	111.00
2	B	174	LYS	N-CA-C	5.51	125.88	111.00
3	G	5	HIS	N-CA-C	5.44	125.68	111.00
4	D	204	HIS	N-CA-C	5.27	125.22	111.00
4	D	174	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	144	TYR	Sidechain
3	C	9	TYR	Sidechain
4	D	35	TYR	Sidechain
4	H	150	TYR	Sidechain

## 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	1476	0	1402	86	0
1	E	1464	0	1394	102	0
2	B	1797	0	1703	125	0
2	F	1870	0	1765	133	0
3	C	1459	0	1386	120	0
3	G	1459	0	1386	101	0
4	D	1594	0	1534	169	0
4	H	1594	0	1534	156	0
5	A	1	0	0	0	0
5	E	2	0	0	0	0
All	All	12716	0	12104	876	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 35.

All (876) 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)
3:C:3:ALA:HB1	4:H:164:GLU:H	0.97	1.10
3:C:109:PHE:HE2	3:C:111:ASP:HB2	1.16	1.08
3:C:2:GLU:HA	4:D:45:ASN:OD1	1.55	1.05
3:C:71:LEU:HD23	4:D:35:TYR:HB2	1.40	1.03
4:H:116:THR:HG23	4:H:117:SER:H	1.17	1.02
3:G:15:GLN:HE22	3:G:117:VAL:HG23	1.25	1.02
2:B:7:ARG:HH21	2:B:103:PRO:HB2	1.23	1.00
4:D:5:LYS:HD3	4:D:5:LYS:H	1.27	1.00
2:F:5:SER:HB3	2:F:6:PRO:HD3	1.42	1.00
2:F:7:ARG:HH21	2:F:103:PRO:HB2	1.27	0.98
4:D:151:PRO:HG3	4:D:205:PRO:HA	1.41	0.98
1:A:99:ILE:HD12	2:B:99:GLN:HE21	1.29	0.97
3:C:3:ALA:HB1	4:H:164:GLU:N	1.78	0.96
4:D:52:TYR:H	4:D:68:SER:HB2	1.29	0.96
2:B:5:SER:HB3	2:B:6:PRO:HD3	1.44	0.95
2:F:147:PHE:HB3	2:F:148:PRO:HD3	1.50	0.94
4:D:151:PRO:HG3	4:D:205:PRO:CA	1.98	0.94
3:C:15:GLN:HG2	4:D:34:VAL:HG22	1.46	0.93
1:E:99:ILE:HD12	2:F:99:GLN:HE21	1.31	0.93
4:D:123:GLN:NE2	4:D:123:GLN:H	1.68	0.92
4:D:172:THR:O	4:D:173:GLN:HG2	1.69	0.92
3:G:71:LEU:HD23	4:H:35:TYR:HB2	1.54	0.90
4:H:172:THR:O	4:H:173:GLN:HB3	1.72	0.90
4:D:202:VAL:HB	4:D:211:ILE:HG23	1.54	0.89
1:E:124:LYS:HA	1:E:131:SER:HB3	1.55	0.89
1:A:123:LEU:HD23	1:A:133:LEU:HD12	1.56	0.88
4:H:202:VAL:HB	4:H:211:ILE:HG23	1.54	0.87
4:H:122:GLU:HB2	4:H:150:TYR:H	1.40	0.86
3:C:67:VAL:HG13	4:D:35:TYR:HD2	1.40	0.86
3:C:109:PHE:CE2	3:C:111:ASP:HB2	2.07	0.85
4:D:199:THR:HG23	4:D:214:GLU:HG3	1.59	0.84
4:H:4:GLN:HG3	4:H:5:LYS:H	1.42	0.84
3:C:46:LEU:O	3:C:49:PHE:HB2	1.77	0.84
3:G:15:GLN:HE22	3:G:117:VAL:CG2	1.90	0.84
2:B:121:VAL:HG12	2:B:227:ILE:HG22	1.59	0.84
1:E:28:THR:HG21	4:H:2:GLU:OE2	1.78	0.84
3:C:15:GLN:NE2	3:C:115:PRO:HB2	1.93	0.83
1:A:28:THR:HG21	4:D:2:GLU:OE2	1.79	0.83
3:C:2:GLU:HA	4:D:45:ASN:CG	1.98	0.83
4:H:101:LEU:O	4:H:105:CYS:HB2	1.80	0.82
3:C:67:VAL:HG13	4:D:35:TYR:CD2	2.14	0.82
1:E:99:ILE:HD12	2:F:99:GLN:NE2	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:147:THR:HG22	4:D:183:GLN:HG3	1.61	0.81
1:E:20:LEU:HD22	1:E:105:THR:HG21	1.60	0.80
4:H:116:THR:HG23	4:H:117:SER:N	1.97	0.80
3:G:1:ILE:O	4:H:45:ASN:HA	1.82	0.80
3:G:161:ILE:HG21	3:G:178:HIS:NE2	1.97	0.80
1:A:60:ARG:HG3	1:A:60:ARG:HH11	1.46	0.80
1:A:20:LEU:HD22	1:A:105:THR:HG21	1.63	0.79
4:D:112:PRO:O	4:D:116:THR:HG22	1.82	0.79
3:G:16:SER:HB2	3:G:71:LEU:HD11	1.65	0.79
1:E:60:ARG:HG3	1:E:60:ARG:HH11	1.48	0.79
3:C:99:LEU:HD23	3:C:102:GLN:OE1	1.82	0.79
2:F:48:TYR:OH	3:G:58:GLN:HG3	1.83	0.78
2:B:114:ARG:NH1	2:B:114:ARG:HB2	1.98	0.78
4:H:151:PRO:HG3	4:H:205:PRO:HA	1.64	0.78
4:D:52:TYR:H	4:D:68:SER:CB	1.97	0.77
1:A:99:ILE:HD12	2:B:99:GLN:NE2	1.98	0.77
1:A:154:PHE:CZ	2:B:175:GLU:HG2	2.19	0.77
1:A:148:THR:HG22	1:A:150:GLU:H	1.47	0.77
2:F:34:ARG:HB2	2:F:44:ILE:HD11	1.64	0.77
3:C:110:VAL:HG21	3:C:120:ILE:HD13	1.66	0.77
4:D:124:PRO:HD3	4:D:205:PRO:HG2	1.67	0.77
2:B:84:THR:HG23	2:B:108:THR:HA	1.67	0.76
1:A:113:ILE:HG13	1:A:140:ASP:HA	1.67	0.75
1:E:99:ILE:CD1	2:F:99:GLN:HE21	1.99	0.75
2:F:84:THR:HG23	2:F:108:THR:HA	1.68	0.75
2:B:34:ARG:HB2	2:B:44:ILE:HD11	1.68	0.75
2:B:147:PHE:HB3	2:B:148:PRO:HD3	1.67	0.75
1:A:148:THR:H	1:A:155:ILE:HD12	1.50	0.75
4:H:204:HIS:CG	4:H:204:HIS:O	2.39	0.75
4:D:96:ARG:HG3	4:D:96:ARG:HH11	1.49	0.74
1:E:19:ILE:HG22	1:E:75:HIS:ND1	2.02	0.74
4:D:123:GLN:HE21	4:D:123:GLN:H	1.33	0.74
2:F:147:PHE:HE1	2:F:178:TYR:HA	1.51	0.74
2:F:5:SER:CB	2:F:6:PRO:HD3	2.15	0.74
2:B:128:LYS:O	2:B:131:ILE:HG13	1.88	0.74
3:C:74:LEU:HD11	4:D:63:TYR:CE2	2.22	0.74
4:D:4:GLN:HG3	4:D:5:LYS:N	2.00	0.74
1:E:56:LYS:HG2	1:E:57:GLU:H	1.52	0.74
1:A:19:ILE:HG22	1:A:75:HIS:ND1	2.02	0.74
3:C:3:ALA:CB	4:H:164:GLU:H	1.90	0.73
1:A:99:ILE:CD1	2:B:99:GLN:HE21	2.00	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:202:VAL:HB	4:H:211:ILE:CG2	2.18	0.73
3:G:67:VAL:HG13	4:H:35:TYR:HD2	1.54	0.73
2:F:209:LEU:HB3	2:F:213:ASP:OD1	1.87	0.73
1:A:6:SER:HB3	1:A:7:PRO:HD3	1.69	0.73
2:B:5:SER:CB	2:B:6:PRO:HD3	2.16	0.73
1:E:6:SER:HB3	1:E:7:PRO:HD3	1.69	0.72
1:A:56:LYS:HG2	1:A:57:GLU:H	1.55	0.72
3:C:110:VAL:HG21	3:C:120:ILE:CD1	2.19	0.72
4:D:78:GLU:HG3	4:D:81:ARG:HD2	1.70	0.72
1:E:26:ASP:HB3	1:E:29:PHE:CE2	2.25	0.72
4:H:174:LEU:HD13	4:H:184:VAL:HB	1.69	0.72
4:H:78:GLU:HG3	4:H:81:ARG:HD2	1.72	0.72
4:D:149:PHE:HB2	4:D:151:PRO:HD2	1.71	0.72
3:G:97:PRO:HG3	4:H:127:VAL:HG11	1.71	0.72
3:C:180:GLU:HG3	3:C:182:GLU:HB2	1.71	0.71
2:F:31:TYR:HB3	2:F:43:LEU:HD11	1.72	0.71
4:H:5:LYS:HD3	4:H:5:LYS:N	2.05	0.71
2:B:113:LEU:HD13	2:B:113:LEU:O	1.90	0.71
2:F:191:THR:HA	2:F:194:HIS:NE2	2.05	0.71
3:G:90:ALA:HA	3:G:109:PHE:O	1.90	0.71
2:B:54:GLU:HG2	3:C:58:GLN:NE2	2.04	0.71
4:H:73:HIS:HB2	4:H:88:ASN:HD21	1.56	0.71
3:C:97:PRO:HG3	4:D:127:VAL:HG11	1.70	0.71
1:E:14:GLU:HG3	1:E:111:PRO:HA	1.71	0.71
4:D:160:ARG:NH2	4:D:163:GLN:OE1	2.23	0.71
2:F:5:SER:HB3	2:F:6:PRO:CD	2.20	0.71
2:F:54:GLU:HG2	3:G:58:GLN:NE2	2.06	0.71
2:B:121:VAL:HG12	2:B:227:ILE:CG2	2.21	0.70
4:D:4:GLN:HG3	4:D:5:LYS:H	1.57	0.70
4:H:197:VAL:HG12	4:H:216:LYS:HB3	1.71	0.70
1:E:161:LEU:HB2	2:F:185:ARG:HH12	1.54	0.70
3:G:118:ILE:HD11	3:G:166:VAL:HG13	1.73	0.70
