Full wwPDB X-ray Structure Validation Report (i)

Jun 22, 2024 – 06:28 PM EDT

PDB ID	:	5CJQ
Title	:	Crystal structure of a trimeric influenza hemagglutinin stem in complex with an broadly neutralizing antibody CR9114
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2015-07-14
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

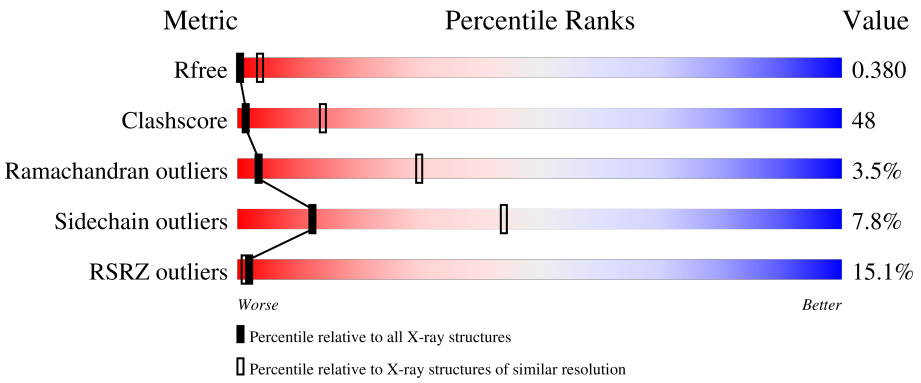
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	L	215	25%; 34%; 48%; 13%; • •
2	H	230	13%; 49%; 40%; • • 6%
3	A	66	3%; 30%; 45%; • 21%
4	B	193	6%; 34%; 39%; 6% • 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4812 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 CR9114 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	1568	978	266	320	4	0	0	0

- Molecule 2 is a protein called CR9114 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	217	1613	1017	269	320	7	0	0	0

- Molecule 3 is a protein called Designed influenza hemagglutinin stem #4900, HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	52	397	242	72	80	3	0	0	0

- Molecule 4 is a protein called Designed influenza hemagglutinin stem #4900, HA2.

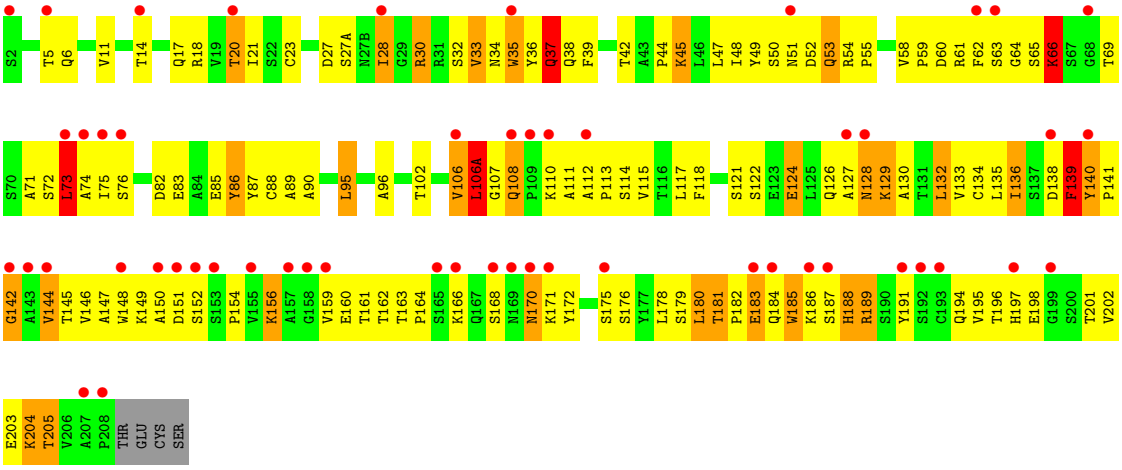
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	154	1234	767	208	251	8	0	0	0

3 Residue-property plots (i)

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

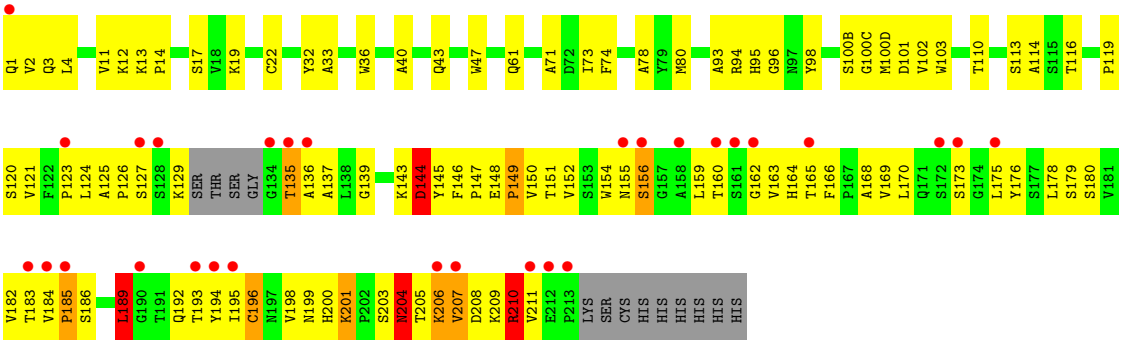
• Molecule 1: CR9114 light chain

Chain L:



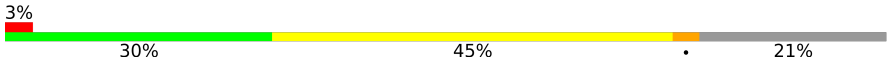
• Molecule 2: CR9114 heavy chain

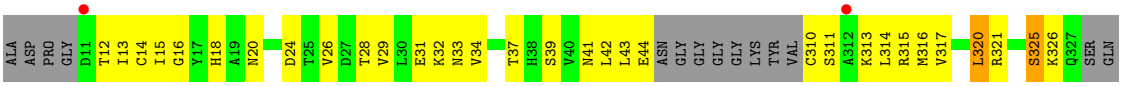
Chain H:



• Molecule 3: Designed influenza hemagglutinin stem #4900, HA1

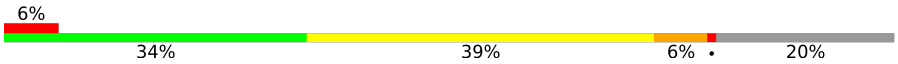
Chain A:

