Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:09 AM GMT

PDB ID	:	3HFM
Title	:	STRUCTURE OF AN ANTIBODY-ANTIGEN COMPLEX. CRYSTAL STRUCTURE OF THE HY/HEL-10 FAB-LYSOZYME COMPLEX
Authors	:	Padlan, E.A.; Davies, D.R.
Deposited on	:	1988-08-11
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

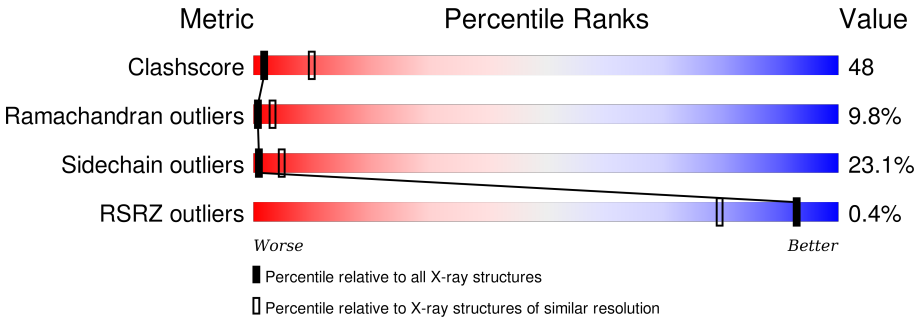
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	214	27% 52% 19% ·
2	H	215	% 30% 45% 19% 6%
3	Y	129	22% 56% 19% ·

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4297 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 HYHEL-10 IGG1 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1655	1026	281	341	7			

- Molecule 2 is a protein called HYHEL-10 IGG1 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1640	1032	266	335	7			

- Molecule 3 is a protein called HEN EGG WHITE LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	129	Total	C	N	O	S	0	0	0
			1001	613	193	185	10			

- Molecule 4 is water.

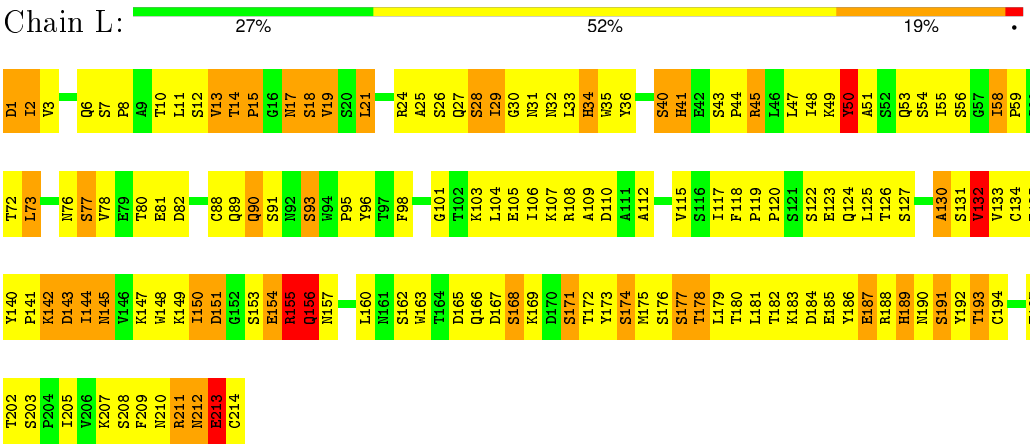
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Y	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

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

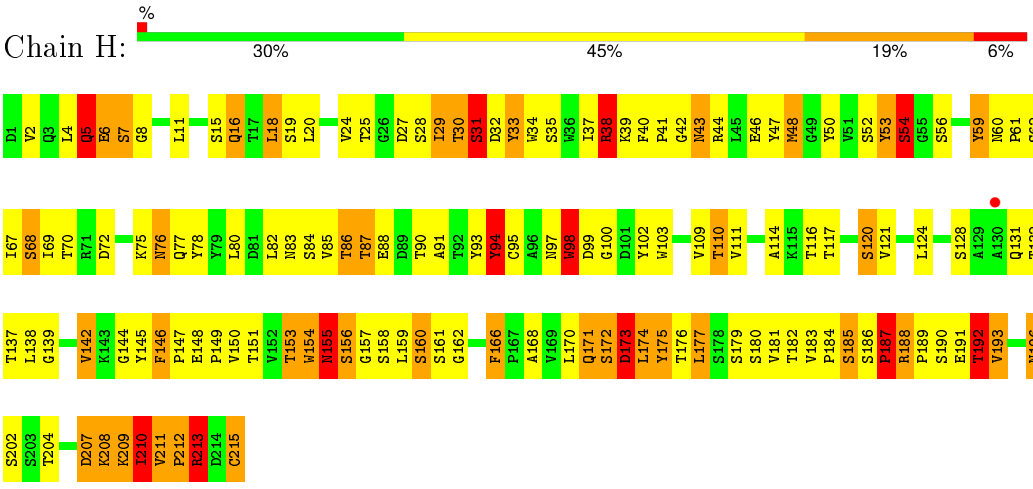
- Molecule 1: HYHEL-10 IGG1 FAB (LIGHT CHAIN)