1:A:26:ASP:HB3	1:A:29:PHE:CE2	2.27	0.70
1:A:51:PRO:O	1:A:52:VAL:HG23	1.91	0.70
4:D:113:GLU:O	4:D:115:HIS:N	2.24	0.70
1:E:28:THR:HB	4:H:4:GLN:HE22	1.56	0.70
4:H:116:THR:CG2	4:H:117:SER:H	1.99	0.70
3:C:172:GLU:OE2	3:C:173:GLU:HG2	1.92	0.69
2:F:213:ASP:HB3	2:F:221:LYS:HD2	1.74	0.69
3:G:2:GLU:HG3	4:H:45:ASN:ND2	2.07	0.69
1:E:52:VAL:HG12	1:E:52:VAL:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:112:PRO:O	4:H:116:THR:HG22	1.93	0.69
1:A:52:VAL:HG12	1:A:52:VAL:O	1.92	0.69
3:C:81:THR:O	4:D:33:PHE:CE1	2.46	0.69
4:H:96:ARG:HH11	4:H:96:ARG:HG3	1.57	0.69
2:B:31:TYR:HB3	2:B:43:LEU:HD11	1.74	0.68
3:C:103:PRO:HG3	3:C:155:ILE:CD1	2.22	0.68
1:E:133:LEU:HD11	2:F:140:VAL:HG11	1.75	0.68
1:A:126:PRO:HB3	2:B:234:ARG:HH12	1.59	0.68
3:C:15:GLN:HE22	3:C:117:VAL:HG23	1.58	0.68
2:F:50:ALA:HA	2:F:66:ARG:HG3	1.76	0.68
4:H:63:TYR:CD2	4:H:64:VAL:HG23	2.29	0.68
4:D:126:VAL:HG21	4:D:202:VAL:HG21	1.76	0.67
2:F:141:CYS:HB2	2:F:155:TRP:CH2	2.29	0.67
4:D:202:VAL:HB	4:D:211:ILE:CG2	2.24	0.67
4:D:164:GLU:N	3:G:3:ALA:HB1	2.09	0.67
2:B:147:PHE:CB	2:B:148:PRO:HD3	2.23	0.67
2:B:199:HIS:HE1	2:B:230:GLU:HB2	1.59	0.67
2:B:50:ALA:HA	2:B:66:ARG:HG3	1.75	0.67
3:C:11:ILE:HB	3:C:24:THR:HG23	1.76	0.67
3:G:58:GLN:NE2	3:G:61:LEU:HD22	2.09	0.67
4:H:124:PRO:HG3	4:H:205:PRO:HG3	1.77	0.67
2:B:5:SER:HB3	2:B:6:PRO:CD	2.23	0.66
4:D:35:TYR:OH	4:D:56:TYR:HB3	1.96	0.66
4:D:52:TYR:N	4:D:68:SER:HB2	2.07	0.66
1:E:51:PRO:O	1:E:52:VAL:HG23	1.94	0.66
1:E:148:THR:HG22	1:E:150:GLU:H	1.61	0.66
2:F:153:LEU:HD21	2:F:168:THR:HG21	1.76	0.66
4:H:124:PRO:HD3	4:H:205:PRO:HG2	1.78	0.66
2:B:114:ARG:HB2	2:B:114:ARG:HH11	1.60	0.66
4:D:158:TRP:HD1	4:D:169:VAL:HG12	1.61	0.66
4:H:160:ARG:HH11	4:H:190:MET:HE1	1.61	0.66
4:D:43:PHE:O	4:H:163:GLN:NE2	2.23	0.66
2:B:191:THR:HA	2:B:194:HIS:NE2	2.10	0.66
3:C:61:LEU:H	3:C:61:LEU:HD12	1.61	0.66
3:G:34:TYR:CE1	3:G:43:VAL:HB	2.30	0.65
2:B:148:PRO:O	2:B:150:HIS:N	2.26	0.65
3:G:30:ASP:HB3	4:H:180:TRP:CE2	2.30	0.65
1:E:47:ILE:HB	1:E:63:ILE:HD11	1.79	0.65
2:F:128:LYS:HG3	2:F:131:ILE:HD11	1.78	0.65
3:C:133:VAL:HG22	3:C:152:LEU:HD23	1.79	0.65
2:F:147:PHE:HB3	2:F:148:PRO:CD	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:TYR:CE1	3:C:62:GLN:HG2	2.32	0.65
4:H:4:GLN:HG3	4:H:5:LYS:N	2.10	0.64
4:D:5:LYS:CD	4:D:5:LYS:H	2.05	0.64
4:D:164:GLU:H	3:G:3:ALA:HB1	1.62	0.64
4:H:5:LYS:HD3	4:H:5:LYS:H	1.62	0.64
2:F:95:TRP:CH2	3:G:62:GLN:HB3	2.32	0.64
4:H:108:ASN:HA	4:H:112:PRO:HD2	1.78	0.64
2:B:153:LEU:HD22	2:B:182:LEU:HD21	1.78	0.64
2:F:97:TYR:C	2:F:98:GLU:HG3	2.18	0.64
2:B:139:LEU:H	2:B:139:LEU:HD12	1.63	0.64
3:G:109:PHE:HD1	3:G:149:LEU:HD21	1.62	0.64
4:H:151:PRO:HG3	4:H:205:PRO:CA	2.27	0.64
2:B:209:LEU:H	2:B:209:LEU:HD12	1.63	0.64
4:D:117:SER:O	4:D:118:LEU:C	2.36	0.64
4:D:160:ARG:HH11	4:D:160:ARG:HG3	1.63	0.64
2:F:111:GLU:HG2	2:F:112:ASP:H	1.61	0.64
4:D:116:THR:HG23	4:D:117:SER:H	1.61	0.63
4:D:44:THR:O	4:D:45:ASN:HB2	1.99	0.63
4:D:65:ARG:HG2	4:D:66:TYR:N	2.12	0.63
2:F:7:ARG:NH1	2:F:7:ARG:HB3	2.13	0.63
2:F:147:PHE:CB	2:F:148:PRO:HD3	2.27	0.63
4:H:193:ARG:CB	4:H:193:ARG:HH11	2.11	0.63
2:F:126:PRO:HD2	2:F:193:TRP:CH2	2.33	0.63
2:B:7:ARG:HB3	2:B:7:ARG:NH1	2.13	0.63
1:E:182:PHE:CZ	1:E:184:CYS:SG	2.93	0.62
2:F:44:ILE:O	2:F:45:HIS:ND1	2.33	0.62
4:D:66:TYR:HB2	4:D:73:HIS:ND1	2.15	0.62
4:H:44:THR:O	4:H:45:ASN:HB2	1.98	0.62
3:C:15:GLN:HE21	3:C:115:PRO:HB2	1.64	0.62
3:C:98:VAL:HG13	3:C:156:PRO:HB3	1.82	0.62
3:C:16:SER:OG	4:D:33:PHE:HB2	1.99	0.62
3:G:161:ILE:CG2	3:G:178:HIS:NE2	2.62	0.62
2:F:134:LYS:O	2:F:135:GLN:HB2	2.00	0.62
2:B:97:TYR:C	2:B:98:GLU:HG3	2.19	0.62
3:G:138:PHE:CE1	3:G:148:LYS:HE2	2.35	0.62
3:C:90:ALA:HA	3:C:109:PHE:O	2.00	0.62
4:D:165:GLU:O	4:D:166:THR:HG23	2.00	0.62
1:A:125:ASP:C	1:A:127:ARG:H	2.03	0.62
1:A:174:ILE:HD11	2:B:185:ARG:HD2	1.81	0.62
3:C:97:PRO:O	3:C:99:LEU:HD22	1.99	0.61
4:D:173:GLN:O	4:D:173:GLN:CG	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:168:THR:HG23	2:F:184:SER:HB2	1.82	0.61
1:A:56:LYS:O	1:A:57:GLU:O	2.18	0.61
2:F:225:GLN:NE2	2:F:227:ILE:HD11	2.14	0.61
3:G:58:GLN:HE22	3:G:61:LEU:HD22	1.63	0.61
1:A:60:ARG:HG3	1:A:60:ARG:NH1	2.15	0.61
2:F:153:LEU:HD22	2:F:182:LEU:HD21	1.81	0.61
4:H:65:ARG:HG2	4:H:66:TYR:N	2.14	0.61
3:C:55:PHE:O	3:C:57:PRO:HD3	1.99	0.61
3:G:70:ASN:O	3:G:71:LEU:C	2.37	0.61
4:H:122:GLU:HB2	4:H:150:TYR:N	2.15	0.61
4:H:160:ARG:HH11	4:H:160:ARG:HG3	1.66	0.61
4:H:165:GLU:O	4:H:166:THR:HG23	2.00	0.61
2:B:95:TRP:CH2	3:C:62:GLN:HB3	2.35	0.61
4:D:151:PRO:CG	4:D:205:PRO:HA	2.26	0.61
2:B:16:LYS:HZ1	2:B:77:GLU:HG3	1.66	0.61
2:B:203:GLN:NE2	2:B:226:ASP:HB2	2.16	0.61
3:G:36:ASP:OD2	3:G:39:LYS:HE3	2.01	0.61
1:E:33:PRO:HG2	1:E:90:ALA:HB3	1.83	0.60
3:G:95:LYS:HE3	4:H:179:ASP:OD1	2.01	0.60
4:D:78:GLU:O	4:D:81:ARG:HG3	2.01	0.60
1:E:124:LYS:HA	1:E:131:SER:CB	2.30	0.60
2:B:121:VAL:CG1	2:B:227:ILE:HG22	2.30	0.60
2:B:49:GLY:O	2:B:52:SER:HB3	2.02	0.60
1:E:113:ILE:HD12	1:E:138:ASP:O	2.00	0.60
4:D:36:GLN:HB2	4:D:57:ILE:HB	1.82	0.60
3:G:123:LEU:HD22	3:G:126:SER:O	2.01	0.60
4:H:173:GLN:HG2	4:H:174:LEU:O	2.01	0.60
2:F:148:PRO:O	2:F:150:HIS:N	2.30	0.60
2:F:213:ASP:O	2:F:215:TRP:N	2.35	0.60
2:F:31:TYR:CD1	2:F:31:TYR:N	2.70	0.60
4:D:100:GLU:HA	4:D:103:THR:OG1	2.02	0.60
4:D:150:TYR:N	4:D:151:PRO:CD	2.65	0.60
4:D:116:THR:O	4:D:117:SER:O	2.20	0.60
2:F:209:LEU:HD12	2:F:222:PRO:HG2	1.84	0.60
2:B:134:LYS:O	2:B:135:GLN:HB2	2.01	0.59
2:B:153:LEU:HD22	2:B:182:LEU:CD2	2.31	0.59
1:A:124:LYS:HA	1:A:131:SER:HB3	1.83	0.59
1:E:46:LEU:HG	1:E:47:ILE:HG13	1.84	0.59
2:F:123:LEU:HD23	2:F:124:PHE:N	2.17	0.59
2:F:211:GLU:O	2:F:213:ASP:N	2.35	0.59
