



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:58 AM GMT

PDB ID : 1D9K  
Title : CRYSTAL STRUCTURE OF COMPLEX BETWEEN D10 TCR AND PMHC I-AK/CA  
Authors : Reinherz, E.L.; Tan, K.; Tang, L.; Kern, P.; Liu, J.-H.; Xiong, Y.; Hussey, R.E.; Smolyar, A.; Hare, B.; Zhang, R.; Joachimiak, A.; Chang, H.-C.; Wagner, G.; Wang, J-H.  
Deposited on : 1999-10-28  
Resolution : 3.20 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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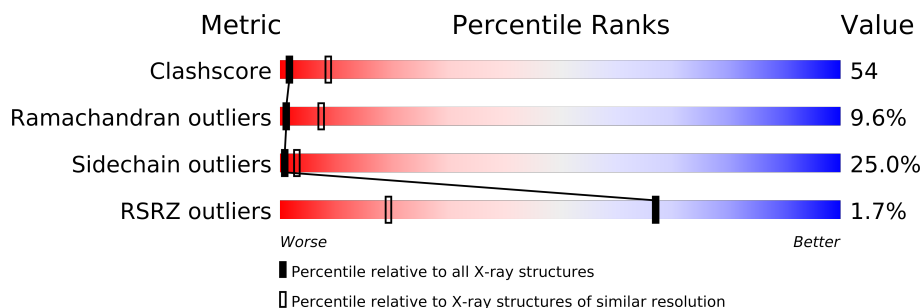
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 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	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	110	
1	E	110	
2	B	112	
2	F	112	
3	C	183	
3	G	183	
4	D	188	
4	H	188	
5	P	16	
5	Q	16	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9962 atoms, of which 0 are hydrogen and 0 are deuterium.

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 T-CELL RECEPTOR D10 (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	0	0
			877	563	145	167	2			
1	E	110	Total	C	N	O	S	0	0	0
			877	563	145	167	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	SER	CYS	ENGINEERED	GB 5724764
E	115	SER	CYS	ENGINEERED	GB 5724764

- Molecule 2 is a protein called T-CELL RECEPTOR D10 (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	112	Total	C	N	O	S	0	0	0
			854	528	155	168	3			
2	F	112	Total	C	N	O	S	0	0	0
			854	528	155	168	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	116B	GLY	GLU	SEE REMARK 999	GB 1791255
B	116C	SER	ASP	SEE REMARK 999	GB 1791255
F	116B	GLY	GLU	SEE REMARK 999	GB 1791255
F	116C	SER	ASP	SEE REMARK 999	GB 1791255

- Molecule 3 is a protein called MHC I-AK A CHAIN (ALPHA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	183	Total	C	N	O	S	0	0	0
			1485	959	237	286	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	183	Total	C	N	O	S	0	0	0
			1485	959	237	286	3			

- Molecule 4 is a protein called MHC I-AK B CHAIN (BETA CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	188	Total	C	N	O	S	0	0	0
			1575	991	287	291	6			
4	H	188	Total	C	N	O	S	0	0	0
			1575	991	287	291	6			

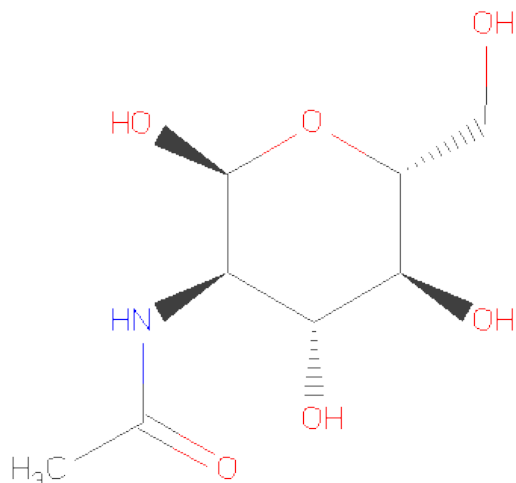
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	GLY	ASN	CONFLICT	UNP P06343
H	2	GLY	ASN	CONFLICT	UNP P06343

- Molecule 5 is a protein called CONALBUMIN PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	16	Total	C	N	O	0	0	0
			120	71	23	26			
5	Q	16	Total	C	N	O	0	0	0
			120	71	23	26			

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is a polymer of unknown type called SUGAR (NAG-NAG).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	2	Total	C	N	O	0	0
			28	16	2	10		
7	D	2	Total	C	N	O	0	0
			28	16	2	10		
7	G	2	Total	C	N	O	0	0
			28	16	2	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	GLY	ASN	CONFLICT	UNP P06343

- Molecule 8 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	2	Total	C	N	O	0	0
			28	16	2	10		

There is a discrepancy between the modelled and reference sequences:

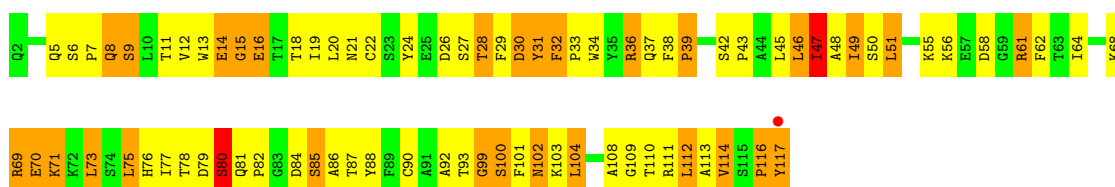
Chain	Residue	Modelled	Actual	Comment	Reference
H	2	GLY	ASN	CONFLICT	UNP P06343

### 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 errors 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.

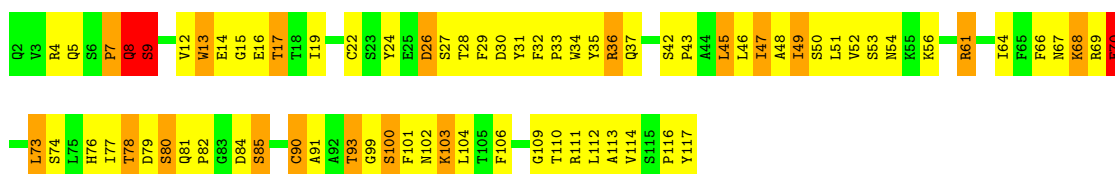
- Molecule 1: T-CELL RECEPTOR D10 (ALPHA CHAIN)

Chain A:



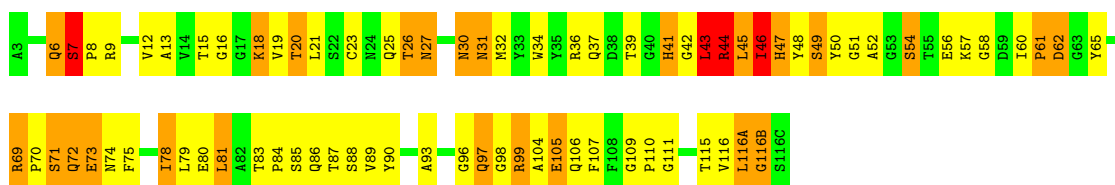
- Molecule 1: T-CELL RECEPTOR D10 (ALPHA CHAIN)

Chain E:



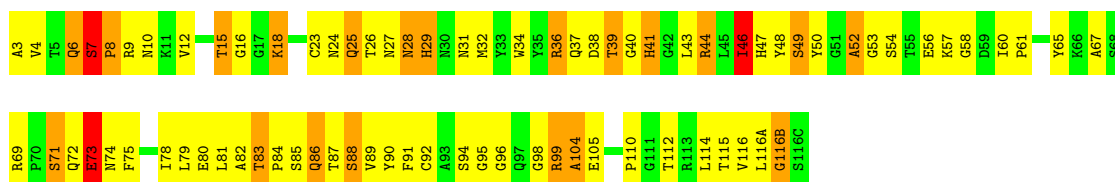
- Molecule 2: T-CELL RECEPTOR D10 (BETA CHAIN)

Chain B:



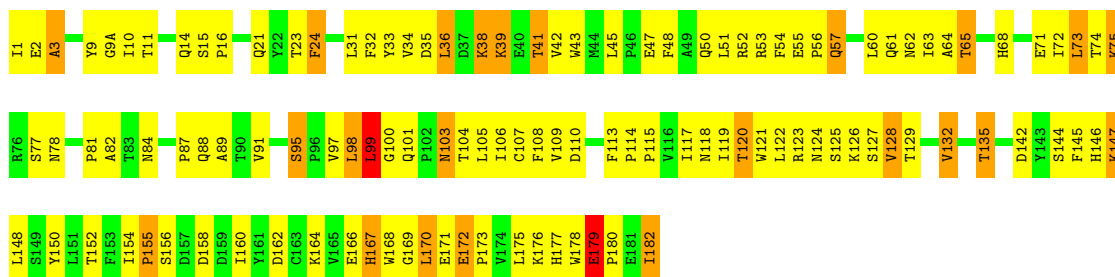
- Molecule 2: T-CELL RECEPTOR D10 (BETA CHAIN)

Chain F:



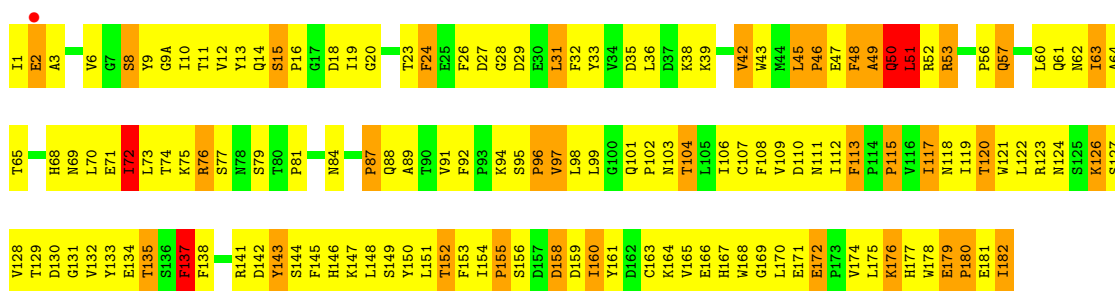
- Molecule 3: MHC I-AK A CHAIN (ALPHA CHAIN)

## Chain C:



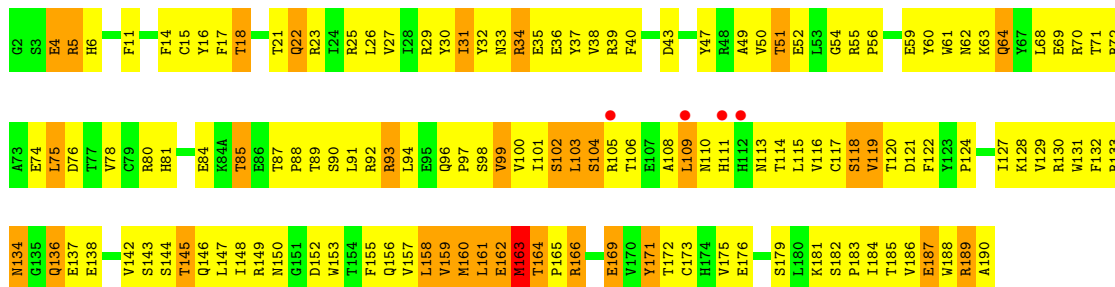
- Molecule 3: MHC I-AK A CHAIN (ALPHA CHAIN)

## Chain G:



- Molecule 4: MHC I-AK B CHAIN (BETA CHAIN)

## Chain D:





● Molecule 5: CONALBUMIN PEPTIDE



● Molecule 5: CONALBUMIN PEPTIDE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.60Å 345.30Å 97.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.02 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (15.00-3.20) 91.5 (15.02-3.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 3.19Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.247 , 0.293 0.243 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	61.1	Xtriage
Anisotropy	0.840	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.8	EDS
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 50029 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.61	0/901	0.88	3/1220 (0.2%)
1	E	0.57	0/901	0.88	3/1220 (0.2%)
2	B	0.54	0/873	0.92	5/1181 (0.4%)
2	F	0.44	1/873 (0.1%)	0.80	2/1181 (0.2%)
3	C	0.29	0/1530	0.56	0/2087
3	G	0.31	0/1530	0.56	0/2087
4	D	0.30	0/1615	0.58	0/2191
4	H	0.33	0/1615	0.56	0/2191
5	P	0.40	0/122	0.66	0/161
5	Q	0.37	0/122	0.88	0/161
All	All	0.41	1/10082 (0.0%)	0.69	13/13680 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	53	GLY	CA-C	5.04	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	52	ALA	O-C-N	-8.58	108.62	123.20
2	B	43	LEU	O-C-N	-7.59	110.56	122.70
2	B	47	HIS	CB-CA-C	-7.36	95.67	110.40
2	B	44	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	A	70	GLU	N-CA-C	-6.87	92.45	111.00
1	E	111	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	A	47	ILE	O-C-N	6.37	132.90	122.70
1	E	70	GLU	CB-CA-C	6.06	122.51	110.40
1	E	69	ARG	NE-CZ-NH2	5.91	123.25	120.30
2	B	46	ILE	CB-CA-C	-5.89	99.83	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	43	LEU	CA-CB-CG	-5.47	102.71	115.30
1	A	16	GLU	N-CA-CB	-5.21	101.22	110.60
2	F	29	HIS	N-CA-C	-5.17	97.05	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	877	0	848	95	0
1	E	877	0	848	99	0
2	B	854	0	813	101	0
2	F	854	0	813	93	0
3	C	1485	0	1413	120	0
3	G	1485	0	1413	206	0
4	D	1575	0	1518	151	0
4	H	1575	0	1517	259	0
5	P	120	0	102	15	0
5	Q	120	0	102	38	0
6	C	14	0	13	0	0
6	G	14	0	13	0	0
7	C	28	0	25	3	0
7	D	28	0	25	0	0
7	G	28	0	25	0	0
8	H	28	0	25	4	0
All	All	9962	0	9513	1043	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 54.

