



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:38 PM GMT

PDB ID : 1BQH  
Title : MURINE CD8AA ECTODOMAIN FRAGMENT IN COMPLEX WITH H-2KB/VSV8  
Authors : Wang, J.H.; Reinherz, E.L.; Kern, P.S.; Chang, H.C.  
Deposited on : 1998-08-16  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

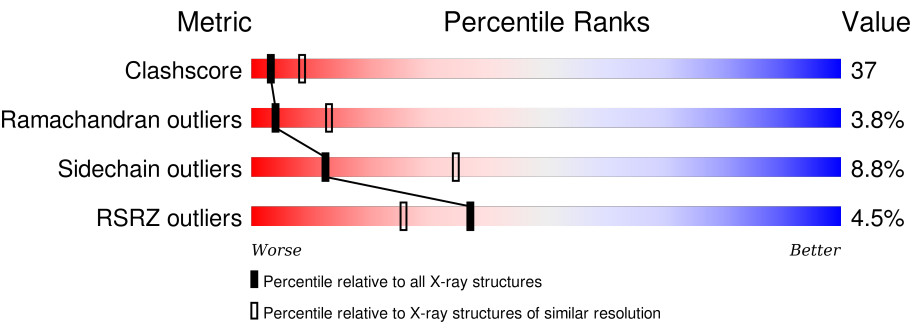
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	274	<div><div></div><div><div></div><div>50%</div><div>45%</div><div>6%</div></div></div>
1	D	274	<div><div></div><div><div></div><div>50%</div><div>43%</div><div>6%</div><div>.</div></div></div>
2	B	99	<div><div></div><div><div></div><div>51%</div><div>46%</div><div>.</div></div></div>
2	E	99	<div><div></div><div><div></div><div>51%</div><div>45%</div><div>.</div></div></div>
3	C	8	<div><div></div><div><div></div><div>63%</div><div>38%</div></div></div>
3	F	8	<div><div></div><div><div></div><div>25%</div><div>63%</div><div>13%</div></div></div>
4	G	129	<div><div>16%</div><div><div></div><div>38%</div><div>44%</div><div>11%</div><div>.</div><div>5%</div></div></div>

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Mol	Chain	Length	Quality of chain
4	H	129	
4	I	129	
4	K	129	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NDG	G	130	-	-	X	X
6	NAG	I	130	X	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10204 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 PROTEIN (H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			
1	D	274	Total	C	N	O	S	0	0	0
			2232	1408	393	422	9			

- Molecule 2 is a protein called PROTEIN (BETA-2-MICROGLOBULIN ).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called PROTEIN (VSV8).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			68	44	12	12			
3	F	8	Total	C	N	O	0	0	0
			68	44	12	12			

- Molecule 4 is a protein called PROTEIN (CD8A OR LYT2 OR LYT-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	122	Total	C	N	O	S	0	0	0
			970	623	158	182	7			
4	H	125	Total	C	N	O	S	0	0	0
			987	632	161	187	7			
4	I	122	Total	C	N	O	S	0	0	0
			962	616	156	183	7			

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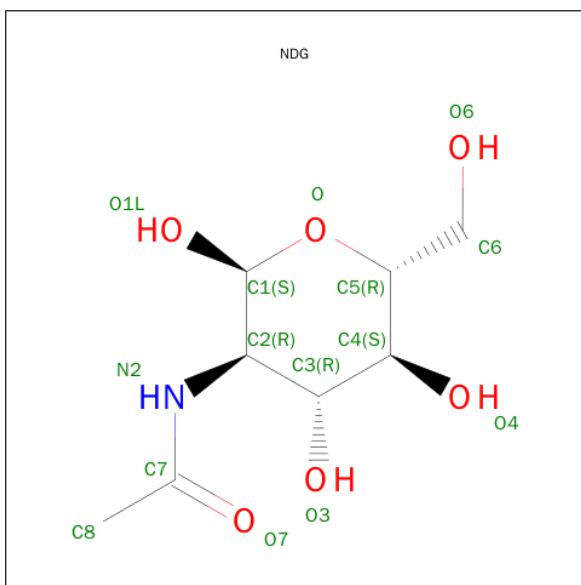
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	125	Total	C	N	O	S	0	0	0
			987	632	161	187	7			

There are 20 discrepancies between the modelled and reference sequences:

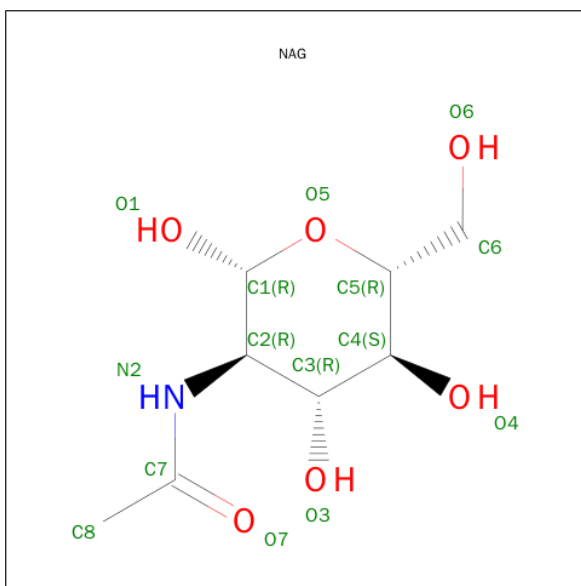
Chain	Residue	Modelled	Actual	Comment	Reference
G	123	SER	ASN	CONFLICT	UNP P01731
G	125	ALA	THR	CONFLICT	UNP P01731
G	126	ASP	THR	CONFLICT	UNP P01731
G	127	LEU	THR	CONFLICT	UNP P01731
G	128	VAL	LYS	CONFLICT	UNP P01731
H	123	SER	ASN	CONFLICT	UNP P01731
H	125	ALA	THR	CONFLICT	UNP P01731
H	126	ASP	THR	CONFLICT	UNP P01731
H	127	LEU	THR	CONFLICT	UNP P01731
H	128	VAL	LYS	CONFLICT	UNP P01731
I	123	SER	ASN	CONFLICT	UNP P01731
I	125	ALA	THR	CONFLICT	UNP P01731
I	126	ASP	THR	CONFLICT	UNP P01731
I	127	LEU	THR	CONFLICT	UNP P01731
I	128	VAL	LYS	CONFLICT	UNP P01731
K	123	SER	ASN	CONFLICT	UNP P01731
K	125	ALA	THR	CONFLICT	UNP P01731
K	126	ASP	THR	CONFLICT	UNP P01731
K	127	LEU	THR	CONFLICT	UNP P01731
K	128	VAL	LYS	CONFLICT	UNP P01731

- Molecule 5 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

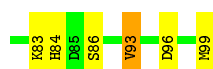
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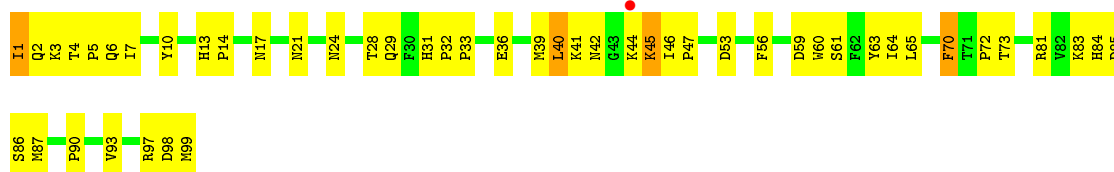
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	K	1	Total	C	N	O	0	0
			14	8	1	5		



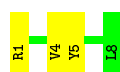




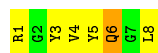
- Molecule 2: PROTEIN (BETA-2-MICROGLOBULIN )



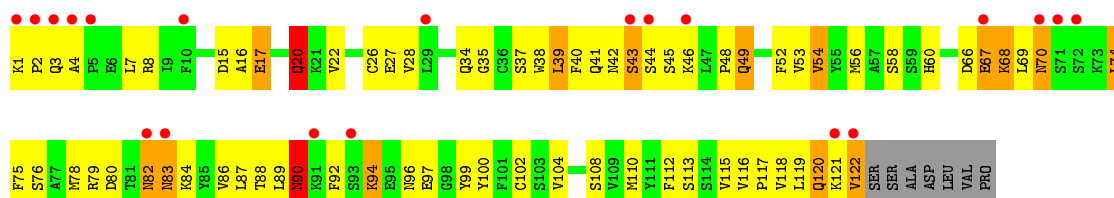
- Molecule 3: PROTEIN (VSV8)



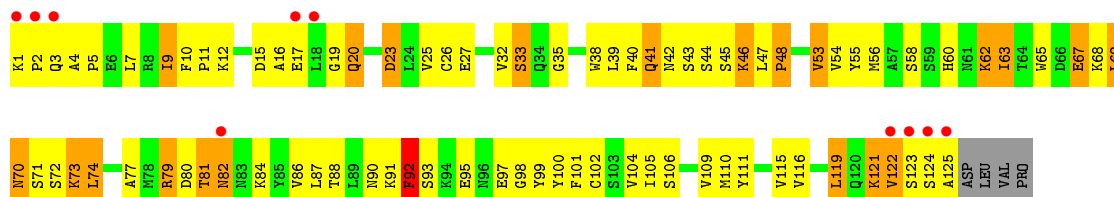
- Molecule 3: PROTEIN (VSV8)



- Molecule 4: PROTEIN (CD8A OR LYT2 OR LYT-2)

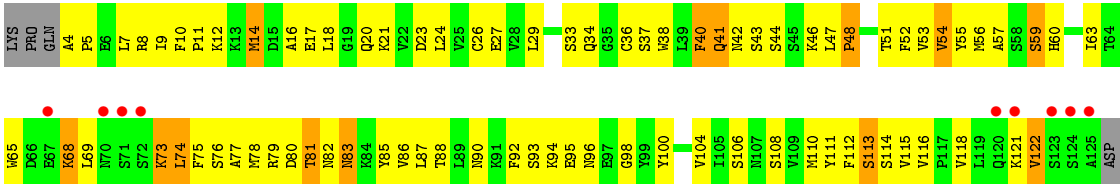


- Molecule 4: PROTEIN (CD8A OR LYT2 OR LYT-2)



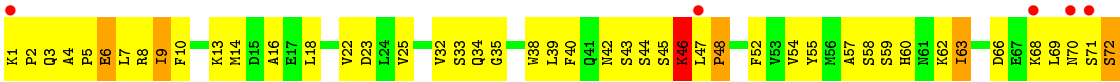
- Molecule 4: PROTEIN (CD8A OR LYT2 OR LYT-2)





LEU  
VAL  
PRO

● Molecule 4: PROTEIN (CD8A OR LYT2 OR LYT-2)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.90 Å 98.40 Å 170.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 28.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.5 (15.00-2.80) 89.6 (28.84-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.80 Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.212 , 0.296 0.225 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 32529 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10204	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.24 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.3207e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.44	0/2293	0.60	0/3113
1	D	0.44	0/2293	0.60	0/3113
2	B	0.48	0/847	0.67	0/1148
2	E	0.45	0/847	0.64	1/1148 (0.1%)
3	C	0.55	0/69	0.66	0/90
3	F	0.51	0/69	0.64	0/90
4	G	0.51	0/992	0.82	2/1340 (0.1%)
4	H	0.52	0/1009	0.80	1/1363 (0.1%)
4	I	0.56	0/983	0.75	0/1328
4	K	0.51	0/1009	0.79	1/1363 (0.1%)
All	All	0.48	0/10411	0.69	5/14096 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	122	VAL	N-CA-C	7.27	130.64	111.00
4	G	20	GLN	N-CA-C	5.71	126.43	111.00
4	H	53	VAL	CB-CA-C	-5.51	100.93	111.40
2	E	1	ILE	CA-C-N	-5.12	105.94	117.20
4	K	122	VAL	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2232	0	2123	146	2
1	D	2232	0	2123	140	0
2	B	821	0	796	54	0
2	E	821	0	796	62	0
3	C	68	0	67	13	0
3	F	68	0	67	13	0
4	G	970	0	972	115	0
4	H	987	0	988	102	2
4	I	962	0	956	96	0
4	K	987	0	988	91	0
5	G	14	0	13	10	0
6	H	14	0	13	5	0
6	I	14	0	13	3	0
6	K	14	0	13	3	0
All	All	10204	0	9928	751	2

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 37.