4:H:55:ARG:HH11	4:H:55:ARG:HG2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:GLU:HG2	4:D:76:VAL:HG11	1.84	0.59
1:E:56:LYS:HG2	1:E:57:GLU:N	2.17	0.59
2:F:209:LEU:HB3	2:F:213:ASP:CG	2.22	0.59
3:G:16:SER:HB2	3:G:71:LEU:CD1	2.33	0.59
4:H:193:ARG:HH11	4:H:193:ARG:HB3	1.67	0.59
2:B:7:ARG:NH2	2:B:103:PRO:HB2	2.06	0.59
3:G:63:ASN:O	3:G:67:VAL:HG23	2.03	0.59
3:G:120:ILE:HD12	3:G:148:LYS:HD2	1.83	0.59
1:A:125:ASP:OD1	1:A:131:SER:HA	2.02	0.59
3:C:33:PHE:HB2	3:C:43:VAL:O	2.02	0.59
3:G:89:GLN:O	3:G:110:VAL:HA	2.03	0.59
4:H:148:ASP:HA	4:H:181:THR:HB	1.85	0.59
3:C:118:ILE:HD11	3:C:166:VAL:HG13	1.84	0.59
2:B:119:PRO:O	2:B:227:ILE:HG13	2.02	0.59
3:C:103:PRO:HG3	3:C:155:ILE:HD11	1.84	0.59
1:E:135:LEU:O	1:E:135:LEU:HG	2.02	0.59
2:F:207:HIS:HA	2:F:224:THR:HG23	1.84	0.58
2:B:44:ILE:O	2:B:45:HIS:ND1	2.36	0.58
3:C:124:ARG:HG3	3:C:162:TYR:CE1	2.37	0.58
1:A:47:ILE:HB	1:A:63:ILE:HD11	1.83	0.58
4:D:173:GLN:O	4:D:173:GLN:HG3	2.03	0.58
1:E:60:ARG:HG3	1:E:60:ARG:NH1	2.17	0.58
4:H:143:VAL:HG22	4:H:187:MET:CG	2.33	0.58
4:H:189:GLU:HA	4:H:189:GLU:OE1	2.03	0.58
4:H:197:VAL:HG23	4:H:197:VAL:O	2.03	0.58
4:D:81:ARG:N	4:D:82:PRO:CD	2.66	0.58
1:E:56:LYS:O	1:E:57:GLU:O	2.21	0.58
3:G:17:PRO:HG3	4:H:32:HIS:HA	1.84	0.58
4:H:143:VAL:HG22	4:H:187:MET:HG3	1.85	0.58
4:D:122:GLU:HB2	4:D:150:TYR:H	1.68	0.58
3:G:15:GLN:HG2	4:H:34:VAL:HG22	1.84	0.58
3:G:46:LEU:HD23	3:G:49:PHE:CE1	2.39	0.58
2:B:31:TYR:CD1	2:B:31:TYR:N	2.72	0.58
4:H:197:VAL:HG12	4:H:216:LYS:CB	2.33	0.58
2:B:225:GLN:HE21	2:B:227:ILE:HD11	1.69	0.58
4:D:160:ARG:HD2	4:D:161:ASN:N	2.18	0.58
4:D:96:ARG:HG3	4:D:96:ARG:NH1	2.17	0.58
2:F:7:ARG:NH2	2:F:103:PRO:HB2	2.10	0.58
1:A:53:SER:O	1:A:54:ASN:HB3	2.04	0.58
2:B:117:THR:HB	2:B:145:GLY:O	2.03	0.58
3:C:15:GLN:HE21	3:C:116:PRO:HD2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:204:HIS:O	4:D:204:HIS:CG	2.53	0.58
1:E:28:THR:HG21	4:H:2:GLU:CD	2.23	0.58
3:C:16:SER:N	3:C:17:PRO:HD2	2.19	0.57
1:E:19:ILE:HG13	1:E:19:ILE:O	2.03	0.57
2:F:47:SER:HB3	2:F:66:ARG:HH11	1.69	0.57
2:F:26:ASN:O	4:H:10:LYS:NZ	2.37	0.57
2:B:153:LEU:H	2:B:153:LEU:HD23	1.69	0.57
4:D:160:ARG:NH1	4:D:160:ARG:HG3	2.19	0.57
1:A:56:LYS:HG2	1:A:57:GLU:N	2.20	0.57
2:B:47:SER:HB3	2:B:66:ARG:HH11	1.68	0.57
4:D:120:ARG:O	4:D:120:ARG:HG2	2.01	0.57
2:F:193:TRP:C	2:F:193:TRP:CD1	2.78	0.57
4:D:173:GLN:HA	4:H:169:VAL:O	2.04	0.57
1:A:17:THR:HG22	1:A:77:ALA:HA	1.86	0.57
3:C:16:SER:HB3	3:C:71:LEU:CD1	2.34	0.57
3:G:86:GLU:HG3	4:H:60:ARG:HH12	1.69	0.57
1:A:33:PRO:HG2	1:A:90:ALA:HB3	1.87	0.57
3:G:124:ARG:O	3:G:125:ASN:HB2	2.05	0.57
4:H:3:ALA:HB2	4:H:112:PRO:HG2	1.87	0.57
4:D:36:GLN:N	4:D:57:ILE:O	2.38	0.57
4:H:141:THR:HG23	4:H:188:LEU:O	2.04	0.57
3:C:118:ILE:HG13	3:C:167:GLU:O	2.05	0.57
3:C:151:TYR:OH	4:D:178:GLY:HA3	2.05	0.56
4:D:184:VAL:C	4:D:185:LEU:HD12	2.25	0.56
4:D:113:GLU:C	4:D:115:HIS:H	2.09	0.56
2:F:116:VAL:HG13	2:F:148:PRO:CD	2.34	0.56
2:F:49:GLY:O	2:F:52:SER:HB3	2.04	0.56
3:G:109:PHE:HD1	3:G:149:LEU:CD2	2.19	0.56
2:B:23:GLN:HG2	2:B:24:THR:N	2.19	0.56
3:C:175:VAL:O	3:C:175:VAL:HG23	2.04	0.56
4:D:158:TRP:CD1	4:D:169:VAL:HG12	2.39	0.56
2:F:111:GLU:H	2:F:111:GLU:CD	2.09	0.56
3:G:2:GLU:HA	4:H:45:ASN:CG	2.26	0.56
4:D:114:THR:HG22	4:D:114:THR:O	2.04	0.56
1:E:53:SER:O	1:E:54:ASN:HB3	2.04	0.56
4:H:76:VAL:HG13	4:H:77:THR:HG23	1.88	0.56
1:E:49:ILE:HD13	1:E:65:PHE:HB2	1.87	0.56
4:H:52:TYR:H	4:H:68:SER:HB2	1.71	0.56
3:C:15:GLN:NE2	3:C:116:PRO:HD2	2.20	0.56
3:C:165:LYS:HA	3:C:176:LEU:HA	1.86	0.56
3:C:17:PRO:HG3	4:D:32:HIS:ND1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:ILE:HD11	2:F:185:ARG:HD2	1.87	0.56
4:H:193:ARG:HB2	4:H:196:GLU:OE2	2.05	0.56
1:A:46:LEU:HG	1:A:47:ILE:HG13	1.86	0.56
1:E:123:LEU:HD21	1:E:135:LEU:HB2	1.88	0.56
1:E:126:PRO:HD3	2:F:125:GLU:OE1	2.05	0.56
3:G:73:VAL:HG21	4:H:11:ALA:HB3	1.86	0.56
4:D:72:GLU:HB2	4:D:88:ASN:OD1	2.06	0.56
2:F:153:LEU:HD22	2:F:182:LEU:CD2	2.36	0.56
2:F:16:LYS:HZ1	2:F:77:GLU:HG3	1.71	0.56
4:D:160:ARG:CD	4:D:161:ASN:H	2.19	0.55
4:D:187:MET:SD	4:D:187:MET:N	2.78	0.55
3:G:17:PRO:HG3	4:H:32:HIS:ND1	2.21	0.55
4:H:194:ARG:HG3	4:H:217:ALA:OXT	2.06	0.55
4:H:67:ASP:HB3	4:H:70:VAL:HG23	1.88	0.55
2:B:5:SER:CB	2:B:6:PRO:CD	2.83	0.55
4:D:63:TYR:CD2	4:D:64:VAL:HG23	2.41	0.55
2:F:16:LYS:NZ	2:F:77:GLU:HG3	2.21	0.55
3:G:74:LEU:HD21	4:H:63:TYR:OH	2.06	0.55
2:B:174:LYS:HD3	2:B:175:GLU:N	2.21	0.55
3:C:95:LYS:NZ	4:D:148:ASP:OD1	2.34	0.55
1:E:81:PRO:CG	1:E:111:PRO:HB3	2.37	0.55
4:D:216:LYS:HG2	4:D:217:ALA:H	1.70	0.55
4:D:81:ARG:NH1	4:D:81:ARG:HB3	2.22	0.55
1:E:20:LEU:CD2	1:E:105:THR:HG21	2.33	0.55
1:E:123:LEU:HD23	1:E:133:LEU:HD12	1.89	0.55
1:E:113:ILE:CD1	1:E:138:ASP:O	2.55	0.55
2:F:141:CYS:HB2	2:F:155:TRP:CZ2	2.42	0.55
3:G:46:LEU:O	3:G:47:PRO:C	2.44	0.55
1:A:49:ILE:HD13	1:A:65:PHE:HB2	1.89	0.55
2:B:165:GLY:O	2:B:186:LEU:HD12	2.07	0.55
3:C:86:GLU:HB3	3:C:112:ASN:HD21	1.72	0.55
2:F:147:PHE:CE1	2:F:178:TYR:HA	2.38	0.55
4:D:8:ALA:HB2	4:D:37:PHE:CD2	2.41	0.55
3:C:37:LEU:HD21	3:C:64:ILE:HG13	1.89	0.54
2:F:48:TYR:CE1	3:G:62:GLN:HG2	2.42	0.54
3:G:16:SER:HB3	4:H:33:PHE:HB2	1.90	0.54
4:D:51:ARG:HG3	4:D:68:SER:HB3	1.89	0.54
2:F:23:GLN:HG2	2:F:24:THR:N	2.21	0.54
2:B:128:LYS:HA	2:B:131:ILE:HD11	1.89	0.54
1:A:161:LEU:HB2	2:B:185:ARG:HH12	1.72	0.54
3:C:86:GLU:HB3	3:C:112:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:5:SER:CB	2:F:6:PRO:CD	2.81	0.54
4:H:150:TYR:O	4:H:150:TYR:CG	2.59	0.54
1:A:19:ILE:O	1:A:19:ILE:HG13	2.07	0.54
3:C:2:GLU:O	3:C:3:ALA:O	2.26	0.54
3:G:42:THR:OG1	3:G:57:PRO:HG3	2.07	0.54
2:B:199:HIS:CE1	2:B:230:GLU:HB2	2.42	0.54
2:F:147:PHE:HD1	2:F:179:SER:H	1.55	0.54