Chain L:



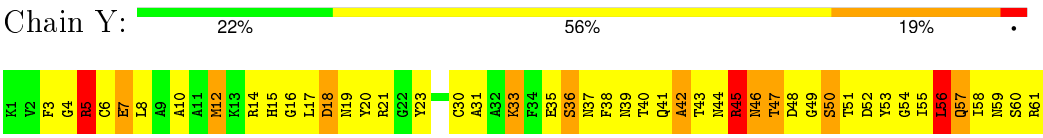
- Molecule 2: HYHEL-10 IGG1 FAB (HEAVY CHAIN)

Chain H:



- Molecule 3: HEN EGG WHITE LYSOZYME

Chain Y:




T69
P70
G71
S72
R73
N74
L75
C76
N77
I78
P79
C80
S81
A82
L83
L84
S85
S86
D87
I88
T89
V92
N93
C94
A95
K96
K97
I98
V99
S100
D101
G102
N103
G104
M105
N106
V109
A110
W111
R112
N113
R114
C115
K116
G117
T118
D119
V120
Q121
A122
W123
I124
R125
R128
L129

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.47Å 118.73Å 137.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 9.99 – 2.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.00) 65.0 (9.99-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.246 , (Not available) 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 38.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 12501 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	4297	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality

5.1 Standard geometry

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	0.81	0/1693	1.72	21/2297 (0.9%)
2	H	0.83	0/1684	1.70	29/2310 (1.3%)
3	Y	0.79	0/1021	1.62	16/1379 (1.2%)
All	All	0.81	0/4398	1.69	66/5986 (1.1%)