All (1043) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:67:ASN:OD1	1:E:70:GLU:HB2	1.25	1.36

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:7:PRO:HB2	1:A:110:THR:HG21	1.20	1.17
3:C:179:GLU:H	3:C:180:PRO:CD	1.59	1.16
1:E:102:ASN:HA	2:F:104:ALA:HA	1.24	1.15
1:E:26:ASP:HB3	1:E:29:PHE:CD1	1.84	1.13
3:C:179:GLU:H	3:C:180:PRO:HD2	0.92	1.07
4:H:56:PRO:HB2	5:Q:143:ILE:HG21	1.36	1.06
3:G:118:ASN:HB2	3:G:166:GLU:HB2	1.30	1.06
1:A:47:ILE:HD11	1:A:58:ASP:HB3	1.36	1.04
2:F:69:ARG:HH11	2:F:72:GLN:HA	1.21	1.03
3:G:81:PRO:HB3	4:H:5:ARG:HG2	1.36	1.03
2:B:7:SER:HB3	2:B:8:PRO:HD3	1.39	1.03
2:F:7:SER:HB3	2:F:8:PRO:HD3	1.38	1.03
2:F:87:THR:HG23	2:F:115:THR:HA	1.37	1.01
4:D:34:ARG:HH11	4:D:34:ARG:HG2	1.20	1.01
4:H:134:ASN:HA	4:H:170:VAL:HB	1.38	1.00
3:C:179:GLU:N	3:C:180:PRO:HD2	1.75	0.99
4:H:176:GLU:HG3	4:H:183:PRO:HG3	1.42	0.99
2:F:69:ARG:NH1	2:F:72:GLN:HA	1.79	0.97
1:A:85:SER:HB3	1:A:113:ALA:HA	1.45	0.96
1:A:13:TRP:O	1:A:15:GLY:N	1.97	0.96
4:H:174:HIS:HA	4:H:185:THR:HG22	1.48	0.95
4:D:108:ALA:HB1	4:D:111:HIS:HB2	1.43	0.95
4:H:113:ASN:HB2	4:H:165:PRO:HD3	1.49	0.94
1:A:45:LEU:HD12	1:A:46:LEU:H	1.30	0.94
4:H:108:ALA:HB1	4:H:111:HIS:HB2	1.49	0.94
4:H:33:ASN:O	4:H:34:ARG:HG2	1.65	0.93
2:F:6:GLN:HG3	2:F:110:PRO:HD2	1.48	0.93
1:A:30:ASP:HA	1:A:51:LEU:HD21	1.50	0.93
1:E:26:ASP:CB	1:E:29:PHE:CE1	2.53	0.91
3:G:119:ILE:HG12	3:G:165:VAL:HG22	1.49	0.91
2:F:15:THR:OG1	2:F:116(B):GLY:HA3	1.70	0.90
3:G:181:GLU:HG3	3:G:182:ILE:H	1.36	0.90
3:C:103:ASN:HD22	3:C:104:THR:H	1.17	0.90
4:H:172:THR:HG23	4:H:187:GLU:HG3	1.53	0.89
2:B:32:MET:HG3	2:B:69:ARG:HH21	1.38	0.89
1:E:26:ASP:HB3	1:E:29:PHE:HD1	1.36	0.89
3:C:160:ILE:HA	3:C:179:GLU:HB3	1.55	0.88
3:C:180:PRO:HB2	3:C:182:ILE:HG13	1.55	0.88
3:C:118:ASN:HB2	3:C:166:GLU:HB3	1.54	0.88
4:D:99:VAL:HG13	4:D:119:VAL:HG13	1.55	0.88
3:G:120:THR:HG23	3:G:164:LYS:HB3	1.54	0.87
4:D:128:LYS:HE2	4:D:130:ARG:HD2	1.54	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:87:THR:HA	4:D:91:LEU:HD12	1.56	0.86
4:H:104:SER:HB2	4:H:114:THR:HB	1.57	0.86
1:A:7:PRO:HB2	1:A:110:THR:CG2	2.05	0.86
3:G:144:SER:HB3	4:H:34:ARG:HH12	1.40	0.86
4:H:134:ASN:CA	4:H:170:VAL:HB	2.06	0.86
2:B:6:GLN:HG3	2:B:110:PRO:HD2	1.57	0.86
2:F:65:TYR:CE2	2:F:79:LEU:HD21	2.11	0.85
4:D:34:ARG:NH1	4:D:34:ARG:HG2	1.87	0.85
4:D:116:VAL:HG22	4:D:160:MET:HG2	1.59	0.85
3:G:1:ILE:HG22	3:G:2:GLU:H	1.42	0.85
4:H:76:ASP:HA	4:H:80:ARG:HB3	1.59	0.85
4:H:37:TYR:HA	4:H:51:THR:HG23	1.57	0.85
1:A:47:ILE:HD12	1:A:62:PHE:CB	2.06	0.84
1:E:8:GLN:O	1:E:8:GLN:HG3	1.78	0.84
1:E:5:GLN:HE22	1:E:90:CYS:H	1.25	0.83
3:G:45:LEU:O	3:G:48:PHE:HB2	1.78	0.83
3:C:171:GLU:CD	3:C:171:GLU:H	1.80	0.83
1:E:102:ASN:HA	2:F:104:ALA:CA	2.08	0.83
1:E:67:ASN:O	1:E:68:LYS:O	1.97	0.83
2:B:44:ARG:HG2	2:B:60:ILE:HD11	1.59	0.83
1:A:30:ASP:HA	1:A:51:LEU:CD2	2.09	0.82
1:E:26:ASP:HB3	1:E:29:PHE:CE1	2.13	0.82
3:C:53:ARG:O	5:P:134:HIS:HB2	1.80	0.82
2:F:36:ARG:HH21	2:F:86:GLN:HA	1.43	0.81
2:B:87:THR:HG23	2:B:115:THR:HA	1.63	0.81
5:Q:143:ILE:HD12	5:Q:144:GLU:H	1.46	0.81
1:A:16:GLU:O	1:A:80:SER:OG	1.99	0.81
2:F:31:ASN:HB3	2:F:50:TYR:HA	1.63	0.81
1:A:61:ARG:HB3	1:A:78:THR:HB	1.62	0.81
4:D:131:TRP:CD1	4:D:161:LEU:HB2	2.16	0.80
3:G:45:LEU:H	3:G:45:LEU:HD12	1.47	0.80
3:G:135:THR:HG21	3:G:148:LEU:HB2	1.62	0.80
2:F:16:GLY:HA2	2:F:81:LEU:HA	1.62	0.80
3:C:71:GLU:HG2	3:C:75:LYS:HE3	1.63	0.80
3:G:3:ALA:HA	4:H:18:THR:HG23	1.64	0.80
2:F:7:SER:HB3	2:F:8:PRO:CD	2.12	0.79
1:E:51:LEU:HD23	1:E:66:PHE:CE2	2.16	0.79
2:F:98:GLY:O	4:H:67:TYR:CE1	2.36	0.79
4:H:41:ASP:HB3	4:H:44:VAL:HG23	1.63	0.78
2:B:32:MET:HE2	2:B:69:ARG:HH21	1.48	0.78
1:E:36:ARG:HG2	1:E:46:LEU:HD13	1.64	0.78
4:H:68:LEU:HG	4:H:69:GLU:N	1.98	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:71:GLU:HB3	3:G:75:LYS:NZ	1.99	0.78
1:A:47:ILE:HD12	1:A:62:PHE:HB3	1.65	0.78
4:H:109:LEU:O	4:H:110:ASN:HB2	1.82	0.78
2:B:57:LYS:HB3	2:B:61:PRO:HG3	1.65	0.78
4:D:36:GLU:HG2	4:D:50:VAL:HG21	1.66	0.78
1:E:26:ASP:CB	1:E:29:PHE:CD1	2.67	0.78
2:B:26:THR:O	2:B:27:ASN:HB2	1.83	0.77
4:H:74:GLU:HA	4:H:77:THR:OG1	1.84	0.77
4:H:93:ARG:HG3	4:H:93:ARG:HH11	1.50	0.77
2:B:7:SER:HB3	2:B:8:PRO:CD	2.15	0.77
1:E:81:GLN:O	1:E:84:ASP:HB2	1.85	0.77
1:A:14:GLU:O	1:A:14:GLU:HG2	1.85	0.76
3:G:14:GLN:HB3	3:G:19:ILE:HB	1.66	0.76
3:G:134:GLU:HG2	3:G:135:THR:H	1.48	0.76
2:F:43:LEU:O	2:F:44:ARG:HG2	1.85	0.76
4:D:99:VAL:HG11	4:D:175:VAL:HG21	1.68	0.75
2:F:60:ILE:N	2:F:61:PRO:HD3	2.00	0.75
1:A:18:THR:HG21	1:A:112:LEU:HD22	1.68	0.75
3:G:60:LEU:HD12	3:G:60:LEU:H	1.51	0.75
3:G:53:ARG:HH21	5:Q:131:GLY:HA3	1.52	0.75
3:G:10:ILE:HG13	4:H:13:PRO:HD2	1.68	0.75
1:E:67:ASN:OD1	1:E:70:GLU:CB	2.21	0.75
5:Q:143:ILE:CG1	5:Q:144:GLU:H	1.97	0.75
1:A:47:ILE:CD1	1:A:58:ASP:HB3	2.16	0.75
1:A:102:ASN:HA	2:B:104:ALA:HA	1.67	0.74
4:H:22:GLN:HE22	8:H:201:NAG:H2	1.52	0.74
1:E:5:GLN:NE2	1:E:90:CYS:H	1.84	0.74
5:Q:143:ILE:CD1	5:Q:144:GLU:H	2.00	0.74
2:B:49:SER:HB2	2:B:54:SER:O	1.88	0.74
3:G:113:PHE:CZ	4:H:33:ASN:O	2.40	0.74
1:A:47:ILE:HD12	1:A:62:PHE:HB2	1.70	0.74
3:G:8:SER:HB3	3:G:10:ILE:HD11	1.68	0.74
2:B:41:HIS:HB2	2:B:44:ARG:HD2	1.68	0.73
4:D:172:THR:HA	4:D:187:GLU:HA	1.71	0.73
4:D:160:MET:H	4:D:160:MET:HE3	1.54	0.73
2:B:15:THR:OG1	2:B:116(B):GLY:HA3	1.87	0.73
1:E:82:PRO:HA	1:E:114:VAL:HB	1.69	0.73
3:G:65:THR:HG23	5:Q:140:TRP:O	1.89	0.73
4:H:103:LEU:HD21	4:H:188:TRP:CZ2	2.24	0.73
2:B:46:ILE:HG23	2:B:60:ILE:O	1.87	0.73
4:D:129:VAL:HG11	4:D:159:VAL:HG21	1.70	0.73
2:F:3:ALA:HB3	2:F:26:THR:HB	1.70	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:37:GLN:HB2	1:E:43:PRO:HB3	1.70	0.72
3:G:128:VAL:HG11	3:G:151:LEU:HD11	1.70	0.72
3:C:81:PRO:HB3	4:D:5:ARG:HG2	1.72	0.72
4:D:85:THR:O	4:D:88:PRO:HD2	1.90	0.72
4:D:160:MET:H	4:D:160:MET:CE	2.01	0.72
2:B:15:THR:HG23	2:B:84:PRO:HD3	1.71	0.72
3:C:179:GLU:N	3:C:180:PRO:CD	2.36	0.72
3:G:135:THR:O	3:G:147:LYS:HD3	1.89	0.72
3:C:135:THR:O	3:C:147:LYS:HE2	1.90	0.72
1:A:82:PRO:HG3	1:A:116:PRO:HB3	1.72	0.72
3:G:123:ARG:HG2	3:G:124:ASN:HD22	1.55	0.71
1:E:93:THR:HG22	1:E:99:GLY:H	1.55	0.71
1:E:101:PHE:H	4:H:70:ARG:HH22	1.38	0.71
4:H:56:PRO:HB2	5:Q:143:ILE:CG2	2.18	0.71
3:G:65:THR:HG21	5:Q:139:GLU:HB3	1.72	0.71
1:A:87:THR:HA	1:A:111:ARG:HA	1.73	0.71
4:D:103:LEU:HD23	4:D:114:THR:O	1.91	0.71
3:G:142:ASP:HB2	4:H:34:ARG:HH22	1.54	0.71
2:B:69:ARG:HG2	2:B:75:PHE:CD1	2.26	0.71
3:C:68:HIS:NE2	3:C:72:ILE:HD11	2.06	0.70
2:B:6:GLN:CG	2:B:110:PRO:HD2	2.21	0.70
2:F:25:GLN:O	2:F:25:GLN:HG2	1.90	0.70
4:H:71:THR:O	4:H:74:GLU:HG3	1.92	0.70
1:E:51:LEU:HD23	1:E:66:PHE:HE2	1.57	0.70
2:B:47:HIS:O	2:B:48:TYR:HB3	1.90	0.70
4:H:75:LEU:O	4:H:79:CYS:HB2	1.92	0.70
4:H:108:ALA:CB	4:H:111:HIS:HB2	2.22	0.70
4:H:93:ARG:HG3	4:H:93:ARG:NH1	2.04	0.69
3:G:43:TRP:HH2	5:Q:134:HIS:HE1	1.39	0.69
3:G:117:ILE:HG21	3:G:119:ILE:HD12	1.74	0.69
3:G:118:ASN:CB	3:G:166:GLU:HB2	2.18	0.69
1:E:61:ARG:HG3	1:E:78:THR:O	1.92	0.69
3:C:52:ARG:HD3	4:D:89:THR:HG21	1.74	0.69
3:C:103:ASN:ND2	3:C:104:THR:H	1.90	0.69
1:A:8:GLN:O	1:A:8:GLN:HG3	1.91	0.69
1:E:22:CYS:HB3	1:E:73:LEU:HD23	1.75	0.69
1:A:6:SER:N	1:A:7:PRO:HD2	2.07	0.69
3:G:8:SER:HA	4:H:13:PRO:O	1.93	0.69
3:G:1:ILE:HG22	3:G:2:GLU:N	2.07	0.69
4:D:114:THR:HA	4:D:162:GLU:HA	1.74	0.69
4:H:118:SER:HA	4:H:158:LEU:HB3	1.74	0.69
1:E:102:ASN:CA	2:F:104:ALA:HA	2.14	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:72:GLN:O	2:F:74:ASN:N	2.26	0.69
3:C:120:THR:HG23	3:C:164:LYS:HB3	1.73	0.69
2:B:52:ALA:O	2:B:69:ARG:HB3	1.93	0.69
1:A:5:GLN:NE2	1:A:109:GLY:H	1.91	0.68
4:H:49:ALA:HB2	4:H:58:ALA:HB2	1.74	0.68
3:G:144:SER:HB3	4:H:34:ARG:NH1	2.07	0.68
2:F:87:THR:HG22	2:F:87:THR:O	1.92	0.68
3:G:181:GLU:CG	3:G:182:ILE:H	2.06	0.68
2:F:36:ARG:NH2	2:F:86:GLN:HA	2.06	0.68
3:C:57:GLN:HA	3:C:57:GLN:HE21	1.59	0.68
1:A:29:PHE:HD2	1:A:92:ALA:HB1	1.58	0.68
4:H:188:TRP:O	4:H:189:ARG:HB2	1.94	0.68
2:B:32:MET:HG3	2:B:69:ARG:NH2	2.08	0.68
5:Q:143:ILE:CG1	5:Q:144:GLU:N	2.56	0.68
1:A:45:LEU:CD1	1:A:46:LEU:H	2.04	0.68
1:E:14:GLU:HG2	1:E:82:PRO:HD3	1.76	0.68
4:D:131:TRP:HB3	4:D:161:LEU:HD13	1.75	0.67
4:H:134:ASN:HA	4:H:170:VAL:CB	2.22	0.67
3:C:56:PRO:O	3:C:60:LEU:HD12	1.95	0.67
4:H:56:PRO:CB	5:Q:143:ILE:HG21	2.19	0.67
3:G:148:LEU:HB3	3:G:150:TYR:HE2	1.60	0.67
4:D:164:THR:O	4:D:166:ARG:HG3	1.94	0.67
3:G:147:LYS:C	3:G:148:LEU:HD12	2.15	0.67
4:D:85:THR:C	4:D:88:PRO:HD2	2.15	0.67
1:A:22:CYS:HB3	1:A:73:LEU:HD23	1.77	0.67
4:H:12:GLN:HB2	4:H:29:ARG:HB2	1.76	0.67
3:C:135:THR:HG23	3:C:148:LEU:O	1.93	0.67
3:G:142:ASP:HB2	4:H:34:ARG:NH2	2.10	0.67
2:B:32:MET:HE2	2:B:69:ARG:NH2	2.09	0.67
2:B:44:ARG:CG	2:B:60:ILE:HD11	2.25	0.67
4:H:138:GLU:O	4:H:142:VAL:HG21	1.95	0.67
4:H:115:LEU:O	4:H:160:MET:HA	1.95	0.67
1:E:26:ASP:CB	1:E:29:PHE:HE1	2.06	0.66
2:F:28:ASN:HB2	2:F:72:GLN:OE1	1.95	0.66
1:A:26:ASP:HB3	1:A:29:PHE:CD1	2.29	0.66
3:G:43:TRP:HH2	5:Q:134:HIS:CE1	2.14	0.66
4:H:133:ARG:HB3	4:H:133:ARG:HH11	1.61	0.66
4:H:133:ARG:HB2	4:H:138:GLU:HG3	1.77	0.66
3:G:156:SER:HB3	3:G:159:ASP:OD2	1.95	0.66
1:E:26:ASP:HB2	1:E:29:PHE:CE1	2.31	0.66
4:H:111:HIS:O	4:H:165:PRO:HD2	1.95	0.66
7:C:211:NDG:H6C1	7:C:212:NDG:C8	2.25	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:98:GLY:O	4:H:67:TYR:HE1	1.78	0.66
3:G:49:ALA:O	3:G:51:LEU:N	2.28	0.66
3:G:123:ARG:HA	3:G:161:TYR:HD2	1.61	0.66
5:Q:143:ILE:O	5:Q:144:GLU:HB2	1.95	0.65
3:C:162:ASP:HB3	3:C:175:LEU:HD22	1.78	0.65
5:Q:134:HIS:CD2	5:Q:134:HIS:N	2.65	0.65
4:D:130:ARG:HB3	4:D:132:PHE:HE1	1.62	0.65
4:H:47:TYR:HB2	4:H:62:ASN:OD1	1.97	0.65
1:A:43:PRO:HG2	2:B:43:LEU:HD21	1.79	0.65
2:F:49:SER:HB2	2:F:54:SER:O	1.96	0.64
2:B:7:SER:CB	2:B:8:PRO:HD3	2.23	0.64
1:A:11:THR:HB	1:E:9:SER:HB2	1.79	0.64
3:G:137:PHE:HB3	3:G:145:PHE:HB3	1.79	0.64
4:H:16:TYR:O	4:H:24:ILE:HA	1.97	0.64
4:H:29:ARG:HA	4:H:39:ARG:HB2	1.79	0.64
3:G:147:LYS:O	3:G:148:LEU:HD12	1.97	0.64
1:E:34:TRP:HE1	1:E:73:LEU:HD21	1.61	0.64
4:H:134:ASN:HD21	4:H:169:GLU:HG3	1.62	0.64
3:G:137:PHE:H	3:G:137:PHE:HD2	1.43	0.64
2:B:72:GLN:O	2:B:74:ASN:N	2.31	0.64
4:H:175:VAL:HB	4:H:184:ILE:O	1.97	0.64
4:H:86:GLU:OE1	4:H:86:GLU:HA	1.98	0.64
2:B:52:ALA:O	2:B:69:ARG:O	2.15	0.64
2:F:44:ARG:HG3	2:F:60:ILE:CD1	2.27	0.64
3:G:107:CYS:HB2	3:G:121:TRP:CZ2	2.33	0.64
3:G:129:THR:HG22	3:G:129:THR:O	1.98	0.64
7:C:211:NDG:H6C1	7:C:212:NDG:C7	2.28	0.63
2:F:8:PRO:O	2:F:112:THR:HG23	1.98	0.63
4:H:132:PHE:HB2	4:H:172:THR:HB	1.80	0.63
4:H:50:VAL:HG23	4:H:51:THR:H	1.63	0.63
1:E:116:PRO:O	1:E:117:TYR:HB2	1.97	0.63
4:H:119:VAL:HG21	4:H:129:VAL:HG21	1.80	0.63
2:B:49:SER:OG	2:B:69:ARG:HG3	1.98	0.63
2:F:31:ASN:HA	2:F:69:ARG:NH2	2.12	0.63
4:H:114:THR:HA	4:H:161:LEU:O	1.99	0.63
2:F:46:ILE:O	2:F:58:GLY:HA3	1.98	0.63
2:F:32:MET:HG3	2:F:69:ARG:NH2	2.14	0.63
1:E:34:TRP:CZ2	1:E:90:CYS:HB2	2.34	0.63
2:F:44:ARG:HG3	2:F:60:ILE:HD11	1.81	0.63
3:G:110:ASP:OD1	3:G:111:ASN:N	2.28	0.63
1:A:47:ILE:CD1	1:A:62:PHE:HB2	2.29	0.63
1:E:68:LYS:O	1:E:70:GLU:N	2.32	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:ARG:O	1:A:36:ARG:HG3	1.99	0.62
1:E:100:SER:O	1:E:101:PHE:HB3	1.98	0.62
4:D:163:MET:N	4:D:163:MET:SD	2.71	0.62
7:C:211:NDG:H6C1	7:C:212:NDG:H8C3	1.82	0.62
4:D:11:PHE:CD1	5:P:139:GLU:HG3	2.34	0.62
4:D:149:ARG:HG3	4:D:155:PHE:CE2	2.34	0.62
4:H:144:SER:HB2	4:H:159:VAL:HG13	1.82	0.62
2:F:6:GLN:CG	2:F:110:PRO:HD2	2.25	0.62