4:D:216:LYS:O	4:D:217:ALA:HB3	2.08	0.54
3:G:71:LEU:C	3:G:71:LEU:HD13	2.28	0.54
4:D:120:ARG:HD3	4:D:150:TYR:CD1	2.44	0.54
3:G:2:GLU:HG3	4:H:45:ASN:HD21	1.73	0.54
1:A:36:HIS:O	1:A:36:HIS:ND1	2.41	0.53
4:D:172:THR:O	4:D:173:GLN:CG	2.49	0.53
4:H:188:LEU:HD12	4:H:189:GLU:N	2.24	0.53
1:E:123:LEU:HD12	2:F:126:PRO:HA	1.89	0.53
3:G:81:THR:O	4:H:33:PHE:HE1	1.91	0.53
1:A:93:ASP:CG	1:A:97:ASN:H	2.11	0.53
1:A:123:LEU:HD12	2:B:126:PRO:HA	1.89	0.53
2:B:16:LYS:NZ	2:B:77:GLU:HG3	2.23	0.53
2:B:16:LYS:HD2	2:B:77:GLU:HA	1.91	0.53
2:F:118:PRO:HD3	2:F:222:PRO:HB3	1.91	0.53
2:F:168:THR:HG23	2:F:183:SER:O	2.09	0.53
2:B:146:PHE:CE1	2:B:180:TYR:O	2.62	0.53
4:D:122:GLU:HB2	4:D:150:TYR:N	2.24	0.53
3:C:37:LEU:N	3:C:37:LEU:HD12	2.24	0.53
2:B:199:HIS:HE1	2:B:230:GLU:CB	2.22	0.52
3:C:136:THR:O	3:C:148:LYS:NZ	2.40	0.52
2:F:94:ALA:CB	3:G:62:GLN:HE22	2.22	0.52
4:H:160:ARG:NH1	4:H:190:MET:HE1	2.24	0.52
1:A:33:PRO:HA	1:A:48:ALA:HA	1.91	0.52
4:D:176:ARG:HG3	4:D:182:PHE:HE1	1.73	0.52
3:G:15:GLN:HE21	3:G:115:PRO:HB2	1.74	0.52
3:G:33:PHE:HB2	3:G:43:VAL:O	2.10	0.52
4:D:124:PRO:HG3	4:D:205:PRO:HG3	1.91	0.52
1:E:3:VAL:C	1:E:4:ARG:HD2	2.29	0.52
1:A:3:VAL:C	1:A:4:ARG:HD2	2.30	0.52
4:D:76:VAL:HG13	4:D:77:THR:HG23	1.92	0.52
1:E:33:PRO:HA	1:E:48:ALA:HA	1.91	0.52
2:F:94:ALA:HB1	3:G:62:GLN:NE2	2.25	0.52
2:F:29:ASN:HB2	2:F:92:GLY:O	2.10	0.52
1:A:174:ILE:N	1:A:174:ILE:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:VAL:HG12	2:B:204:VAL:O	2.09	0.52
1:E:93:ASP:CG	1:E:97:ASN:H	2.12	0.52
3:G:36:ASP:OD2	3:G:39:LYS:CE	2.58	0.52
4:D:207:LEU:HD23	4:D:207:LEU:N	2.24	0.52
4:D:201:HIS:NE2	4:D:210:PRO:HB3	2.25	0.52
2:F:16:LYS:HD2	2:F:77:GLU:HA	1.91	0.52
2:F:27:HIS:ND1	2:F:91:SER:OG	2.42	0.52
4:H:150:TYR:CD1	4:H:150:TYR:O	2.63	0.52
4:H:188:LEU:HD12	4:H:189:GLU:H	1.75	0.52
2:F:210:SER:O	2:F:211:GLU:C	2.48	0.52
4:D:100:GLU:HB3	4:D:104:VAL:CG2	2.40	0.51
4:D:162:GLY:O	3:G:3:ALA:HB2	2.10	0.51
4:D:148:ASP:HA	4:D:181:THR:HB	1.91	0.51
2:F:209:LEU:HD13	2:F:213:ASP:OD2	2.10	0.51
3:C:98:VAL:HG13	3:C:156:PRO:CB	2.41	0.51
4:D:160:ARG:HD2	4:D:161:ASN:H	1.73	0.51
1:E:36:HIS:ND1	1:E:36:HIS:O	2.43	0.51
4:H:189:GLU:O	4:H:190:MET:O	2.28	0.51
4:D:128:ILE:HG22	4:D:129:SER:N	2.25	0.51
1:E:36:HIS:HD2	1:E:46:LEU:HB2	1.76	0.51
4:H:88:ASN:OD1	4:H:94:LEU:HD13	2.10	0.51
2:B:113:LEU:HD11	2:B:209:LEU:CD2	2.41	0.51
2:B:184:SER:OG	2:B:185:ARG:N	2.44	0.51
4:D:163:GLN:HA	3:G:3:ALA:HB1	1.91	0.51
4:D:171:SER:HB2	4:H:171:SER:HB3	1.93	0.51
4:D:170:SER:HB2	4:D:187:MET:HB2	1.92	0.51
4:D:124:PRO:CD	4:D:205:PRO:HG2	2.40	0.51
3:C:81:THR:O	4:D:33:PHE:HE1	1.92	0.51
3:G:178:HIS:CD2	3:G:179:TRP:H	2.28	0.51
3:G:15:GLN:HA	4:H:33:PHE:O	2.09	0.51
4:D:144:CYS:HB2	4:D:158:TRP:CZ2	2.46	0.51
2:B:174:LYS:HD3	2:B:174:LYS:C	2.30	0.51
3:C:34:TYR:CE1	3:C:43:VAL:HB	2.46	0.51
1:E:4:ARG:O	1:E:22:CYS:HA	2.10	0.51
4:H:120:ARG:HG3	4:H:120:ARG:HH11	1.75	0.51
4:H:47:THR:HG22	4:H:106:ARG:HH12	1.76	0.51
4:D:160:ARG:HG3	4:D:190:MET:HE2	1.93	0.50
4:D:79:LEU:HG	4:D:79:LEU:O	2.10	0.50
2:B:121:VAL:HG22	2:B:122:SER:N	2.25	0.50
3:C:124:ARG:O	3:C:125:ASN:HB2	2.12	0.50
2:B:36:ASP:OD2	2:B:85:SER:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:197:VAL:HG23	4:D:197:VAL:O	2.12	0.50
2:B:153:LEU:N	2:B:153:LEU:HD23	2.27	0.50
3:C:123:LEU:HD23	3:C:128:SER:HA	1.93	0.50
4:D:4:GLN:CG	4:D:5:LYS:N	2.72	0.50
3:C:47:PRO:C	3:C:49:PHE:H	2.14	0.50
4:D:207:LEU:HD23	4:D:207:LEU:H	1.77	0.50
4:D:62:GLU:OE1	4:D:65:ARG:NE	2.40	0.50
3:G:176:LEU:HD12	3:G:176:LEU:O	2.11	0.50
4:D:2:GLU:O	4:D:107:HIS:HE1	1.94	0.50
2:F:175:GLU:O	2:F:176:SER:HB3	2.11	0.50
3:G:114:PHE:CD1	3:G:114:PHE:C	2.85	0.50
4:H:160:ARG:NH1	4:H:160:ARG:HG3	2.25	0.50
2:F:128:LYS:HD3	2:F:236:ASP:HB3	1.92	0.50
4:H:193:ARG:CB	4:H:193:ARG:NH1	2.74	0.50
4:H:193:ARG:NH1	4:H:193:ARG:HB2	2.27	0.50
1:A:92:SER:HB2	1:A:99:ILE:HG12	1.93	0.50
2:B:153:LEU:CD2	2:B:182:LEU:HD21	2.41	0.50
2:B:48:TYR:HE2	3:C:58:GLN:HE21	1.60	0.50
4:D:116:THR:HG23	4:D:117:SER:N	2.27	0.50
1:E:92:SER:HB2	1:E:99:ILE:HG12	1.93	0.50
3:G:61:LEU:HD12	3:G:61:LEU:H	1.76	0.50
3:G:168:HIS:CD2	3:G:170:GLY:H	2.29	0.49
2:B:79:ALA:HA	2:B:83:GLN:OE1	2.12	0.49
1:A:177:SER:OG	1:A:182:PHE:HD2	1.95	0.49
3:C:16:SER:HB3	3:C:71:LEU:HD11	1.93	0.49
4:H:190:MET:CE	4:H:198:TYR:HE2	2.26	0.49
1:A:11:THR:HG22	1:A:108:VAL:HB	1.93	0.49
2:B:27:HIS:ND1	2:B:91:SER:OG	2.44	0.49
4:H:156:VAL:HA	4:H:201:HIS:O	2.13	0.49
2:B:203:GLN:HE21	2:B:226:ASP:HB2	1.77	0.49
4:D:174:LEU:HD13	4:D:184:VAL:HB	1.95	0.49
2:F:114:ARG:HG2	2:F:215:TRP:CZ2	2.48	0.49
4:H:126:VAL:HG21	4:H:202:VAL:HG21	1.95	0.49
2:F:125:GLU:OE2	2:F:234:ARG:NH2	2.46	0.49
2:B:148:PRO:C	2:B:150:HIS:H	2.13	0.49
3:C:151:TYR:CD1	3:C:151:TYR:N	2.81	0.49
3:C:180:GLU:CG	3:C:182:GLU:HB2	2.42	0.49
1:A:20:LEU:CD2	1:A:105:THR:HG21	2.38	0.49
2:B:29:ASN:HB2	2:B:92:GLY:O	2.11	0.49
4:D:168:GLY:HA2	4:H:173:GLN:HG3	1.95	0.49
1:E:17:THR:HG22	1:E:77:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:GLN:NE2	2:F:88:PHE:HE2	2.11	0.49
4:D:5:LYS:N	4:D:5:LYS:HD3	2.06	0.49
1:A:4:ARG:O	1:A:22:CYS:HA	2.13	0.49
4:D:167:VAL:HG23	4:D:168:GLY:N	2.28	0.49
3:C:17:PRO:HG3	4:D:32:HIS:HA	1.94	0.48
2:B:206:PHE:O	2:B:224:THR:HA	2.13	0.48
3:G:96:SER:HB3	3:G:97:PRO:HD2	1.95	0.48
4:H:190:MET:HE2	4:H:198:TYR:HE2	1.78	0.48
1:E:28:THR:CB	4:H:4:GLN:HE22	2.23	0.48
1:A:93:ASP:OD2	1:A:97:ASN:N	2.43	0.48
3:C:106:LEU:HB2	3:C:154:PHE:CE1	2.48	0.48
3:C:15:GLN:NE2	3:C:116:PRO:CD	2.76	0.48
4:D:120:ARG:HG3	4:D:120:ARG:HH11	1.77	0.48
4:D:45:ASN:HB2	4:D:48:GLN:HB3	1.94	0.48
4:H:81:ARG:HB2	4:H:82:PRO:HD3	1.95	0.48
1:A:184:CYS:O	1:A:185:GLN:HB2	2.13	0.48
2:B:174:LYS:HA	2:B:180:TYR:HD1	1.77	0.48