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	45	ARG	CD-NE-CZ	20.15	151.81	123.60
1	L	155	ARG	NE-CZ-NH1	13.40	127.00	120.30
2	H	162	GLY	N-CA-C	10.52	139.39	113.10
2	H	44	ARG	NE-CZ-NH2	-9.41	115.59	120.30
3	Y	45	ARG	NE-CZ-NH1	8.92	124.76	120.30
3	Y	114	ARG	NE-CZ-NH1	8.39	124.49	120.30
1	L	145	ASN	CA-CB-CG	8.23	131.50	113.40
1	L	155	ARG	CD-NE-CZ	8.11	134.96	123.60
2	H	38	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	L	212	ASN	CA-CB-CG	8.06	131.14	113.40
2	H	94	TYR	CA-CB-CG	7.99	128.57	113.40
1	L	24	ARG	CD-NE-CZ	7.49	134.09	123.60
2	H	208	LYS	C-N-CA	7.10	139.45	121.70
3	Y	128	ARG	NE-CZ-NH2	-7.07	116.77	120.30
3	Y	45	ARG	CD-NE-CZ	6.91	133.28	123.60
1	L	50	TYR	CA-CB-CG	-6.77	100.54	113.40
2	H	38	ARG	NE-CZ-NH2	-6.69	116.96	120.30
2	H	133	ASN	CA-CB-CG	6.64	128.02	113.40
3	Y	5	ARG	NE-CZ-NH1	6.59	123.60	120.30
3	Y	46	ASN	CB-CA-C	6.34	123.08	110.40
1	L	213	GLU	N-CA-C	6.27	127.94	111.00
3	Y	20	TYR	N-CA-CB	6.21	121.79	110.60
2	H	38	ARG	CA-CB-CG	6.20	127.03	113.40
3	Y	21	ARG	CD-NE-CZ	-6.11	115.05	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	211	VAL	N-CA-C	-6.08	94.58	111.00
3	Y	14	ARG	NE-CZ-NH2	-6.04	117.28	120.30
3	Y	101	ASP	CB-CG-OD1	6.01	123.71	118.30
2	H	175	TYR	N-CA-C	6.00	127.21	111.00
3	Y	112	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	L	155	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	H	174	LEU	C-N-CA	5.90	136.45	121.70
1	L	153	SER	C-N-CA	5.86	136.36	121.70
2	H	187	PRO	CA-N-CD	-5.82	103.35	111.50
2	H	187	PRO	N-CA-C	5.80	127.17	112.10
2	H	48	MET	CB-CA-C	5.75	121.90	110.40
1	L	36	TYR	CA-CB-CG	5.71	124.26	113.40
2	H	211	VAL	CB-CA-C	5.66	122.15	111.40
1	L	1	ASP	CB-CG-OD1	5.61	123.35	118.30
2	H	5	GLN	CB-CG-CD	5.61	126.18	111.60
3	Y	18	ASP	CB-CG-OD1	5.61	123.35	118.30
2	H	33	TYR	CB-CG-CD1	5.44	124.26	121.00
1	L	188	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	Y	56	LEU	CA-CB-CG	5.41	127.73	115.30
1	L	132	VAL	CB-CA-C	5.39	121.64	111.40
1	L	132	VAL	N-CA-C	-5.35	96.55	111.00
2	H	207	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	L	189	HIS	CA-CB-CG	-5.32	104.56	113.60
2	H	171	GLN	CA-CB-CG	5.32	125.10	113.40
2	H	154	TRP	CB-CA-C	5.30	121.00	110.40
2	H	160	SER	N-CA-CB	5.29	118.43	110.50
1	L	188	ARG	CA-CB-CG	5.27	125.00	113.40
2	H	59	TYR	CA-CB-CG	5.26	123.40	113.40
3	Y	114	ARG	NE-CZ-NH2	-5.25	117.67	120.30
3	Y	128	ARG	NE-CZ-NH1	5.23	122.91	120.30
3	Y	45	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	L	13	VAL	C-N-CA	5.15	134.58	121.70
2	H	33	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	L	150	ILE	N-CA-C	-5.10	97.23	111.00
1	L	138	ASN	N-CA-CB	-5.09	101.44	110.60
2	H	207	ASP	CB-CA-C	5.05	120.50	110.40
2	H	213	ARG	CA-CB-CG	5.05	124.50	113.40
2	H	120	SER	N-CA-C	-5.04	97.39	111.00
1	L	205	ILE	N-CA-C	-5.03	97.43	111.00
2	H	196	ASN	CA-CB-CG	-5.01	102.38	113.40
2	H	128	SER	CB-CA-C	5.00	119.61	110.10
2	H	65	SER	N-CA-CB	5.00	118.00	110.50