All (751) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:NH1	2:B:53:ASP:HB3	1.45	1.30
1:D:121:CYS:SG	2:E:1:ILE:HG21	1.76	1.25
4:H:95:GLU:HG3	6:H:130:NAG:O3	1.35	1.22
1:A:35:ARG:NH1	2:B:53:ASP:CB	2.02	1.22
1:A:35:ARG:HH12	2:B:53:ASP:CB	1.58	1.14
1:A:198:LYS:O	1:A:199:VAL:HG23	1.46	1.10
4:G:99:TYR:CE1	4:G:117:PRO:HB3	1.87	1.10
4:K:91:LYS:HG3	4:K:91:LYS:O	1.43	1.09
1:A:169:ARG:CG	1:A:169:ARG:HH11	1.66	1.07
4:G:76:SER:HB2	4:G:88:THR:HG23	1.30	1.07
4:I:44:SER:OG	6:I:130:NAG:H82	1.51	1.06
4:G:2:PRO:O	4:G:4:ALA:N	1.88	1.04
1:A:224:LEU:HA	4:G:34:GLN:HE22	1.22	1.04
4:G:99:TYR:HB3	4:G:115:VAL:CG2	1.88	1.03
1:A:187:ALA:HB1	1:A:272:LEU:HD11	1.36	1.03
4:G:94:LYS:H	4:G:94:LYS:HD2	1.23	1.03
1:D:108:ARG:O	1:D:109:LEU:HD12	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:GLY:HA3	1:D:110:LEU:HD22	1.02	1.01
2:B:96:ASP:HB3	2:B:99:MET:HG3	1.42	1.01
1:D:121:CYS:SG	2:E:1:ILE:HD13	2.02	1.00
4:G:40:PHE:HE1	4:G:42:ASN:OD1	1.44	1.00
1:D:104:GLY:CA	1:D:110:LEU:HD22	1.92	1.00
1:A:169:ARG:HG2	1:A:169:ARG:HH11	1.23	1.00
1:A:9:VAL:HG22	1:A:97:VAL:HG13	1.41	0.99
1:A:130:LEU:HD23	1:A:157:ARG:HG3	1.44	0.97
4:H:79:ARG:HB3	4:H:79:ARG:HH11	1.26	0.97
1:A:35:ARG:NH2	2:B:54:MET:O	1.98	0.96
4:I:42:ASN:OD1	4:I:43:SER:O	1.84	0.95
4:I:4:ALA:HB1	4:I:5:PRO:HD2	1.48	0.95
4:G:40:PHE:CE1	4:G:42:ASN:OD1	2.18	0.95
4:H:95:GLU:HG3	6:H:130:NAG:HO3	1.28	0.95
4:H:95:GLU:CB	6:H:130:NAG:O3	2.15	0.95
4:G:49:GLN:HE21	4:G:49:GLN:HA	1.26	0.95
4:G:99:TYR:HB3	4:G:115:VAL:HG22	1.49	0.95
4:I:59:SER:OG	4:I:60:HIS:ND1	1.99	0.94
1:A:204:TRP:HH2	2:B:99:MET:O	1.50	0.94
4:G:16:ALA:HB1	4:G:20:GLN:CD	1.87	0.94
1:D:108:ARG:C	1:D:109:LEU:HD12	1.89	0.93
1:A:204:TRP:CH2	2:B:99:MET:O	2.21	0.93
4:G:2:PRO:C	4:G:4:ALA:H	1.69	0.93
1:D:104:GLY:HA3	1:D:110:LEU:CD2	1.98	0.93
4:G:22:VAL:HG12	4:G:89:LEU:HB2	1.49	0.93
1:D:28:VAL:HG23	1:D:33:PHE:CD1	2.04	0.93
2:E:36:GLU:HB3	2:E:83:LYS:HB3	1.52	0.92
1:A:70:ASN:HD22	3:C:5:TYR:HD1	1.17	0.92
1:A:70:ASN:ND2	3:C:5:TYR:HD1	1.68	0.91
1:D:106:ASP:N	1:D:106:ASP:OD1	2.04	0.90
4:H:60:HIS:ND1	4:H:62:LYS:HB3	1.85	0.89
1:A:35:ARG:NH1	2:B:53:ASP:HB2	1.86	0.89
2:E:7:ILE:H	2:E:7:ILE:HD12	1.38	0.89
4:I:40:PHE:HE1	4:I:42:ASN:HB3	1.38	0.88
1:A:9:VAL:HG22	1:A:97:VAL:CG1	2.04	0.87
1:A:121:CYS:SG	2:B:1:ILE:HG22	2.15	0.87
1:A:19:GLU:HB3	1:A:20:PRO:HD2	1.54	0.87
4:I:115:VAL:HG11	4:K:48:PRO:O	1.74	0.87
4:G:94:LYS:HD2	4:G:94:LYS:N	1.90	0.86
4:I:106:SER:HB3	4:I:111:TYR:HE2	1.40	0.86
1:A:155:ARG:HH21	3:C:4:VAL:HG13	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:122:VAL:HG23	4:I:122:VAL:O	1.74	0.86
1:D:263:HIS:CD2	1:D:265:GLY:H	1.94	0.86
4:H:63:ILE:H	4:H:63:ILE:HD13	1.39	0.86
1:A:192:HIS:HB2	1:A:200:THR:HG23	1.58	0.85
1:D:87:GLN:NE2	1:D:118:TYR:OH	2.10	0.85
4:K:91:LYS:CG	4:K:91:LYS:O	2.25	0.85
2:E:5:PRO:HG2	2:E:87:MET:CE	2.06	0.85
2:B:2:GLN:HE22	2:B:32:PRO:HD3	1.42	0.85
1:A:35:ARG:HH12	2:B:53:ASP:HB2	1.39	0.85
4:K:120:GLN:O	4:K:122:VAL:HG23	1.77	0.84
4:I:79:ARG:HD3	4:I:85:TYR:CE2	2.11	0.84
4:H:23:ASP:HB3	4:H:88:THR:HG22	1.60	0.84
4:H:53:VAL:HG12	4:H:54:VAL:N	1.93	0.84
2:E:3:LYS:HE3	2:E:29:GLN:HG3	1.59	0.84
4:I:59:SER:HG	4:I:60:HIS:H	1.26	0.84
4:H:53:VAL:HG12	4:H:54:VAL:HB	1.60	0.83
1:D:224:LEU:HA	4:I:34:GLN:HE22	1.42	0.83
4:I:44:SER:HG	6:I:130:NAG:H82	1.40	0.83
4:H:97:GLU:HG3	4:H:119:LEU:HA	1.58	0.83
4:H:46:LYS:H	4:H:46:LYS:HD2	1.43	0.83
1:A:35:ARG:HH12	2:B:53:ASP:HB3	1.18	0.83
4:I:74:LEU:HD23	4:I:74:LEU:H	1.44	0.82
4:G:82:ASN:O	4:G:84:LYS:HG2	1.80	0.82
4:H:60:HIS:CE1	4:H:62:LYS:HB3	2.15	0.82
1:D:224:LEU:HA	4:I:34:GLN:NE2	1.93	0.81
4:G:83:ASN:C	4:G:83:ASN:HD22	1.84	0.81
2:B:36:GLU:HB3	2:B:83:LYS:HB3	1.62	0.81
4:G:99:TYR:CD1	4:G:117:PRO:HB3	2.15	0.81
4:G:97:GLU:HG2	4:G:119:LEU:HD23	1.63	0.81
4:H:99:TYR:HB3	4:H:115:VAL:HG21	1.64	0.80
4:K:63:ILE:HD13	4:K:63:ILE:H	1.46	0.80
1:A:73:SER:O	1:A:76:VAL:HG22	1.81	0.80
1:A:198:LYS:O	1:A:199:VAL:CG2	2.28	0.80
4:G:78:MET:HG2	4:G:86:VAL:CG1	2.11	0.80
4:H:99:TYR:HB3	4:H:115:VAL:CG2	2.12	0.80
4:G:115:VAL:CG1	4:H:47:LEU:HB3	2.12	0.79
4:G:43:SER:O	4:G:45:SER:N	2.16	0.79
1:D:14:ARG:HB3	1:D:17:LEU:HB3	1.64	0.79
4:G:118:VAL:HG23	4:G:118:VAL:O	1.83	0.79
4:G:94:LYS:H	4:G:94:LYS:CD	1.95	0.78
4:G:7:LEU:HD11	4:G:104:VAL:HG22	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:ARG:HH21	2:E:90:PRO:HG3	1.47	0.78
4:I:43:SER:O	4:I:44:SER:HB2	1.83	0.78
1:D:109:LEU:HG	1:D:165:VAL:HG11	1.66	0.77
4:H:5:PRO:HG3	4:H:32:VAL:HG23	1.66	0.76
1:A:215:LEU:HD23	1:A:261:VAL:HG22	1.67	0.76
4:I:40:PHE:CE1	4:I:42:ASN:HB3	2.20	0.76
1:D:56:GLY:HA3	1:D:58:GLU:OE2	1.85	0.76
1:D:73:SER:O	1:D:76:VAL:HG22	1.86	0.76
4:I:73:LYS:HD3	4:I:73:LYS:H	1.49	0.76
2:E:3:LYS:CE	2:E:29:GLN:HG3	2.16	0.76
1:A:224:LEU:HA	4:G:34:GLN:NE2	2.01	0.76
1:A:187:ALA:CB	1:A:272:LEU:HD11	2.14	0.75
4:K:92:PHE:CE1	4:K:118:VAL:HG12	2.22	0.75
1:D:155:ARG:NH2	3:F:4:VAL:O	2.19	0.75
4:I:63:ILE:HD12	4:I:65:TRP:HE1	1.49	0.75
4:I:63:ILE:O	4:I:63:ILE:HG13	1.85	0.74
4:K:18:LEU:HD21	4:K:120:GLN:HE22	1.50	0.74
4:G:43:SER:OG	5:G:130:NDG:C8	2.35	0.74
4:I:106:SER:HB3	4:I:111:TYR:CE2	2.21	0.74
2:B:46:ILE:HG23	2:B:47:PRO:HD2	1.70	0.74
2:B:96:ASP:HB3	2:B:99:MET:CG	2.17	0.73
1:D:234:ARG:NH1	1:D:242:GLN:OE1	2.22	0.73
4:K:40:PHE:HE1	4:K:98:GLY:HA3	1.53	0.73
1:D:182:THR:HB	1:D:264:GLN:HE21	1.54	0.73
4:H:95:GLU:HA	6:H:130:NAG:O3	1.89	0.72
4:I:53:VAL:HG12	4:I:54:VAL:HG22	1.71	0.72
4:H:9:ILE:HD12	4:H:9:ILE:H	1.53	0.72
1:A:121:CYS:SG	2:B:1:ILE:CG2	2.77	0.72
1:D:5:LEU:HB2	1:D:168:LEU:HD13	1.71	0.72
1:A:169:ARG:CG	1:A:169:ARG:NH1	2.39	0.72
1:A:192:HIS:HB2	1:A:200:THR:CG2	2.21	0.71
4:G:40:PHE:HZ	5:G:130:NDG:H6C2	1.56	0.71
4:I:54:VAL:HG21	4:I:87:LEU:HD13	1.72	0.71
4:K:43:SER:HB2	4:K:98:GLY:HA2	1.73	0.71
4:G:115:VAL:HG11	4:H:47:LEU:HB3	1.73	0.71
1:D:28:VAL:HG23	1:D:33:PHE:CE1	2.25	0.70
4:K:18:LEU:HD21	4:K:120:GLN:NE2	2.06	0.70
1:D:35:ARG:NH1	2:E:53:ASP:HB3	2.06	0.70
4:G:16:ALA:HB1	4:G:20:GLN:OE1	1.91	0.70
4:H:53:VAL:HG12	4:H:54:VAL:CB	2.21	0.70
4:K:124:SER:O	4:K:125:ALA:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:95:GLU:CA	6:H:130:NAG:O3	2.40	0.69
1:A:138:MET:HA	1:A:141:LEU:HD23	1.73	0.69
1:D:44:ARG:HG2	1:D:45:TYR:N	2.08	0.69
1:D:121:CYS:SG	2:E:1:ILE:CD1	2.79	0.69
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.74	0.69
2:E:41:LYS:HB2	2:E:46:ILE:HD11	1.73	0.69
4:G:66:ASP:HB3	4:G:69:LEU:HB2	1.75	0.68
4:H:109:VAL:HG23	4:H:111:TYR:CE2	2.28	0.68
1:D:70:ASN:ND2	3:F:5:TYR:CD1	2.61	0.68
1:A:169:ARG:HG2	1:A:169:ARG:NH1	2.04	0.68
4:K:71:SER:O	4:K:73:LYS:N	2.27	0.68
2:E:7:ILE:N	2:E:7:ILE:HD12	2.09	0.68
1:D:108:ARG:C	1:D:109:LEU:CD1	2.62	0.68
1:D:70:ASN:ND2	3:F:5:TYR:HD1	1.91	0.68
4:I:76:SER:HB2	4:I:88:THR:OG1	1.94	0.67
1:A:155:ARG:NH2	3:C:4:VAL:HG13	2.08	0.67
4:G:22:VAL:HG13	4:G:89:LEU:HD13	1.75	0.67
4:K:106:SER:HB3	4:K:111:TYR:HE2	1.58	0.67
4:I:46:LYS:H	4:I:46:LYS:HD3	1.59	0.67
4:G:68:LYS:HE3	4:G:69:LEU:HD22	1.75	0.66
4:I:78:MET:HG3	4:I:86:VAL:CG1	2.25	0.66
4:I:59:SER:OG	4:I:60:HIS:N	2.28	0.66
4:I:44:SER:OG	6:I:130:NAG:C8	2.37	0.66
1:D:104:GLY:H	1:D:110:LEU:HB2	1.60	0.66
4:I:78:MET:HG3	4:I:86:VAL:HG12	1.75	0.66
1:A:135:ALA:HB1	1:A:140:ALA:HB3	1.77	0.66
1:D:29:ASP:O	1:D:30:ASP:HB2	1.95	0.66
4:H:121:LYS:O	4:H:121:LYS:HG3	1.95	0.66
4:H:63:ILE:HD13	4:H:63:ILE:N	2.08	0.66
2:E:32:PRO:CB	2:E:33:PRO:HD2	2.26	0.66
4:H:92:PHE:C	4:H:92:PHE:CD1	2.69	0.66
4:G:80:ASP:HB3	4:G:84:LYS:HB2	1.76	0.66
4:G:43:SER:OG	5:G:130:NDG:H8C1	1.96	0.66
4:G:1:LYS:N	4:G:2:PRO:HD3	2.12	0.65
4:I:57:ALA:HB1	4:I:59:SER:OG	1.95	0.65
4:H:79:ARG:HB3	4:H:79:ARG:NH1	2.06	0.65
4:I:73:LYS:CD	4:I:73:LYS:H	2.09	0.65
4:I:42:ASN:CG	4:I:43:SER:O	2.34	0.65
2:E:5:PRO:HG2	2:E:87:MET:HE1	1.79	0.65
1:D:114:GLN:NE2	1:D:156:LEU:HD21	2.12	0.65
4:K:40:PHE:CE1	4:K:98:GLY:HA3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:97:GLU:HG3	4:K:119:LEU:HA	1.78	0.65
1:A:189:VAL:HG23	1:A:274:TRP:HE3	1.61	0.65
4:H:77:ALA:HB2	4:H:87:LEU:HD12	1.78	0.65
1:D:95:ILE:HA	1:D:117:ALA:O	1.97	0.64
4:K:1:LYS:N	4:K:2:PRO:CD	2.60	0.64