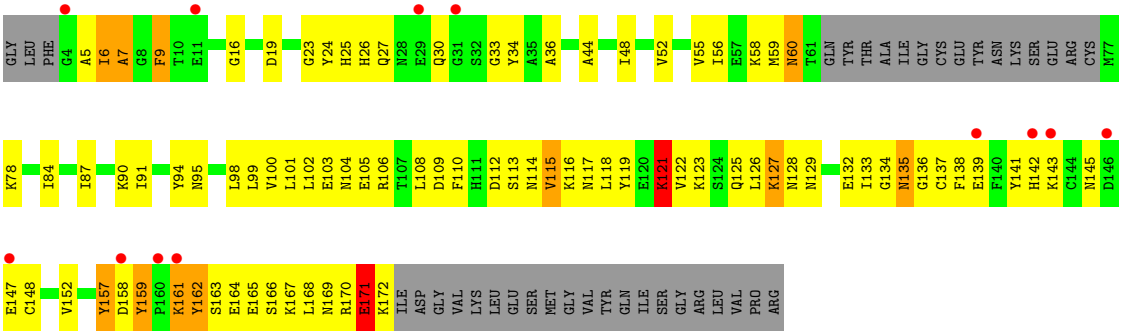




• Molecule 4: Designed influenza hemagglutinin stem #4900, HA2

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	157.70Å 157.70Å 202.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.85 – 3.60 28.32 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.85-3.60) 99.6 (28.32-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.55Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.346 , 0.369 0.349 , 0.380	Depositor DCC
R_{free} test set	550 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	138.2	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 125.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.030 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.003 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.000 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	4812	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	L	0.75	1/1606 (0.1%)	1.43	20/2193 (0.9%)
2	H	0.69	5/1652 (0.3%)	1.08	9/2251 (0.4%)
3	A	0.61	0/399	1.02	1/539 (0.2%)
4	B	0.44	0/1256	0.75	0/1687
All	All	0.65	6/4913 (0.1%)	1.14	30/6670 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
2	H	0	2
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	206	LYS	CA-CB	7.92	1.71	1.53
2	H	206	LYS	CD-CE	6.83	1.68	1.51
2	H	206	LYS	CB-CG	5.88	1.68	1.52
2	H	207	VAL	CB-CG2	-5.75	1.40	1.52
1	L	35	TRP	CB-CG	-5.61	1.40	1.50
2	H	196	CYS	CB-SG	-5.31	1.73	1.81

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	142	GLY	N-CA-C	13.49	146.82	113.10
2	H	206	LYS	CB-CG-CD	12.76	144.77	111.60
1	L	139	PHE	CB-CA-C	-8.75	92.90	110.40
1	L	132	LEU	CB-CG-CD1	-8.52	96.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	206	LYS	N-CA-C	-8.29	88.61	111.00
1	L	37	GLN	CB-CA-C	-7.94	94.52	110.40
1	L	73	LEU	CA-CB-CG	-7.75	97.47	115.30
1	L	140	TYR	C-N-CD	-7.68	103.70	120.60
1	L	95	LEU	CB-CG-CD2	-7.27	98.64	111.00
2	H	210	ARG	CG-CD-NE	7.25	127.03	111.80
2	H	189	LEU	CA-CB-CG	6.85	131.06	115.30
1	L	86	TYR	CA-CB-CG	6.79	126.29	113.40
1	L	170	ASN	N-CA-C	6.77	129.28	111.00
1	L	66	LYS	CD-CE-NZ	6.74	127.21	111.70
1	L	139	PHE	CB-CG-CD2	-6.73	116.09	120.80
1	L	162	THR	CA-CB-CG2	-6.33	103.53	112.40
2	H	185	PRO	CA-C-N	-6.22	103.53	117.20
2	H	144	ASP	CB-CG-OD1	6.07	123.76	118.30
1	L	35	TRP	CA-CB-CG	6.00	125.09	113.70
1	L	136	ILE	N-CA-C	-5.88	95.12	111.00
1	L	66	LYS	CG-CD-CE	-5.88	94.27	111.90
1	L	185	TRP	CA-CB-CG	-5.85	102.58	113.70
2	H	208	ASP	CB-CG-OD1	5.85	123.56	118.30
1	L	170	ASN	N-CA-CB	-5.85	100.08	110.60
1	L	140	TYR	C-N-CA	5.62	145.62	122.00
2	H	101	ASP	CB-CG-OD2	5.59	123.33	118.30
1	L	64	GLY	N-CA-C	5.54	126.96	113.10
2	H	210	ARG	CB-CG-CD	5.14	124.97	111.60
1	L	144	VAL	CA-CB-CG1	-5.12	103.21	110.90
3	A	33	ASN	N-CA-CB	5.08	119.73	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	203	SER	Peptide
2	H	206	LYS	Mainchain
1	L	129	LYS	Peptide
1	L	188	HIS	Peptide