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	L	1655	0	1572	138	0
2	H	1640	0	1582	176	0
3	Y	1001	0	959	102	0
4	Y	1	0	0	0	0
All	All	4297	0	4113	401	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 (401) 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:L:214:CYS:HA	2:H:215:CYS:CB	1.80	1.11
1:L:214:CYS:CA	2:H:215:CYS:HB3	1.79	1.10
2:H:183:VAL:HB	2:H:184:PRO:HD2	1.27	1.08
2:H:53:TYR:O	2:H:54:SER:HB3	1.35	1.08
1:L:156:GLN:HG3	1:L:157:ASN:H	1.17	1.07
1:L:30:GLY:O	1:L:31:ASN:HB3	1.54	1.05
2:H:188:ARG:CB	2:H:189:PRO:HD3	1.88	1.03
1:L:150:ILE:HD11	1:L:155:ARG:HH11	1.24	1.03
1:L:112:ALA:HB2	1:L:200:THR:HG21	1.40	1.02
2:H:188:ARG:HB3	2:H:189:PRO:CD	1.90	1.01
2:H:155:ASN:HD21	2:H:193:VAL:HA	1.25	1.01
2:H:146:PHE:HD2	2:H:147:PRO:HA	1.25	1.00
2:H:64:LYS:H	2:H:64:LYS:HD2	1.22	1.00
2:H:188:ARG:HB3	2:H:189:PRO:HD3	1.01	0.99
2:H:2:VAL:HG22	2:H:27:ASP:HB2	1.41	0.99
1:L:151:ASP:N	1:L:191:SER:O	1.95	0.98
3:Y:45:ARG:HH11	3:Y:45:ARG:HB2	1.28	0.94
1:L:156:GLN:HG3	1:L:157:ASN:N	1.84	0.93
3:Y:121:GLN:HB3	3:Y:125:ARG:HE	1.30	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:TRP:CE3	2:H:98:TRP:HA	2.03	0.92
2:H:186:SER:HA	2:H:188:ARG:N	1.84	0.91
2:H:132:THR:O	2:H:133:ASN:HB2	1.68	0.90
3:Y:53:TYR:CD1	3:Y:84:LEU:HD11	2.07	0.90
2:H:98:TRP:HE3	2:H:98:TRP:HA	1.36	0.89
3:Y:53:TYR:HD1	3:Y:84:LEU:HD11	1.37	0.89
1:L:156:GLN:CG	1:L:157:ASN:H	1.80	0.89
1:L:213:GLU:HG2	1:L:214:CYS:H	1.37	0.88
3:Y:111:TRP:HA	3:Y:115:CYS:HB2	1.54	0.88
1:L:149:LYS:HB2	1:L:193:THR:HG22	1.55	0.88
1:L:186:TYR:O	1:L:192:TYR:OH	1.91	0.88
2:H:121:VAL:HG21	2:H:197:VAL:HG11	1.55	0.87
3:Y:62:TRP:O	3:Y:75:LEU:HG	1.74	0.87
2:H:18:LEU:CD2	2:H:82:LEU:HB3	2.04	0.86
1:L:49:LYS:HG3	1:L:55:ILE:HD11	1.56	0.86
2:H:146:PHE:HD2	2:H:147:PRO:CA	1.89	0.86
3:Y:5:ARG:NH1	3:Y:123:TRP:O	2.09	0.85
1:L:143:ASP:O	1:L:144:ILE:HB	1.75	0.84
3:Y:59:ASN:ND2	3:Y:60:SER:H	1.75	0.84
1:L:213:GLU:CG	1:L:214:CYS:H	1.89	0.84
2:H:18:LEU:HD21	2:H:82:LEU:HB3	1.59	0.83
1:L:155:ARG:HE	1:L:155:ARG:HA	1.42	0.83
3:Y:12:MET:HG2	3:Y:17:LEU:HD12	1.59	0.83
1:L:47:LEU:HD22	1:L:58:ILE:HD12	1.59	0.82
1:L:132:VAL:HG22	1:L:179:LEU:HB3	1.60	0.82
3:Y:115:CYS:O	3:Y:118:THR:HG23	1.80	0.82
2:H:30:THR:HB	3:Y:73:ARG:NH1	1.96	0.81
2:H:183:VAL:HB	2:H:184:PRO:CD	2.10	0.80