1:A:35:ARG:HH11	2:B:53:ASP:CB	2.08	0.64
1:D:156:LEU:O	1:D:160:LEU:HG	1.97	0.64
1:A:171:TYR:OH	3:C:1:ARG:HB3	1.97	0.64
2:B:7:ILE:HG21	2:B:93:VAL:HG11	1.80	0.64
1:D:194:ARG:HB3	1:D:195:PRO:HD2	1.80	0.64
4:G:121:LYS:O	4:G:122:VAL:HG12	1.99	0.63
1:D:133:TRP:NE1	1:D:153:ALA:HB2	2.13	0.63
4:K:63:ILE:O	4:K:63:ILE:HG12	1.98	0.63
4:H:92:PHE:C	4:H:92:PHE:HD1	2.02	0.63
4:K:100:TYR:O	4:K:116:VAL:HG12	1.98	0.63
1:D:272:LEU:HD22	1:D:272:LEU:H	1.63	0.63
1:A:76:VAL:HG23	1:A:77:ASP:N	2.14	0.62
4:K:101:PHE:HB3	4:K:115:VAL:HA	1.81	0.62
1:A:250:PRO:HG2	1:A:253:LYS:HB3	1.81	0.62
1:D:121:CYS:SG	2:E:1:ILE:CG2	2.70	0.62
2:E:45:LYS:HG3	2:E:46:ILE:N	2.15	0.62
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.81	0.62
2:E:5:PRO:HG2	2:E:87:MET:HE2	1.80	0.62
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.30	0.62
4:G:99:TYR:CB	4:G:115:VAL:CG2	2.73	0.62
4:G:43:SER:HB2	5:G:130:NDG:C7	2.30	0.62
4:I:59:SER:HG	4:I:60:HIS:CE1	2.10	0.62
4:K:92:PHE:HE1	4:K:118:VAL:HG12	1.64	0.62
4:H:82:ASN:O	4:H:84:LYS:HG2	1.99	0.62
4:G:97:GLU:HG2	4:G:119:LEU:CD2	2.30	0.62
1:D:230:LEU:HD12	1:D:230:LEU:C	2.19	0.62
1:A:169:ARG:HG3	1:A:169:ARG:HH11	1.57	0.62
4:G:99:TYR:HB3	4:G:115:VAL:HG23	1.80	0.61
1:D:135:ALA:HB1	1:D:140:ALA:HB3	1.81	0.61
1:A:20:PRO:CG	1:A:75:ARG:HG2	2.31	0.61
2:B:73:THR:HG22	2:B:75:THR:H	1.64	0.61
4:G:40:PHE:CZ	5:G:130:NDG:H6C2	2.36	0.61
4:H:116:VAL:O	4:H:116:VAL:HG23	1.99	0.61
4:G:49:GLN:NE2	4:G:49:GLN:HA	2.08	0.61
4:I:74:LEU:N	4:I:74:LEU:HD23	2.14	0.61
1:D:97:VAL:HG13	1:D:115:GLN:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:106:SER:O	4:H:109:VAL:HG22	2.01	0.60
1:A:98:ILE:HG13	2:B:60:TRP:CZ3	2.35	0.60
4:G:116:VAL:O	4:G:116:VAL:HG23	2.01	0.60
1:A:191:HIS:NE2	1:A:254:GLU:OE1	2.33	0.60
4:H:35:GLY:H	4:H:58:SER:HB3	1.67	0.60
4:I:110:MET:HE2	4:I:112:PHE:CZ	2.37	0.60
1:A:187:ALA:HB1	1:A:272:LEU:CD1	2.22	0.60
1:A:20:PRO:HG2	1:A:75:ARG:HG2	1.82	0.60
4:G:83:ASN:ND2	4:G:83:ASN:C	2.53	0.60
1:A:168:LEU:O	1:A:172:LEU:HB2	2.01	0.60
2:E:13:HIS:HB3	2:E:14:PRO:HD2	1.83	0.60
1:D:173:LYS:O	1:D:176:ASN:ND2	2.35	0.60
4:K:6:GLU:HG3	4:K:6:GLU:O	2.01	0.60
1:A:155:ARG:NH2	3:C:4:VAL:O	2.34	0.60
2:E:32:PRO:O	2:E:84:HIS:HE1	1.85	0.60
4:G:78:MET:HG2	4:G:86:VAL:HG13	1.83	0.60
4:I:4:ALA:HB1	4:I:5:PRO:CD	2.28	0.60
2:E:2:GLN:HE21	2:E:85:ASP:C	2.05	0.60
2:B:46:ILE:CG2	2:B:47:PRO:HD2	2.31	0.60
2:B:32:PRO:O	2:B:84:HIS:HE1	1.84	0.60
4:I:36:CYS:HA	4:I:104:VAL:HG12	1.84	0.59
1:D:25:VAL:HG22	1:D:27:TYR:CE1	2.37	0.59
4:G:67:GLU:OE2	4:H:4:ALA:HB2	2.02	0.59
4:G:120:GLN:HG2	4:G:121:LYS:N	2.17	0.59
1:A:25:VAL:HG22	1:A:27:TYR:CE1	2.37	0.59
4:G:39:LEU:HD23	4:G:52:PHE:HA	1.84	0.59
2:B:84:HIS:HD2	2:B:86:SER:OG	1.86	0.59
4:G:22:VAL:CG1	4:G:89:LEU:HB2	2.29	0.59
2:B:32:PRO:CB	2:B:33:PRO:HD2	2.33	0.59
1:D:175:GLY:O	1:D:179:LEU:HD23	2.03	0.59
4:G:49:GLN:OE1	4:H:115:VAL:HG12	2.02	0.59
4:I:122:VAL:CG2	4:I:122:VAL:O	2.46	0.59
1:D:96:GLN:NE2	2:E:60:TRP:HB3	2.18	0.59
4:I:108:SER:HB3	4:K:55:TYR:CD2	2.38	0.58
4:H:17:GLU:OE1	4:H:20:GLN:NE2	2.35	0.58
1:D:10:THR:HG23	1:D:23:MET:HG3	1.85	0.58
4:K:8:ARG:HB3	4:K:10:PHE:CZ	2.38	0.58
4:K:106:SER:HB3	4:K:111:TYR:CE2	2.37	0.58
1:A:3:HIS:CG	1:A:172:LEU:HD21	2.38	0.58
1:D:176:ASN:HA	1:D:180:LEU:HD23	1.84	0.58
1:D:119:ASP:O	2:E:1:ILE:HD12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:7:ILE:CD1	2:E:7:ILE:H	2.13	0.58
4:H:23:ASP:CB	4:H:88:THR:HG22	2.32	0.58
1:A:184:SER:O	1:A:186:LYS:HE3	2.03	0.58
4:H:91:LYS:NZ	4:H:93:SER:HA	2.19	0.58
4:K:1:LYS:H3	4:K:2:PRO:CD	2.16	0.58
1:A:106:ASP:OD2	1:A:108:ARG:HD3	2.04	0.58
4:I:41:GLN:NE2	4:K:48:PRO:HB2	2.18	0.58
4:K:35:GLY:H	4:K:58:SER:HB3	1.68	0.58
4:H:46:LYS:H	4:H:46:LYS:CD	2.14	0.58
4:G:16:ALA:HB1	4:G:20:GLN:NE2	2.18	0.58
4:H:33:SER:HB3	4:H:106:SER:HB2	1.86	0.58
4:H:121:LYS:O	4:H:123:SER:N	2.37	0.58
1:A:19:GLU:HB3	1:A:20:PRO:CD	2.31	0.57
1:A:163:THR:HG22	3:C:1:ARG:N	2.19	0.57
1:D:96:GLN:HE21	2:E:60:TRP:HB3	1.67	0.57
4:K:16:ALA:O	4:K:120:GLN:HA	2.03	0.57
4:I:94:LYS:C	4:I:96:ASN:H	2.06	0.57
2:E:28:THR:HG22	2:E:63:TYR:HB2	1.86	0.57
4:G:1:LYS:H2	4:G:2:PRO:HD3	1.69	0.57
4:G:28:VAL:HG13	4:G:28:VAL:O	2.04	0.57
4:K:72:SER:O	4:K:73:LYS:HB2	2.04	0.57
4:G:42:ASN:O	4:G:45:SER:OG	2.14	0.57
1:A:164:CYS:O	1:A:168:LEU:HB2	2.05	0.57
4:I:11:PRO:O	4:I:116:VAL:HG11	2.04	0.57
1:A:251:LEU:HD12	1:A:254:GLU:OE2	2.04	0.57
4:K:75:PHE:CD1	4:K:89:LEU:CD2	2.88	0.57
4:K:22:VAL:O	4:K:88:THR:HA	2.05	0.57
1:A:207:GLY:HA2	1:A:240:THR:HB	1.87	0.57
1:A:194:ARG:HG3	1:A:194:ARG:HH11	1.68	0.57
4:I:48:PRO:O	4:K:115:VAL:HG11	2.04	0.57
2:E:3:LYS:HE2	2:E:29:GLN:HE21	1.70	0.57
4:G:43:SER:OG	5:G:130:NDG:H8C3	2.05	0.56
1:A:5:LEU:HB2	1:A:168:LEU:HG	1.87	0.56
1:D:189:VAL:HA	1:D:202:ARG:O	2.05	0.56
1:A:216:THR:O	1:A:259:CYS:HA	2.05	0.56
4:I:40:PHE:O	4:I:51:THR:OG1	2.20	0.56
4:I:54:VAL:HG13	4:I:65:TRP:CD2	2.40	0.56
2:B:57:SER:O	2:B:60:TRP:N	2.35	0.56
4:K:92:PHE:HE2	4:K:120:GLN:HB3	1.70	0.56
4:G:7:LEU:HD23	4:G:28:VAL:HA	1.88	0.56
1:D:152:GLU:HG2	3:F:6:GLN:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:GLU:CG	3:F:6:GLN:HG3	2.36	0.56
1:D:123:TYR:HD2	1:D:124:ILE:HG22	1.70	0.56
4:K:44:SER:CB	6:K:130:NAG:H62	2.36	0.56
1:A:28:VAL:HG23	1:A:33:PHE:CD1	2.41	0.56
4:H:19:GLY:HA2	4:H:91:LYS:HG2	1.87	0.56
1:A:51:TRP:CD1	1:A:178:THR:HG21	2.40	0.56
2:B:73:THR:HG22	2:B:74:GLU:N	2.20	0.56
4:K:57:ALA:HB3	4:K:60:HIS:CD2	2.40	0.56
4:G:1:LYS:N	4:G:2:PRO:CD	2.68	0.56
4:K:66:ASP:OD2	4:K:68:LYS:HB3	2.06	0.56
1:A:187:ALA:O	1:A:188:HIS:HB3	2.06	0.56
4:G:43:SER:CB	5:G:130:NDG:C8	2.83	0.55
1:A:70:ASN:ND2	3:C:5:TYR:CD1	2.60	0.55
4:G:2:PRO:C	4:G:4:ALA:N	2.41	0.55
1:D:35:ARG:HB3	1:D:48:ARG:HD3	1.88	0.55
4:G:43:SER:CB	5:G:130:NDG:C7	2.84	0.55
4:G:22:VAL:O	4:G:22:VAL:HG13	2.06	0.55
1:A:137:ASP:O	1:A:141:LEU:HD22	2.06	0.55
1:D:22:TYR:HB3	1:D:71:GLU:HG3	1.87	0.55
4:H:56:MET:HG2	4:H:63:ILE:HG22	1.87	0.55
4:G:80:ASP:HB3	4:G:84:LYS:CB	2.36	0.55
2:B:40:LEU:N	2:B:40:LEU:HD12	2.21	0.55
1:D:228:MET:HE2	1:D:230:LEU:HD23	1.88	0.55
4:G:7:LEU:HD22	4:G:26:CYS:SG	2.47	0.55
1:D:234:ARG:HD3	2:E:10:TYR:CZ	2.42	0.55
4:I:7:LEU:HD11	4:I:104:VAL:HG22	1.88	0.55
2:E:2:GLN:NE2	2:E:85:ASP:C	2.61	0.55
2:E:81:ARG:HH21	2:E:90:PRO:CG	2.18	0.55
1:D:133:TRP:HE1	1:D:153:ALA:HB2	1.71	0.55
1:A:76:VAL:CG2	1:A:77:ASP:N	2.69	0.54
4:K:8:ARG:HB3	4:K:10:PHE:CE2	2.42	0.54
1:D:230:LEU:O	1:D:230:LEU:HD12	2.08	0.54
1:A:238:ASP:HB2	2:B:12:ARG:HD3	1.89	0.54
4:H:60:HIS:ND1	4:H:62:LYS:CB	2.66	0.54
1:D:97:VAL:HG12	1:D:98:ILE:N	2.23	0.54
4:K:75:PHE:HD1	4:K:89:LEU:CD2	2.19	0.54
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.43	0.54
2:E:24:ASN:HB3	2:E:65:LEU:HD11	1.90	0.54
4:G:115:VAL:O	4:G:115:VAL:HG13	2.08	0.54
4:G:90:ASN:HD22	4:G:90:ASN:N	2.05	0.54
4:I:11:PRO:HD2	4:I:24:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1:LYS:N	4:H:1:LYS:HD2	2.23	0.54
1:A:49:ALA:HB1	1:A:51:TRP:NE1	2.23	0.53
4:I:40:PHE:HE1	4:I:42:ASN:CB	2.16	0.53
4:G:118:VAL:O	4:G:118:VAL:CG2	2.55	0.53
1:A:169:ARG:HG3	1:A:169:ARG:NH1	2.18	0.53
1:D:75:ARG:O	1:D:79:ARG:HG2	2.08	0.53
1:D:252:GLY:N	1:D:254:GLU:OE1	2.41	0.53
4:I:116:VAL:HG23	4:I:116:VAL:O	2.07	0.53
1:D:202:ARG:HD3	1:D:246:SER:HB3	1.90	0.53
4:H:109:VAL:HG21	4:H:111:TYR:OH	2.08	0.53
4:G:22:VAL:HG11	4:G:89:LEU:HD22	1.89	0.53
4:I:54:VAL:HG13	4:I:65:TRP:CE3	2.44	0.53
4:G:83:ASN:ND2	4:G:83:ASN:O	2.39	0.53
1:A:29:ASP:O	1:A:30:ASP:HB2	2.07	0.53
2:B:12:ARG:HG2	2:B:13:HIS:CE1	2.44	0.53
4:I:74:LEU:HG	4:I:75:PHE:CD1	2.43	0.53
1:A:168:LEU:CD2	1:A:172:LEU:HD22	2.38	0.53
1:D:187:ALA:HA	1:D:204:TRP:O	2.09	0.53
4:G:68:LYS:C	4:G:70:ASN:H	2.11	0.53
4:H:40:PHE:CZ	4:H:42:ASN:HA	2.44	0.53
1:A:169:ARG:N	1:A:169:ARG:HD3	2.24	0.53
4:I:8:ARG:HG3	4:I:29:LEU:HD13	1.90	0.53
1:A:11:ALA:HB3	1:A:95:ILE:HG23	1.91	0.52
4:I:55:TYR:CD2	4:K:108:SER:HB3	2.44	0.52
1:D:156:LEU:O	1:D:156:LEU:HD22	2.09	0.52
4:K:103:SER:HA	4:K:111:TYR:O	2.08	0.52
1:A:42:ASN:O	1:A:44:ARG:HG2	2.09	0.52
1:A:51:TRP:HB2	1:A:174:ASN:O	2.09	0.52
2:E:39:MET:O	2:E:46:ILE:HG12	2.10	0.52
2:B:7:ILE:CG2	2:B:93:VAL:HG11	2.39	0.52