3:C:22:GLN:HE21	3:C:24:THR:HG22	1.77	0.48
4:D:160:ARG:HH11	4:D:190:MET:HE1	1.78	0.48
2:F:121:VAL:HG12	2:F:227:ILE:HG22	1.95	0.48
2:F:79:ALA:HA	2:F:83:GLN:OE1	2.13	0.48
4:H:160:ARG:HD2	4:H:161:ASN:ND2	2.28	0.48
4:H:172:THR:OG1	4:H:185:LEU:HB2	2.14	0.48
1:E:11:THR:HG22	1:E:108:VAL:HB	1.95	0.48
1:A:15:GLY:HA2	1:A:78:ASP:HA	1.95	0.48
4:D:203:GLU:O	4:D:205:PRO:HD3	2.14	0.48
2:F:123:LEU:HD23	2:F:123:LEU:C	2.33	0.48
3:C:129:VAL:HG22	3:C:130:ALA:N	2.29	0.48
3:C:69:HIS:HD2	4:D:10:LYS:HG3	1.78	0.48
3:C:92:VAL:HG12	3:C:93:PHE:N	2.29	0.48
4:H:54:THR:OG1	4:H:66:TYR:HB3	2.13	0.48
1:E:163:MET:HE1	2:F:188:VAL:HA	1.96	0.48
3:G:22:GLN:HE22	3:G:138:PHE:HB2	1.79	0.48
2:B:147:PHE:HB3	2:B:148:PRO:CD	2.40	0.47
2:F:119:PRO:HD3	2:F:206:PHE:CD2	2.49	0.47
2:F:114:ARG:NH2	2:F:215:TRP:CZ3	2.82	0.47
2:F:23:GLN:HG2	2:F:25:ASN:H	1.79	0.47
2:F:53:THR:HG23	2:F:53:THR:O	2.14	0.47
3:G:105:THR:HA	3:G:153:THR:HA	1.96	0.47
1:A:177:SER:OG	1:A:182:PHE:CD2	2.68	0.47
2:B:147:PHE:CE1	2:B:178:TYR:HA	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:PHE:O	3:C:106:LEU:HD12	2.14	0.47
4:D:100:GLU:HB3	4:D:104:VAL:HG21	1.96	0.47
2:F:209:LEU:HB3	2:F:213:ASP:OD2	2.15	0.47
2:B:194:HIS:HB2	2:B:235:ALA:HA	1.96	0.47
4:D:114:THR:CG2	4:D:114:THR:O	2.62	0.47
1:E:174:ILE:N	1:E:174:ILE:HD12	2.29	0.47
1:A:126:PRO:HB3	2:B:234:ARG:NH1	2.27	0.47
3:C:114:PHE:CZ	4:D:60:ARG:HG3	2.49	0.47
1:E:81:PRO:HG2	1:E:111:PRO:HB3	1.95	0.47
3:G:69:HIS:CD2	4:H:10:LYS:HG3	2.49	0.47
2:B:123:LEU:HD23	2:B:123:LEU:C	2.35	0.47
2:F:84:THR:O	2:F:85:SER:HB3	2.15	0.47
2:B:201:ARG:HD3	2:B:228:SER:OG	2.14	0.47
3:C:69:HIS:CD2	4:D:10:LYS:HG3	2.50	0.47
2:B:119:PRO:HG3	2:B:204:VAL:HG11	1.97	0.47
2:B:23:GLN:HG2	2:B:25:ASN:H	1.78	0.47
2:F:36:ASP:OD2	2:F:85:SER:CB	2.62	0.47
2:B:189:SER:O	2:B:190:ALA:C	2.53	0.47
3:C:176:LEU:H	3:C:176:LEU:HD23	1.79	0.47
3:C:119:ASN:HD22	3:C:167:GLU:CD	2.17	0.47
4:D:165:GLU:O	4:D:166:THR:CG2	2.62	0.47
4:D:37:PHE:HA	4:D:55:ARG:O	2.15	0.47
4:D:73:HIS:CE1	4:D:97:THR:HG21	2.50	0.47
4:H:172:THR:O	4:H:173:GLN:CB	2.50	0.47
2:B:128:LYS:HA	2:B:131:ILE:CG1	2.45	0.47
2:B:153:LEU:H	2:B:153:LEU:CD2	2.28	0.47
2:B:174:LYS:HE2	2:B:176:SER:H	1.80	0.47
1:E:15:GLY:HA2	1:E:78:ASP:OD1	2.14	0.47
2:F:123:LEU:HD21	2:F:139:LEU:HD23	1.96	0.47
2:F:34:ARG:CB	2:F:44:ILE:HD11	2.41	0.47
1:A:165:ALA:O	1:A:166:MET:C	2.52	0.46
3:C:106:LEU:HB2	3:C:154:PHE:CD1	2.50	0.46
3:G:101:GLY:H	3:G:156:PRO:HG2	1.79	0.46
4:H:100:GLU:O	4:H:104:VAL:HB	2.15	0.46
2:B:34:ARG:NH1	2:B:62:TYR:OH	2.47	0.46
3:C:119:ASN:ND2	3:C:167:GLU:OE2	2.47	0.46
1:E:120:VAL:O	1:E:120:VAL:HG12	2.15	0.46
4:H:56:TYR:CD1	4:H:56:TYR:N	2.83	0.46
1:A:15:GLY:HA2	1:A:78:ASP:OD1	2.16	0.46
3:C:77:ARG:NH2	4:D:79:LEU:O	2.46	0.46
4:D:156:VAL:HG11	4:D:186:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:153:LEU:HD11	2:F:184:SER:HB2	1.98	0.46
3:G:2:GLU:HA	4:H:45:ASN:OD1	2.15	0.46
2:F:94:ALA:CB	3:G:62:GLN:NE2	2.78	0.46
4:H:113:GLU:HA	4:H:116:THR:HG22	1.97	0.46
4:H:81:ARG:N	4:H:82:PRO:CD	2.78	0.46
1:A:38:PHE:O	1:A:40:GLY:N	2.49	0.46
3:C:165:LYS:O	3:C:165:LYS:HG3	2.15	0.46
3:C:25:PHE:CG	3:C:33:PHE:CZ	3.03	0.46
2:F:114:ARG:CZ	2:F:215:TRP:CZ3	2.98	0.46
4:H:47:THR:HG22	4:H:47:THR:O	2.15	0.46
1:A:130:ASP:O	1:A:130:ASP:OD1	2.34	0.46
2:B:153:LEU:HD21	2:B:168:THR:HG21	1.97	0.46
3:C:124:ARG:HG3	3:C:162:TYR:HE1	1.79	0.46
4:D:38:MET:CE	4:D:40:GLU:CD	2.84	0.46
1:E:125:ASP:OD1	1:E:131:SER:HA	2.15	0.46
4:H:160:ARG:HG3	4:H:190:MET:HE2	1.98	0.46
1:A:125:ASP:C	1:A:127:ARG:N	2.68	0.46
2:B:84:THR:HG23	2:B:107:LEU:O	2.15	0.46
3:G:69:HIS:NE2	4:H:10:LYS:HE3	2.30	0.46
4:H:52:TYR:H	4:H:68:SER:CB	2.28	0.46
2:B:84:THR:O	2:B:85:SER:HB3	2.16	0.46
3:C:163:ASP:HB3	3:C:176:LEU:HD12	1.98	0.46
4:D:123:GLN:NE2	4:D:123:GLN:N	2.50	0.46
2:F:114:ARG:H	2:F:114:ARG:CD	2.29	0.46
4:H:55:ARG:HG2	4:H:55:ARG:NH1	2.30	0.46
1:A:177:SER:HG	1:A:182:PHE:HD2	1.61	0.46
4:D:92:GLU:O	4:D:96:ARG:HB2	2.16	0.46
2:F:128:LYS:HD3	2:F:236:ASP:CG	2.36	0.46
3:G:143:ASP:C	3:G:143:ASP:OD2	2.53	0.46
1:A:120:VAL:O	1:A:120:VAL:HG12	2.15	0.46
2:B:113:LEU:HD11	2:B:209:LEU:HD21	1.96	0.46
2:B:84:THR:HG21	2:B:108:THR:HG23	1.97	0.46
2:B:35:GLN:NE2	2:B:88:PHE:HE2	2.13	0.46
4:D:212:THR:O	4:D:212:THR:HG22	2.16	0.46
1:E:137:THR:OG1	1:E:138:ASP:N	2.49	0.46
1:E:97:ASN:OD1	3:G:59:GLY:HA2	2.15	0.46
3:G:135:GLU:CD	3:G:148:LYS:HD3	2.36	0.46
1:A:64:PHE:CD1	1:A:75:HIS:HD2	2.34	0.45
2:B:141:CYS:HB2	2:B:155:TRP:CZ2	2.51	0.45
2:B:121:VAL:HA	2:B:142:LEU:O	2.15	0.45
4:D:111:GLY:HA3	4:D:112:PRO:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:ARG:NH1	4:D:190:MET:HE1	2.31	0.45
1:E:13:TRP:HH2	1:E:142:GLN:N	2.14	0.45
1:E:33:PRO:HD2	1:E:90:ALA:O	2.15	0.45
2:F:174:LYS:HG2	2:F:175:GLU:N	2.31	0.45
1:E:136:PHE:HB3	1:E:173:ALA:HB3	1.98	0.45
3:C:64:ILE:HD13	3:C:64:ILE:HA	1.73	0.45
4:H:12:VAL:HG12	4:H:12:VAL:O	2.16	0.45
1:A:117:GLU:HG2	1:A:117:GLU:O	2.17	0.45
3:C:33:PHE:CD1	3:C:33:PHE:C	2.90	0.45
1:E:123:LEU:HD22	1:E:123:LEU:N	2.32	0.45
1:E:3:VAL:HG12	1:E:4:ARG:N	2.32	0.45
2:F:34:ARG:NH1	2:F:62:TYR:OH	2.48	0.45
2:F:48:TYR:HE2	3:G:58:GLN:HE21	1.63	0.45
1:A:47:ILE:HD12	1:A:47:ILE:N	2.32	0.45
1:A:51:PRO:O	1:A:52:VAL:CG2	2.63	0.45
2:B:48:TYR:OH	3:C:58:GLN:HG3	2.17	0.45
3:C:88:PRO:HD3	3:C:168:HIS:HD2	1.81	0.45
1:A:37:GLN:HE22	2:B:35:GLN:HE22	1.65	0.45
3:C:118:ILE:HD11	3:C:166:VAL:CG1	2.47	0.45
4:D:189:GLU:O	4:D:190:MET:C	2.54	0.45
4:H:169:VAL:HG23	4:H:169:VAL:O	2.16	0.45
2:B:80:THR:HB	2:B:81:PRO:HD2	1.99	0.45
4:D:52:TYR:O	4:D:68:SER:N	2.49	0.45
3:G:16:SER:N	3:G:17:PRO:HD2	2.31	0.45
1:E:47:ILE:CG2	1:E:57:GLU:HB3	2.46	0.45
1:E:62:THR:OG1	1:E:75:HIS:HB2	2.17	0.45