2:H:147:PRO:O	2:H:199:HIS:NE2	2.13	0.80
2:H:146:PHE:CD2	2:H:147:PRO:HA	2.13	0.80
2:H:48:MET:CE	2:H:63:LEU:HD11	2.12	0.80
2:H:136:VAL:HG13	2:H:183:VAL:HG23	1.63	0.80
2:H:90:THR:HG22	2:H:111:VAL:H	1.45	0.80
3:Y:55:ILE:HG22	3:Y:56:LEU:HD13	1.64	0.79
2:H:199:HIS:ND1	2:H:202:SER:HB2	1.98	0.79
2:H:172:SER:O	2:H:173:ASP:HB2	1.84	0.78
2:H:154:TRP:HE1	2:H:179:SER:HG	1.31	0.78
2:H:64:LYS:HB2	2:H:66:ARG:CG	2.13	0.78
2:H:6:GLU:OE1	2:H:94:TYR:HA	1.83	0.78
2:H:156:SER:O	2:H:158:SER:N	2.16	0.77
2:H:148:GLU:HB3	2:H:149:PRO:HA	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:74:ASN:OD1	3:Y:77:ASN:HA	1.85	0.77
2:H:53:TYR:O	2:H:54:SER:CB	2.25	0.76
2:H:64:LYS:HD3	2:H:66:ARG:HE	1.49	0.76
2:H:29:ILE:O	2:H:31:SER:N	2.18	0.75
1:L:155:ARG:O	1:L:156:GLN:HB3	1.86	0.74
3:Y:46:ASN:ND2	3:Y:52:ASP:OD1	2.19	0.74
2:H:64:LYS:HB2	2:H:66:ARG:HG3	1.68	0.74
2:H:188:ARG:HG2	2:H:212:PRO:HB2	1.67	0.74
2:H:16:GLN:HA	2:H:16:GLN:HE21	1.52	0.74
2:H:183:VAL:CB	2:H:184:PRO:HD2	2.13	0.74
1:L:33:LEU:HD21	1:L:88:CYS:HB2	1.69	0.74
1:L:17:ASN:O	1:L:78:VAL:HG13	1.90	0.72
2:H:90:THR:CG2	2:H:111:VAL:H	2.03	0.71
2:H:148:GLU:HB3	2:H:149:PRO:CA	2.19	0.71
1:L:190:ASN:HA	1:L:211:ARG:HG3	1.70	0.71
1:L:90:GLN:NE2	1:L:93:SER:H	1.88	0.71
2:H:86:THR:OG1	2:H:87:THR:N	2.24	0.71
1:L:26:SER:O	1:L:27:GLN:HG2	1.91	0.70
2:H:64:LYS:HD2	2:H:64:LYS:N	2.04	0.70
2:H:168:ALA:HB2	2:H:177:LEU:HB3	1.73	0.69
3:Y:45:ARG:HD3	3:Y:50:SER:O	1.92	0.69
2:H:34:TRP:O	2:H:50:TYR:HB2	1.93	0.69
1:L:132:VAL:HG23	1:L:148:TRP:CH2	2.28	0.69
1:L:112:ALA:HB2	1:L:200:THR:CG2	2.19	0.69
1:L:198:HIS:ND1	1:L:200:THR:OG1	2.22	0.69
2:H:134:SER:O	2:H:185:SER:HB2	1.91	0.69
2:H:186:SER:HA	2:H:188:ARG:H	1.57	0.69
1:L:95:PRO:HG3	2:H:61:PRO:HD2	1.75	0.68
2:H:142:VAL:HG23	2:H:177:LEU:O	1.94	0.68
1:L:90:GLN:HE22	1:L:93:SER:H	1.39	0.68
1:L:120:PRO:HD3	1:L:132:VAL:HG12	1.75	0.68
1:L:198:HIS:HD1	1:L:200:THR:HG1	1.40	0.67
3:Y:12:MET:O	3:Y:15:HIS:N	2.23	0.67
3:Y:85:SER:OG	3:Y:87:ASP:N	2.26	0.67
2:H:40:PHE:HD1	2:H:91:ALA:HB2	1.59	0.67
2:H:48:MET:HE2	2:H:63:LEU:HD11	1.76	0.67
1:L:40:SER:O	1:L:41:HIS:HB2	1.93	0.67
1:L:18:SER:OG	1:L:76:ASN:HA	1.95	0.67
2:H:172:SER:O	2:H:173:ASP:CB	2.43	0.66
2:H:40:PHE:HB3	2:H:41:PRO:HD2	1.76	0.66
2:H:39:LYS:HE2	2:H:43:ASN:HA	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:LEU:HG	2:H:24:VAL:HG12	1.77	0.66