4:K:39:LEU:HD22	4:K:52:PHE:HA	1.91	0.52
1:A:57:PRO:O	1:A:61:GLU:HG3	2.10	0.52
4:H:39:LEU:HB2	4:H:101:PHE:CE1	2.45	0.52
4:G:115:VAL:HG13	4:H:47:LEU:HB3	1.91	0.52
1:A:74:PHE:HE1	3:C:5:TYR:HB2	1.75	0.52
2:E:2:GLN:HE21	2:E:86:SER:N	2.08	0.52
2:E:41:LYS:CB	2:E:46:ILE:HD11	2.40	0.52
1:D:114:GLN:HE22	1:D:156:LEU:HD21	1.74	0.52
4:K:1:LYS:N	4:K:2:PRO:HD2	2.24	0.52
1:D:71:GLU:O	1:D:75:ARG:HG3	2.09	0.52
1:D:3:HIS:HA	1:D:29:ASP:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:92:PHE:O	4:G:92:PHE:CD2	2.63	0.52
4:H:74:LEU:HA	4:H:90:ASN:HB2	1.92	0.52
4:I:42:ASN:OD1	4:I:42:ASN:C	2.47	0.52
4:K:1:LYS:H3	4:K:2:PRO:HD3	1.75	0.52
2:E:6:GLN:NE2	4:K:1:LYS:O	2.43	0.52
1:D:98:ILE:HG12	2:E:60:TRP:HZ3	1.75	0.52
4:G:76:SER:HB2	4:G:88:THR:CG2	2.21	0.51
2:B:28:THR:HG22	2:B:63:TYR:HB2	1.91	0.51
1:D:202:ARG:HD2	1:D:244:TRP:CE3	2.45	0.51
2:B:27:VAL:HG11	2:B:35:ILE:HD11	1.91	0.51
4:G:45:SER:OG	4:G:45:SER:O	2.29	0.51
4:K:23:ASP:CG	4:K:88:THR:HG22	2.29	0.51
4:H:115:VAL:HG22	4:H:116:VAL:N	2.25	0.51
1:A:191:HIS:HD2	1:A:274:TRP:NE1	2.08	0.51
4:G:68:LYS:C	4:G:70:ASN:N	2.64	0.51
2:B:6:GLN:OE1	4:H:2:PRO:HA	2.10	0.51
1:D:176:ASN:OD1	1:D:177:ALA:N	2.44	0.51
4:G:99:TYR:CD1	4:G:117:PRO:CB	2.91	0.51
4:I:110:MET:HB2	4:K:52:PHE:CD1	2.45	0.51
4:H:91:LYS:NZ	4:H:93:SER:CB	2.74	0.51
4:K:58:SER:HB3	4:K:85:TYR:OH	2.11	0.51
2:B:27:VAL:HG11	2:B:35:ILE:CD1	2.40	0.51
1:D:185:PRO:HB3	1:D:208:PHE:HB3	1.92	0.51
1:A:202:ARG:HG3	1:A:246:SER:HB3	1.92	0.51
4:K:25:VAL:HG22	4:K:86:VAL:HG13	1.93	0.51
4:G:43:SER:HB3	5:G:130:NDG:N2	2.25	0.51
1:D:135:ALA:HB1	1:D:140:ALA:CB	2.41	0.51
1:A:126:LEU:HD22	1:A:156:LEU:HD23	1.93	0.51
1:D:263:HIS:HD2	1:D:265:GLY:H	1.55	0.50
1:D:224:LEU:CA	4:I:34:GLN:HE22	2.18	0.50
3:F:3:TYR:O	3:F:5:TYR:CD1	2.64	0.50
4:I:16:ALA:HB1	4:I:20:GLN:CD	2.32	0.50
1:D:35:ARG:CZ	2:E:53:ASP:HB3	2.41	0.50
2:B:73:THR:HB	2:B:76:ASP:HB2	1.92	0.50
4:K:7:LEU:HD21	4:K:104:VAL:HB	1.94	0.50
4:I:68:LYS:O	4:I:69:LEU:HD22	2.12	0.50
2:E:84:HIS:HB3	2:E:87:MET:HE2	1.93	0.50
1:D:34:VAL:HG13	1:D:45:TYR:HE1	1.77	0.50
2:E:41:LYS:O	2:E:42:ASN:HB2	2.12	0.50
4:H:19:GLY:HA2	4:H:91:LYS:CG	2.40	0.50
1:A:91:GLY:O	1:A:93:HIS:CD2	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:58:SER:C	4:H:79:ARG:HH21	2.14	0.50
4:H:3:GLN:CB	4:H:32:VAL:HG11	2.41	0.50
4:H:32:VAL:O	4:H:33:SER:HB3	2.10	0.50
1:D:262:TYR:CD2	4:K:59:SER:HB2	2.47	0.50
4:G:22:VAL:CG1	4:G:89:LEU:HD13	2.40	0.50
4:H:81:THR:HG22	4:H:82:ASN:N	2.27	0.50
4:K:75:PHE:HD1	4:K:89:LEU:HD23	1.74	0.50
2:B:17:ASN:HA	2:B:72:PRO:O	2.12	0.50
4:K:121:LYS:C	4:K:122:VAL:HG23	2.32	0.50
4:G:89:LEU:N	4:G:89:LEU:HD12	2.27	0.50
4:K:110:MET:HE2	4:K:112:PHE:CZ	2.47	0.50
2:E:64:ILE:HG12	2:E:65:LEU:N	2.27	0.50
1:A:144:LYS:O	1:A:148:GLU:HG3	2.11	0.50
4:G:40:PHE:HB2	4:G:99:TYR:O	2.12	0.49
1:D:158:ALA:O	1:D:162:GLY:N	2.41	0.49
4:H:122:VAL:HG22	4:H:122:VAL:O	2.12	0.49
4:I:79:ARG:HD3	4:I:85:TYR:CZ	2.47	0.49
4:H:9:ILE:CD1	4:H:12:LYS:HE3	2.42	0.49
4:K:119:LEU:N	4:K:119:LEU:HD13	2.28	0.49
1:D:72:GLN:HA	1:D:75:ARG:HD3	1.93	0.49
4:I:92:PHE:CE1	4:I:118:VAL:HG12	2.47	0.49
1:D:198:LYS:HD3	1:D:250:PRO:HA	1.94	0.49
2:E:2:GLN:NE2	2:E:86:SER:HA	2.27	0.49
2:B:55:SER:O	2:B:63:TYR:CD2	2.65	0.49
4:H:91:LYS:HZ2	4:H:93:SER:CA	2.26	0.49
1:A:28:VAL:O	1:A:29:ASP:HB2	2.12	0.49
4:I:27:GLU:OE1	4:I:29:LEU:HD11	2.13	0.49
4:K:105:ILE:CD1	4:K:110:MET:HG2	2.43	0.49
1:D:228:MET:CE	1:D:230:LEU:HD23	2.42	0.49
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.78	0.49
1:D:98:ILE:HG12	2:E:60:TRP:CZ3	2.48	0.49
2:B:32:PRO:CB	2:B:33:PRO:CD	2.91	0.49
4:I:59:SER:OG	4:I:60:HIS:CE1	2.64	0.49
4:H:46:LYS:HG2	4:H:47:LEU:HG	1.95	0.48
4:H:9:ILE:HD12	4:H:12:LYS:HE3	1.95	0.48
1:D:19:GLU:CD	1:D:75:ARG:HH22	2.17	0.48
4:H:25:VAL:HG12	4:H:86:VAL:HG22	1.94	0.48
1:D:109:LEU:N	1:D:109:LEU:CD1	2.76	0.48
4:K:124:SER:O	4:K:125:ALA:CB	2.59	0.48
4:G:43:SER:CB	5:G:130:NDG:N2	2.76	0.48
4:I:93:SER:OG	4:I:94:LYS:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:O	1:A:92:SER:HB2	2.13	0.48
4:K:116:VAL:O	4:K:116:VAL:HG13	2.13	0.48
1:D:271:THR:HG23	1:D:271:THR:O	2.14	0.48
1:A:271:THR:HG22	1:A:271:THR:O	2.12	0.48
4:G:27:GLU:HG3	4:G:83:ASN:HD21	1.79	0.48
1:D:70:ASN:O	1:D:73:SER:HB3	2.13	0.48
4:H:91:LYS:NZ	4:H:93:SER:CA	2.77	0.48
1:D:201:LEU:O	1:D:246:SER:HA	2.14	0.48
1:D:234:ARG:HD2	1:D:242:GLN:HG3	1.96	0.48
4:I:42:ASN:HA	4:I:98:GLY:HA3	1.96	0.48
2:E:2:GLN:NE2	2:E:85:ASP:O	2.47	0.48
2:E:21:ASN:HB3	2:E:70:PHE:CE1	2.49	0.48
4:K:59:SER:OG	4:K:60:HIS:N	2.47	0.48
4:G:74:LEU:HG	4:G:75:PHE:CD1	2.49	0.48
4:K:74:LEU:O	4:K:90:ASN:ND2	2.47	0.47
4:I:17:GLU:O	4:I:20:GLN:HG2	2.14	0.47
1:D:217:TRP:CD2	1:D:259:CYS:HB2	2.48	0.47
1:D:192:HIS:HB2	1:D:200:THR:HB	1.97	0.47
1:A:70:ASN:ND2	3:C:5:TYR:H	2.11	0.47
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.49	0.47
1:D:141:LEU:HA	1:D:141:LEU:HD13	1.78	0.47
1:D:51:TRP:O	1:D:54:GLN:HG2	2.15	0.47
4:H:124:SER:O	4:H:125:ALA:HB3	2.14	0.47
4:H:70:ASN:C	4:H:70:ASN:OD1	2.52	0.47
4:G:108:SER:HB3	4:H:55:TYR:CD2	2.49	0.47
1:A:163:THR:HG22	3:C:1:ARG:H3	1.77	0.47
1:D:243:LYS:HG2	1:D:244:TRP:N	2.29	0.47
1:D:98:ILE:HD11	2:E:56:PHE:CE2	2.50	0.47
4:K:39:LEU:CD2	4:K:52:PHE:HA	2.45	0.47
1:A:149:GLN:O	1:A:149:GLN:HG2	2.14	0.47
1:A:252:GLY:C	1:A:254:GLU:H	2.17	0.47
4:I:54:VAL:HG22	4:I:65:TRP:CZ3	2.50	0.47
4:K:66:ASP:O	4:K:70:ASN:HA	2.15	0.47
4:K:9:ILE:HD12	4:K:9:ILE:O	2.15	0.47
4:G:100:TYR:O	4:G:116:VAL:HG22	2.14	0.47
4:I:26:CYS:HB2	4:I:38:TRP:CZ2	2.49	0.47
1:A:126:LEU:HD22	1:A:156:LEU:CD2	2.44	0.47
4:G:58:SER:O	4:G:79:ARG:NH1	2.48	0.47
1:D:81:LEU:HD21	3:F:8:LEU:HD13	1.97	0.47
4:K:45:SER:O	4:K:46:LYS:O	2.33	0.47
1:A:216:THR:HG23	1:A:228:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PHE:CE1	1:A:34:VAL:HG22	2.50	0.46
1:A:42:ASN:HB3	1:A:44:ARG:NH1	2.29	0.46
4:H:63:ILE:CD1	4:H:63:ILE:N	2.78	0.46
2:E:32:PRO:HB3	2:E:33:PRO:HD2	1.97	0.46
2:B:40:LEU:H	2:B:40:LEU:HD12	1.80	0.46
4:H:72:SER:O	4:H:73:LYS:HG2	2.16	0.46
4:K:57:ALA:CB	4:K:60:HIS:CD2	2.98	0.46
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.50	0.46
1:A:6:ARG:NH1	1:A:30:ASP:OD1	2.48	0.46
1:A:258:THR:HG22	1:A:273:ARG:HB2	1.96	0.46
2:E:32:PRO:CB	2:E:33:PRO:CD	2.93	0.46
1:D:228:MET:CE	1:D:245:ALA:HB1	2.46	0.46
1:A:121:CYS:SG	2:B:1:ILE:HG23	2.55	0.46
4:K:47:LEU:HB3	4:K:48:PRO:HD2	1.98	0.46
4:H:74:LEU:N	4:H:74:LEU:HD23	2.31	0.46
4:H:46:LYS:HG2	4:H:47:LEU:N	2.31	0.46
4:K:4:ALA:HB1	4:K:111:TYR:CE1	2.50	0.46
4:K:68:LYS:HB3	4:K:68:LYS:HE2	1.74	0.46
3:F:3:TYR:O	3:F:5:TYR:CE1	2.69	0.46
2:B:13:HIS:HB2	2:B:21:ASN:HD21	1.81	0.46
1:A:32:GLU:OE2	1:A:35:ARG:HD2	2.16	0.45
4:G:22:VAL:O	4:G:88:THR:HA	2.15	0.45
1:A:13:SER:HA	1:A:20:PRO:HB3	1.98	0.45
4:H:91:LYS:NZ	4:H:93:SER:HB3	2.30	0.45
1:A:194:ARG:HG3	1:A:194:ARG:NH1	2.30	0.45
1:A:94:THR:HG21	2:B:31:HIS:CE1	2.51	0.45
1:A:231:VAL:O	1:A:243:LYS:NZ	2.41	0.45
1:A:32:GLU:OE2	1:A:48:ARG:HG3	2.15	0.45
4:H:79:ARG:CB	4:H:79:ARG:HH11	2.13	0.45
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.16	0.45
4:G:1:LYS:H2	4:G:2:PRO:CD	2.27	0.45
1:D:95:ILE:HG12	1:D:95:ILE:O	2.16	0.45
1:D:176:ASN:O	1:D:180:LEU:HB2	2.16	0.45
1:D:6:ARG:HH21	1:D:8:PHE:HZ	1.65	0.45
2:B:21:ASN:OD1	2:B:22:ILE:N	2.45	0.45
2:B:52:SER:O	2:B:64:ILE:HD11	2.17	0.45
1:A:169:ARG:N	1:A:169:ARG:CD	2.80	0.45
2:E:2:GLN:HG2	2:E:86:SER:HB3	1.97	0.45
4:H:68:LYS:O	4:H:69:LEU:C	2.55	0.45
1:A:168:LEU:HD22	1:A:172:LEU:HD22	1.98	0.45
1:D:226:GLN:NE2	4:I:37:SER:OG	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:LEU:HA	1:D:110:LEU:HD12	1.77	0.45
4:H:121:LYS:C	4:H:123:SER:H	2.20	0.45
1:D:175:GLY:O	1:D:179:LEU:CD2	2.65	0.45
1:A:67:ALA:O	1:A:71:GLU:HB3	2.17	0.45
4:I:8:ARG:HD2	4:I:27:GLU:OE1	2.17	0.45
4:I:42:ASN:C	4:I:43:SER:O	2.53	0.45
1:D:70:ASN:ND2	3:F:5:TYR:CE1	2.85	0.45
4:I:52:PHE:HZ	4:I:55:TYR:HB2	1.81	0.45
1:A:95:ILE:HD11	1:A:116:TYR:HD2	1.82	0.44
4:G:15:ASP:O	4:G:121:LYS:HE2	2.17	0.44
1:A:20:PRO:HG3	1:A:75:ARG:HG2	1.98	0.44
4:I:73:LYS:O	4:I:73:LYS:HG2	2.18	0.44
4:G:69:LEU:N	4:G:69:LEU:HD22	2.32	0.44
4:G:38:TRP:HB3	4:G:87:LEU:HD22	1.98	0.44