4:H:148:ILE:HB	4:H:156:GLN:O	2.00	0.62
3:G:181:GLU:HG3	3:G:182:ILE:N	2.09	0.62
4:D:122:PHE:CE2	4:D:155:PHE:HB2	2.35	0.62
4:D:166:ARG:O	4:D:169:GLU:HG3	1.99	0.62
2:B:87:THR:CG2	2:B:115:THR:HA	2.27	0.62
2:F:16:GLY:HA2	2:F:81:LEU:CA	2.29	0.62
3:C:52:ARG:CD	4:D:89:THR:HG21	2.27	0.62
1:A:26:ASP:OD1	1:A:28:THR:HB	1.99	0.62
3:G:108:PHE:CZ	3:G:110:ASP:HB2	2.35	0.62
4:H:116:VAL:HG13	4:H:160:MET:HG3	1.80	0.62
4:H:147:LEU:HD11	4:H:155:PHE:HB3	1.79	0.62
4:D:40:PHE:HB2	4:D:47:TYR:CD1	2.34	0.62
2:F:37:GLN:HE21	2:F:43:LEU:H	1.46	0.62
4:D:25:ARG:HD2	4:D:43:ASP:OD2	2.00	0.62
3:G:135:THR:HG23	3:G:148:LEU:O	2.00	0.61
2:B:83:THR:HG22	2:B:85:SER:H	1.65	0.61
3:G:107:CYS:HB2	3:G:121:TRP:CH2	2.35	0.61
4:D:127:ILE:HG13	4:D:176:GLU:O	2.00	0.61
4:H:164:THR:O	4:H:166:ARG:HG3	2.00	0.61
1:E:61:ARG:HH22	1:E:81:GLN:HB2	1.65	0.61
4:D:152:ASP:O	4:D:153:TRP:HB2	2.00	0.61
4:H:129:VAL:HA	4:H:174:HIS:O	2.01	0.61
1:A:104:LEU:HD21	2:B:104:ALA:O	2.00	0.61
1:E:30:ASP:OD1	4:H:70:ARG:HD2	2.01	0.61
1:A:8:GLN:HE21	1:E:12:VAL:HA	1.65	0.61
3:G:48:PHE:CZ	4:H:89:THR:HB	2.36	0.61
4:H:97:PRO:HB3	4:H:122:PHE:HB3	1.81	0.61
4:D:36:GLU:O	4:D:50:VAL:HB	2.01	0.61
1:E:30:ASP:HB3	4:H:77:THR:HG21	1.82	0.61
4:H:147:LEU:HD12	4:H:148:ILE:N	2.16	0.60
2:F:83:THR:O	2:F:86:GLN:HG3	2.00	0.60
4:H:103:LEU:HD22	4:H:115:LEU:HD23	1.83	0.60
1:E:19:ILE:HG23	1:E:76:HIS:HE1	1.65	0.60
2:F:38:ASP:C	2:F:40:GLY:H	2.05	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:32:TYR:O	4:D:33:ASN:HB2	2.00	0.60
3:G:71:GLU:HB3	3:G:75:LYS:HZ2	1.66	0.60
4:H:87:THR:HB	4:H:88:PRO:HD3	1.83	0.60
1:E:34:TRP:N	1:E:47:ILE:O	2.35	0.60
1:E:14:GLU:CG	1:E:82:PRO:HD3	2.31	0.60
4:D:60:TYR:CD2	5:P:143:ILE:HG12	2.37	0.60
3:G:71:GLU:HB3	3:G:75:LYS:HZ1	1.66	0.60
4:D:108:ALA:O	4:D:165:PRO:HG2	2.01	0.60
4:H:21:THR:HG21	4:H:84:GLU:CG	2.31	0.60
4:H:21:THR:HG21	4:H:84:GLU:OE2	2.02	0.60
1:E:102:ASN:HD21	2:F:95:GLY:HA3	1.67	0.60
4:H:149:ARG:NH1	4:H:149:ARG:HG3	2.17	0.60
2:B:65:TYR:CE2	2:B:79:LEU:HD21	2.36	0.60
2:F:47:HIS:O	2:F:48:TYR:HB3	2.01	0.60
4:H:72:ARG:O	4:H:75:LEU:HB2	2.01	0.59
2:F:71:SER:O	2:F:72:GLN:C	2.40	0.59
2:B:84:PRO:HA	2:B:116:VAL:HB	1.83	0.59
4:H:134:ASN:N	4:H:170:VAL:HB	2.16	0.59
4:H:130:ARG:HD3	4:H:174:HIS:HB3	1.84	0.59
3:C:171:GLU:CD	3:C:171:GLU:N	2.54	0.59
3:C:3:ALA:HA	4:D:18:THR:HG23	1.85	0.59
4:H:113:ASN:HB2	4:H:165:PRO:CD	2.29	0.59
4:D:99:VAL:HG11	4:D:175:VAL:CG2	2.32	0.59
2:F:60:ILE:N	2:F:61:PRO:CD	2.64	0.59
4:H:19:ASN:ND2	8:H:201:NAG:C6	2.64	0.59
4:D:25:ARG:HH11	4:D:43:ASP:HB2	1.66	0.59
3:C:61:GLN:O	3:C:64:ALA:HB3	2.03	0.59
4:H:57:ASP:OD1	5:Q:142:GLY:HA3	2.02	0.59
3:C:45:LEU:O	3:C:48:PHE:HB2	2.03	0.59
1:A:93:THR:HG23	1:A:99:GLY:N	2.18	0.59
4:D:76:ASP:OD1	4:D:80:ARG:HD2	2.02	0.59
4:H:149:ARG:HG3	4:H:149:ARG:HH11	1.66	0.59
4:D:132:PHE:CZ	4:D:137:GLU:HB2	2.38	0.59
3:C:32:PHE:HB2	3:C:42:VAL:O	2.02	0.59
3:G:134:GLU:HG2	3:G:135:THR:N	2.17	0.59
4:H:33:ASN:O	4:H:34:ARG:CG	2.46	0.59
4:H:144:SER:CB	4:H:159:VAL:HG13	2.33	0.59
4:D:134:ASN:HD21	4:D:169:GLU:HB3	1.68	0.59
1:A:45:LEU:HD12	1:A:46:LEU:N	2.10	0.59
4:D:144:SER:HB2	4:D:159:VAL:HG12	1.85	0.59
3:C:108:PHE:HE2	3:C:110:ASP:HB2	1.68	0.59
4:H:41:ASP:HB3	4:H:44:VAL:CG2	2.30	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:14:GLN:HE21	4:H:6:HIS:HB3	1.67	0.59
2:B:37:GLN:O	2:B:88:SER:HB2	2.02	0.59
1:E:28:THR:HG23	5:Q:135:ARG:HB3	1.83	0.59
4:H:184:ILE:HG22	4:H:184:ILE:O	2.02	0.59
2:B:87:THR:HG23	2:B:116:VAL:H	1.68	0.59
1:A:101:PHE:HB2	5:P:138:ILE:HG21	1.84	0.59
4:D:108:ALA:HB1	4:D:111:HIS:CB	2.25	0.58
3:G:159:ASP:O	3:G:180:PRO:HD3	2.03	0.58
4:D:16:TYR:HB2	4:D:25:ARG:HB3	1.85	0.58
3:C:180:PRO:CB	3:C:182:ILE:HG13	2.31	0.58
1:A:104:LEU:HD11	2:B:106:GLN:HG3	1.84	0.58
3:G:124:ASN:OD1	3:G:159:ASP:HA	2.02	0.58
2:F:84:PRO:HA	2:F:116:VAL:HB	1.85	0.58
2:B:20:THR:HG23	2:B:78:ILE:HG23	1.84	0.58
3:G:117:ILE:HD12	3:G:167:HIS:ND1	2.19	0.58
2:B:31:ASN:HB3	2:B:50:TYR:HA	1.85	0.58
4:H:38:VAL:HA	4:H:49:ALA:HA	1.85	0.58
5:Q:143:ILE:HG13	5:Q:144:GLU:N	2.18	0.58
3:G:12:VAL:O	3:G:20:GLY:HA2	2.02	0.58
2:B:31:ASN:HB2	2:B:49:SER:O	2.03	0.58
1:E:85:SER:HB3	1:E:113:ALA:HA	1.84	0.58
1:A:24:TYR:CZ	1:A:71:LYS:HG2	2.39	0.58
4:D:71:THR:HA	4:D:74:GLU:HG3	1.86	0.58
4:H:113:ASN:CB	4:H:165:PRO:HD3	2.29	0.58
1:E:116:PRO:O	1:E:117:TYR:CB	2.52	0.58
1:E:101:PHE:N	4:H:70:ARG:HH22	2.01	0.58
3:C:57:GLN:CA	3:C:57:GLN:HE21	2.15	0.58
1:E:7:PRO:HB2	1:E:110:THR:HG21	1.85	0.58
1:E:31:TYR:HB2	4:H:70:ARG:HD3	1.83	0.57
3:C:99:LEU:HA	3:C:155:PRO:HB2	1.86	0.57
3:G:6:VAL:HG22	4:H:16:TYR:CE1	2.38	0.57
4:H:152:ASP:O	4:H:153:TRP:HB2	2.03	0.57
3:C:73:LEU:O	3:C:77:SER:HB3	2.04	0.57
2:F:7:SER:CB	2:F:8:PRO:HD3	2.23	0.57
4:H:133:ARG:HA	4:H:170:VAL:O	2.04	0.57
4:H:18:THR:O	4:H:19:ASN:HB3	2.04	0.57
4:H:115:LEU:HD21	4:H:188:TRP:CD2	2.40	0.57
4:H:129:VAL:HG22	4:H:175:VAL:HA	1.87	0.57
4:D:102:SER:O	4:D:115:LEU:HD22	2.02	0.57
3:G:32:PHE:HB2	3:G:42:VAL:O	2.04	0.57
2:F:83:THR:HG22	2:F:85:SER:H	1.69	0.57
2:F:29:HIS:HB3	2:F:95:GLY:O	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:62:ASP:O	2:B:62:ASP:OD1	2.22	0.57
4:H:68:LEU:O	4:H:71:THR:HB	2.05	0.57
3:G:84:ASN:HD21	3:G:168:TRP:HB3	1.69	0.57
4:H:111:HIS:O	4:H:164:THR:HA	2.03	0.57
3:G:45:LEU:N	3:G:45:LEU:HD12	2.18	0.57
4:H:21:THR:HA	4:H:24:ILE:HD11	1.86	0.57
3:G:52:ARG:HA	5:Q:132:ASN:HB3	1.86	0.57
2:F:15:THR:HG1	2:F:116(B):GLY:HA3	1.70	0.57
3:G:24:PHE:O	3:G:31:LEU:HB2	2.05	0.56
2:B:32:MET:CE	2:B:69:ARG:HH21	2.18	0.56
2:F:57:LYS:HD3	2:F:61:PRO:HB3	1.87	0.56
1:A:61:ARG:HD2	1:A:78:THR:O	2.05	0.56
3:G:124:ASN:HA	3:G:160:ILE:O	2.05	0.56
4:D:39:ARG:HG2	4:D:40:PHE:N	2.19	0.56
4:D:56:PRO:O	5:P:143:ILE:HD11	2.05	0.56
2:F:71:SER:O	2:F:73:GLU:HG2	2.04	0.56
4:D:34:ARG:CG	4:D:34:ARG:HH11	2.04	0.56
3:G:121:TRP:CG	3:G:151:LEU:HD22	2.40	0.56
3:C:32:PHE:HD1	3:C:33:TYR:N	2.04	0.56
1:A:32:PHE:N	1:A:32:PHE:CD1	2.73	0.56
3:G:135:THR:CG2	3:G:148:LEU:HB2	2.33	0.56
1:E:17:THR:HA	1:E:77:ILE:O	2.05	0.56
2:F:50:TYR:CE2	3:G:61:GLN:HG2	2.40	0.56
4:H:127:ILE:HG13	4:H:176:GLU:O	2.05	0.56
3:C:95:SER:H	3:C:103:ASN:HD21	1.53	0.56
4:D:25:ARG:NH1	4:D:43:ASP:HB2	2.20	0.56
2:F:41:HIS:CD2	2:F:41:HIS:N	2.73	0.56
3:G:72:ILE:HG22	3:G:73:LEU:HD22	1.88	0.56
2:F:24:ASN:HA	2:F:73:GLU:O	2.06	0.56
2:F:36:ARG:O	2:F:36:ARG:HG2	2.06	0.56
1:A:37:GLN:O	1:A:86:ALA:HB1	2.06	0.56
1:A:81:GLN:O	1:A:114:VAL:HG21	2.06	0.56
3:C:89:ALA:HB3	3:C:176:LYS:HG3	1.87	0.56
3:C:122:LEU:HA	3:C:126:LYS:O	2.06	0.56
3:G:13:TYR:HA	3:G:19:ILE:O	2.06	0.56
4:H:93:ARG:HH11	4:H:93:ARG:CG	2.17	0.56
3:G:84:ASN:ND2	3:G:168:TRP:HB3	2.20	0.56
1:E:24:TYR:HE1	1:E:26:ASP:O	1.89	0.55
4:H:96:GLN:HA	4:H:179:SER:OG	2.06	0.55
3:G:10:ILE:N	3:G:10:ILE:HD12	2.21	0.55
2:B:71:SER:O	2:B:72:GLN:C	2.43	0.55
1:E:19:ILE:HG23	1:E:76:HIS:CE1	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:93:ARG:O	4:D:94:LEU:HD23	2.05	0.55
1:A:101:PHE:HB2	5:P:138:ILE:CG2	2.36	0.55
2:F:6:GLN:HG3	2:F:110:PRO:CD	2.28	0.55
3:G:65:THR:CG2	5:Q:139:GLU:HB3	2.37	0.55
4:D:114:THR:OG1	4:D:162:GLU:HB2	2.07	0.55
4:H:78:VAL:O	4:H:82:ASN:HB2	2.06	0.55
4:H:116:VAL:HA	4:H:159:VAL:O	2.07	0.55
3:G:91:VAL:HA	3:G:106:ILE:O	2.07	0.55
1:E:33:PRO:HA	1:E:48:ALA:HA	1.88	0.54
3:G:112:ILE:O	3:G:113:PHE:HB2	2.07	0.54
4:H:36:GLU:HG2	4:H:50:VAL:HG21	1.90	0.54
3:G:170:LEU:HD13	3:G:174:VAL:HG23	1.88	0.54
4:H:21:THR:CA	4:H:24:ILE:HD11	2.37	0.54
2:B:42:GLY:O	2:B:44:ARG:N	2.41	0.54
4:D:55:ARG:HB3	4:D:56:PRO:HD3	1.88	0.54
3:G:72:ILE:HD12	5:Q:142:GLY:O	2.06	0.54
2:F:18:LYS:HA	2:F:79:LEU:O	2.07	0.54
3:C:113:PHE:HA	3:C:114:PRO:C	2.27	0.54
2:F:16:GLY:CA	2:F:81:LEU:HA	2.34	0.54
4:D:129:VAL:CG1	4:D:159:VAL:HG21	2.36	0.54
3:G:91:VAL:HG13	3:G:106:ILE:O	2.07	0.54
3:C:105:LEU:HD11	3:C:178:TRP:CE3	2.43	0.54
4:H:113:ASN:HB3	4:H:163:MET:SD	2.47	0.54
4:D:116:VAL:HG13	4:D:160:MET:HG3	1.89	0.54
1:A:8:GLN:N	1:A:110:THR:HG23	2.23	0.54
3:G:76:ARG:HH22	4:H:57:ASP:CG	2.11	0.54
3:C:110:ASP:OD1	3:C:146:HIS:HB3	2.08	0.54
3:C:24:PHE:O	3:C:31:LEU:HB2	2.08	0.54
3:G:81:PRO:CB	4:H:5:ARG:HG2	2.25	0.54
2:B:43:LEU:O	2:B:44:ARG:C	2.44	0.54
3:C:109:VAL:HG21	3:C:119:ILE:HG12	1.90	0.54
3:G:171:GLU:C	3:G:172:GLU:HG3	2.28	0.54
1:E:17:THR:HG23	1:E:78:THR:HG23	1.90	0.54
2:F:41:HIS:CD2	2:F:41:HIS:H	2.26	0.54
2:B:16:GLY:HA2	2:B:81:LEU:HD12	1.89	0.54
1:A:7:PRO:HG3	1:A:21:ASN:H	1.74	0.53
4:H:21:THR:HB	4:H:24:ILE:HD11	1.89	0.53
3:G:113:PHE:HZ	4:H:33:ASN:O	1.91	0.53
4:H:188:TRP:CG	4:H:189:ARG:N	2.76	0.53
2:B:70:PRO:O	2:B:71:SER:HB3	2.08	0.53
3:C:123:ARG:H	3:C:128:VAL:HG22	1.73	0.53
1:A:11:THR:HA	1:A:113:ALA:O	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:22:GLN:HG3	4:D:23:ARG:N	2.23	0.53
3:G:6:VAL:HG13	4:H:16:TYR:HE1	1.73	0.53
3:G:160:ILE:HD12	3:G:160:ILE:O	2.09	0.53
1:A:26:ASP:HB3	1:A:29:PHE:CE1	2.44	0.53
1:E:51:LEU:HD23	1:E:66:PHE:CZ	2.42	0.53
1:A:47:ILE:O	1:A:64:ILE:HD11	2.09	0.53
1:E:112:LEU:HG	1:E:113:ALA:N	2.24	0.53
3:G:137:PHE:CD2	3:G:137:PHE:N	2.76	0.53
1:A:61:ARG:HB2	1:A:78:THR:H	1.74	0.53
3:G:65:THR:HG22	5:Q:139:GLU:OE2	2.08	0.53
4:H:134:ASN:H	4:H:170:VAL:HB	1.73	0.53
4:H:116:VAL:HG22	4:H:160:MET:HG2	1.89	0.53
2:B:98:GLY:C	2:B:104:ALA:H	2.12	0.53
2:F:38:ASP:OD1	2:F:88:SER:HB2	2.08	0.53
1:A:31:TYR:HB2	4:D:70:ARG:HD3	1.91	0.53
4:H:95:GLU:OE1	4:H:95:GLU:HA	2.09	0.53
3:C:68:HIS:CE1	3:C:72:ILE:HD11	2.43	0.53
4:H:11:PHE:O	4:H:13:PRO:HD3	2.08	0.52
4:D:129:VAL:HG11	4:D:159:VAL:CG2	2.39	0.52
1:A:100:SER:O	1:A:101:PHE:HB3	2.09	0.52
4:D:148:ILE:HB	4:D:156:GLN:HG2	1.89	0.52
1:A:69:ARG:O	1:A:70:GLU:HB3	2.09	0.52
4:D:132:PHE:CE2	4:D:137:GLU:HB2	2.45	0.52
3:G:123:ARG:HG2	3:G:124:ASN:ND2	2.24	0.52
2:F:98:GLY:O	2:F:99:ARG:HG3	2.10	0.52
4:H:12:GLN:HG3	4:H:31:ILE:CD1	2.40	0.52
4:H:57:ASP:O	4:H:60:TYR:HB3	2.10	0.52
1:A:18:THR:HB	1:A:77:ILE:HB	1.92	0.52
3:G:10:ILE:HG13	4:H:13:PRO:CD	2.37	0.52
3:G:28:GLY:HA3	4:H:149:ARG:NH2	2.25	0.52
3:C:106:ILE:HG12	3:C:150:TYR:CD1	2.43	0.52
1:E:28:THR:HG23	5:Q:135:ARG:CB	2.40	0.52
3:G:117:ILE:HG23	3:G:119:ILE:H	1.74	0.52
4:H:73:ALA:O	4:H:77:THR:HG23	2.10	0.52
3:C:154:ILE:O	3:C:156:SER:N	2.42	0.52
2:F:60:ILE:HG22	2:F:60:ILE:O	2.09	0.52
3:C:65:THR:O	3:C:68:HIS:HB3	2.09	0.52
2:F:6:GLN:NE2	2:F:34:TRP:CH2	2.76	0.52
4:D:18:THR:HG21	4:D:23:ARG:HH11	1.75	0.52
2:B:20:THR:CG2	2:B:78:ILE:HD13	2.39	0.52
4:H:82:ASN:HD21	5:Q:134:HIS:HB2	1.74	0.52
3:C:148:LEU:HD12	3:C:148:LEU:N	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:37:TYR:HA	4:D:51:THR:HG23	1.92	0.52
4:H:78:VAL:HG13	5:Q:135:ARG:O	2.10	0.52
4:H:166:ARG:O	4:H:190:ALA:HB1	2.10	0.52
4:D:164:THR:HG21	4:D:166:ARG:NH2	2.24	0.52
2:B:49:SER:CB	2:B:69:ARG:HG3	2.39	0.52
3:C:43:TRP:CH2	3:C:52:ARG:HG3	2.44	0.52
1:A:19:ILE:HG12	1:A:76:HIS:CE1	2.45	0.52
4:H:25:ARG:HD2	4:H:43:ASP:OD1	2.10	0.51
2:B:60:ILE:HG22	2:B:60:ILE:O	2.09	0.51
3:C:11:THR:HB	4:D:11:PHE:HB3	1.92	0.51
3:C:117:ILE:HG12	3:C:118:ASN:H	1.74	0.51
3:G:1:ILE:CG2	3:G:2:GLU:H	2.19	0.51
2:F:36:ARG:NH2	2:F:85:SER:O	2.44	0.51
3:C:146:HIS:NE2	4:D:149:ARG:NH2	2.59	0.51
3:C:167:HIS:ND1	3:C:168:TRP:N	2.57	0.51
3:C:15:SER:OG	3:C:16:PRO:HA	2.09	0.51
4:D:188:TRP:CG	4:D:189:ARG:N	2.78	0.51
1:E:26:ASP:CG	1:E:29:PHE:HE1	2.12	0.51
4:H:163:MET:HE3	4:H:188:TRP:HZ3	1.75	0.51
3:G:158:ASP:OD1	3:G:158:ASP:N	2.42	0.51
5:Q:134:HIS:N	5:Q:134:HIS:HD2	2.09	0.51