1:E:15:GLY:HA2	1:E:78:ASP:HA	1.98	0.45
4:H:150:TYR:N	4:H:151:PRO:CD	2.79	0.45
4:H:167:VAL:HG23	4:H:168:GLY:H	1.81	0.45
3:G:30:ASP:HB3	4:H:180:TRP:NE1	2.32	0.45
1:A:64:PHE:O	1:A:72:PHE:HA	2.16	0.45
2:F:114:ARG:NH1	2:F:215:TRP:CH2	2.85	0.45
3:G:144:TYR:CE1	4:H:62:GLU:HB2	2.52	0.45
1:A:16:GLU:HG2	1:A:17:THR:N	2.32	0.44
1:A:47:ILE:CG2	1:A:57:GLU:HB3	2.47	0.44
3:C:13:VAL:HG12	3:C:14:TYR:N	2.32	0.44
4:D:113:GLU:C	4:D:115:HIS:N	2.68	0.44
1:E:93:ASP:OD2	1:E:97:ASN:N	2.48	0.44
4:H:47:THR:CG2	4:H:106:ARG:NH1	2.80	0.44
4:H:121:LEU:O	4:H:122:GLU:HG2	2.17	0.44
2:B:34:ARG:CB	2:B:44:ILE:HD11	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:ASN:HB2	3:C:167:GLU:HB3	1.98	0.44
4:D:63:TYR:CE2	4:D:64:VAL:HG23	2.53	0.44
4:H:130:LEU:HD23	4:H:140:ASN:HB2	1.99	0.44
3:C:73:VAL:HG12	3:C:77:ARG:HD3	1.99	0.44
1:E:38:PHE:O	1:E:40:GLY:N	2.50	0.44
2:F:80:THR:HB	2:F:81:PRO:HD2	1.98	0.44
4:H:73:HIS:HB2	4:H:88:ASN:ND2	2.29	0.44
3:C:93:PHE:HB2	3:C:94:PRO:HD2	1.99	0.44
3:G:15:GLN:NE2	3:G:117:VAL:CG2	2.71	0.44
3:C:3:ALA:O	3:C:4:ASP:OD2	2.36	0.44
4:D:177:ASN:HA	4:D:177:ASN:HD22	1.59	0.44
2:F:130:GLU:OE2	2:F:136:LYS:O	2.35	0.44
2:F:214:LYS:HD2	2:F:214:LYS:H	1.83	0.44
2:F:225:GLN:HE21	2:F:227:ILE:HD11	1.81	0.44
1:A:118:PRO:HB2	1:A:187:ILE:CG2	2.47	0.44
1:A:47:ILE:HD12	1:A:47:ILE:H	1.83	0.44
2:B:124:PHE:N	2:B:124:PHE:CD1	2.86	0.44
3:C:61:LEU:HD12	3:C:61:LEU:N	2.30	0.44
1:E:123:LEU:CD1	2:F:126:PRO:HA	2.47	0.44
3:G:33:PHE:C	3:G:33:PHE:CD1	2.90	0.44
3:C:91:THR:HG22	3:C:91:THR:O	2.17	0.44
1:E:154:PHE:HE2	2:F:174:LYS:O	2.00	0.44
3:G:111:ASP:OD1	3:G:112:ASN:N	2.45	0.44
3:G:168:HIS:CG	3:G:169:TRP:N	2.86	0.44
4:H:64:VAL:HG12	4:H:65:ARG:N	2.32	0.44
2:B:175:GLU:O	2:B:177:ASN:N	2.51	0.44
2:B:36:ASP:OD2	2:B:85:SER:HB2	2.18	0.44
1:E:79:SER:HB2	1:E:109:VAL:HG21	2.00	0.44
4:H:184:VAL:O	4:H:185:LEU:HD12	2.18	0.44
1:E:161:LEU:HD13	1:E:161:LEU:C	2.39	0.44
2:F:125:GLU:HA	2:F:126:PRO:HD3	1.88	0.44
3:G:37:LEU:N	3:G:37:LEU:HD12	2.33	0.44
4:H:207:LEU:H	4:H:207:LEU:HD23	1.83	0.44
1:A:6:SER:O	1:A:8:GLN:N	2.51	0.43
1:E:16:GLU:HG2	1:E:17:THR:H	1.83	0.43
1:E:64:PHE:CD1	1:E:75:HIS:HD2	2.36	0.43
2:F:175:GLU:HB3	2:F:179:SER:O	2.17	0.43
3:G:61:LEU:N	3:G:61:LEU:HD12	2.33	0.43
4:H:3:ALA:HA	4:H:108:ASN:OD1	2.17	0.43
3:C:25:PHE:CD1	3:C:33:PHE:CZ	3.06	0.43
4:D:167:VAL:HG23	4:D:168:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:124:PRO:CD	4:H:205:PRO:HG2	2.47	0.43
3:C:88:PRO:HA	3:C:112:ASN:O	2.18	0.43
3:C:165:LYS:HE3	3:C:165:LYS:HB2	1.81	0.43
3:C:46:LEU:HA	3:C:47:PRO:HD2	1.86	0.43
4:D:165:GLU:OE1	4:D:167:VAL:HG22	2.18	0.43
4:D:197:VAL:HG12	4:D:216:LYS:HA	2.00	0.43
4:H:143:VAL:HG22	4:H:187:MET:HG2	1.99	0.43
1:A:118:PRO:HB2	1:A:187:ILE:HG22	2.01	0.43
1:A:62:THR:OG1	1:A:75:HIS:HB2	2.18	0.43
2:B:53:THR:O	2:B:53:THR:HG23	2.17	0.43
3:C:105:THR:HA	3:C:153:THR:HA	2.01	0.43
2:F:166:VAL:HG12	2:F:167:SER:N	2.32	0.43
3:G:34:TYR:CG	3:G:34:TYR:O	2.71	0.43
1:A:111:PRO:HG3	1:A:160:VAL:CG2	2.49	0.43
2:B:235:ALA:O	2:B:236:ASP:OXT	2.37	0.43
4:D:150:TYR:O	4:D:150:TYR:CG	2.70	0.43
2:F:35:GLN:HE21	2:F:88:PHE:HE2	1.66	0.43
4:H:1:PHE:CE2	4:H:115:HIS:CD2	3.07	0.43
4:H:193:ARG:O	4:H:196:GLU:HG3	2.19	0.43
3:C:151:TYR:HH	4:D:178:GLY:HA3	1.83	0.43
1:E:16:GLU:HG2	1:E:17:THR:N	2.32	0.43
2:F:95:TRP:CE3	2:F:95:TRP:HA	2.53	0.43
3:G:92:VAL:HG12	3:G:93:PHE:N	2.33	0.43
1:A:34:TRP:HB2	1:A:47:ILE:HD12	2.01	0.43
1:E:58:ASP:O	1:E:60:ARG:N	2.51	0.43
2:F:114:ARG:NH1	2:F:114:ARG:HG2	2.34	0.43
2:F:153:LEU:CD2	2:F:182:LEU:HD21	2.48	0.43
2:F:206:PHE:O	2:F:224:THR:HG23	2.18	0.43
1:A:38:PHE:C	1:A:40:GLY:H	2.22	0.43
4:D:117:SER:HB2	4:D:118:LEU:H	1.68	0.43
4:D:156:VAL:CG1	4:D:186:VAL:HG21	2.49	0.43
4:D:65:ARG:CG	4:D:66:TYR:N	2.81	0.43
2:B:166:VAL:HG22	2:B:186:LEU:HD13	1.99	0.43
4:D:191:THR:O	3:G:142:ARG:HD3	2.19	0.43
4:D:5:LYS:CD	4:D:5:LYS:N	2.75	0.43
1:E:176:TRP:CE2	2:F:142:LEU:HD11	2.54	0.43
2:B:119:PRO:HD3	2:B:206:PHE:CD2	2.54	0.43
3:C:110:VAL:HG21	3:C:120:ILE:HD11	1.98	0.43
2:B:48:TYR:CZ	3:C:62:GLN:HG2	2.53	0.43
1:E:64:PHE:O	1:E:72:PHE:HA	2.19	0.43
2:F:194:HIS:HA	2:F:234:ARG:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:114:THR:HG22	4:H:114:THR:O	2.17	0.43
3:G:144:TYR:OH	4:H:55:ARG:HD3	2.19	0.43
4:D:118:LEU:H	4:D:118:LEU:HD12	1.82	0.42
2:F:174:LYS:HG2	2:F:175:GLU:H	1.84	0.42
3:G:91:THR:HB	3:G:109:PHE:HB3	2.01	0.42
2:B:147:PHE:HE1	2:B:178:TYR:HA	1.84	0.42
4:D:189:GLU:HA	4:D:189:GLU:OE1	2.19	0.42
1:E:60:ARG:CG	1:E:60:ARG:NH1	2.82	0.42
2:F:193:TRP:CD1	2:F:194:HIS:N	2.88	0.42
1:A:132:THR:HG22	1:A:182:PHE:CD1	2.54	0.42
1:A:34:TRP:CZ3	1:A:89:CYS:HB3	2.54	0.42
3:C:15:GLN:NE2	3:C:116:PRO:HG2	2.34	0.42
3:C:177:LYS:HD2	3:C:177:LYS:HA	1.76	0.42
4:D:73:HIS:HE1	4:D:97:THR:HG21	1.84	0.42
4:D:81:ARG:HB3	4:D:81:ARG:CZ	2.48	0.42
1:A:58:ASP:O	1:A:60:ARG:N	2.51	0.42
3:C:15:GLN:HE22	3:C:115:PRO:HB2	1.79	0.42
4:D:144:CYS:O	4:D:144:CYS:SG	2.77	0.42
4:D:45:ASN:HB2	4:D:48:GLN:CB	2.49	0.42
2:F:209:LEU:H	2:F:209:LEU:HG	1.66	0.42
2:F:223:VAL:O	2:F:224:THR:C	2.56	0.42
3:C:15:GLN:HA	4:D:33:PHE:O	2.19	0.42
1:E:14:GLU:C	1:E:16:GLU:H	2.23	0.42
2:B:225:GLN:NE2	2:B:227:ILE:HD11	2.32	0.42
3:G:61:LEU:H	3:G:61:LEU:CD1	2.33	0.42
3:G:99:LEU:HB2	3:G:102:GLN:HB3	2.01	0.42
1:A:111:PRO:HG3	1:A:160:VAL:HG21	2.00	0.42
1:A:53:SER:O	1:A:54:ASN:CB	2.67	0.42
2:B:35:GLN:HE21	2:B:88:PHE:HE2	1.68	0.42
3:C:16:SER:HB3	3:C:71:LEU:HD12	2.02	0.42
1:E:161:LEU:HD13	1:E:162:ASP:N	2.34	0.42
2:F:153:LEU:HD23	2:F:153:LEU:H	1.85	0.42
2:F:36:ASP:OD2	2:F:85:SER:HB3	2.20	0.42
3:G:49:PHE:CD2	4:H:116:THR:OG1	2.72	0.42
2:B:206:PHE:C	2:B:206:PHE:CD1	2.93	0.42