4:K:86:VAL:HG12	4:K:87:LEU:N	2.33	0.44
4:H:23:ASP:HA	4:H:88:THR:HA	1.98	0.44
4:G:66:ASP:OD2	4:G:69:LEU:HD23	2.18	0.44
4:I:94:LYS:C	4:I:96:ASN:N	2.71	0.44
1:A:213:ILE:HG12	1:A:214:THR:N	2.33	0.44
1:A:78:LEU:HD21	1:A:95:ILE:HG22	1.98	0.44
2:E:73:THR:O	2:E:97:ARG:NH2	2.50	0.44
2:E:98:ASP:O	2:E:99:MET:HB2	2.17	0.44
1:A:35:ARG:O	1:A:45:TYR:HA	2.17	0.44
4:I:56:MET:HG2	4:I:63:ILE:HG22	1.99	0.44
4:G:27:GLU:HG3	4:G:83:ASN:ND2	2.32	0.44
1:D:175:GLY:C	1:D:179:LEU:HD23	2.38	0.44
4:G:53:VAL:HG12	4:G:54:VAL:CG2	2.48	0.44
1:A:242:GLN:O	1:A:243:LYS:HB2	2.18	0.44
4:I:14:MET:HA	4:I:14:MET:CE	2.48	0.44
1:D:9:VAL:HG22	1:D:24:GLU:HB3	2.00	0.44
1:D:96:GLN:NE2	2:E:60:TRP:O	2.51	0.43
1:A:201:LEU:O	1:A:246:SER:HB2	2.18	0.43
1:A:191:HIS:HB2	1:A:274:TRP:CZ2	2.53	0.43
1:D:156:LEU:HD23	3:F:3:TYR:CZ	2.53	0.43
1:A:88:SER:OG	1:A:89:LYS:N	2.49	0.43
1:A:234:ARG:HD2	2:B:10:TYR:CE1	2.52	0.43
2:E:84:HIS:HD2	2:E:86:SER:H	1.66	0.43
4:H:100:TYR:O	4:H:116:VAL:HG22	2.19	0.43
1:A:11:ALA:HB3	1:A:95:ILE:CG2	2.47	0.43
4:K:121:LYS:O	4:K:122:VAL:CG2	2.67	0.43
4:K:119:LEU:H	4:K:119:LEU:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:MET:HE1	1:D:245:ALA:HB1	1.99	0.43
4:K:23:ASP:OD1	4:K:88:THR:HG22	2.19	0.43
1:D:247:VAL:O	1:D:247:VAL:HG13	2.17	0.43
4:H:41:GLN:HE21	4:H:41:GLN:HB3	1.56	0.43
4:G:7:LEU:CD1	4:G:104:VAL:HG22	2.42	0.43
4:I:110:MET:HE2	4:I:112:PHE:CE2	2.53	0.43
1:A:59:TYR:HE2	1:A:167:TRP:CZ3	2.37	0.43
4:G:35:GLY:HA3	4:G:56:MET:O	2.19	0.43
1:A:14:ARG:HD2	1:A:92:SER:HB3	2.00	0.43
4:G:78:MET:O	4:G:86:VAL:HG12	2.18	0.43
1:D:160:LEU:O	1:D:164:CYS:HB3	2.17	0.43
4:H:26:CYS:HB2	4:H:38:TRP:CZ2	2.53	0.43
4:K:90:ASN:N	4:K:90:ASN:HD22	2.16	0.43
4:H:104:VAL:HG12	4:H:105:ILE:N	2.34	0.43
4:I:80:ASP:CG	4:I:81:THR:N	2.72	0.43
1:A:217:TRP:HA	1:A:259:CYS:HA	2.01	0.43
4:I:113:SER:HB2	4:I:114:SER:H	1.70	0.43
4:G:40:PHE:CD1	4:G:41:GLN:N	2.87	0.43
4:G:68:LYS:O	4:G:70:ASN:N	2.52	0.43
4:K:100:TYR:HB2	4:K:116:VAL:HG13	2.00	0.43
1:D:98:ILE:HD11	2:E:56:PHE:HE2	1.84	0.43
2:E:13:HIS:HB2	2:E:21:ASN:HD21	1.84	0.43
1:D:127:ASN:HB3	1:D:129:ASP:OD2	2.19	0.43
1:A:189:VAL:HG23	1:A:274:TRP:CE3	2.48	0.42
4:G:37:SER:O	4:G:102:CYS:HA	2.19	0.42
1:D:229:GLU:O	1:D:229:GLU:HG3	2.19	0.42
1:A:58:GLU:H	1:A:58:GLU:CD	2.22	0.42
4:G:99:TYR:CE1	4:G:117:PRO:CB	2.80	0.42
2:E:31:HIS:ND1	2:E:32:PRO:HA	2.34	0.42
4:I:56:MET:SD	4:I:77:ALA:HB1	2.60	0.42
4:I:18:LEU:HA	4:I:92:PHE:O	2.19	0.42
4:G:110:MET:HE2	4:G:112:PHE:CZ	2.53	0.42
1:A:225:ILE:HG13	1:A:225:ILE:H	1.66	0.42
4:G:89:LEU:HD23	4:G:96:ASN:OD1	2.18	0.42
1:A:224:LEU:CA	4:G:34:GLN:HE22	2.10	0.42
4:I:121:LYS:C	4:I:122:VAL:HG22	2.40	0.42
2:E:5:PRO:CG	2:E:87:MET:HE2	2.48	0.42
4:K:1:LYS:H2	4:K:2:PRO:HD2	1.84	0.42
4:H:10:PHE:CD1	4:H:11:PRO:HA	2.54	0.42
1:A:8:PHE:HD2	2:B:56:PHE:CE2	2.37	0.42
4:H:91:LYS:HZ2	4:H:93:SER:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:GLU:HB3	1:D:20:PRO:HD2	2.00	0.42
4:H:74:LEU:H	4:H:74:LEU:HD23	1.85	0.42
4:I:80:ASP:CG	4:I:81:THR:H	2.23	0.42
1:A:218:GLN:HA	1:A:222:GLU:O	2.20	0.42
4:I:74:LEU:HG	4:I:75:PHE:CE1	2.53	0.42
4:I:75:PHE:HE2	4:I:100:TYR:HE2	1.67	0.42
1:D:79:ARG:HG2	1:D:79:ARG:H	1.72	0.42
1:D:185:PRO:CA	1:D:208:PHE:HB3	2.50	0.42
4:H:122:VAL:HG13	4:H:124:SER:OG	2.19	0.42
3:F:8:LEU:HD12	3:F:8:LEU:C	2.40	0.42
1:D:12:VAL:HG13	1:D:12:VAL:O	2.19	0.42
1:A:249:VAL:HB	1:A:250:PRO:HD2	2.02	0.42
4:H:27:GLU:OE1	4:H:84:LYS:HE2	2.20	0.42
4:I:94:LYS:O	4:I:96:ASN:N	2.52	0.42
4:G:92:PHE:CG	4:G:92:PHE:O	2.72	0.42
2:E:59:ASP:OD2	2:E:61:SER:OG	2.32	0.42
1:A:110:LEU:HD22	1:A:110:LEU:HA	1.81	0.42
1:D:103:VAL:HG22	1:D:165:VAL:HG12	2.01	0.42
4:K:117:PRO:HB2	4:K:119:LEU:HD21	2.02	0.42
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.54	0.42
4:H:7:LEU:HD23	4:H:102:CYS:O	2.19	0.42
4:I:21:LYS:HB3	4:I:21:LYS:NZ	2.35	0.42
4:K:92:PHE:CE2	4:K:120:GLN:HB3	2.53	0.42
4:K:44:SER:HB3	6:K:130:NAG:H62	2.01	0.42
4:H:110:MET:HB3	4:H:110:MET:HE2	1.75	0.42
1:D:130:LEU:HB3	1:D:157:ARG:HG3	2.02	0.42
1:A:84:TYR:OH	1:A:146:LYS:NZ	2.43	0.42
4:K:5:PRO:HG3	4:K:32:VAL:HG23	2.02	0.42
1:A:74:PHE:HE1	3:C:5:TYR:CB	2.33	0.42
4:I:115:VAL:O	4:I:115:VAL:HG23	2.19	0.42
4:K:121:LYS:C	4:K:122:VAL:CG2	2.88	0.42
4:I:56:MET:CE	4:I:85:TYR:HB3	2.50	0.42
1:D:126:LEU:HD22	1:D:156:LEU:CD1	2.50	0.42
4:I:9:ILE:HG21	4:I:114:SER:O	2.19	0.42
2:B:56:PHE:HA	2:B:62:PHE:HA	2.02	0.42
4:G:17:GLU:N	4:G:17:GLU:OE1	2.52	0.42
4:H:9:ILE:CD1	4:H:9:ILE:H	2.21	0.42
4:H:40:PHE:HE1	4:H:98:GLY:HA3	1.85	0.42
4:K:46:LYS:H	4:K:46:LYS:HE2	1.84	0.42
1:D:151:GLY:O	1:D:154:GLU:HB2	2.20	0.42
1:D:15:PRO:HG2	1:D:90:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:LEU:HA	2:E:44:LYS:O	2.20	0.42
1:D:34:VAL:HG22	1:D:45:TYR:CD1	2.55	0.41
1:D:44:ARG:HD2	1:D:46:GLU:HG2	2.01	0.41
1:A:135:ALA:HB1	1:A:140:ALA:CB	2.47	0.41
4:G:117:PRO:O	4:G:119:LEU:N	2.52	0.41
1:D:102:GLU:O	1:D:110:LEU:HB3	2.20	0.41
3:C:4:VAL:O	3:C:4:VAL:HG13	2.20	0.41
2:B:84:HIS:CD2	2:B:86:SER:H	2.39	0.41
1:D:8:PHE:CE2	1:D:98:ILE:HD12	2.55	0.41
1:A:17:LEU:N	1:A:17:LEU:HD23	2.35	0.41
4:K:33:SER:OG	4:K:34:GLN:N	2.53	0.41
4:H:115:VAL:CG2	4:H:116:VAL:N	2.83	0.41
4:H:63:ILE:HG13	4:H:65:TRP:HE1	1.85	0.41
1:D:70:ASN:CG	3:F:5:TYR:HD1	2.24	0.41
1:A:172:LEU:O	1:A:176:ASN:HB2	2.21	0.41
4:I:12:LYS:O	4:I:116:VAL:HG12	2.20	0.41
1:A:206:LEU:HD23	1:A:242:GLN:HB3	2.00	0.41
4:H:105:ILE:HG12	4:H:110:MET:HG2	2.02	0.41
1:A:183:ASP:O	1:A:208:PHE:HA	2.20	0.41
4:G:46:LYS:HA	4:G:46:LYS:HD3	1.64	0.41
4:H:54:VAL:HG22	4:H:55:TYR:N	2.35	0.41
1:A:103:VAL:HG13	1:A:108:ARG:O	2.21	0.41
4:H:43:SER:HB2	4:H:98:GLY:HA2	2.01	0.41
1:A:101:CYS:HB2	1:A:109:LEU:HD11	2.03	0.41
1:A:199:VAL:HG21	1:A:251:LEU:HD13	2.03	0.41
2:E:29:GLN:OE1	4:K:3:GLN:NE2	2.53	0.41
4:K:103:SER:HB2	4:K:112:PHE:CD1	2.56	0.41
4:H:16:ALA:HB1	4:H:20:GLN:NE2	2.36	0.41
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.55	0.41
4:H:69:LEU:O	4:H:70:ASN:C	2.59	0.41
4:K:81:THR:HB	4:K:82:ASN:H	1.61	0.41
1:D:225:ILE:H	1:D:225:ILE:HG13	1.69	0.41
1:D:182:THR:HB	1:D:264:GLN:NE2	2.29	0.41
1:D:209:TYR:HA	1:D:210:PRO:C	2.40	0.41
4:G:60:HIS:ND1	4:G:60:HIS:N	2.68	0.41
4:G:8:ARG:HB2	4:G:27:GLU:HB3	2.01	0.41
4:H:38:TRP:HB2	4:H:54:VAL:HG12	2.02	0.41
4:H:5:PRO:HD2	4:H:111:TYR:CE2	2.56	0.41
1:D:97:VAL:CG1	1:D:98:ILE:N	2.84	0.41
4:K:42:ASN:C	4:K:44:SER:H	2.23	0.41
4:I:43:SER:O	4:I:44:SER:CB	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:5:PRO:HA	4:I:29:LEU:O	2.21	0.41
1:D:194:ARG:HH11	1:D:194:ARG:HG2	1.85	0.41
1:D:98:ILE:CG1	2:E:60:TRP:CZ3	3.04	0.41
1:D:214:THR:HB	1:D:262:TYR:HB2	2.02	0.41
2:B:23:LEU:O	2:B:67:HIS:HA	2.20	0.41
1:D:167:TRP:CZ2	3:F:1:ARG:NE	2.88	0.41
1:D:118:TYR:O	1:D:119:ASP:HB2	2.20	0.41
2:E:4:THR:HA	2:E:86:SER:OG	2.20	0.41
4:K:92:PHE:HE2	4:K:120:GLN:CB	2.34	0.41
4:H:80:ASP:HB3	4:H:81:THR:H	1.54	0.41
4:G:39:LEU:HA	4:G:53:VAL:HG23	2.01	0.41
4:I:10:PHE:CG	4:I:11:PRO:HA	2.56	0.41
4:I:10:PHE:CD2	4:I:11:PRO:HA	2.56	0.41
1:A:216:THR:HG21	1:A:223:GLU:HG2	2.03	0.41
1:D:22:TYR:CB	1:D:71:GLU:HG3	2.51	0.41
4:G:66:ASP:C	4:G:68:LYS:H	2.24	0.40
4:I:47:LEU:HA	4:I:48:PRO:HD3	1.98	0.40
4:K:69:LEU:CD1	6:K:130:NAG:C8	3.00	0.40
4:I:74:LEU:N	4:I:74:LEU:CD2	2.81	0.40
4:K:71:SER:O	4:K:74:LEU:N	2.54	0.40
4:K:38:TRP:O	4:K:39:LEU:HD23	2.21	0.40
4:G:53:VAL:HG12	4:G:54:VAL:HG22	2.03	0.40
4:K:54:VAL:HG22	4:K:55:TYR:N	2.35	0.40
2:B:49:VAL:HG22	2:B:68:THR:HB	2.03	0.40
4:G:43:SER:C	4:G:45:SER:N	2.74	0.40
4:G:89:LEU:N	4:G:89:LEU:CD1	2.84	0.40
1:A:98:ILE:HG13	2:B:60:TRP:HZ3	1.84	0.40
4:I:54:VAL:HG21	4:I:87:LEU:CD1	2.48	0.40
4:H:44:SER:O	4:H:45:SER:HB2	2.21	0.40
1:A:173:LYS:HA	1:A:173:LYS:HD3	1.61	0.40
2:B:84:HIS:CD2	2:B:86:SER:OG	2.71	0.40
4:G:38:TRP:O	4:G:53:VAL:HB	2.21	0.40
4:H:91:LYS:HZ2	4:H:93:SER:CB	2.34	0.40
4:H:71:SER:HB3	4:H:74:LEU:HD11	2.04	0.40
4:K:77:ALA:HB2	4:K:87:LEU:HD12	2.03	0.40
2:B:10:TYR:OH	2:B:26:TYR:HB2	2.21	0.40
2:E:17:ASN:HA	2:E:72:PRO:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:NH1	4:H:69:LEU:C[4_555]	2.02	0.18
1:A:169:ARG:NH1	4:H:70:ASN:N[4_555]	2.12	0.08