4:D:114:THR:HG22	4:D:115:LEU:N	2.25	0.51
1:E:93:THR:HG1	1:E:104:LEU:HA	1.76	0.51
5:Q:143:ILE:O	5:Q:144:GLU:CB	2.57	0.51
4:H:114:THR:HG23	4:H:161:LEU:C	2.31	0.51
1:E:112:LEU:HD21	1:E:114:VAL:HG22	1.92	0.51
4:D:103:LEU:HD23	4:D:114:THR:C	2.30	0.51
4:D:26:LEU:HB2	4:D:75:LEU:HD13	1.92	0.51
1:A:79:ASP:O	1:A:80:SER:C	2.48	0.51
4:H:35:GLU:HG2	4:H:51:THR:HG21	1.92	0.51
2:F:88:SER:OG	2:F:89:VAL:N	2.40	0.51
3:G:95:SER:O	3:G:103:ASN:ND2	2.44	0.51
4:H:104:SER:CB	4:H:114:THR:HB	2.35	0.51
4:H:93:ARG:HD3	4:H:123:TYR:CD1	2.46	0.51
4:D:74:GLU:OE2	5:P:135:ARG:NH2	2.44	0.51
3:G:181:GLU:CG	3:G:182:ILE:N	2.73	0.51
1:E:15:GLY:HA2	1:E:79:ASP:HA	1.92	0.51
3:G:121:TRP:CZ3	3:G:163:CYS:HB2	2.46	0.51
4:D:103:LEU:CD2	4:D:114:THR:HB	2.41	0.51
3:C:48:PHE:HZ	4:D:90:SER:HA	1.76	0.51
1:A:101:PHE:H	4:D:70:ARG:HH22	1.58	0.51
3:C:103:ASN:HD22	3:C:104:THR:N	1.96	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:43:LEU:O	2:B:44:ARG:O	2.29	0.51
2:F:26:THR:O	2:F:27:ASN:HB2	2.10	0.51
1:A:29:PHE:HA	1:A:93:THR:O	2.11	0.51
4:H:97:PRO:HD2	4:H:180:LEU:HD21	1.93	0.50
3:G:98:LEU:O	3:G:155:PRO:HG2	2.10	0.50
3:G:120:THR:CG2	3:G:164:LYS:HB3	2.34	0.50
2:B:57:LYS:HD3	2:B:61:PRO:HB2	1.92	0.50
4:D:72:ARG:O	4:D:75:LEU:HB2	2.10	0.50
1:E:93:THR:HG21	1:E:103:LYS:O	2.10	0.50
3:G:123:ARG:HA	3:G:161:TYR:CD2	2.44	0.50
1:A:28:THR:HG23	5:P:135:ARG:CD	2.41	0.50
3:G:92:PHE:CZ	3:G:106:ILE:HG21	2.46	0.50
1:A:7:PRO:HG3	1:A:20:LEU:HA	1.94	0.50
3:G:9(A):GLY:N	3:G:24:PHE:CD1	2.80	0.50
1:A:61:ARG:CB	1:A:78:THR:HB	2.36	0.50
1:E:47:ILE:HG21	1:E:64:ILE:HG13	1.92	0.50
3:G:74:THR:HA	4:H:32:TYR:OH	2.12	0.50
2:F:43:LEU:O	2:F:44:ARG:CG	2.59	0.50
3:C:142:ASP:OD1	3:C:144:SER:HB3	2.11	0.50
3:G:45:LEU:HD21	4:H:153:TRP:CD2	2.46	0.50
2:B:36:ARG:HB3	2:B:46:ILE:HD11	1.93	0.50
1:E:24:TYR:CE1	1:E:26:ASP:O	2.65	0.49
2:B:32:MET:HE3	2:B:69:ARG:HE	1.76	0.49
1:E:34:TRP:CD1	1:E:64:ILE:HD11	2.46	0.49
4:H:133:ARG:O	4:H:134:ASN:HB2	2.11	0.49
2:B:97:GLN:C	2:B:98:GLY:O	2.48	0.49
2:F:44:ARG:CG	2:F:60:ILE:HD11	2.42	0.49
3:G:91:VAL:HG12	3:G:92:PHE:N	2.26	0.49
2:B:16:GLY:CA	2:B:81:LEU:HD12	2.42	0.49
1:E:12:VAL:HG12	1:E:13:TRP:H	1.76	0.49
3:G:14:GLN:HB2	4:H:8:VAL:HG13	1.94	0.49
3:C:47:GLU:O	3:C:50:GLN:HG3	2.12	0.49
3:G:14:GLN:CG	4:H:8:VAL:HG13	2.42	0.49
3:G:52:ARG:HD3	4:H:89:THR:HG21	1.94	0.49
4:D:99:VAL:HA	4:D:118:SER:O	2.12	0.49
2:F:37:GLN:HG3	2:F:91:PHE:CE1	2.47	0.49
3:G:57:GLN:HA	3:G:57:GLN:HE21	1.77	0.49
2:B:37:GLN:HG2	2:B:43:LEU:CD1	2.42	0.49
2:B:45:LEU:HG	2:B:46:ILE:N	2.27	0.49
3:C:32:PHE:CD1	3:C:33:TYR:N	2.80	0.49
5:Q:140:TRP:O	5:Q:141:GLU:HB3	2.12	0.49
3:G:26:PHE:O	3:G:27:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:83:TYR:HA	4:H:86:GLU:HB2	1.95	0.49
2:B:6:GLN:HG3	2:B:110:PRO:CD	2.36	0.49
3:C:1:ILE:HG21	4:D:16:TYR:CZ	2.48	0.49
3:G:130:ASP:OD1	3:G:131:GLY:N	2.44	0.49
4:H:171:TYR:HD2	4:H:190:ALA:HB2	1.78	0.49
4:H:148:ILE:HB	4:H:156:GLN:HG2	1.94	0.49
4:H:178:PRO:C	4:H:180:LEU:H	2.15	0.49
4:D:61:TRP:NE1	5:P:141:GLU:O	2.41	0.49
1:E:93:THR:HG22	1:E:100:SER:OG	2.12	0.49
4:H:32:TYR:C	4:H:32:TYR:CD1	2.86	0.49
3:G:14:GLN:HG3	4:H:7:PHE:O	2.11	0.49
4:H:173:CYS:O	4:H:185:THR:HA	2.13	0.49
1:A:46:LEU:O	1:A:46:LEU:HD23	2.13	0.49
2:F:57:LYS:HB3	2:F:61:PRO:CG	2.43	0.49
1:A:33:PRO:HB3	1:A:48:ALA:HB2	1.95	0.49
2:F:99:ARG:O	2:F:104:ALA:HB3	2.13	0.48
3:G:6:VAL:HG13	4:H:16:TYR:CE1	2.48	0.48
2:B:51:GLY:C	2:B:69:ARG:HH11	2.17	0.48
2:B:36:ARG:HH21	2:B:88:SER:HB3	1.77	0.48
2:B:83:THR:O	2:B:116:VAL:HG21	2.12	0.48
2:B:61:PRO:O	2:B:62:ASP:OD1	2.31	0.48
3:G:70:LEU:HD12	4:H:9:HIS:HB2	1.95	0.48
2:B:32:MET:O	2:B:48:TYR:HB2	2.12	0.48
4:H:118:SER:OG	4:H:158:LEU:HD23	2.13	0.48
1:A:5:GLN:NE2	1:A:90:CYS:H	2.11	0.48
4:D:74:GLU:HA	4:D:78:VAL:HG23	1.94	0.48
1:A:75:LEU:HD12	1:A:76:HIS:N	2.29	0.48
1:A:34:TRP:CH2	1:A:90:CYS:HB2	2.48	0.48
4:D:87:THR:HB	4:D:88:PRO:HD3	1.95	0.48
2:B:37:GLN:HB2	2:B:89:VAL:HB	1.95	0.48
3:C:87:PRO:HD3	3:C:167:HIS:CD2	2.48	0.48
4:H:62:ASN:O	4:H:68:LEU:HB3	2.13	0.48
4:D:134:ASN:OD1	4:D:169:GLU:HA	2.14	0.48
4:D:148:ILE:HD12	4:D:148:ILE:N	2.28	0.48
4:H:122:PHE:O	4:H:155:PHE:HB2	2.14	0.48
1:E:34:TRP:CH2	1:E:90:CYS:HB2	2.48	0.48
1:E:47:ILE:HG22	1:E:64:ILE:CD1	2.44	0.48
1:A:42:SER:HB3	2:B:109:GLY:O	2.13	0.48
3:G:104:THR:HG23	3:G:152:THR:HA	1.95	0.48
3:G:89:ALA:HA	3:G:109:VAL:HG22	1.95	0.48
3:G:84:ASN:HD22	3:G:168:TRP:C	2.17	0.48
3:G:142:ASP:O	3:G:143:TYR:HB2	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:113:ASN:O	4:H:162:GLU:HA	2.13	0.48
3:G:10:ILE:HG23	4:H:11:PHE:O	2.14	0.48
2:F:116(A):LEU:O	2:F:116(B):GLY:C	2.52	0.48
1:E:32:PHE:CD1	1:E:32:PHE:N	2.81	0.48
3:C:129:THR:HA	3:C:132:VAL:HG21	1.94	0.48
1:E:93:THR:OG1	1:E:104:LEU:HA	2.14	0.48
3:C:91:VAL:HA	3:C:106:ILE:O	2.14	0.48
2:B:36:ARG:HG3	2:B:36:ARG:O	2.14	0.48
4:H:163:MET:HE1	4:H:165:PRO:HA	1.96	0.47
4:D:31:ILE:HG23	4:D:35:GLU:C	2.34	0.47
2:F:114:LEU:HD12	2:F:115:THR:N	2.28	0.47
2:B:116(A):LEU:O	2:B:116(B):GLY:C	2.52	0.47
4:H:126:LYS:NZ	4:H:178:PRO:HG3	2.29	0.47
4:D:97:PRO:HB2	4:D:119:VAL:HG12	1.96	0.47
1:E:67:ASN:O	1:E:68:LYS:C	2.53	0.47
3:G:73:LEU:HB3	4:H:32:TYR:CD2	2.49	0.47
4:H:131:TRP:CD1	4:H:161:LEU:HB2	2.49	0.47
3:C:87:PRO:HD3	3:C:167:HIS:HD2	1.79	0.47
4:H:52:GLU:O	4:H:55:ARG:HB3	2.15	0.47
4:H:164:THR:O	4:H:166:ARG:N	2.47	0.47
4:H:128:LYS:HE2	4:H:130:ARG:HH12	1.79	0.47
4:D:114:THR:O	4:D:115:LEU:HD23	2.14	0.47
3:C:84:ASN:HD21	3:C:168:TRP:HB3	1.79	0.47
4:D:133:ARG:N	4:D:136:GLN:O	2.36	0.47
4:H:123:TYR:CG	4:H:124:PRO:HA	2.49	0.47
4:D:29:ARG:HD3	4:D:36:GLU:OE2	2.14	0.47
1:A:13:TRP:CH2	1:E:8:GLN:HB2	2.50	0.47
3:G:29:ASP:HB3	4:H:153:TRP:NE1	2.30	0.47
3:G:28:GLY:HA3	4:H:149:ARG:HH22	1.78	0.47
1:E:47:ILE:HG22	1:E:64:ILE:HD11	1.95	0.47
4:D:31:ILE:HG23	4:D:36:GLU:N	2.30	0.47
3:G:60:LEU:N	3:G:60:LEU:HD12	2.26	0.47
1:E:35:TYR:CE2	1:E:45:LEU:HD12	2.50	0.47
3:C:115:PRO:HB3	3:C:145:PHE:CD1	2.50	0.47
2:F:32:MET:H	2:F:69:ARG:HH21	1.61	0.47
3:G:14:GLN:HB3	3:G:19:ILE:CB	2.39	0.47
2:B:26:THR:O	2:B:27:ASN:CB	2.58	0.47
3:G:63:ILE:HG22	3:G:64:ALA:N	2.30	0.47
3:G:123:ARG:H	3:G:128:VAL:HG23	1.80	0.47
4:D:47:TYR:HB2	4:D:62:ASN:OD1	2.15	0.47
3:G:15:SER:OG	3:G:16:PRO:HA	2.15	0.47
4:H:157:VAL:HG13	4:H:157:VAL:O	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:46:GLU:HG3	4:H:47:TYR:O	2.14	0.47
3:C:97:VAL:HG12	3:C:155:PRO:HB3	1.97	0.47
3:G:164:LYS:HE2	3:G:166:GLU:CG	2.45	0.47
1:E:36:ARG:O	1:E:36:ARG:HG3	2.14	0.47
4:H:177:HIS:CE1	4:H:179:SER:HB3	2.50	0.47
4:H:150:ASN:HB2	4:H:154:THR:OG1	2.15	0.47
1:E:12:VAL:HG12	1:E:13:TRP:N	2.30	0.47
3:C:178:TRP:C	3:C:179:GLU:HG3	2.35	0.47
4:D:15:CYS:HB3	4:D:17:PHE:CZ	2.50	0.47
3:C:32:PHE:CD1	3:C:32:PHE:C	2.87	0.47
1:A:11:THR:HB	1:E:9:SER:CB	2.43	0.46
1:E:49:ILE:HG23	1:E:50:SER:N	2.30	0.46
3:C:125:SER:H	3:C:160:ILE:HD11	1.80	0.46
4:H:31:ILE:HG22	4:H:32:TYR:N	2.30	0.46
2:F:38:ASP:C	2:F:40:GLY:N	2.68	0.46
3:G:50:GLN:HG2	3:G:50:GLN:H	1.41	0.46
3:C:41:THR:HG21	3:C:54:PHE:O	2.15	0.46
3:G:76:ARG:HE	5:Q:143:ILE:HD13	1.81	0.46
3:G:138:PHE:HB2	3:G:146:HIS:NE2	2.29	0.46
4:H:130:ARG:O	4:H:174:HIS:N	2.46	0.46
3:G:65:THR:O	3:G:68:HIS:HB3	2.15	0.46
1:E:102:ASN:ND2	2:F:95:GLY:HA3	2.30	0.46
3:G:73:LEU:HD12	4:H:32:TYR:HD2	1.80	0.46
4:H:32:TYR:C	4:H:32:TYR:HD1	2.19	0.46
3:G:179:GLU:CD	3:G:179:GLU:H	2.19	0.46
3:G:71:GLU:O	3:G:72:ILE:C	2.54	0.46
3:G:9:TYR:OH	4:H:86:GLU:HG2	2.15	0.46
4:H:19:ASN:ND2	4:H:22:GLN:NE2	2.63	0.46
3:G:60:LEU:HA	3:G:63:ILE:HB	1.98	0.46
3:C:9:TYR:HB3	3:C:24:PHE:CZ	2.50	0.46
3:G:150:TYR:HE1	4:H:152:ASP:HB3	1.81	0.46
1:E:106:PHE:CG	2:F:43:LEU:HD12	2.51	0.46
4:H:63:LYS:O	4:H:63:LYS:HE2	2.15	0.46
1:E:51:LEU:HD22	1:E:68:LYS:HD2	1.96	0.46
2:F:114:LEU:HD12	2:F:115:THR:H	1.81	0.46
3:C:34:VAL:O	3:C:36:LEU:HD23	2.16	0.46
4:H:14:PHE:N	4:H:27:VAL:O	2.38	0.46
3:C:52:ARG:NH1	4:D:89:THR:OG1	2.48	0.46
2:B:105:GLU:OE1	2:B:107:PHE:CZ	2.69	0.46
4:D:38:VAL:CA	4:D:50:VAL:HG23	2.46	0.46
3:C:82:ALA:HB1	3:C:113:PHE:HE2	1.79	0.46
3:G:43:TRP:CH2	5:Q:134:HIS:HE1	2.27	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:98:LEU:HD23	3:C:98:LEU:HA	1.82	0.46
4:H:114:THR:HG23	4:H:162:GLU:N	2.30	0.46
4:H:133:ARG:CB	4:H:138:GLU:HG3	2.45	0.46
1:A:112:LEU:HD12	1:A:113:ALA:H	1.80	0.46
4:D:130:ARG:HB3	4:D:132:PHE:CE1	2.47	0.46
1:E:15:GLY:O	1:E:17:THR:N	2.46	0.46
3:G:123:ARG:HG3	3:G:161:TYR:HE2	1.80	0.46
4:H:145:THR:HG21	4:H:158:LEU:HD12	1.98	0.46
3:C:35:ASP:CG	3:C:38:LYS:HB2	2.37	0.46
3:C:154:ILE:O	3:C:155:PRO:C	2.55	0.45
4:D:25:ARG:HH11	4:D:43:ASP:CB	2.28	0.45
4:D:18:THR:HG21	4:D:23:ARG:NH1	2.30	0.45
1:A:101:PHE:HD2	1:A:101:PHE:O	1.98	0.45
4:D:163:MET:HG2	4:D:171:TYR:CE1	2.51	0.45
4:D:131:TRP:HB2	4:D:142:VAL:HG22	1.99	0.45
1:A:55:LYS:HG2	1:A:56:LYS:N	2.31	0.45
2:F:32:MET:HE2	2:F:69:ARG:NH1	2.32	0.45
3:G:45:LEU:HA	3:G:46:PRO:HD2	1.82	0.45
4:D:49:ALA:HB2	4:D:55:ARG:HA	1.98	0.45
4:D:100:VAL:O	4:D:117:CYS:O	2.35	0.45
1:A:7:PRO:HG3	1:A:21:ASN:N	2.31	0.45
3:G:137:PHE:HB3	3:G:145:PHE:CB	2.45	0.45
2:F:16:GLY:HA2	2:F:81:LEU:C	2.36	0.45
3:G:176:LYS:HA	3:G:176:LYS:HD3	1.54	0.45
3:C:162:ASP:OD1	3:C:177:HIS:ND1	2.50	0.45
4:D:100:VAL:O	4:D:100:VAL:HG23	2.17	0.45
4:D:104:SER:C	4:D:106:THR:H	2.20	0.45
3:C:51:LEU:HD12	4:D:89:THR:HG22	1.98	0.45
4:D:52:GLU:OE1	4:D:55:ARG:NH1	2.50	0.45
1:A:101:PHE:CZ	5:P:141:GLU:HG2	2.51	0.45
4:H:32:TYR:C	4:H:34:ARG:H	2.20	0.45
3:C:135:THR:O	3:C:147:LYS:HG3	2.16	0.45
3:G:123:ARG:NH1	3:G:161:TYR:HE2	2.14	0.45
2:B:23:CYS:O	2:B:74:ASN:HA	2.16	0.45
3:G:106:ILE:HD12	3:G:106:ILE:N	2.32	0.45
4:H:63:LYS:O	4:H:64:GLN:CG	2.65	0.45
3:C:35:ASP:OD1	3:C:38:LYS:HB2	2.16	0.45
3:G:76:ARG:HH21	5:Q:143:ILE:CG2	2.30	0.45
3:G:81:PRO:HA	4:H:7:PHE:CD1	2.52	0.45
4:H:131:TRP:HD1	4:H:142:VAL:HG13	1.82	0.45
4:H:97:PRO:CB	4:H:122:PHE:HB3	2.45	0.45
4:H:19:ASN:ND2	8:H:201:NAG:H62	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:18:LYS:HE3	2:B:80:GLU:HG2	1.98	0.45
4:D:146:GLN:O	4:D:148:ILE:HD12	2.17	0.45
1:A:16:GLU:HG3	1:A:16:GLU:H	1.24	0.45
4:H:128:LYS:HE2	4:H:130:ARG:NH1	2.31	0.45
4:D:62:ASN:O	4:D:68:LEU:HB2	2.15	0.45
3:G:95:SER:HB2	3:G:101:GLN:HE22	1.82	0.45
4:H:167:ARG:HA	4:H:190:ALA:O	2.16	0.45
3:G:9:TYR:HD1	3:G:24:PHE:CD2	2.34	0.45
3:G:46:PRO:O	3:G:48:PHE:N	2.50	0.45
4:D:166:ARG:HG2	4:D:166:ARG:NH1	2.31	0.45
4:H:109:LEU:O	4:H:110:ASN:CB	2.59	0.45
3:C:47:GLU:HG2	3:C:48:PHE:H	1.82	0.45
4:H:145:THR:HG21	4:H:158:LEU:CD1	2.47	0.45
4:H:52:GLU:HG3	4:H:55:ARG:NH2	2.32	0.45
1:E:54:ASN:HB2	1:E:66:PHE:O	2.17	0.44
4:H:87:THR:CB	4:H:88:PRO:HD3	2.46	0.44
4:H:26:LEU:HB3	4:H:75:LEU:HD13	1.98	0.44
2:B:43:LEU:HA	2:B:43:LEU:HD12	1.40	0.44
2:B:44:ARG:HB3	2:B:60:ILE:HD11	1.99	0.44
2:F:58:GLY:N	2:F:61:PRO:HG3	2.32	0.44
3:G:87:PRO:HB2	3:G:109:VAL:CG1	2.48	0.44
1:E:26:ASP:OD2	1:E:29:PHE:HE1	2.01	0.44
3:C:101:GLN:O	3:C:155:PRO:HD2	2.16	0.44
4:D:130:ARG:CB	4:D:132:PHE:HE1	2.29	0.44
4:D:142:VAL:HG12	4:D:142:VAL:O	2.15	0.44
3:C:3:ALA:HB1	4:D:17:PHE:O	2.17	0.44
1:A:33:PRO:HA	1:A:48:ALA:HA	1.99	0.44
1:A:13:TRP:O	1:A:14:GLU:C	2.53	0.44
4:D:158:LEU:O	4:D:160:MET:HE2	2.17	0.44
3:G:68:HIS:CD2	3:G:69:ASN:N	2.86	0.44
1:A:116:PRO:O	1:A:117:TYR:HB2	2.15	0.44
3:G:33:TYR:O	3:G:42:VAL:HG23	2.18	0.44
3:C:9(A):GLY:O	3:C:10:ILE:C	2.55	0.44
4:H:32:TYR:CE1	4:H:33:ASN:ND2	2.86	0.44
4:D:94:LEU:CD2	4:D:124:PRO:HD3	2.48	0.44