3:C:113:ILE:O	3:C:114:PHE:HB2	2.20	0.42
3:C:22:GLN:HE21	3:C:24:THR:CG2	2.32	0.42
1:A:97:ASN:OD1	3:C:59:GLY:HA2	2.19	0.42
1:E:138:ASP:HA	1:E:170:SER:HB2	2.01	0.42
4:H:31:ARG:O	4:H:31:ARG:HG3	2.20	0.42
4:H:40:GLU:OE2	4:H:55:ARG:NE	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:GLU:O	2:B:231:ALA:HB2	2.20	0.42
2:B:80:THR:OG1	2:B:83:GLN:HG3	2.20	0.42
4:D:48:GLN:HE21	4:D:48:GLN:HA	1.84	0.42
3:C:66:VAL:HG11	4:D:8:ALA:O	2.19	0.42
1:E:132:THR:HB	1:E:182:PHE:CE2	2.55	0.42
2:F:7:ARG:HH11	2:F:7:ARG:HB3	1.84	0.42
4:D:165:GLU:C	4:D:166:THR:HG23	2.40	0.42
1:E:37:GLN:HE22	2:F:35:GLN:HE22	1.68	0.42
1:A:161:LEU:HB2	2:B:185:ARG:NH1	2.33	0.41
1:A:41:GLU:HB2	1:A:42:SER:H	1.48	0.41
3:C:111:ASP:OD1	3:C:112:ASN:N	2.46	0.41
4:D:151:PRO:HG3	4:D:205:PRO:C	2.38	0.41
4:D:43:PHE:CE2	4:D:109:TYR:HB2	2.55	0.41
4:D:72:GLU:HG2	4:D:73:HIS:N	2.34	0.41
1:E:137:THR:O	1:E:138:ASP:HB2	2.19	0.41
1:E:19:ILE:HG22	1:E:75:HIS:CE1	2.54	0.41
3:G:168:HIS:CG	3:G:169:TRP:H	2.38	0.41
3:G:25:PHE:CG	3:G:33:PHE:CZ	3.07	0.41
3:G:95:LYS:HZ3	4:H:148:ASP:CG	2.23	0.41
3:C:142:ARG:O	4:H:193:ARG:HD3	2.20	0.41
4:D:193:ARG:O	4:D:194:ARG:C	2.58	0.41
1:E:180:THR:HB	1:E:181:SER:H	1.47	0.41
1:E:47:ILE:N	1:E:47:ILE:HD12	2.34	0.41
2:F:84:THR:HG21	2:F:108:THR:HG23	2.02	0.41
1:A:113:ILE:HB	1:A:140:ASP:CG	2.41	0.41
1:A:3:VAL:HG12	1:A:4:ARG:N	2.34	0.41
2:B:62:TYR:N	2:B:62:TYR:CD1	2.88	0.41
1:E:24:TYR:CE2	1:E:32:PHE:CE2	3.09	0.41
2:F:116:VAL:HG13	2:F:148:PRO:HD2	2.01	0.41
4:H:126:VAL:CG2	4:H:202:VAL:HG21	2.51	0.41
4:H:189:GLU:O	4:H:190:MET:C	2.58	0.41
2:B:33:TYR:CZ	2:B:43:LEU:HD13	2.55	0.41
2:B:44:ILE:HG22	2:B:45:HIS:ND1	2.36	0.41
3:C:96:SER:HB3	3:C:97:PRO:HD2	2.01	0.41
4:D:169:VAL:O	4:H:173:GLN:HA	2.21	0.41
4:D:63:TYR:H	4:D:63:TYR:HD1	1.68	0.41
3:G:15:GLN:NE2	3:G:115:PRO:HB2	2.35	0.41
2:B:84:THR:CG2	2:B:108:THR:HA	2.46	0.41
4:D:157:ARG:HD2	4:D:164:GLU:OE1	2.20	0.41
1:E:161:LEU:HD23	2:F:167:SER:HB2	2.01	0.41
4:H:128:ILE:HG22	4:H:129:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:63:ASN:O	3:G:67:VAL:CG2	2.68	0.41
4:H:193:ARG:O	4:H:194:ARG:C	2.59	0.41
1:A:16:GLU:HG2	1:A:17:THR:H	1.85	0.41
4:D:108:ASN:O	4:D:109:TYR:C	2.58	0.41
1:E:42:SER:HB3	2:F:102:GLY:O	2.19	0.41
2:F:62:TYR:CD1	2:F:62:TYR:N	2.89	0.41
3:G:123:LEU:HB2	3:G:163:ASP:HB2	2.02	0.41
4:H:207:LEU:N	4:H:207:LEU:HD23	2.35	0.41
2:B:95:TRP:HA	2:B:95:TRP:CE3	2.56	0.41
1:E:34:TRP:CZ3	1:E:89:CYS:HB3	2.56	0.41
2:F:215:TRP:HA	2:F:215:TRP:CE3	2.55	0.41
2:F:84:THR:HG23	2:F:107:LEU:O	2.21	0.41
4:H:97:THR:HA	4:H:100:GLU:HG3	2.03	0.41
2:B:128:LYS:HA	2:B:131:ILE:CD1	2.50	0.41
2:B:36:ASP:OD2	2:B:85:SER:HB3	2.20	0.41
1:E:60:ARG:HD2	1:E:77:ALA:O	2.20	0.41
2:F:95:TRP:CH2	3:G:62:GLN:CB	3.03	0.41
1:A:79:SER:HB2	1:A:109:VAL:HG21	2.03	0.41
1:A:112:ASN:CG	1:A:112:ASN:O	2.60	0.41
2:F:128:LYS:HB2	2:F:128:LYS:HE3	1.93	0.41
2:F:128:LYS:O	2:F:131:ILE:HG13	2.21	0.41
4:H:160:ARG:HG3	4:H:190:MET:CE	2.50	0.41
4:H:70:VAL:HG12	4:H:70:VAL:O	2.21	0.41
1:E:123:LEU:HB3	2:F:124:PHE:HB3	2.02	0.41
1:E:123:LEU:HD23	1:E:133:LEU:O	2.21	0.41
3:G:135:GLU:OE2	3:G:148:LYS:HD3	2.21	0.41
3:G:140:VAL:HG12	4:H:36:GLN:OE1	2.21	0.41
3:G:69:HIS:O	3:G:73:VAL:HG23	2.20	0.41
3:C:2:GLU:HB3	3:C:3:ALA:H	1.69	0.40
3:G:74:LEU:HD11	4:H:63:TYR:CE2	2.56	0.40
4:H:123:GLN:H	4:H:123:GLN:HE21	1.69	0.40
4:H:209:SER:O	4:H:210:PRO:C	2.60	0.40
1:E:28:THR:CG2	4:H:2:GLU:CD	2.90	0.40
4:H:96:ARG:HH11	4:H:96:ARG:CG	2.27	0.40
1:E:38:PHE:C	1:E:40:GLY:H	2.25	0.40
1:E:51:PRO:O	1:E:52:VAL:CG2	2.65	0.40
4:H:1:PHE:CE2	4:H:115:HIS:NE2	2.90	0.40
4:H:179:ASP:OD2	4:H:179:ASP:N	2.53	0.40
4:H:192:PRO:HA	4:H:198:TYR:OH	2.21	0.40
1:A:33:PRO:HD2	1:A:90:ALA:O	2.20	0.40
4:D:59:ASN:HB3	4:D:60:ARG:H	1.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ILE:HG22	1:E:100:PHE:N	2.35	0.40
1:E:41:GLU:HB2	1:E:42:SER:H	1.49	0.40
1:E:6:SER:O	1:E:8:GLN:N	2.54	0.40
2:B:12:VAL:HG22	2:B:13:THR:N	2.36	0.40
2:B:148:PRO:C	2:B:150:HIS:N	2.74	0.40
2:B:119:PRO:HG3	2:B:204:VAL:CG1	2.52	0.40
3:C:172:GLU:H	3:C:172:GLU:CD	2.25	0.40
3:C:37:LEU:N	3:C:37:LEU:CD1	2.84	0.40
4:D:160:ARG:HH11	4:D:190:MET:CE	2.34	0.40
1:E:129:GLN:HB2	1:E:129:GLN:HE21	1.68	0.40
4:H:150:TYR:N	4:H:151:PRO:HD3	2.36	0.40
4:D:199:THR:HG23	4:D:214:GLU:CG	2.41	0.40
4:H:122:GLU:HB3	4:H:149:PHE:HA	2.03	0.40
3:C:5:HIS:O	4:H:163:GLN:NE2	2.55	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	183/185 (99%)	135 (74%)	29 (16%)	19 (10%)	0	5
1	E	182/185 (98%)	135 (74%)	30 (16%)	17 (9%)	1	7
2	B	223/236 (94%)	177 (79%)	31 (14%)	15 (7%)	1	13
2	F	234/236 (99%)	189 (81%)	27 (12%)	18 (8%)	1	10
3	C	180/182 (99%)	154 (86%)	19 (11%)	7 (4%)	3	26
3	G	180/182 (99%)	149 (83%)	24 (13%)	7 (4%)	3	26
4	D	186/217 (86%)	151 (81%)	20 (11%)	15 (8%)	1	9
4	H	186/217 (86%)	150 (81%)	25 (13%)	11 (6%)	2	16
All	All	1554/1640 (95%)	1240 (80%)	205 (13%)	109 (7%)	1	12

All (109) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	53	SER
1	A	57	GLU
1	A	60	ARG
1	A	128	SER
1	A	180	THR
1	A	181	SER
2	B	126	PRO
2	B	149	ASP
2	B	174	LYS
3	C	3	ALA
3	C	5	HIS
4	D	114	THR
4	D	117	SER
1	E	52	VAL
1	E	53	SER
1	E	57	GLU
1	E	60	ARG
1	E	128	SER
2	F	115	ASP
2	F	209	LEU
3	G	3	ALA
3	G	5	HIS
4	H	190	MET
4	H	206	SER
1	A	59	GLY
1	A	130	ASP
1	A	185	GLN
2	B	5	SER
2	B	96	GLY
2	B	115	ASP
2	B	175	GLU
2	B	179	SER
2	B	209	LEU
3	C	100	LEU
4	D	118	LEU
4	D	154	ILE
4	D	190	MET
4	D	204	HIS
4	D	206	SER
4	D	210	PRO
1	E	14	GLU

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Mol	Chain	Res	Type
1	E	59	GLY
1	E	130	ASP
1	E	180	THR
1	E	181	SER
2	F	5	SER
2	F	85	SER
2	F	96	GLY
2	F	126	PRO
2	F	149	ASP
2	F	211	GLU
2	F	212	GLU
2	F	214	LYS
4	H	105	CYS