## 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	272/274 (99%)	245 (90%)	23 (8%)	4 (2%)	13	40
1	D	272/274 (99%)	245 (90%)	22 (8%)	5 (2%)	11	34
2	B	97/99 (98%)	86 (89%)	10 (10%)	1 (1%)	19	52
2	E	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	19	52
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
4	G	120/129 (93%)	91 (76%)	21 (18%)	8 (7%)	1	4
4	H	123/129 (95%)	97 (79%)	15 (12%)	11 (9%)	1	2
4	I	120/129 (93%)	96 (80%)	17 (14%)	7 (6%)	2	5
4	K	123/129 (95%)	99 (80%)	14 (11%)	10 (8%)	1	2
All	All	1236/1278 (97%)	1059 (86%)	130 (10%)	47 (4%)	4	13

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	47	PRO
1	D	110	LEU
4	G	3	GLN
4	G	43	SER
4	G	44	SER
4	H	73	LYS
4	H	81	THR
4	I	59	SER

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Mol	Chain	Res	Type
4	I	82	ASN
4	K	46	LYS
4	K	72	SER
4	K	81	THR
4	K	91	LYS
1	A	150	ALA
4	H	67	GLU
4	H	70	ASN
4	H	92	PHE
4	H	122	VAL
4	I	95	GLU
4	I	122	VAL
1	D	88	SER
1	D	106	ASP
4	G	67	GLU
4	H	33	SER
4	H	82	ASN
4	H	121	LYS
4	K	92	PHE
4	K	124	SER
2	E	47	PRO
4	H	69	LEU
4	I	83	ASN
4	I	90	ASN
4	K	13	LYS
1	A	199	VAL
4	G	82	ASN
4	G	90	ASN
4	I	48	PRO
4	K	48	PRO
4	K	122	VAL
1	A	43	PRO
1	D	90	GLY
4	G	113	SER
4	K	90	ASN
1	D	43	PRO
4	G	48	PRO
1	A	90	GLY
4	H	48	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	232/232 (100%)	215 (93%)	17 (7%)	17	44
1	D	232/232 (100%)	209 (90%)	23 (10%)	10	28
2	B	94/94 (100%)	91 (97%)	3 (3%)	46	80
2	E	94/94 (100%)	90 (96%)	4 (4%)	35	70
3	C	6/6 (100%)	6 (100%)	0	100	100
3	F	6/6 (100%)	5 (83%)	1 (17%)	3	8
4	G	114/120 (95%)	102 (90%)	12 (10%)	8	24
4	H	116/120 (97%)	102 (88%)	14 (12%)	6	18
4	I	113/120 (94%)	101 (89%)	12 (11%)	8	24
4	K	116/120 (97%)	103 (89%)	13 (11%)	7	22
All	All	1123/1144 (98%)	1024 (91%)	99 (9%)	12	35