2:B:81:LEU:HD12	2:B:81:LEU:HA	1.88	0.44
3:C:14:GLN:OE1	3:C:115:PRO:HD2	2.17	0.44
4:H:115:LEU:HD11	4:H:188:TRP:CE3	2.52	0.44
3:C:57:GLN:HA	3:C:57:GLN:NE2	2.28	0.44
2:B:58:GLY:C	2:B:61:PRO:HD3	2.37	0.44
3:C:15:SER:HA	3:C:16:PRO:C	2.38	0.44
3:G:122:LEU:HB3	3:G:126:LYS:H	1.83	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:GLY:O	1:A:79:ASP:HA	2.17	0.44
4:H:75:LEU:HA	4:H:75:LEU:HD12	1.88	0.44
2:B:47:HIS:O	2:B:48:TYR:CB	2.49	0.44
3:C:117:ILE:HG23	3:C:118:ASN:N	2.33	0.44
2:B:87:THR:O	2:B:87:THR:HG22	2.18	0.44
3:G:121:TRP:CD2	3:G:151:LEU:HD22	2.53	0.44
3:C:11:THR:HG23	3:C:63:ILE:HD13	2.00	0.44
3:G:132:VAL:HG12	3:G:133:TYR:H	1.82	0.44
2:F:90:TYR:N	2:F:90:TYR:CD1	2.86	0.44
4:H:74:GLU:HA	4:H:78:VAL:HG23	2.00	0.43
4:H:4:GLU:O	4:H:5:ARG:HB2	2.18	0.43
2:B:34:TRP:CD1	2:B:75:PHE:CE2	3.06	0.43
3:G:39:LYS:HG2	3:G:60:LEU:HD21	2.00	0.43
1:E:8:GLN:O	1:E:9:SER:HB2	2.17	0.43
4:H:120:THR:HA	4:H:156:GLN:HB2	1.99	0.43
1:E:91:ALA:HB2	1:E:106:PHE:CD2	2.52	0.43
1:E:61:ARG:HH21	1:E:84:ASP:CG	2.22	0.43
1:A:116:PRO:O	1:A:117:TYR:CB	2.65	0.43
4:D:109:LEU:O	4:D:110:ASN:HB2	2.17	0.43
3:G:35:ASP:OD2	3:G:38:LYS:HB2	2.18	0.43
1:A:112:LEU:HD12	1:A:113:ALA:N	2.33	0.43
4:H:83:TYR:CE2	4:H:91:LEU:HD11	2.52	0.43
3:C:53:ARG:HH12	5:P:131:GLY:N	2.15	0.43
3:C:97:VAL:HG21	3:C:178:TRP:CZ2	2.54	0.43
3:G:71:GLU:O	3:G:74:THR:N	2.51	0.43
3:G:167:HIS:CD2	3:G:169:GLY:H	2.37	0.43
4:H:129:VAL:HG22	4:H:175:VAL:HG22	2.00	0.43
4:D:85:THR:HG21	5:P:134:HIS:CE1	2.53	0.43
4:H:36:GLU:O	4:H:50:VAL:CG2	2.66	0.43
4:D:56:PRO:CB	5:P:143:ILE:HD12	2.48	0.43
4:D:22:GLN:CG	4:D:23:ARG:N	2.81	0.43
1:A:81:GLN:O	1:A:84:ASP:HB2	2.18	0.43
3:C:100:GLY:O	3:C:154:ILE:HG23	2.17	0.43
2:F:54:SER:HB2	2:F:56:GLU:OE2	2.19	0.43
4:H:53:LEU:O	4:H:56:PRO:HD2	2.18	0.43
1:A:108:ALA:HA	2:B:42:GLY:H	1.84	0.43
4:D:25:ARG:HD2	4:D:43:ASP:CG	2.39	0.43
2:F:67:ALA:HB1	2:F:75:PHE:CE1	2.54	0.43
2:F:47:HIS:CB	2:F:67:ALA:HB2	2.49	0.43
3:G:99:LEU:HD12	3:G:155:PRO:O	2.19	0.43
4:D:101:ILE:HD11	4:D:173:CYS:HB2	2.00	0.43
4:H:82:ASN:ND2	5:Q:134:HIS:CB	2.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:H:32:TYR:O	4:H:34:ARG:N	2.51	0.43
4:H:141:GLY:O	4:H:161:LEU:HA	2.17	0.43
3:G:26:PHE:CE1	4:H:86:GLU:HG3	2.53	0.43
2:B:30:ASN:O	2:B:69:ARG:NH2	2.36	0.43
4:D:145:THR:HG22	4:D:158:LEU:O	2.19	0.43
1:A:29:PHE:CD2	1:A:92:ALA:HB1	2.44	0.43
2:B:20:THR:HG21	2:B:78:ILE:HD13	2.01	0.43
3:C:105:LEU:HA	3:C:105:LEU:HD23	1.76	0.43
3:G:76:ARG:NH2	5:Q:143:ILE:HG12	2.34	0.43
4:H:26:LEU:O	4:H:41:ASP:HA	2.18	0.43
3:G:148:LEU:HD22	4:H:151:GLY:HA3	2.00	0.43
4:H:37:TYR:HA	4:H:51:THR:CG2	2.39	0.43
2:B:80:GLU:O	2:B:81:LEU:CB	2.67	0.43
1:E:100:SER:O	1:E:101:PHE:CB	2.65	0.43
3:C:124:ASN:HA	3:C:160:ILE:HG13	2.01	0.43
1:E:102:ASN:HD21	2:F:95:GLY:CA	2.29	0.43
3:G:115:PRO:HG3	3:G:145:PHE:CE1	2.54	0.43
3:G:9(A):GLY:O	4:H:13:PRO:HG3	2.19	0.43
4:H:149:ARG:CG	4:H:149:ARG:HH11	2.31	0.43
1:E:34:TRP:CE2	1:E:90:CYS:HB2	2.53	0.43
3:G:121:TRP:CD1	3:G:151:LEU:HB2	2.53	0.43
4:D:74:GLU:CA	4:D:78:VAL:HG23	2.49	0.43
4:H:57:ASP:OD1	5:Q:143:ILE:HG23	2.18	0.43
4:H:134:ASN:ND2	4:H:169:GLU:HG3	2.32	0.43
3:G:102:PRO:HA	3:G:154:ILE:HG12	2.01	0.43
4:H:26:LEU:HD11	4:H:28:ILE:HG12	2.01	0.42
4:D:40:PHE:HB2	4:D:47:TYR:CE1	2.54	0.42
3:C:158:ASP:N	3:C:158:ASP:OD1	2.45	0.42
3:C:125:SER:N	3:C:160:ILE:HD11	2.34	0.42
3:G:117:ILE:HG13	3:G:166:GLU:O	2.19	0.42
3:G:1:ILE:HG13	4:H:25:ARG:NH2	2.34	0.42
3:G:60:LEU:CD1	3:G:60:LEU:H	2.26	0.42
4:D:144:SER:HB2	4:D:159:VAL:CG1	2.49	0.42
3:G:89:ALA:HB3	3:G:176:LYS:HG2	2.01	0.42
4:D:74:GLU:O	4:D:78:VAL:HG23	2.19	0.42
1:A:8:GLN:HE21	1:E:12:VAL:CA	2.32	0.42
4:H:10:GLN:HB2	4:H:31:ILE:HB	2.01	0.42
4:D:88:PRO:HA	4:D:92:ARG:NH1	2.34	0.42
3:C:48:PHE:CE1	4:D:89:THR:HB	2.54	0.42
4:D:74:GLU:HB3	4:D:78:VAL:HG21	2.02	0.42
3:G:96:PRO:HG3	4:H:100:VAL:HG21	2.01	0.42
2:F:28:ASN:OD1	2:F:28:ASN:C	2.57	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:131:TRP:CB	4:D:161:LEU:HD13	2.46	0.42
2:B:57:LYS:HD3	2:B:61:PRO:CB	2.50	0.42
4:D:38:VAL:HA	4:D:50:VAL:HG23	2.02	0.42
3:G:124:ASN:OD1	3:G:160:ILE:HG13	2.20	0.42
2:B:20:THR:HG23	2:B:78:ILE:HD13	2.01	0.42
2:B:80:GLU:O	2:B:81:LEU:HB2	2.19	0.42
4:D:96:GLN:HA	4:D:179:SER:OG	2.19	0.42
3:C:98:LEU:O	3:C:99:LEU:C	2.57	0.42
2:B:97:GLN:O	2:B:98:GLY:O	2.37	0.42
3:C:118:ASN:CB	3:C:166:GLU:HB3	2.36	0.42
1:E:5:GLN:HE22	1:E:90:CYS:N	2.04	0.42
4:D:89:THR:OG1	4:D:90:SER:N	2.50	0.42
2:F:31:ASN:CB	2:F:49:SER:O	2.68	0.42
4:H:105:ARG:CG	4:H:113:ASN:HA	2.50	0.42
2:B:47:HIS:N	2:B:47:HIS:CD2	2.86	0.42
4:D:160:MET:H	4:D:160:MET:HE2	1.84	0.42
3:G:62:ASN:CG	5:Q:139:GLU:H	2.23	0.42
4:H:30:TYR:HB2	4:H:38:VAL:O	2.20	0.42
4:H:63:LYS:O	4:H:64:GLN:HG3	2.19	0.42
2:F:32:MET:N	2:F:69:ARG:HH21	2.17	0.42
3:G:29:ASP:HB3	4:H:153:TRP:CD1	2.54	0.42
2:B:36:ARG:HA	2:B:89:VAL:O	2.19	0.42
2:B:74:ASN:OD1	2:B:74:ASN:C	2.58	0.42
4:D:37:TYR:O	4:D:54:GLY:HA3	2.19	0.42
4:H:39:ARG:HG2	4:H:40:PHE:N	2.33	0.42
4:H:44:VAL:HG11	4:H:48:ARG:HG3	2.01	0.42
3:G:46:PRO:C	3:G:48:PHE:H	2.23	0.42
3:C:104:THR:CG2	3:C:150:TYR:HB3	2.50	0.42
2:F:43:LEU:HB3	2:F:44:ARG:H	1.50	0.42
1:A:38:PHE:HA	1:A:39:PRO:HD2	1.90	0.42
3:C:169:GLY:C	3:C:170:LEU:HG	2.39	0.42
1:A:102:ASN:HD22	2:B:31:ASN:HD21	1.67	0.42
2:F:37:GLN:HG3	2:F:91:PHE:CD1	2.55	0.42
3:G:107:CYS:O	3:G:109:VAL:HG23	2.20	0.42
3:C:122:LEU:HD12	3:C:175:LEU:HD21	2.00	0.42
1:E:19:ILE:HG12	1:E:76:HIS:CE1	2.54	0.42
4:D:60:TYR:HB2	5:P:143:ILE:HD11	2.01	0.42
3:G:15:SER:HB2	3:G:70:LEU:CD2	2.49	0.42
4:H:142:VAL:HG22	4:H:161:LEU:HD12	2.02	0.42
4:H:50:VAL:HG23	4:H:51:THR:N	2.33	0.42
3:C:172:GLU:H	3:C:172:GLU:HG3	1.63	0.42
3:C:160:ILE:C	3:C:160:ILE:HD12	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:135:THR:OG1	3:G:138:PHE:HE1	2.02	0.41
3:G:135:THR:OG1	3:G:147:LYS:HG2	2.20	0.41
1:A:45:LEU:CG	1:A:46:LEU:N	2.83	0.41
1:E:34:TRP:NE1	1:E:73:LEU:HD21	2.31	0.41
2:B:83:THR:C	2:B:85:SER:H	2.22	0.41
2:B:18:LYS:HG2	2:B:80:GLU:HA	2.02	0.41
1:A:38:PHE:O	1:A:39:PRO:C	2.58	0.41
3:G:6:VAL:O	3:G:26:PHE:HA	2.19	0.41
4:H:119:VAL:O	4:H:156:GLN:HA	2.20	0.41
4:H:87:THR:HG22	4:H:88:PRO:N	2.35	0.41
4:D:87:THR:CA	4:D:91:LEU:HD12	2.39	0.41
1:E:47:ILE:CG2	1:E:64:ILE:HG13	2.49	0.41
1:A:22:CYS:CB	1:A:73:LEU:HD23	2.48	0.41
4:D:149:ARG:HG3	4:D:155:PHE:HE2	1.82	0.41
1:A:101:PHE:HZ	5:P:141:GLU:HG2	1.85	0.41
2:F:23:CYS:O	2:F:74:ASN:HA	2.20	0.41
4:D:34:ARG:CG	4:D:34:ARG:NH1	2.66	0.41
4:H:151:GLY:C	4:H:153:TRP:H	2.23	0.41
2:B:83:THR:C	2:B:85:SER:N	2.74	0.41
4:H:45:GLY:O	4:H:46:GLU:HB3	2.21	0.41
3:C:104:THR:HA	3:C:152:THR:HA	2.01	0.41
4:H:18:THR:OG1	4:H:23:ARG:HD3	2.21	0.41
3:G:56:PRO:O	3:G:57:GLN:C	2.57	0.41
3:C:107:CYS:HB2	3:C:121:TRP:CH2	2.56	0.41
8:H:202:NDG:O6	8:H:202:NDG:C1	2.68	0.41
1:E:101:PHE:HA	4:H:70:ARG:NH2	2.35	0.41
4:H:27:VAL:HG22	4:H:41:ASP:OD1	2.21	0.41
4:H:12:GLN:O	4:H:28:ILE:HA	2.20	0.41
3:G:119:ILE:HA	3:G:164:LYS:O	2.21	0.41
4:H:171:TYR:CD2	4:H:190:ALA:HB2	2.56	0.41
2:B:98:GLY:O	2:B:99:ARG:HB2	2.21	0.41
2:B:93:ALA:HA	2:B:107:PHE:O	2.19	0.41
4:H:140:VAL:C	4:H:142:VAL:H	2.24	0.41
4:H:87:THR:HA	4:H:91:LEU:HB2	2.03	0.41
4:D:163:MET:HB2	4:D:164:THR:H	1.66	0.41
4:D:30:TYR:HB2	4:D:38:VAL:HG12	2.02	0.41
1:A:49:ILE:HD11	1:A:55:LYS:C	2.41	0.41
3:G:101:GLN:O	3:G:155:PRO:HD2	2.20	0.41
4:H:59:GLU:H	4:H:59:GLU:HG3	1.63	0.41
1:E:26:ASP:OD2	1:E:28:THR:HB	2.20	0.41
4:H:12:GLN:HB3	4:H:14:PHE:CE2	2.56	0.41
3:G:144:SER:CB	4:H:34:ARG:NH1	2.81	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:164:LYS:HE2	3:G:166:GLU:HG3	2.01	0.41
3:G:48:PHE:CE2	4:H:89:THR:HB	2.55	0.41
2:F:36:ARG:O	2:F:43:LEU:O	2.39	0.41
4:H:118:SER:HA	4:H:158:LEU:HA	2.03	0.41
4:D:26:LEU:HD12	4:D:27:VAL:N	2.36	0.41
4:H:106:THR:HG22	4:H:107:GLU:HG2	2.01	0.41
2:B:12:VAL:HG12	2:B:13:ALA:N	2.35	0.41
4:H:21:THR:HG21	4:H:84:GLU:HG2	2.02	0.41
4:H:21:THR:CB	4:H:24:ILE:HD11	2.49	0.41
4:H:20:GLY:HA2	4:H:83:TYR:OH	2.21	0.41
3:G:26:PHE:CZ	4:H:86:GLU:HG3	2.55	0.41
2:B:6:GLN:HG3	2:B:111:GLY:H	1.86	0.41
2:F:18:LYS:HG3	2:F:80:GLU:HA	2.02	0.41
4:H:25:ARG:HD2	4:H:43:ASP:CG	2.41	0.41
3:G:36:LEU:HD13	3:G:63:ILE:HG13	2.01	0.41
4:D:14:PHE:N	4:D:27:VAL:O	2.54	0.41
3:C:121:TRP:CD1	3:C:132:VAL:HG13	2.56	0.41
3:C:35:ASP:O	3:C:39:LYS:N	2.54	0.41
3:G:77:SER:HB3	4:H:32:TYR:CE2	2.56	0.41
4:H:99:VAL:HG22	4:H:175:VAL:HG21	2.03	0.41
3:G:52:ARG:HH12	4:H:86:GLU:HA	1.86	0.41
4:D:169:GLU:HG3	4:D:169:GLU:H	1.76	0.41
3:C:135:THR:CG2	3:C:150:TYR:HE2	2.33	0.41
2:B:9:ARG:NH2	2:B:110:PRO:HB2	2.35	0.41
2:B:37:GLN:HG2	2:B:43:LEU:HD11	2.02	0.41
3:G:129:THR:CG2	3:G:129:THR:O	2.66	0.41
3:C:82:ALA:HB2	4:D:33:ASN:OD1	2.20	0.41
2:F:38:ASP:O	2:F:40:GLY:N	2.54	0.41
2:B:65:TYR:HE2	2:B:90:TYR:CE2	2.39	0.41
1:A:31:TYR:HA	1:A:49:ILE:O	2.21	0.41
1:E:51:LEU:HD12	4:H:77:THR:CG2	2.51	0.41
3:G:120:THR:O	3:G:164:LYS:N	2.51	0.41
3:G:137:PHE:CE2	3:G:147:LYS:HE2	2.56	0.41
4:D:111:HIS:O	4:D:164:THR:HG23	2.20	0.41
4:D:145:THR:CG2	4:D:158:LEU:O	2.68	0.41
3:G:68:HIS:CD2	5:Q:141:GLU:HB2	2.56	0.41
4:D:21:THR:HG21	4:D:84:GLU:CD	2.42	0.41
1:E:31:TYR:CD1	4:H:70:ARG:HD3	2.56	0.40
3:G:76:ARG:NH2	4:H:57:ASP:CG	2.74	0.40
1:A:34:TRP:O	1:A:45:LEU:HD12	2.21	0.40
3:C:150:TYR:N	3:C:150:TYR:CD2	2.89	0.40
3:C:104:THR:OG1	3:C:152:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:14:GLN:HB3	4:D:6:HIS:NE2	2.36	0.40
3:G:132:VAL:HG12	3:G:133:TYR:N	2.36	0.40
5:Q:135:ARG:HG2	5:Q:136:GLY:O	2.21	0.40
3:G:142:ASP:O	3:G:143:TYR:CB	2.69	0.40
4:H:125:ALA:O	4:H:126:LYS:C	2.60	0.40
4:H:147:LEU:HD11	4:H:155:PHE:CG	2.57	0.40
2:F:18:LYS:CG	2:F:80:GLU:HA	2.52	0.40
3:C:2:GLU:HG2	3:C:3:ALA:H	1.86	0.40
4:H:134:ASN:HD21	4:H:169:GLU:CG	2.31	0.40
4:H:124:PRO:HB2	4:H:125:ALA:H	1.66	0.40
1:A:30:ASP:CA	1:A:51:LEU:HD21	2.36	0.40
3:G:123:ARG:HG3	3:G:161:TYR:CE2	2.56	0.40
4:H:118:SER:HA	4:H:158:LEU:CB	2.47	0.40
3:C:84:ASN:ND2	3:C:168:TRP:HB3	2.36	0.40
4:D:189:ARG:O	4:D:190:ALA:O	2.39	0.40
3:G:177:HIS:CD2	3:G:178:TRP:N	2.89	0.40
3:G:53:ARG:N	5:Q:134:HIS:NE2	2.69	0.40
3:G:48:PHE:CZ	4:H:90:SER:N	2.90	0.40
1:A:45:LEU:CD1	1:A:46:LEU:N	2.80	0.40
2:F:12:VAL:HG13	2:F:116(A):LEU:HG	2.04	0.40
3:G:65:THR:CG2	5:Q:140:TRP:O	2.66	0.40
3:C:68:HIS:NE2	3:C:72:ILE:CD1	2.81	0.40
3:C:1:ILE:CD1	4:D:25:ARG:HH21	2.35	0.40
3:G:84:ASN:ND2	3:G:168:TRP:CB	2.83	0.40
4:H:121:ASP:OD1	4:H:121:ASP:N	2.54	0.40
1:E:29:PHE:CD1	1:E:29:PHE:N	2.90	0.40
3:G:150:TYR:N	3:G:150:TYR:CD2	2.89	0.40
3:G:26:PHE:C	3:G:28:GLY:H	2.24	0.40
4:H:149:ARG:HA	4:H:155:PHE:CD2	2.56	0.40
3:C:148:LEU:HD22	4:D:150:ASN:O	2.21	0.40
2:B:48:TYR:HH	3:C:57:GLN:CD	2.25	0.40
4:D:99:VAL:CG1	4:D:175:VAL:HG21	2.45	0.40
3:G:156:SER:O	3:G:180:PRO:HG2	2.21	0.40
4:D:114:THR:HG23	4:D:162:GLU:CA	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	108/110 (98%)	80 (74%)	12 (11%)	16 (15%)	0	1
1	E	108/110 (98%)	82 (76%)	17 (16%)	9 (8%)	1	9
2	B	110/112 (98%)	77 (70%)	19 (17%)	14 (13%)	0	3
2	F	110/112 (98%)	79 (72%)	15 (14%)	16 (14%)	0	2
3	C	181/183 (99%)	161 (89%)	15 (8%)	5 (3%)	8	44
3	G	181/183 (99%)	133 (74%)	33 (18%)	15 (8%)	1	9
4	D	186/188 (99%)	145 (78%)	30 (16%)	11 (6%)	2	20
4	H	186/188 (99%)	129 (69%)	33 (18%)	24 (13%)	0	3
5	P	14/16 (88%)	12 (86%)	1 (7%)	1 (7%)	2	13
5	Q	14/16 (88%)	9 (64%)	1 (7%)	4 (29%)	0	0
All	All	1198/1218 (98%)	907 (76%)	176 (15%)	115 (10%)	1	7