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	L	1568	0	1517	213	0
2	H	1613	0	1568	123	0
3	A	397	0	401	40	0
4	B	1234	0	1153	112	0
All	All	4812	0	4639	455	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (455) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:114:ALA:HB1	2:H:146:PHE:CE2	1.56	1.40
2:H:114:ALA:CB	2:H:146:PHE:HE2	1.43	1.32
2:H:114:ALA:CB	2:H:146:PHE:CE2	2.21	1.19
1:L:140:TYR:CE1	1:L:171:LYS:HD2	1.82	1.14
2:H:146:PHE:HB2	2:H:175:LEU:HD11	1.28	1.10
1:L:124:GLU:HG2	1:L:129:LYS:HB2	1.45	0.98
2:H:114:ALA:HB1	2:H:146:PHE:HE2	0.92	0.91
4:B:121:LYS:HZ3	4:B:122:VAL:HG22	1.36	0.90
1:L:136:ILE:HG22	1:L:139:PHE:CZ	2.08	0.89
2:H:120:SER:HB2	2:H:143:LYS:HD3	1.55	0.88
1:L:51:ASN:HA	1:L:66:LYS:HD2	1.56	0.88
1:L:21:ILE:HD12	1:L:86:TYR:CZ	2.10	0.86
1:L:142:GLY:HA2	1:L:172:TYR:CZ	2.11	0.85
2:H:195:ILE:HG23	2:H:210:ARG:HE	1.39	0.85
1:L:144:VAL:HG21	1:L:197:HIS:CD2	2.10	0.85
2:H:168:ALA:HA	2:H:178:LEU:HG	1.59	0.84
4:B:121:LYS:HG3	4:B:122:VAL:HG13	1.60	0.83
1:L:135:LEU:HD22	2:H:166:PHE:CE2	2.15	0.81
2:H:165:THR:HG22	2:H:180:SER:HB3	1.61	0.81
2:H:163:VAL:HG13	2:H:182:VAL:HB	1.61	0.81
1:L:149:LYS:HD3	1:L:152:SER:HA	1.61	0.81
2:H:13:LYS:HG3	2:H:14:PRO:HD2	1.62	0.81
1:L:150:ALA:HB1	1:L:188:HIS:CE1	2.16	0.80
1:L:150:ALA:HB1	1:L:188:HIS:HE1	1.46	0.80
4:B:164:GLU:OE1	4:B:164:GLU:N	2.14	0.80
1:L:146:VAL:HG22	1:L:148:TRP:HE1	1.47	0.79
4:B:162:TYR:CE2	4:B:165:GLU:HG2	2.17	0.79
1:L:144:VAL:HG21	1:L:197:HIS:HD2	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:GLN:HE22	1:L:188:HIS:CE1	1.99	0.79
1:L:130:ALA:HB3	1:L:180:LEU:O	1.83	0.79
4:B:122:VAL:O	4:B:126:LEU:N	2.17	0.78
3:A:39:SER:OG	3:A:315:ARG:CZ	2.32	0.77
1:L:196:THR:HA	1:L:201:THR:HA	1.66	0.77
1:L:75:ILE:HD11	1:L:86:TYR:HE2	1.50	0.76
1:L:37:GLN:HE22	1:L:47:LEU:HB2	1.50	0.76
1:L:45:LYS:HZ3	1:L:47:LEU:HD13	1.51	0.76
2:H:195:ILE:HG23	2:H:210:ARG:NE	2.00	0.76
2:H:201:LYS:HD2	2:H:201:LYS:H	1.50	0.76
3:A:325:SER:O	3:A:326:LYS:HG2	1.85	0.76
1:L:110:LYS:HD2	1:L:111:ALA:N	2.00	0.75
1:L:181:THR:HG22	1:L:182:PRO:HD2	1.67	0.75
1:L:188:HIS:CG	1:L:189:ARG:HD2	2.23	0.74
3:A:321:ARG:HD3	4:B:108:LEU:HG	1.69	0.74
4:B:158:ASP:OD1	4:B:159:TYR:N	2.20	0.74
1:L:122:SER:O	1:L:126:GLN:NE2	2.20	0.74
1:L:11:VAL:HG11	1:L:21:ILE:HD11	1.68	0.73
4:B:9:PHE:HZ	4:B:115:VAL:HG11	1.54	0.73
1:L:124:GLU:OE2	1:L:130:ALA:HA	1.88	0.72
2:H:209:LYS:C	2:H:210:ARG:HH11	1.92	0.72
1:L:195:VAL:O	1:L:202:VAL:N	2.19	0.72
3:A:26:VAL:HG13	3:A:315:ARG:HH11	1.54	0.71
4:B:162:TYR:CD2	4:B:165:GLU:HG2	2.25	0.71
1:L:28:ILE:HD11	1:L:69:THR:O	1.90	0.71
1:L:118:PHE:HB3	2:H:124:LEU:HD22	1.71	0.71
2:H:114:ALA:HB3	2:H:146:PHE:HE2	1.50	0.70
1:L:37:GLN:HE22	1:L:47:LEU:CB	2.04	0.70
2:H:182:VAL:HG22	2:H:184:VAL:HG23	1.74	0.70
2:H:146:PHE:HB2	2:H:175:LEU:CD1	2.17	0.70
1:L:49:TYR:O	1:L:53:GLN:HB2	1.90	0.69
1:L:188:HIS:HA	1:L:189:ARG:HH11	1.58	0.69
1:L:144:VAL:HG11	1:L:196:THR:O	1.93	0.69
1:L:144:VAL:HG12	1:L:145:THR:H	1.58	0.69
1:L:35:TRP:CZ2	1:L:73:LEU:HD13	2.28	0.69
3:A:28:THR:HB	4:B:105:GLU:HG2	1.74	0.68
4:B:129:ASN:O	4:B:141:TYR:N	2.16	0.68
4:B:122:VAL:HA	4:B:125:GLN:HB2	1.75	0.68
1:L:75:ILE:HD11	1:L:86:TYR:CE2	2.29	0.68
2:H:209:LYS:N	2:H:210:ARG:NH1	2.41	0.67
4:B:23:GLY:HA3	4:B:36:ALA:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:316:MET:HE1	4:B:55:VAL:HG11	1.75	0.67
2:H:146:PHE:CB	2:H:175:LEU:HD11	2.18	0.67
2:H:13:LYS:CG	2:H:14:PRO:HD2	2.24	0.66
2:H:195:ILE:HG22	2:H:210:ARG:HH21	1.60	0.66
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.77	0.66
3:A:26:VAL:HG13	3:A:315:ARG:NH1	2.11	0.66
1:L:151:ASP:N	1:L:189:ARG:HD3	2.11	0.66
2:H:11:VAL:HG13	2:H:110:THR:O	1.94	0.66
2:H:149:PRO:O	2:H:200:HIS:HB2	1.96	0.66
2:H:11:VAL:HG22	2:H:110:THR:HB	1.77	0.65
2:H:123:PRO:HD3	2:H:209:LYS:HG2	1.78	0.65
1:L:118:PHE:CD1	2:H:124:LEU:HB3	2.31	0.65
1:L:166:LYS:CE	1:L:170:ASN:OD1	2.44	0.65
2:H:148:GLU:HG3	2:H:149:PRO:HA	1.78	0.64
1:L:35:TRP:HZ2	1:L:73:LEU:HD22	1.62	0.64
1:L:146:VAL:CG2	1:L:148:TRP:HE1	2.10	0.64
1:L:6:GLN:NE2	1:L:88:CYS:H	1.94	0.64