1:L:190:ASN:O	1:L:210:ASN:HA	1.95	0.66
1:L:150:ILE:CD1	1:L:155:ARG:HD2	2.26	0.66
1:L:142:LYS:O	1:L:163:TRP:HZ3	1.79	0.66
1:L:139:PHE:O	1:L:173:TYR:N	2.30	0.65
2:H:30:THR:HB	3:Y:73:ARG:CZ	2.26	0.65
1:L:49:LYS:O	1:L:51:ALA:N	2.29	0.65
1:L:120:PRO:HB3	1:L:130:ALA:HA	1.79	0.65
3:Y:59:ASN:ND2	3:Y:60:SER:N	2.44	0.64
2:H:37:ILE:HG12	2:H:47:TYR:CD1	2.33	0.64
1:L:134:CYS:HB2	1:L:148:TRP:CZ2	2.33	0.63
3:Y:80:CYS:O	3:Y:81:SER:C	2.36	0.63
1:L:124:GLN:NE2	1:L:130:ALA:H	1.96	0.63
2:H:192:THR:HB	2:H:211:VAL:HG13	1.81	0.63
1:L:182:THR:HG23	1:L:185:GLU:OE1	1.99	0.63
3:Y:4:GLY:O	3:Y:7:GLU:N	2.31	0.62
2:H:98:TRP:CE3	2:H:98:TRP:CA	2.81	0.62
3:Y:111:TRP:O	3:Y:116:LYS:HB2	1.99	0.62
3:Y:88:ILE:HG13	3:Y:92:VAL:HG23	1.82	0.62
2:H:177:LEU:HD12	2:H:177:LEU:C	2.20	0.62
2:H:188:ARG:HG2	2:H:212:PRO:CB	2.30	0.62
3:Y:10:ALA:HA	3:Y:129:LEU:HD23	1.81	0.61
2:H:202:SER:HB3	2:H:204:THR:OG1	1.99	0.61
2:H:136:VAL:CG1	2:H:183:VAL:HG23	2.30	0.61
3:Y:94:CYS:O	3:Y:97:LYS:HB3	2.01	0.61
1:L:115:VAL:HG22	1:L:136:LEU:HD23	1.83	0.61
2:H:116:THR:HA	2:H:146:PHE:O	2.00	0.60
1:L:11:LEU:HD13	1:L:19:VAL:HG22	1.82	0.60
1:L:58:ILE:HG13	1:L:59:PRO:HD2	1.84	0.60
3:Y:33:LYS:NZ	3:Y:37:ASN:OD1	2.34	0.60
1:L:108:ARG:HG2	1:L:109:ALA:H	1.66	0.60
2:H:5:GLN:HE22	2:H:25:THR:CG2	2.14	0.60
2:H:5:GLN:NE2	2:H:25:THR:HG23	2.17	0.60
2:H:29:ILE:HG21	2:H:76:ASN:O	2.02	0.60
3:Y:37:ASN:O	3:Y:38:PHE:HB2	2.01	0.60
3:Y:23:TYR:CE1	3:Y:105:MET:HG3	2.36	0.60
1:L:122:SER:N	1:L:123:GLU:OE2	2.35	0.60
1:L:208:SER:OG	1:L:209:PHE:N	2.35	0.59
2:H:2:VAL:CG2	2:H:27:ASP:HB2	2.25	0.59
3:Y:40:THR:O	3:Y:54:GLY:HA2	2.02	0.59
1:L:40:SER:O	1:L:41:HIS:CB	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:ARG:HB2	1:L:171:SER:HB2	1.85	0.59
2:H:39:LYS:O	2:H:91:ALA:HB1	2.03	0.58
1:L:11:LEU:HD13	1:L:19:VAL:CG2	2.33	0.58
3:Y:18:ASP:O	3:Y:19:ASN:HB2	2.03	0.58
3:Y:84:LEU:HD12	3:Y:84:LEU:N	2.18	0.58
2:H:16:GLN:HA	2:H:16:GLN:NE2	2.15	0.58
3:Y:85:SER:OG	3:Y:86:SER:N	2.33	0.58
1:L:28:SER:O	1:L:29:ILE:C	2.42	0.58
2:H:48:MET:HE3	2:H:63:LEU:HD11	1.84	0.58
2:H:52:SER:OG	3:Y:101:ASP:HB2	2.03	0.58
1:L:125:LEU:O	1:L:183:LYS:HD2	2.03	0.58
1:L:175:MET:HG3	1:L:176:SER:N	2.19	0.58
1:L:214:CYS:HA	2:H:215:CYS:HB3	0.84	0.58
1:L:150:ILE:CD1	1:L:155:ARG:HH11	2.09	0.57