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	14	GLU
1	A	68	LYS
1	A	71	LYS
1	A	103	LYS
2	B	43	LEU
2	B	73	GLU
3	C	179	GLU
1	E	16	GLU
1	E	68	LYS
2	F	7	SER
2	F	28	ASN
2	F	52	ALA
2	F	71	SER
2	F	73	GLU
2	F	99	ARG

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Mol	Chain	Res	Type
2	F	116(B)	GLY
3	G	49	ALA
3	G	50	GLN
3	G	51	LEU
3	G	180	PRO
4	H	34	ARG
4	H	58	ALA
4	H	79	CYS
4	H	97	PRO
4	H	108	ALA
4	H	110	ASN
4	H	126	LYS
4	H	188	TRP
4	H	189	ARG
5	Q	144	GLU
1	A	31	TYR
1	A	46	LEU
1	A	47	ILE
1	A	88	TYR
1	A	99	GLY
1	A	102	ASN
2	B	27	ASN
2	B	39	THR
2	B	44	ARG
2	B	62	ASP
2	B	71	SER
2	B	116(B)	GLY
3	C	3	ALA
4	D	4	GLU
4	D	102	SER
4	D	103	LEU
1	E	8	GLN
2	F	82	ALA
3	G	46	PRO
3	G	47	GLU
4	H	5	ARG
4	H	64	GLN
4	H	80	ARG
4	H	121	ASP
4	H	165	PRO
1	A	9	SER
1	A	80	SER