1:L:184:GLN:HE22	1:L:188:HIS:CD2	2.15	0.64
1:L:5:THR:O	1:L:23:CYS:HA	1.98	0.64
1:L:47:LEU:HD12	1:L:58:VAL:HG22	1.79	0.64
1:L:166:LYS:HE3	1:L:170:ASN:OD1	1.98	0.64
2:H:148:GLU:HG3	2:H:149:PRO:CA	2.28	0.64
1:L:47:LEU:HD12	1:L:58:VAL:CG2	2.27	0.64
2:H:2:VAL:HG11	2:H:94:ARG:NH1	2.12	0.64
4:B:103:GLU:OE1	4:B:103:GLU:N	2.31	0.64
2:H:209:LYS:N	2:H:210:ARG:HH11	1.96	0.63
1:L:188:HIS:CD2	1:L:189:ARG:NH1	2.66	0.63
1:L:35:TRP:CZ2	1:L:73:LEU:HD22	2.33	0.63
1:L:33:VAL:HG11	1:L:66:LYS:HZ3	1.64	0.63
3:A:39:SER:HB2	3:A:316:MET:O	1.99	0.63
4:B:103:GLU:HA	4:B:106:ARG:CG	2.29	0.63
1:L:136:ILE:CG2	1:L:139:PHE:CZ	2.82	0.62
1:L:156:LYS:O	1:L:159:VAL:HG12	1.99	0.62
1:L:37:GLN:NE2	1:L:47:LEU:HB2	2.15	0.62
1:L:14:THR:HG22	1:L:106(A):LEU:HD12	1.82	0.62
1:L:144:VAL:HG11	1:L:197:HIS:HA	1.81	0.62
1:L:61:ARG:HH22	1:L:82:ASP:CG	2.02	0.62
1:L:171:LYS:N	1:L:171:LYS:HD3	2.14	0.61
2:H:3:GLN:OE1	2:H:4:LEU:N	2.32	0.61
2:H:204:ASN:OD1	2:H:204:ASN:N	2.33	0.61
1:L:33:VAL:HG11	1:L:66:LYS:NZ	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:VAL:HG22	1:L:89:ALA:O	2.00	0.61
1:L:110:LYS:HZ1	1:L:112:ALA:HA	1.65	0.61
2:H:200:HIS:N	2:H:205:THR:O	2.33	0.61
2:H:150:VAL:HG23	2:H:200:HIS:HB3	1.82	0.61
2:H:201:LYS:H	2:H:201:LYS:CD	2.10	0.61
4:B:9:PHE:HZ	4:B:115:VAL:CG1	2.14	0.61
1:L:52:ASP:OD1	1:L:53:GLN:NE2	2.33	0.60
1:L:85:GLU:HG2	1:L:102:THR:O	2.01	0.60
4:B:162:TYR:HE2	4:B:165:GLU:HG2	1.65	0.60
1:L:28:ILE:HG22	1:L:33:VAL:HG23	1.83	0.60
1:L:124:GLU:HG2	1:L:129:LYS:CB	2.28	0.60
2:H:186:SER:O	2:H:189:LEU:HG	2.02	0.60
1:L:23:CYS:N	1:L:71:ALA:O	2.34	0.60
4:B:121:LYS:CG	4:B:122:VAL:HG13	2.31	0.60
1:L:33:VAL:HG23	1:L:90:ALA:HB2	1.83	0.60
1:L:27(A):SER:HA	1:L:30:ARG:HH11	1.65	0.60
2:H:184:VAL:HG13	2:H:185:PRO:HD2	1.83	0.60
1:L:54:ARG:NH1	1:L:58:VAL:O	2.35	0.59
1:L:184:GLN:O	1:L:184:GLN:NE2	2.35	0.59
2:H:201:LYS:HD2	2:H:201:LYS:N	2.16	0.59
2:H:114:ALA:CB	2:H:146:PHE:CZ	2.83	0.59
1:L:144:VAL:HG12	1:L:145:THR:N	2.15	0.59
2:H:170:LEU:HD13	2:H:176:TYR:CE1	2.38	0.59
4:B:102:LEU:HB3	4:B:106:ARG:NH1	2.17	0.59
4:B:94:TYR:O	4:B:98:LEU:HG	2.03	0.59
1:L:186:LYS:HG2	1:L:187:SER:N	2.18	0.58
2:H:195:ILE:CG2	2:H:210:ARG:HH21	2.16	0.58
1:L:6:GLN:HE22	1:L:88:CYS:H	1.52	0.58
1:L:83:GLU:OE2	1:L:106:VAL:CG2	2.51	0.58
4:B:103:GLU:HA	4:B:106:ARG:HG2	1.85	0.58
4:B:119:TYR:O	4:B:123:LYS:HE2	2.03	0.58
1:L:83:GLU:HG3	1:L:106:VAL:HG22	1.85	0.58
1:L:66:LYS:HB3	1:L:71:ALA:HB2	1.85	0.58
1:L:175:SER:OG	2:H:166:PHE:CD2	2.54	0.58
3:A:13:ILE:HA	4:B:26:HIS:HA	1.86	0.58
1:L:118:PHE:HE2	1:L:135:LEU:HD12	1.69	0.58
1:L:160:GLU:HB3	2:H:169:VAL:HG21	1.86	0.58
4:B:19:ASP:HB2	4:B:36:ALA:HB3	1.85	0.58
1:L:115:VAL:HG22	1:L:136:ILE:HG23	1.86	0.57
1:L:188:HIS:ND1	1:L:189:ARG:HD2	2.19	0.57
1:L:142:GLY:HA2	1:L:172:TYR:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:ASN:C	1:L:171:LYS:HD3	2.24	0.57
4:B:112:ASP:O	4:B:116:LYS:HG3	2.05	0.57
1:L:141:PRO:C	1:L:172:TYR:CE2	2.78	0.57
2:H:155:ASN:HD21	2:H:195:ILE:H	1.51	0.57
1:L:37:GLN:HG2	1:L:45:LYS:O	2.04	0.56
2:H:13:LYS:HG3	2:H:113:SER:HA	1.86	0.56
1:L:83:GLU:OE2	1:L:106:VAL:HG23	2.05	0.56
1:L:135:LEU:HD22	2:H:166:PHE:CD2	2.39	0.56
1:L:35:TRP:HZ2	1:L:73:LEU:HD13	1.70	0.56
1:L:197:HIS:CE1	1:L:198:GLU:HG2	2.41	0.56
2:H:113:SER:O	2:H:114:ALA:HB2	2.05	0.56
3:A:43:LEU:HD21	3:A:314:LEU:HD12	1.88	0.56
2:H:148:GLU:HB2	2:H:176:TYR:CE2	2.41	0.56
1:L:37:GLN:CG	1:L:45:LYS:HG2	2.36	0.56
1:L:39:PHE:CE1	1:L:42:THR:HG21	2.41	0.56
2:H:94:ARG:O	2:H:100(D):MET:HA	2.06	0.56
3:A:16:GLY:HA2	4:B:9:PHE:CE1	2.41	0.56
1:L:27(A):SER:HA	1:L:30:ARG:NH1	2.21	0.56
1:L:166:LYS:HE3	1:L:170:ASN:O	2.06	0.56
1:L:51:ASN:CA	1:L:66:LYS:HD2	2.34	0.55
1:L:35:TRP:NE1	1:L:73:LEU:HD13	2.21	0.55
3:A:321:ARG:NH1	4:B:108:LEU:HD23	2.20	0.55
4:B:121:LYS:HG2	4:B:122:VAL:N	2.21	0.55
1:L:47:LEU:O	1:L:55:PRO:HD2	2.05	0.55
1:L:23:CYS:O	1:L:71:ALA:N	2.33	0.55
1:L:35:TRP:HE1	1:L:73:LEU:HD13	1.71	0.55
1:L:179:SER:O	1:L:180:LEU:HG	2.07	0.55
4:B:59:MET:SD	4:B:59:MET:N	2.78	0.55
4:B:165:GLU:O	4:B:169:ASN:N	2.33	0.55