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	25	VAL
1	A	45	TYR
1	A	71	GLU
1	A	73	SER
1	A	88	SER
1	A	89	LYS
1	A	97	VAL
1	A	110	LEU
1	A	141	LEU
1	A	169	ARG
1	A	178	THR
1	A	181	ARG
1	A	186	LYS
1	A	206	LEU
1	A	230	LEU

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Mol	Chain	Res	Type
1	A	254	GLU
2	B	40	LEU
2	B	70	PHE
2	B	93	VAL
1	D	10	THR
1	D	14	ARG
1	D	17	LEU
1	D	25	VAL
1	D	30	ASP
1	D	45	TYR
1	D	63	GLU
1	D	88	SER
1	D	95	ILE
1	D	105	SER
1	D	106	ASP
1	D	110	LEU
1	D	128	GLU
1	D	129	ASP
1	D	141	LEU
1	D	149	GLN
1	D	152	GLU
1	D	156	LEU
1	D	181	ARG
1	D	182	THR
1	D	219	LEU
1	D	234	ARG
1	D	272	LEU
2	E	40	LEU
2	E	45	LYS
2	E	70	PHE
2	E	93	VAL
3	F	6	GLN
4	G	17	GLU
4	G	20	GLN
4	G	39	LEU
4	G	49	GLN
4	G	54	VAL
4	G	68	LYS
4	G	70	ASN
4	G	74	LEU
4	G	83	ASN
4	G	90	ASN