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Mol	Chain	Res	Type
2	B	7	SER
2	B	72	GLN
2	B	96	GLY
2	B	116(A)	LEU
3	C	99	LEU
3	C	155	PRO
4	D	64	GLN
4	D	189	ARG
5	P	145	SER
1	E	17	THR
2	F	15	THR
2	F	18	LYS
2	F	104	ALA
3	G	115	PRO
4	H	3	SER
4	H	56	PRO
4	H	104	SER
4	H	118	SER
4	H	183	PRO
5	Q	143	ILE
1	A	116	PRO
2	B	30	ASN
3	C	173	PRO
4	D	5	ARG
1	E	7	PRO
1	E	9	SER
1	E	80	SER
1	E	109	GLY
2	F	39	THR
2	F	44	ARG
2	F	46	ILE
3	G	137	PHE
3	G	143	TYR
4	H	33	ASN
4	H	124	PRO
5	Q	141	GLU
4	D	81	HIS
4	D	134	ASN
4	D	183	PRO
3	G	113	PHE
4	H	19	ASN
4	H	125	ALA

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Mol	Chain	Res	Type
5	Q	137	ALA
1	A	15	GLY
1	A	39	PRO
4	D	118	SER
4	D	163	MET
2	F	10	ASN
2	B	61	PRO
3	G	72	ILE
4	H	100	VAL
1	E	52	VAL
2	F	96	GLY
3	G	96	PRO
3	G	97	VAL
3	G	155	PRO
3	G	87	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	96/96 (100%)	75 (78%)	21 (22%)	1	7
1	E	96/96 (100%)	72 (75%)	24 (25%)	1	3
2	B	91/91 (100%)	66 (72%)	25 (28%)	0	2
2	F	91/91 (100%)	72 (79%)	19 (21%)	1	8
3	C	166/166 (100%)	135 (81%)	31 (19%)	2	11
3	G	166/166 (100%)	126 (76%)	40 (24%)	1	4
4	D	174/174 (100%)	130 (75%)	44 (25%)	1	3
4	H	174/174 (100%)	119 (68%)	55 (32%)	0	1
5	P	11/11 (100%)	5 (46%)	6 (54%)	0	0
5	Q	11/11 (100%)	7 (64%)	4 (36%)	0	0
All	All	1076/1076 (100%)	807 (75%)	269 (25%)	1	3