1:L:30:GLY:O	3:Y:16:GLY:HA3	2.03	0.57
2:H:75:LYS:O	2:H:77:GLN:N	2.38	0.57
2:H:188:ARG:HE	2:H:212:PRO:CB	2.18	0.57
2:H:184:PRO:HG2	2:H:187:PRO:HB3	1.86	0.56
2:H:156:SER:C	2:H:158:SER:H	2.08	0.56
1:L:10:THR:HG22	1:L:103:LYS:HB3	1.87	0.56
2:H:38:ARG:HD3	2:H:93:TYR:CE2	2.41	0.56
3:Y:78:ILE:HG13	3:Y:79:PRO:HD2	1.86	0.56
2:H:59:TYR:HE1	2:H:69:ILE:HG13	1.71	0.56
3:Y:4:GLY:O	3:Y:5:ARG:C	2.44	0.56
3:Y:103:ASN:O	3:Y:106:ASN:N	2.33	0.56
2:H:188:ARG:CG	2:H:212:PRO:HB2	2.35	0.55
1:L:124:GLN:NE2	1:L:130:ALA:N	2.54	0.55
1:L:176:SER:OG	1:L:177:SER:N	2.39	0.55
2:H:38:ARG:NH2	2:H:46:GLU:OE2	2.36	0.55
3:Y:121:GLN:HB3	3:Y:125:ARG:NE	2.11	0.55
3:Y:111:TRP:O	3:Y:116:LYS:N	2.32	0.55
2:H:31:SER:O	2:H:32:ASP:C	2.42	0.55
2:H:52:SER:CB	3:Y:101:ASP:HB2	2.37	0.55
2:H:154:TRP:O	2:H:155:ASN:C	2.45	0.55
2:H:90:THR:HG22	2:H:110:THR:HA	1.87	0.55
1:L:80:THR:HG22	1:L:106:ILE:HG21	1.88	0.55
2:H:52:SER:OG	2:H:56:SER:HB3	2.07	0.55
1:L:112:ALA:CB	1:L:200:THR:HG21	2.27	0.55
3:Y:58:ILE:HB	3:Y:83:LEU:HD13	1.87	0.55
3:Y:74:ASN:HD21	3:Y:78:ILE:N	2.04	0.55
1:L:21:LEU:HD12	1:L:73:LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:59:ASN:HD22	3:Y:60:SER:H	1.53	0.54
2:H:211:VAL:O	2:H:213:ARG:N	2.41	0.54
2:H:16:GLN:H	2:H:85:VAL:HG22	1.72	0.54
2:H:53:TYR:C	2:H:53:TYR:CD2	2.81	0.54
3:Y:45:ARG:NH2	3:Y:68:ARG:HD2	2.22	0.54
3:Y:81:SER:O	3:Y:83:LEU:N	2.41	0.54
1:L:13:VAL:N	1:L:105:GLU:O	2.34	0.54
3:Y:95:ALA:O	3:Y:97:LYS:N	2.41	0.54
2:H:155:ASN:ND2	2:H:193:VAL:HA	2.07	0.54
2:H:72:ASP:OD2	2:H:75:LYS:HB2	2.08	0.53
1:L:33:LEU:CD2	1:L:88:CYS:HB2	2.37	0.53
3:Y:23:TYR:CD1	3:Y:105:MET:HG3	2.42	0.53
2:H:145:TYR:CZ	2:H:175:TYR:HB3	2.43	0.53
1:L:150:ILE:HG22	1:L:192:TYR:CD1	2.43	0.53
3:Y:92:VAL:O	3:Y:95:ALA:N	2.41	0.53
1:L:34:HIS:CD2	1:L:34:HIS:N	2.77	0.53
1:L:2:ILE:HD12	1:L:29:ILE:HG21	1.91	0.53
1:L:31:ASN:HB3	3:Y:16:GLY:HA3	1.91	0.53
2:H:64:LYS:HD3	2:H:66:ARG:NE	2.20	0.53
3:Y:103:ASN:O	3:Y:104:GLY:C	2.47	0.53
2:H:66:ARG:HB2	2:H:82:LEU:HD11	1.91	0.53
2:H:32:ASP:O	2:H:34:TRP:CD1	2.63	0.52
2:H:168:ALA:CB	2:H:177:LEU:HB3	2.39	0.52
2:H:151:THR:HB	2:H:198:ALA:HB3	1.90	0.52
2:H:144:GLY:HA2	2:H:174:LEU:HD21	1.92	0.52
2:H:114:ALA:HB3	2:H:146:PHE:HE1	1.74	0.52
2:H:66:ARG:HB2	2:H:82:LEU:CD1	2.40	0.52
1:L:139:PHE:CZ	1:L:144:ILE:HG21	2.44	0.52
2:H:90:THR:HG22	2:H:111:VAL:N	2.18	0.52