1:L:38:GLN:NE2	1:L:44:PRO:HG3	2.22	0.55
3:A:24:ASP:HB3	3:A:315:ARG:NH2	2.22	0.55
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.42	0.55
1:L:183:GLU:O	1:L:187:SER:OG	2.20	0.55
1:L:183:GLU:HG3	1:L:184:GLN:N	2.22	0.55
2:H:129:LYS:HG3	2:H:135:THR:O	2.07	0.55
3:A:39:SER:OG	3:A:315:ARG:NE	2.39	0.55
4:B:78:LYS:H	4:B:78:LYS:HD2	1.72	0.55
3:A:310:CYS:SG	3:A:311:SER:N	2.80	0.54
1:L:34:ASN:O	1:L:89:ALA:N	2.39	0.54
2:H:156:SER:O	2:H:156:SER:OG	2.18	0.54
4:B:118:LEU:O	4:B:121:LYS:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:110:LYS:HD3	1:L:197:HIS:CE1	2.42	0.54
1:L:48:ILE:HD11	1:L:51:ASN:O	2.07	0.54
1:L:110:LYS:HD2	1:L:111:ALA:H	1.72	0.54
1:L:148:TRP:CZ2	1:L:176:SER:HB3	2.42	0.54
2:H:11:VAL:HG11	2:H:147:PRO:HG3	1.90	0.54
1:L:36:TYR:O	1:L:87:TYR:N	2.37	0.54
1:L:35:TRP:CE2	1:L:73:LEU:HD13	2.43	0.54
2:H:192:GLN:NE2	2:H:193:THR:O	2.41	0.54
4:B:30:GLN:HE22	4:B:145:ASN:HB3	1.72	0.54
1:L:61:ARG:NH2	1:L:82:ASP:OD2	2.41	0.54
1:L:127:ALA:O	1:L:129:LYS:HE3	2.08	0.53
3:A:16:GLY:HA2	4:B:9:PHE:HE1	1.73	0.53
2:H:95:HIS:HB3	2:H:100(B):SER:OG	2.08	0.53
3:A:311:SER:HB3	3:A:313:LYS:NZ	2.24	0.53
1:L:96:ALA:HB3	2:H:47:TRP:CG	2.43	0.53
1:L:186:LYS:CG	1:L:187:SER:N	2.72	0.53
2:H:93:ALA:HB1	2:H:100(D):MET:HB3	1.90	0.53
2:H:159:LEU:HD21	2:H:194:TYR:HD1	1.73	0.53
2:H:121:VAL:HG23	2:H:209:LYS:HB2	1.90	0.53
4:B:90:LYS:HZ2	4:B:94:TYR:HE2	1.57	0.53
1:L:50:SER:HB2	1:L:53:GLN:HG2	1.90	0.53
2:H:198:VAL:O	2:H:207:VAL:N	2.32	0.53
1:L:35:TRP:CH2	1:L:47:LEU:HD23	2.44	0.53
2:H:124:LEU:N	2:H:139:GLY:O	2.26	0.52
1:L:21:ILE:HD12	1:L:86:TYR:OH	2.07	0.52
1:L:37:GLN:NE2	1:L:47:LEU:HD13	2.24	0.52
2:H:4:LEU:HG	2:H:102:VAL:CG1	2.38	0.52
2:H:126:PRO:HA	2:H:137:ALA:O	2.09	0.52
2:H:2:VAL:HG11	2:H:94:ARG:HH12	1.74	0.52
1:L:132:LEU:HD11	1:L:185:TRP:CZ2	2.44	0.52
2:H:119:PRO:HD3	2:H:200:HIS:HE1	1.72	0.52
4:B:134:GLY:O	4:B:135:ASN:HB3	2.09	0.52
1:L:136:ILE:CG2	1:L:139:PHE:HZ	2.23	0.52
3:A:15:ILE:HG13	4:B:24:TYR:HD1	1.75	0.52
1:L:147:ALA:C	1:L:148:TRP:HD1	2.14	0.51
2:H:4:LEU:HB3	2:H:22:CYS:SG	2.51	0.51
1:L:146:VAL:HG22	1:L:148:TRP:NE1	2.20	0.51
1:L:113:PRO:HA	1:L:138:ASP:HB3	1.93	0.51
4:B:159:TYR:CZ	4:B:163:SER:HA	2.46	0.51
2:H:119:PRO:HD3	2:H:200:HIS:CE1	2.45	0.51
2:H:123:PRO:HB2	2:H:211:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:GLN:NE2	1:L:45:LYS:HG2	2.25	0.51
1:L:65:SER:C	1:L:66:LYS:HG2	2.31	0.51
3:A:16:GLY:CA	4:B:9:PHE:HE1	2.24	0.51
1:L:35:TRP:CZ3	1:L:86:TYR:CD1	2.99	0.51
2:H:184:VAL:HG11	2:H:194:TYR:OH	2.11	0.51
2:H:210:ARG:N	2:H:210:ARG:HD2	2.25	0.51
4:B:133:ILE:HG12	4:B:137:CYS:C	2.30	0.51
1:L:66:LYS:NZ	1:L:71:ALA:HB1	2.26	0.50
2:H:155:ASN:ND2	2:H:195:ILE:H	2.09	0.50
3:A:34:VAL:HG21	3:A:321:ARG:HH12	1.76	0.50
2:H:33:ALA:HB2	2:H:98:TYR:O	2.11	0.50
4:B:163:SER:O	4:B:167:LYS:HG2	2.10	0.50
1:L:33:VAL:CG2	1:L:90:ALA:HB2	2.41	0.50
1:L:35:TRP:HE1	1:L:73:LEU:CD1	2.24	0.50
1:L:73:LEU:HD23	1:L:74:ALA:N	2.27	0.50
4:B:6:ILE:HG23	4:B:7:ALA:H	1.76	0.50
4:B:165:GLU:HA	4:B:168:LEU:HG	1.92	0.50
1:L:144:VAL:CG1	1:L:196:THR:O	2.59	0.50
4:B:25:HIS:HB2	4:B:34:TYR:HD1	1.76	0.50
1:L:204:LYS:HD2	1:L:205:THR:H	1.77	0.50
4:B:102:LEU:HB3	4:B:106:ARG:HH12	1.76	0.50
2:H:11:VAL:HG21	2:H:147:PRO:HG2	1.93	0.50
1:L:140:TYR:HA	1:L:172:TYR:HE2	1.76	0.49
2:H:145:TYR:HB2	2:H:200:HIS:CE1	2.47	0.49
1:L:132:LEU:HD11	1:L:185:TRP:HZ2	1.77	0.49
1:L:151:ASP:H	1:L:189:ARG:HD3	1.76	0.49
2:H:40:ALA:HB3	2:H:43:GLN:CD	2.32	0.49
4:B:25:HIS:HB2	4:B:34:TYR:HA	1.94	0.49
4:B:133:ILE:HG12	4:B:137:CYS:O	2.12	0.49
1:L:37:GLN:HE21	1:L:45:LYS:HG2	1.77	0.49
4:B:166:SER:O	4:B:170:ARG:HB2	2.12	0.49
1:L:114:SER:H	1:L:138:ASP:HB3	1.77	0.49
2:H:199:ASN:HA	2:H:205:THR:O	2.12	0.49
4:B:142:HIS:HD2	4:B:143:LYS:H	1.60	0.49
1:L:117:LEU:HD11	1:L:132:LEU:HB3	1.95	0.49
2:H:1:GLN:OE1	2:H:1:GLN:N	2.39	0.49
1:L:132:LEU:HD13	1:L:178:LEU:HB3	1.94	0.49
1:L:204:LYS:CD	1:L:205:THR:H	2.26	0.49
2:H:136:ALA:O	2:H:183:THR:HG23	2.13	0.49
4:B:9:PHE:CE2	4:B:115:VAL:HB	2.48	0.49