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	12	VAL
1	A	27	SER
1	A	28	THR
1	A	30	ASP
1	A	32	PHE
1	A	36	ARG
1	A	49	ILE
1	A	50	SER
1	A	51	LEU
1	A	61	ARG
1	A	69	ARG
1	A	73	LEU
1	A	75	LEU
1	A	80	SER
1	A	85	SER
1	A	100	SER
1	A	104	LEU
1	A	112	LEU
1	A	114	VAL
1	A	117	TYR
2	B	6	GLN
2	B	7	SER
2	B	18	LYS
2	B	19	VAL
2	B	20	THR
2	B	21	LEU
2	B	25	GLN
2	B	26	THR
2	B	31	ASN
2	B	41	HIS
2	B	43	LEU
2	B	44	ARG
2	B	45	LEU
2	B	46	ILE
2	B	49	SER
2	B	54	SER
2	B	56	GLU
2	B	69	ARG
2	B	73	GLU
2	B	78	ILE
2	B	81	LEU
2	B	86	GLN

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Mol	Chain	Res	Type
2	B	97	GLN
2	B	99	ARG
2	B	105	GLU
3	C	21	GLN
3	C	23	THR
3	C	24	PHE
3	C	36	LEU
3	C	38	LYS
3	C	39	LYS
3	C	41	THR
3	C	55	GLU
3	C	57	GLN
3	C	62	ASN
3	C	65	THR
3	C	73	LEU
3	C	74	THR
3	C	75	LYS
3	C	78	ASN
3	C	88	GLN
3	C	95	SER
3	C	98	LEU
3	C	99	LEU
3	C	103	ASN
3	C	120	THR
3	C	127	SER
3	C	128	VAL
3	C	132	VAL
3	C	135	THR
3	C	147	LYS
3	C	167	HIS
3	C	170	LEU
3	C	172	GLU
3	C	179	GLU
3	C	182	ILE
4	D	4	GLU
4	D	18	THR
4	D	22	GLN
4	D	31	ILE
4	D	34	ARG
4	D	51	THR
4	D	59	GLU
4	D	63	LYS

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Mol	Chain	Res	Type
4	D	64	GLN
4	D	69	GLU
4	D	75	LEU
4	D	85	THR
4	D	93	ARG
4	D	98	SER
4	D	99	VAL
4	D	104	SER
4	D	105	ARG
4	D	109	LEU
4	D	113	ASN
4	D	119	VAL
4	D	120	THR
4	D	121	ASP
4	D	136	GLN
4	D	138	GLU
4	D	143	SER
4	D	145	THR
4	D	147	LEU
4	D	157	VAL
4	D	158	LEU
4	D	159	VAL
4	D	160	MET
4	D	161	LEU
4	D	162	GLU
4	D	163	MET
4	D	164	THR
4	D	166	ARG
4	D	169	GLU
4	D	171	TYR
4	D	181	LYS
4	D	182	SER
4	D	184	ILE
4	D	185	THR
4	D	186	VAL
4	D	187	GLU
5	P	133	SER
5	P	134	HIS
5	P	141	GLU
5	P	143	ILE
5	P	144	GLU
5	P	145	SER

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Mol	Chain	Res	Type
1	E	4	ARG
1	E	8	GLN
1	E	9	SER
1	E	13	TRP
1	E	26	ASP
1	E	27	SER
1	E	36	ARG
1	E	42	SER
1	E	45	LEU
1	E	47	ILE
1	E	49	ILE
1	E	53	SER
1	E	56	LYS
1	E	61	ARG
1	E	70	GLU
1	E	73	LEU
1	E	74	SER
1	E	78	THR
1	E	80	SER
1	E	85	SER
1	E	90	CYS
1	E	93	THR
1	E	100	SER
1	E	103	LYS
2	F	4	VAL
2	F	6	GLN
2	F	7	SER
2	F	8	PRO
2	F	9	ARG
2	F	25	GLN
2	F	36	ARG
2	F	39	THR
2	F	41	HIS
2	F	46	ILE
2	F	49	SER
2	F	73	GLU
2	F	78	ILE
2	F	83	THR
2	F	86	GLN
2	F	88	SER
2	F	92	CYS
2	F	94	SER

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Mol	Chain	Res	Type
2	F	105	GLU
3	G	2	GLU
3	G	8	SER
3	G	11	THR
3	G	15	SER
3	G	18	ASP
3	G	23	THR
3	G	24	PHE
3	G	31	LEU
3	G	42	VAL
3	G	45	LEU
3	G	48	PHE
3	G	50	GLN
3	G	51	LEU
3	G	53	ARG
3	G	57	GLN
3	G	63	ILE
3	G	72	ILE
3	G	76	ARG
3	G	79	SER
3	G	88	GLN
3	G	94	LYS
3	G	97	VAL
3	G	104	THR
3	G	117	ILE
3	G	120	THR
3	G	126	LYS
3	G	127	SER
3	G	135	THR
3	G	137	PHE
3	G	141	ARG
3	G	149	SER
3	G	152	THR
3	G	153	PHE
3	G	158	ASP
3	G	160	ILE
3	G	172	GLU
3	G	175	LEU
3	G	176	LYS
3	G	179	GLU
3	G	182	ILE
4	H	3	SER

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Mol	Chain	Res	Type
4	H	4	GLU
4	H	5	ARG
4	H	8	VAL
4	H	18	THR
4	H	22	GLN
4	H	23	ARG
4	H	26	LEU
4	H	28	ILE
4	H	32	TYR
4	H	37	TYR
4	H	39	ARG
4	H	42	SER
4	H	51	THR
4	H	53	LEU
4	H	55	ARG
4	H	59	GLU
4	H	63	LYS
4	H	68	LEU
4	H	72	ARG
4	H	75	LEU
4	H	76	ASP
4	H	86	GLU
4	H	93	ARG
4	H	94	LEU
4	H	95	GLU
4	H	100	VAL
4	H	102	SER
4	H	103	LEU
4	H	105	ARG
4	H	109	LEU
4	H	113	ASN
4	H	118	SER
4	H	120	THR
4	H	121	ASP
4	H	126	LYS
4	H	130	ARG
4	H	132	PHE
4	H	133	ARG
4	H	136	GLN
4	H	137	GLU
4	H	139	THR
4	H	142	VAL

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Mol	Chain	Res	Type
4	H	143	SER
4	H	147	LEU
4	H	158	LEU
4	H	159	VAL
4	H	161	LEU
4	H	162	GLU
4	H	172	THR
4	H	176	GLU
4	H	180	LEU
4	H	182	SER
4	H	184	ILE
4	H	189	ARG
5	Q	133	SER
5	Q	134	HIS
5	Q	135	ARG
5	Q	143	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	8	GLN
1	A	37	GLN
1	A	76	HIS
2	B	25	GLN
2	B	31	ASN
2	B	37	GLN
3	C	57	GLN
3	C	84	ASN
3	C	103	ASN
4	D	82	ASN
4	D	113	ASN
4	D	156	GLN
1	E	5	GLN
1	E	8	GLN
1	E	37	GLN
1	E	76	HIS
1	E	102	ASN
2	F	29	HIS
2	F	41	HIS
3	G	14	GLN
3	G	57	GLN

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Mol	Chain	Res	Type
3	G	84	ASN
4	H	10	GLN
4	H	22	GLN
4	H	82	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NDG	C	211	3,7	12,14,15	0.55	0	15,19,21	0.67	0
7	NDG	C	212	7	12,14,15	0.43	0	15,19,21	0.77	0
7	NDG	D	201	4,7	12,14,15	0.55	0	15,19,21	0.78	0
7	NDG	D	202	7	12,14,15	0.52	0	15,19,21	0.77	0
7	NDG	G	211	3,7	12,14,15	0.65	0	15,19,21	0.70	0
7	NDG	G	212	7	12,14,15	0.47	0	15,19,21	0.76	0
8	NAG	H	201	8,4	12,14,15	0.67	0	15,19,21	1.43	3 (20%)
8	NDG	H	202	8	12,14,15	0.58	0	15,19,21	0.88	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NDG	C	211	3,7	-	0/6/23/26	0/1/1/1
7	NDG	C	212	7	-	0/6/23/26	0/1/1/1
7	NDG	D	201	4,7	-	0/6/23/26	0/1/1/1
7	NDG	D	202	7	-	0/6/23/26	0/1/1/1
7	NDG	G	211	3,7	-	0/6/23/26	0/1/1/1
7	NDG	G	212	7	-	0/6/23/26	0/1/1/1
8	NAG	H	201	8,4	-	0/6/23/26	0/1/1/1
8	NDG	H	202	8	-	0/6/23/26	1/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	201	NAG	C3-C4-C5	3.27	116.04	110.20
8	H	201	NAG	C3-C2-N2	-2.45	108.02	111.76
8	H	201	NAG	C4-C3-C2	2.25	116.83	111.32
8	H	202	NDG	C2-N2-C7	-2.13	119.50	123.09

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	H	202	NDG	C1-C2-C3-C4-C5-O

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NDG	C	201	3	12,14,15	0.43	0	15,19,21	0.71	1 (6%)
6	NDG	G	201	3	12,14,15	0.57	0	15,19,21	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NDG	C	201	3	-	0/6/23/26	1/1/1/1
6	NDG	G	201	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	201	NDG	C2-N2-C7	-2.01	119.72	123.09

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	201	NDG	C1-C2-C3-C4-C5-O

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	110/110 (100%)	-0.30	1 (0%) 81 32	23, 43, 73, 96	0
1	E	110/110 (100%)	-0.26	0 100 100	31, 52, 79, 94	0
2	B	112/112 (100%)	-0.30	0 100 100	29, 48, 69, 91	0
2	F	112/112 (100%)	-0.19	0 100 100	28, 51, 81, 100	0
3	C	183/183 (100%)	-0.33	0 100 100	20, 44, 86, 100	0
3	G	183/183 (100%)	-0.02	1 (0%) 88 46	41, 84, 100, 100	0
4	D	188/188 (100%)	-0.15	4 (2%) 60 15	18, 48, 100, 100	0
4	H	188/188 (100%)	0.16	10 (5%) 25 5	49, 91, 100, 100	0
5	P	16/16 (100%)	0.02	0 100 100	28, 48, 96, 100	0
5	Q	16/16 (100%)	0.17	0 100 100	57, 73, 99, 100	0
All	All	1218/1218 (100%)	-0.14	16 (1%) 67 24	18, 58, 100, 100	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	107	GLU	3.5
4	D	112	HIS	3.4
4	D	111	HIS	3.4
4	H	111	HIS	3.4
4	H	168	GLY	3.1
4	H	106	THR	2.5
4	H	105	ARG	2.5
4	H	167	ARG	2.3
3	G	2	GLU	2.3
4	H	2	GLY	2.3
1	A	117	TYR	2.2
4	H	110	ASN	2.2
4	D	105	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
4	H	108	ALA	2.1
4	H	190	ALA	2.1
4	D	109	LEU	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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	NDG	D	201	14/15	0.40	-	87,97,100,100	0
7	NDG	G	212	14/15	0.52	-	98,100,100,100	0
8	NAG	H	201	14/15	0.66	-	92,100,100,100	0
7	NDG	G	211	14/15	0.36	-	93,100,100,100	0
7	NDG	C	212	14/15	0.36	-	98,100,100,100	0
8	NDG	H	202	14/15	0.69	-	97,100,100,100	0
7	NDG	C	211	14/15	0.32	-	80,90,100,100	0
7	NDG	D	202	14/15	0.70	-	98,100,100,100	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NDG	C	201	14/15	0.64	-	95,100,100,100	0
6	NDG	G	201	14/15	0.65	-	97,100,100,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.