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Mol	Chain	Res	Type
4	G	94	LYS
4	G	120	GLN
4	H	9	ILE
4	H	15	ASP
4	H	20	GLN
4	H	23	ASP
4	H	41	GLN
4	H	46	LYS
4	H	48	PRO
4	H	62	LYS
4	H	63	ILE
4	H	67	GLU
4	H	74	LEU
4	H	79	ARG
4	H	92	PHE
4	H	119	LEU
4	I	14	MET
4	I	23	ASP
4	I	33	SER
4	I	40	PHE
4	I	41	GLN
4	I	54	VAL
4	I	68	LYS
4	I	73	LYS
4	I	74	LEU
4	I	81	THR
4	I	83	ASN
4	I	113	SER
4	K	6	GLU
4	K	9	ILE
4	K	14	MET
4	K	46	LYS
4	K	62	LYS
4	K	63	ILE
4	K	80	ASP
4	K	81	THR
4	K	82	ASN
4	K	90	ASN
4	K	91	LYS
4	K	115	VAL
4	K	119	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	218	GLN
1	A	220	ASN
1	A	260	HIS
2	B	2	GLN
2	B	29	GLN
2	B	34	HIS
2	B	84	HIS
1	D	54	GLN
1	D	87	GLN
1	D	114	GLN
1	D	149	GLN
1	D	220	ASN
1	D	226	GLN
1	D	263	HIS
1	D	264	GLN
2	E	2	GLN
2	E	29	GLN
2	E	84	HIS
4	G	34	GLN
4	G	70	ASN
4	G	83	ASN
4	G	90	ASN
4	G	96	ASN
4	H	3	GLN
4	H	41	GLN
4	H	61	ASN
4	I	34	GLN
4	K	3	GLN
4	K	60	HIS
4	K	90	ASN
4	K	120	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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$
5	NDG	G	130	4	14,14,15	3.17	3 (21%)	15,19,21	1.12	1 (6%)
6	NAG	H	130	4	14,14,15	2.77	5 (35%)	15,19,21	2.06	3 (20%)
6	NAG	I	130	4	14,14,15	1.65	2 (14%)	15,19,21	0.86	0
6	NAG	K	130	1,4	14,14,15	2.74	4 (28%)	15,19,21	0.96	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
5	NDG	G	130	4	-	0/6/23/26	0/1/1/1
6	NAG	H	130	4	-	0/6/23/26	0/1/1/1
6	NAG	I	130	4	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	K	130	1,4	-	0/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	130	NAG	O5-C5	-4.14	1.34	1.43
6	K	130	NAG	O5-C1	-4.02	1.37	1.43
6	K	130	NAG	O5-C5	-3.49	1.35	1.43
6	H	130	NAG	O5-C1	-2.97	1.38	1.43
5	G	130	NDG	O-C1	-2.84	1.39	1.43
6	H	130	NAG	C4-C5	-2.06	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	130	NAG	C4-C5	-2.02	1.48	1.53
6	I	130	NAG	C3-C2	2.36	1.57	1.52
5	G	130	NDG	C3-C2	2.49	1.58	1.52
6	H	130	NAG	C3-C2	2.94	1.59	1.52
6	I	130	NAG	C1-C2	5.19	1.59	1.52
6	H	130	NAG	C1-C2	7.91	1.63	1.52
6	K	130	NAG	C1-C2	8.19	1.63	1.52
5	G	130	NDG	C1-C2	11.02	1.67	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	130	NAG	C3-C2-N2	-3.00	103.37	110.56
5	G	130	NDG	C1-O-C5	-2.83	108.66	112.25
6	H	130	NAG	O5-C5-C6	-2.69	101.51	107.35
6	H	130	NAG	C1-O5-C5	6.32	120.26	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	I	130	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	130	NDG	10	0
6	H	130	NAG	5	0
6	I	130	NAG	3	0
6	K	130	NAG	3	0

## 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	274/274 (100%)	-0.09	2 (0%) 89 84	7, 28, 47, 61	0
1	D	274/274 (100%)	-0.11	4 (1%) 76 68	10, 28, 50, 72	0
2	B	99/99 (100%)	-0.20	1 (1%) 84 77	7, 27, 42, 60	0
2	E	99/99 (100%)	-0.33	1 (1%) 84 77	9, 26, 48, 59	0
3	C	8/8 (100%)	0.13	0 100 100	21, 29, 38, 44	0
3	F	8/8 (100%)	-0.01	0 100 100	23, 29, 32, 35	0
4	G	122/129 (94%)	1.00	20 (16%) 2 1	23, 57, 83, 94	0
4	H	125/129 (96%)	0.57	10 (8%) 15 7	17, 48, 81, 89	0
4	I	122/129 (94%)	0.70	9 (7%) 17 9	27, 46, 73, 96	0
4	K	125/129 (96%)	0.35	10 (8%) 15 7	15, 39, 72, 91	0
All	All	1256/1278 (98%)	0.17	57 (4%) 37 26	7, 33, 70, 96	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	123	SER	7.1
4	K	124	SER	6.6
4	H	125	ALA	6.2
4	G	70	ASN	5.7
4	H	123	SER	5.5
4	H	1	LYS	5.2
4	G	2	PRO	5.0
4	G	4	ALA	4.8
4	G	71	SER	4.7
4	K	70	ASN	4.7
4	H	2	PRO	4.5
4	G	3	GLN	4.4
4	H	18	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
4	I	124	SER	4.2
4	G	82	ASN	4.2
4	I	71	SER	4.2
4	K	123	SER	4.1
4	H	122	VAL	3.9
4	H	124	SER	3.8
4	K	71	SER	3.8
4	G	83	ASN	3.7
2	B	2	GLN	3.7
4	K	125	ALA	3.5
4	I	121	LYS	3.4
4	I	125	ALA	3.4
1	D	105	SER	3.4
4	I	72	SER	3.3
4	G	29	LEU	3.3
4	G	122	VAL	3.2
1	D	108	ARG	3.2
4	G	1	LYS	3.2
1	D	106	ASP	3.1
4	G	44	SER	3.1
4	K	1	LYS	3.0
4	I	67	GLU	2.9
4	I	70	ASN	2.9
4	G	67	GLU	2.7
1	D	107	GLY	2.7
1	A	17	LEU	2.6
4	H	17	GLU	2.5
4	G	10	PHE	2.5
4	I	120	GLN	2.4
4	G	72	SER	2.4
4	G	46	LYS	2.3
4	G	93	SER	2.3
4	K	47	LEU	2.2
4	G	43	SER	2.2
4	K	82	ASN	2.2
4	G	5	PRO	2.2
4	G	121	LYS	2.1
4	H	82	ASN	2.1
4	G	91	LYS	2.1
4	H	3	GLN	2.1
4	K	68	LYS	2.1
4	K	121	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	252	GLY	2.0
2	E	44	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	I	130	14/15	0.65	0.51	6.10	100,100,100,100	0
5	NDG	G	130	14/15	0.53	0.48	2.88	100,100,100,100	0
6	NAG	H	130	14/15	0.67	0.36	1.87	100,100,100,100	0
6	NAG	K	130	14/15	0.76	0.28	0.53	95,99,100,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.