1:L:95:LEU:HA	2:H:61:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:37:GLN:HG3	1:L:45:LYS:HG2	1.94	0.48
1:L:121:SER:O	1:L:124:GLU:HB3	2.12	0.48
1:L:65:SER:O	1:L:66:LYS:HG2	2.13	0.48
1:L:128:ASN:HB2	1:L:129:LYS:HD3	1.96	0.48
1:L:168:SER:C	1:L:170:ASN:H	2.16	0.48
2:H:73:ILE:HG13	2:H:74:PHE:N	2.28	0.48
2:H:209:LYS:H	2:H:210:ARG:NH1	2.10	0.48
1:L:139:PHE:HB3	1:L:172:TYR:CZ	2.48	0.48
4:B:87:ILE:O	4:B:91:ILE:HG13	2.14	0.48
2:H:125:ALA:O	2:H:127:SER:N	2.41	0.48
1:L:151:ASP:CG	1:L:189:ARG:HE	2.17	0.48
4:B:24:TYR:CE1	4:B:121:LYS:HE3	2.48	0.48
2:H:184:VAL:CG1	2:H:185:PRO:HD2	2.43	0.48
2:H:201:LYS:HA	2:H:204:ASN:HA	1.95	0.48
4:B:90:LYS:NZ	4:B:94:TYR:HE2	2.12	0.48
4:B:114:ASN:O	4:B:117:ASN:HB2	2.13	0.48
4:B:159:TYR:C	4:B:161:LYS:N	2.67	0.48
4:B:164:GLU:H	4:B:164:GLU:CD	2.12	0.48
2:H:195:ILE:HG22	2:H:210:ARG:NH2	2.27	0.47
4:B:159:TYR:CE1	4:B:161:LYS:HE2	2.49	0.47
2:H:165:THR:HG22	2:H:180:SER:CB	2.38	0.47
2:H:166:PHE:C	2:H:178:LEU:HD21	2.34	0.47
1:L:44:PRO:HD2	2:H:103:TRP:CE3	2.49	0.47
4:B:109:ASP:O	4:B:113:SER:HB3	2.14	0.47
2:H:148:GLU:HG3	2:H:149:PRO:CB	2.44	0.47
4:B:127:LYS:HB3	4:B:127:LYS:HE3	1.35	0.47
4:B:133:ILE:HD11	4:B:139:GLU:N	2.29	0.47
2:H:74:PHE:CZ	3:A:42:LEU:HA	2.49	0.47
2:H:159:LEU:HD21	2:H:194:TYR:CD1	2.49	0.47
3:A:316:MET:CE	4:B:55:VAL:HG11	2.43	0.47
2:H:154:TRP:CZ3	2:H:196:CYS:SG	3.08	0.47
4:B:52:VAL:O	4:B:56:ILE:HG13	2.14	0.47
1:L:182:PRO:O	1:L:186:LYS:N	2.39	0.47
4:B:128:ASN:ND2	4:B:170:ARG:HH22	2.12	0.47
3:A:13:ILE:HG13	4:B:26:HIS:HB3	1.97	0.47
4:B:121:LYS:NZ	4:B:122:VAL:HG22	2.20	0.47
1:L:114:SER:N	1:L:138:ASP:HB3	2.30	0.46
4:B:59:MET:O	4:B:60:ASN:HB3	2.16	0.46
4:B:84:ILE:O	4:B:87:ILE:HB	2.15	0.46
1:L:14:THR:HG22	1:L:106(A):LEU:CD1	2.43	0.46
1:L:147:ALA:C	1:L:148:TRP:CD1	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:15:ILE:HD11	4:B:121:LYS:NZ	2.30	0.46
3:A:313:LYS:HE2	3:A:313:LYS:HB2	1.80	0.46
4:B:127:LYS:HE2	4:B:159:TYR:CD2	2.50	0.46
1:L:140:TYR:HE1	1:L:171:LYS:HD2	1.68	0.46
2:H:195:ILE:CG2	2:H:210:ARG:NH2	2.77	0.46
4:B:127:LYS:HB3	4:B:128:ASN:H	1.58	0.46
4:B:30:GLN:NE2	4:B:145:ASN:HB3	2.31	0.46
1:L:148:TRP:CE3	1:L:178:LEU:HB2	2.50	0.46
2:H:4:LEU:HG	2:H:102:VAL:HG12	1.98	0.46
2:H:162:GLY:C	2:H:182:VAL:HG23	2.36	0.46
3:A:12:THR:HA	4:B:138:PHE:O	2.16	0.46
4:B:9:PHE:HE2	4:B:115:VAL:HB	1.80	0.46
4:B:159:TYR:CE2	4:B:163:SER:HB3	2.50	0.46
1:L:160:GLU:CB	2:H:169:VAL:HG21	2.45	0.46
3:A:18:HIS:O	3:A:320:LEU:HD11	2.16	0.46
4:B:16:GLY:HA3	4:B:34:TYR:CE2	2.51	0.46
1:L:35:TRP:HB3	1:L:88:CYS:HA	1.98	0.45
1:L:118:PHE:CE2	1:L:135:LEU:HD12	2.51	0.45
4:B:25:HIS:HD2	4:B:33:GLY:C	2.19	0.45
1:L:35:TRP:HA	1:L:87:TYR:O	2.16	0.45
2:H:195:ILE:HG23	2:H:210:ARG:CZ	2.46	0.45
4:B:115:VAL:HA	4:B:118:LEU:HB2	1.99	0.45
1:L:122:SER:O	1:L:126:GLN:HG2	2.16	0.45
1:L:133:VAL:HG11	2:H:179:SER:OG	2.16	0.45
1:L:142:GLY:HA2	1:L:172:TYR:CE1	2.51	0.45
2:H:155:ASN:HD22	2:H:159:LEU:HD22	1.81	0.45
4:B:25:HIS:CD2	4:B:33:GLY:H	2.35	0.45
4:B:58:LYS:HD2	4:B:58:LYS:N	2.32	0.45
1:L:134:CYS:SG	1:L:148:TRP:CZ2	3.10	0.45
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.80	0.45
4:B:157:TYR:OH	4:B:161:LYS:NZ	2.35	0.45
3:A:28:THR:CB	4:B:105:GLU:HG2	2.44	0.45
4:B:159:TYR:CE2	4:B:163:SER:HA	2.51	0.45
1:L:47:LEU:HD12	1:L:58:VAL:HG21	1.99	0.45
4:B:122:VAL:CG2	4:B:126:LEU:HG	2.47	0.45
4:B:163:SER:OG	4:B:164:GLU:OE1	2.33	0.45
1:L:117:LEU:HD13	1:L:134:CYS:SG	2.57	0.45
1:L:139:PHE:CB	1:L:172:TYR:CZ	3.00	0.45
1:L:184:GLN:NE2	1:L:188:HIS:CD2	2.84	0.44
2:H:152:VAL:HG22	2:H:198:VAL:HG13	1.99	0.44
4:B:56:ILE:O	4:B:59:MET:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:TYR:CZ	2:H:94:ARG:NH2	2.84	0.44
3:A:24:ASP:HB3	3:A:315:ARG:CZ	2.46	0.44
1:L:34:ASN:N	1:L:89:ALA:O	2.49	0.44
1:L:85:GLU:HG2	1:L:102:THR:C	2.38	0.44
1:L:132:LEU:CG	1:L:185:TRP:HZ2	2.31	0.44
1:L:183:GLU:OE1	1:L:186:LYS:HE2	2.17	0.44
1:L:188:HIS:HB3	1:L:189:ARG:HB2	1.98	0.44
4:B:135:ASN:OD1	4:B:136:GLY:N	2.51	0.44
2:H:196:CYS:C	2:H:210:ARG:HH22	2.21	0.44
1:L:37:GLN:OE1	1:L:47:LEU:HD22	2.18	0.44
1:L:139:PHE:HB2	1:L:172:TYR:CE2	2.53	0.44