4	H	152	ALA
4	H	154	ILE
4	H	210	PRO
1	A	14	GLU
1	A	166	MET
1	A	169	LYS
2	B	85	SER
2	B	176	SER
2	B	224	THR
3	C	2	GLU
3	C	80	SER
4	D	109	TYR
1	E	15	GLY
1	E	132	THR
2	F	176	SER
2	F	216	PRO
3	G	80	SER
3	G	126	SER
4	H	194	ARG
1	A	7	PRO
1	A	133	LEU
2	B	191	THR
2	B	231	ALA
3	C	126	SER
4	D	151	PRO
4	D	173	GLN
1	E	7	PRO
2	F	53	THR
2	F	179	SER

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Mol	Chain	Res	Type
2	F	217	GLU
2	F	233	GLY
4	H	151	PRO
4	H	173	GLN
1	A	15	GLY
1	A	54	ASN
2	B	53	THR
4	D	48	GLN
1	E	54	ASN
1	E	127	ARG
2	F	175	GLU
3	G	10	GLY
3	G	17	PRO
4	H	150	TYR
4	H	204	HIS
1	A	51	PRO
3	C	142	ARG
1	E	51	PRO
1	A	39	PRO
4	D	150	TYR
1	E	39	PRO
3	G	97	PRO
4	D	82	PRO
4	D	205	PRO
2	F	219	SER

### 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	166/166 (100%)	155 (93%)	11 (7%)	18	54
1	E	165/166 (99%)	154 (93%)	11 (7%)	18	53
2	B	194/202 (96%)	179 (92%)	15 (8%)	14	46
2	F	202/202 (100%)	188 (93%)	14 (7%)	17	52
3	C	163/163 (100%)	155 (95%)	8 (5%)	27	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	163/163 (100%)	154 (94%)	9 (6%)	24	59
4	D	174/189 (92%)	161 (92%)	13 (8%)	15	47
4	H	174/189 (92%)	158 (91%)	16 (9%)	10	37
All	All	1401/1440 (97%)	1304 (93%)	97 (7%)	17	52

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	33	PRO
1	A	41	GLU
1	A	47	ILE
1	A	56	LYS
1	A	60	ARG
1	A	129	GLN
1	A	133	LEU
1	A	159	THR
1	A	163	MET
1	A	187	ILE
2	B	2	VAL
2	B	31	TYR
2	B	34	ARG
2	B	91	SER
2	B	112	ASP
2	B	114	ARG
2	B	147	PHE
2	B	149	ASP
2	B	173	TYR
2	B	174	LYS
2	B	176	SER
2	B	188	VAL
2	B	194	HIS
2	B	223	VAL
2	B	226	ASP
3	C	19	ASP
3	C	24	THR
3	C	25	PHE
3	C	99	LEU
3	C	151	TYR
3	C	167	GLU
3	C	172	GLU

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Mol	Chain	Res	Type
3	C	176	LEU
4	D	5	LYS
4	D	48	GLN
4	D	96	ARG
4	D	120	ARG
4	D	123	GLN
4	D	130	LEU
4	D	160	ARG
4	D	169	VAL
4	D	174	LEU
4	D	187	MET
4	D	199	THR
4	D	205	PRO
4	D	210	PRO
1	E	1	GLN
1	E	33	PRO
1	E	41	GLU
1	E	47	ILE
1	E	56	LYS
1	E	60	ARG
1	E	129	GLN
1	E	133	LEU
1	E	141	SER
1	E	149	MET
1	E	180	THR
2	F	2	VAL
2	F	31	TYR
2	F	34	ARG
2	F	91	SER
2	F	112	ASP
2	F	114	ARG
2	F	115	ASP
2	F	142	LEU
2	F	194	HIS
2	F	213	ASP
2	F	214	LYS
2	F	215	TRP
2	F	226	ASP
2	F	234	ARG
3	G	4	ASP
3	G	19	ASP
3	G	48	GLU

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Mol	Chain	Res	Type
3	G	62	GLN
3	G	100	LEU
3	G	131	ASP
3	G	152	LEU
3	G	172	GLU
3	G	175	VAL
4	H	5	LYS
4	H	44	THR
4	H	48	GLN
4	H	56	TYR
4	H	61	GLU
4	H	96	ARG
4	H	102	ASP
4	H	123	GLN
4	H	155	LYS
4	H	160	ARG
4	H	167	VAL
4	H	187	MET
4	H	199	THR
4	H	205	PRO
4	H	206	SER
4	H	210	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	75	HIS
1	A	115	ASN
1	A	129	GLN
1	A	142	GLN
1	A	171	ASN
2	B	4	GLN
2	B	22	ASN
2	B	23	GLN
2	B	26	ASN
2	B	29	ASN
2	B	35	GLN
2	B	69	GLN
2	B	99	GLN
2	B	133	ASN
2	B	203	GLN

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Mol	Chain	Res	Type
2	B	225	GLN
3	C	15	GLN
3	C	58	GLN
3	C	62	GLN
3	C	69	HIS
3	C	112	ASN
3	C	119	ASN
4	D	48	GLN
4	D	107	HIS
4	D	123	GLN
4	D	177	ASN
1	E	8	GLN
1	E	75	HIS
1	E	129	GLN
1	E	171	ASN
2	F	4	GLN
2	F	22	ASN
2	F	23	GLN
2	F	26	ASN
2	F	29	ASN
2	F	35	GLN
2	F	69	GLN
2	F	99	GLN
2	F	133	ASN
2	F	135	GLN
2	F	203	GLN
2	F	225	GLN
3	G	15	GLN
3	G	58	GLN
3	G	62	GLN
3	G	63	ASN
3	G	85	ASN
3	G	141	ASN
4	H	9	ASN
4	H	48	GLN
4	H	115	HIS
4	H	123	GLN
4	H	173	GLN
4	H	177	ASN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	185/185 (100%)	0.62	21 (11%) 5 6	44, 96, 176, 198	0
1	E	184/185 (99%)	0.76	24 (13%) 3 4	61, 124, 174, 194	0
2	B	227/236 (96%)	0.36	12 (5%) 26 26	50, 98, 156, 186	0
2	F	236/236 (100%)	0.22	6 (2%) 57 55	52, 98, 152, 173	0
3	C	182/182 (100%)	0.15	4 (2%) 62 59	38, 73, 136, 182	0
3	G	182/182 (100%)	0.26	6 (3%) 46 44	44, 78, 142, 178	0
4	D	192/217 (88%)	-0.00	1 (0%) 90 89	43, 77, 122, 153	0
4	H	192/217 (88%)	0.13	9 (4%) 31 31	45, 85, 127, 168	0
All	All	1580/1640 (96%)	0.31	83 (5%) 26 26	38, 91, 160, 198	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	SER	10.2
1	A	182	PHE	7.4
3	G	159	ASP	6.2
2	B	222	PRO	5.8
1	E	166	MET	5.2
1	A	176	TRP	5.1
2	F	176	SER	5.1
2	B	113	LEU	4.6
2	B	208	GLY	4.6
1	A	151	SER	4.5
3	G	82	PRO	4.5
1	A	122	GLN	4.3
1	E	128	SER	4.1
1	E	18	ALA	4.1
1	E	65	PHE	3.8
2	B	116	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
3	C	1	ILE	3.6
1	A	124	LYS	3.6
1	A	6	SER	3.6
3	G	160	ASP	3.6
1	A	181	SER	3.5
1	E	17	THR	3.5
1	E	186	ASP	3.5
1	A	173	ALA	3.5
1	E	144	ASN	3.3
4	H	46	GLY	3.3
1	A	174	ILE	3.3
2	B	236	ASP	3.3
1	E	151	SER	3.3
4	H	140	ASN	3.2
1	E	148	THR	3.2
1	E	129	GLN	3.2
1	E	155	ILE	3.2
1	E	171	ASN	3.2
1	E	145	VAL	3.1
2	B	10	VAL	3.1
3	G	83	ALA	3.1
4	H	33	PHE	3.0
1	E	143	ILE	3.0
2	F	169	ASP	3.0
2	B	221	LYS	2.9
1	E	181	SER	2.9
1	E	180	THR	2.9
2	F	128	LYS	2.9
1	A	183	THR	2.9
1	A	184	CYS	2.8
1	A	133	LEU	2.7
2	F	182	LEU	2.7
1	E	11	THR	2.7
1	E	174	ILE	2.7
1	E	165	ALA	2.7
2	F	1	ALA	2.7
1	A	15	GLY	2.6
1	E	158	LYS	2.6
1	E	64	PHE	2.6
2	B	207	HIS	2.5
1	E	111	PRO	2.5
1	A	186	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	142	GLN	2.5
3	G	1	ILE	2.3
2	B	209	LEU	2.3
3	G	74	LEU	2.3
3	C	80	SER	2.3
4	H	45	ASN	2.3
4	H	32	HIS	2.2
1	A	135	LEU	2.2
2	F	78	LEU	2.2
2	B	96	GLY	2.2
1	E	10	LEU	2.2
1	A	178	ASN	2.2
3	C	81	THR	2.2
4	H	95	GLU	2.2
4	D	159	PHE	2.2
4	H	58	TYR	2.2
1	A	134	CYS	2.1
4	H	47	THR	2.1
4	H	106	ARG	2.1
2	B	11	ALA	2.1
1	A	154	PHE	2.1
1	A	35	TYR	2.1
3	C	159	ASP	2.1
2	B	77	GLU	2.0
1	A	131	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	CA	E	190	1/1	0.92	0.22	85,85,85,85	0
5	CA	A	189	1/1	0.95	0.29	45,45,45,45	0
5	CA	E	189	1/1	0.97	0.15	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.