1:L:17:GLN:HG2	1:L:18:ARG:H	1.81	0.44
1:L:47:LEU:HD21	1:L:62:PHE:CD1	2.53	0.44
1:L:85:GLU:OE1	1:L:87:TYR:CE2	2.70	0.44
2:H:150:VAL:HA	2:H:200:HIS:CB	2.48	0.44
1:L:17:GLN:HG2	1:L:18:ARG:N	2.32	0.44
3:A:29:VAL:N	4:B:101:LEU:HB3	2.33	0.44
4:B:129:ASN:ND2	4:B:159:TYR:CZ	2.86	0.43
4:B:168:LEU:O	4:B:171:GLU:N	2.35	0.43
1:L:132:LEU:CD1	1:L:185:TRP:CZ2	3.01	0.43
1:L:147:ALA:O	1:L:148:TRP:HD1	2.01	0.43
3:A:314:LEU:HD22	4:B:100:VAL:HG21	1.99	0.43
1:L:113:PRO:HA	1:L:138:ASP:O	2.19	0.43
1:L:181:THR:O	1:L:184:GLN:HB3	2.18	0.43
4:B:44:ALA:HA	4:B:110:PHE:HZ	1.82	0.43
4:B:127:LYS:NZ	4:B:159:TYR:CE2	2.80	0.43
1:L:54:ARG:HD2	1:L:58:VAL:O	2.18	0.43
2:H:114:ALA:HB2	2:H:146:PHE:CZ	2.54	0.43
4:B:48:ILE:O	4:B:52:VAL:HG23	2.18	0.43
4:B:171:GLU:HG2	4:B:172:LYS:N	2.34	0.43
1:L:66:LYS:HB3	1:L:71:ALA:CB	2.47	0.43
1:L:140:TYR:CD1	1:L:171:LYS:HB3	2.54	0.43
4:B:148:CYS:O	4:B:152:VAL:HG23	2.18	0.43
4:B:166:SER:HA	4:B:169:ASN:HB2	2.01	0.43
3:A:15:ILE:N	3:A:15:ILE:HD12	2.34	0.43
1:L:163:THR:HA	1:L:164:PRO:HD3	1.85	0.43
3:A:316:MET:HE2	3:A:316:MET:HB2	1.71	0.43
1:L:110:LYS:NZ	1:L:112:ALA:HA	2.33	0.42
1:L:132:LEU:CD1	1:L:185:TRP:HZ2	2.32	0.42
4:B:6:ILE:HG12	4:B:7:ALA:N	2.34	0.42
2:H:71:ALA:HA	2:H:78:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6:GLN:HE22	1:L:88:CYS:N	2.17	0.42
1:L:54:ARG:HA	1:L:55:PRO:HD3	1.84	0.42
1:L:85:GLU:OE1	1:L:85:GLU:C	2.58	0.42
1:L:140:TYR:CD1	1:L:171:LYS:HD2	2.47	0.42
2:H:74:PHE:HZ	3:A:41:ASN:O	2.03	0.42
4:B:165:GLU:HA	4:B:165:GLU:OE1	2.19	0.42
1:L:60:ASP:OD1	1:L:60:ASP:N	2.53	0.42
1:L:27:ASP:O	1:L:30:ARG:HG2	2.20	0.42
1:L:133:VAL:HG12	1:L:135:LEU:CD2	2.49	0.42
4:B:121:LYS:CG	4:B:122:VAL:N	2.82	0.42
1:L:110:LYS:HZ3	1:L:197:HIS:CE1	2.37	0.42
4:B:127:LYS:CE	4:B:129:ASN:HD21	2.33	0.42
1:L:20:THR:HG23	1:L:72:SER:OG	2.19	0.41
4:B:95:ASN:O	4:B:99:LEU:HG	2.20	0.41
3:A:31:GLU:OE1	3:A:34:VAL:HG22	2.20	0.41
1:L:148:TRP:HH2	1:L:176:SER:O	2.03	0.41
3:A:14:CYS:O	4:B:25:HIS:N	2.41	0.41
1:L:108:GLN:HG2	1:L:140:TYR:CE2	2.55	0.41
1:L:110:LYS:CE	1:L:197:HIS:ND1	2.83	0.41
1:L:129:LYS:HZ2	1:L:129:LYS:HG3	1.76	0.41
2:H:175:LEU:HD12	2:H:175:LEU:HA	1.21	0.41
1:L:148:TRP:O	1:L:154:PRO:HA	2.21	0.41
1:L:48:ILE:HD11	1:L:52:ASP:HA	2.01	0.41
1:L:66:LYS:CE	1:L:71:ALA:HB1	2.51	0.41
1:L:166:LYS:HE2	1:L:170:ASN:OD1	2.19	0.41
2:H:178:LEU:HD23	2:H:179:SER:H	1.86	0.41
2:H:209:LYS:O	2:H:210:ARG:NH1	2.54	0.41
1:L:135:LEU:CD2	2:H:166:PHE:CE2	2.96	0.41
2:H:209:LYS:C	2:H:210:ARG:HD2	2.41	0.41
3:A:31:GLU:OE1	3:A:321:ARG:NH2	2.53	0.41
2:H:114:ALA:HB3	2:H:146:PHE:CE2	2.36	0.41
4:B:142:HIS:CD2	4:B:143:LYS:H	2.36	0.41
1:L:18:ARG:HG2	1:L:76:SER:HA	2.02	0.41
1:L:139:PHE:HD1	1:L:172:TYR:O	2.04	0.41
1:L:140:TYR:HA	1:L:172:TYR:CE2	2.53	0.41
1:L:151:ASP:OD1	1:L:189:ARG:NE	2.54	0.41
1:L:194:GLN:NE2	1:L:203:GLU:OE1	2.50	0.41
1:L:204:LYS:HD2	1:L:204:LYS:HA	1.43	0.41
2:H:12:LYS:NZ	2:H:17:SER:O	2.34	0.41
2:H:96:GLY:N	2:H:100(C):GLY:O	2.54	0.41
2:H:148:GLU:HG3	2:H:149:PRO:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:155:ASN:ND2	2:H:159:LEU:HD22	2.36	0.41
2:H:196:CYS:H	2:H:210:ARG:NH1	2.18	0.41
3:A:321:ARG:HD3	4:B:108:LEU:CG	2.44	0.41
4:B:165:GLU:OE1	4:B:168:LEU:HD12	2.20	0.41
1:L:110:LYS:HZ3	1:L:197:HIS:CG	2.39	0.40
2:H:11:VAL:HG11	2:H:147:PRO:CG	2.51	0.40
2:H:143:LYS:O	2:H:144:ASP:OD1	2.39	0.40
4:B:27:GLN:OE1	4:B:27:GLN:HA	2.21	0.40
3:A:317:VAL:HG12	4:B:104:ASN:OD1	2.21	0.40
4:B:143:LYS:HA	4:B:143:LYS:HD3	1.62	0.40
1:L:181:THR:HG22	1:L:182:PRO:CD	2.45	0.40
1:L:132:LEU:HD12	1:L:132:LEU:N	2.36	0.40
2:H:151:THR:HG22	2:H:199:ASN:O	2.21	0.40
3:A:20:ASN:ND2	3:A:37:THR:HB	2.36	0.40
4:B:127:LYS:NZ	4:B:128:ASN:OD1	2.37	0.40
4:B:30:GLN:HE22	4:B:145:ASN:CB	2.33	0.40
4:B:159:TYR:HA	4:B:161:LYS:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	L	209/215 (97%)	200 (96%)	4 (2%)	5 (2%)	6 37
2	H	213/230 (93%)	204 (96%)	6 (3%)	3 (1%)	11 48
3	A	48/66 (73%)	44 (92%)	3 (6%)	1 (2%)	7 40
4	B	150/193 (78%)	112 (75%)	25 (17%)	13 (9%)	1 9
All	All	620/704 (88%)	560 (90%)	38 (6%)	22 (4%)	3 30

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	107	GLY
1	L	128	ASN
2	H	189	LEU
2	H	204	ASN
3	A	325	SER
4	B	5	ALA
4	B	147	GLU
4	B	161	LYS
1	L	106(A)	LEU
1	L	180	LEU
1	L	189	ARG
4	B	9	PHE
4	B	121	LYS
4	B	135	ASN
4	B	157	TYR
4	B	159	TYR
4	B	171	GLU
4	B	6	ILE
4	B	7	ALA
4	B	132	GLU
2	H	149	PRO
4	B	60	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	175/179 (98%)	152 (87%)	23 (13%)	4 23
2	H	181/193 (94%)	170 (94%)	11 (6%)	18 53
3	A	48/56 (86%)	45 (94%)	3 (6%)	18 53
4	B	133/167 (80%)	128 (96%)	5 (4%)	33 66
All	All	537/595 (90%)	495 (92%)	42 (8%)	12 44

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	THR
1	L	28	ILE
1	L	30	ARG
1	L	32	SER
1	L	33	VAL
1	L	37	GLN
1	L	45	LYS
1	L	53	GLN
1	L	63	SER
1	L	66	LYS
1	L	73	LEU
1	L	106	VAL
1	L	106(A)	LEU
1	L	108	GLN
1	L	124	GLU
1	L	139	PHE
1	L	156	LYS
1	L	161	THR
1	L	181	THR
1	L	183	GLU
1	L	191	TYR
1	L	204	LYS
1	L	205	THR
2	H	19	LYS
2	H	116	THR
2	H	135	THR
2	H	144	ASP
2	H	156	SER
2	H	160	THR
2	H	164	HIS
2	H	173	SER
2	H	201	LYS
2	H	204	ASN
2	H	210	ARG
3	A	32	LYS
3	A	44	GLU
3	A	320	LEU
4	B	115	VAL
4	B	121	LYS
4	B	127	LYS
4	B	162	TYR
4	B	171	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	37	GLN
1	L	38	GLN
1	L	184	GLN
1	L	188	HIS
2	H	155	ASN
2	H	192	GLN
2	H	200	HIS
4	B	129	ASN
4	B	145	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	211/215 (98%)	1.35	53 (25%)	0	0	104, 181, 245, 333	0
2	H	217/230 (94%)	0.78	29 (13%)	3	2	74, 135, 238, 337	0
3	A	52/66 (78%)	0.29	2 (3%)	40	26	91, 123, 170, 200	0
4	B	154/193 (79%)	0.31	12 (7%)	13	8	90, 141, 191, 220	0
All	All	634/704 (90%)	0.81	96 (15%)	2	1	74, 160, 234, 337	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	208	PRO	13.6
1	L	169	ASN	12.1
2	H	184	VAL	9.6
2	H	161	SER	7.8
1	L	171	LYS	7.7
2	H	135	THR	6.8
2	H	206	LYS	6.6
1	L	207	ALA	6.4
2	H	212	GLU	5.9
2	H	213	PRO	5.9
1	L	73	LEU	5.2
1	L	128	ASN	5.2
1	L	193	CYS	5.1
2	H	207	VAL	4.8
1	L	142	GLY	4.8
1	L	20	THR	4.8
1	L	74	ALA	4.7
2	H	136	ALA	4.3
1	L	197	HIS	4.3
1	L	68	GLY	4.3
1	L	184	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	134	GLY	3.9
1	L	192	SER	3.8
2	H	175	LEU	3.7
1	L	35	TRP	3.6
1	L	110	LYS	3.4
1	L	165	SER	3.4
2	H	195	ILE	3.4
1	L	183	GLU	3.3
2	H	155	ASN	3.2
1	L	187	SER	3.2
2	H	162	GLY	3.2
2	H	185	PRO	3.1
4	B	142	HIS	3.1
4	B	160	PRO	3.1
3	A	312	ALA	3.1
4	B	147	GLU	3.1
2	H	211	VAL	3.0
2	H	183	THR	3.0
1	L	159	VAL	3.0
4	B	158	ASP	2.9
2	H	165	THR	2.9
2	H	1	GLN	2.9
1	L	191	TYR	2.9
4	B	143	LYS	2.9
4	B	161	LYS	2.9
1	L	148	TRP	2.9
4	B	4	GLY	2.8
1	L	155	VAL	2.8
2	H	158	ALA	2.8
1	L	140	TYR	2.8
2	H	160	THR	2.8
1	L	127	ALA	2.7
1	L	166	LYS	2.7
1	L	158	GLY	2.6
1	L	75	ILE	2.6
2	H	173	SER	2.6
1	L	150	ALA	2.6
1	L	157	ALA	2.5
2	H	156	SER	2.5
1	L	109	PRO	2.5
1	L	152	SER	2.5
1	L	151	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	123	PRO	2.5
1	L	199	GLY	2.4
2	H	127	SER	2.4
1	L	138	ASP	2.4
1	L	186	LYS	2.4
2	H	128	SER	2.4
1	L	153	SER	2.4
1	L	2	SER	2.4
1	L	108	GLN	2.3
1	L	62	PHE	2.3
1	L	76	SER	2.3
1	L	144	VAL	2.3
4	B	146	ASP	2.3
2	H	194	TYR	2.2
1	L	168	SER	2.2
1	L	51	ASN	2.2
1	L	112	ALA	2.2
1	L	63	SER	2.2
4	B	11	GLU	2.2
1	L	175	SER	2.2
2	H	172	SER	2.2
1	L	28	ILE	2.2
1	L	170	ASN	2.1
3	A	11	ASP	2.1
1	L	5	THR	2.1
1	L	143	ALA	2.1
2	H	190	GLY	2.1
2	H	193	THR	2.1
4	B	29	GLU	2.0
1	L	106	VAL	2.0
4	B	31	GLY	2.0
1	L	14	THR	2.0
4	B	139	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.