1:L:150:ILE:HD13	1:L:155:ARG:HD2	1.91	0.52
1:L:61:ARG:NH1	1:L:82:ASP:OD2	2.33	0.52
2:H:7:SER:OG	2:H:8:GLY:N	2.42	0.52
1:L:213:GLU:CG	1:L:214:CYS:N	2.65	0.52
1:L:6:GLN:OE1	1:L:101:GLY:N	2.40	0.52
3:Y:61:ARG:HD3	3:Y:62:TRP:CE2	2.44	0.52
1:L:190:ASN:HD22	1:L:211:ARG:HG3	1.74	0.51
3:Y:124:ILE:O	3:Y:124:ILE:HG13	2.10	0.51
3:Y:36:SER:O	3:Y:39:ASN:HB3	2.10	0.51
1:L:91:SER:HA	1:L:96:TYR:CD1	2.45	0.51
1:L:11:LEU:O	1:L:105:GLU:N	2.27	0.51
2:H:29:ILE:HG23	2:H:76:ASN:OD1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:ILE:CD1	1:L:54:SER:HA	2.41	0.51
2:H:136:VAL:HG13	2:H:183:VAL:CG2	2.36	0.51
1:L:28:SER:O	1:L:30:GLY:N	2.43	0.51
2:H:5:GLN:HE22	2:H:25:THR:HG23	1.76	0.51
1:L:89:GLN:HB2	1:L:98:PHE:CD2	2.46	0.51
3:Y:10:ALA:CA	3:Y:129:LEU:HD23	2.41	0.51
1:L:47:LEU:CD2	1:L:58:ILE:HD12	2.36	0.50
3:Y:101:ASP:CG	3:Y:101:ASP:O	2.49	0.50
1:L:124:GLN:HG2	1:L:124:GLN:O	2.11	0.50
2:H:40:PHE:HB3	2:H:41:PRO:CD	2.40	0.50
1:L:150:ILE:HG22	1:L:192:TYR:HD1	1.77	0.50
2:H:40:PHE:CB	2:H:41:PRO:HD2	2.38	0.50
2:H:67:ILE:HG12	2:H:68:SER:H	1.77	0.49
1:L:190:ASN:ND2	1:L:211:ARG:N	2.61	0.49
2:H:61:PRO:O	2:H:62:SER:C	2.50	0.49
3:Y:63:TRP:CZ3	3:Y:75:LEU:HD12	2.48	0.49
1:L:131:SER:OG	1:L:180:THR:HG22	2.13	0.49
2:H:188:ARG:HG2	2:H:212:PRO:HG2	1.93	0.49
1:L:142:LYS:HD3	1:L:173:TYR:CZ	2.47	0.49
1:L:104:LEU:HD23	1:L:104:LEU:C	2.33	0.49
2:H:188:ARG:HE	2:H:212:PRO:HB3	1.77	0.49
3:Y:121:GLN:OE1	3:Y:125:ARG:NH1	2.45	0.49
3:Y:47:THR:C	3:Y:49:GLY:H	2.15	0.49
2:H:72:ASP:CG	2:H:75:LYS:HB2	2.33	0.49
3:Y:45:ARG:HH12	3:Y:68:ARG:NH2	2.09	0.49
3:Y:18:ASP:OD1	3:Y:19:ASN:ND2	2.46	0.49
3:Y:76:CYS:O	3:Y:78:ILE:N	2.46	0.49
3:Y:45:ARG:HB2	3:Y:45:ARG:NH1	2.12	0.49
3:Y:53:TYR:HE2	3:Y:60:SER:OG	1.96	0.49
3:Y:95:ALA:O	3:Y:96:LYS:C	2.51	0.49
2:H:59:TYR:CE1	2:H:69:ILE:HG13	2.48	0.48
2:H:53:TYR:O	3:Y:101:ASP:OD1	2.31	0.48
1:L:133:VAL:HG21	2:H:124:LEU:HD11	1.95	0.48
2:H:188:ARG:CB	2:H:189:PRO:CD	2.63	0.48
1:L:167:ASP:C	1:L:169:LYS:H	2.17	0.48
1:L:194:CYS:SG	1:L:194:CYS:O	2.71	0.48
2:H:83:ASN:O	2:H:84:SER:C	2.52	0.48
2:H:138:LEU:HD23	2:H:210:ILE:HG13	1.95	0.48
1:L:141:PRO:O	1:L:143:ASP:N	2.47	0.48
3:Y:109:VAL:O	3:Y:112:ARG:N	2.47	0.48
1:L:115:VAL:HG22	1:L:136:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:209:LYS:O	2:H:209:LYS:HG2	2.11	0.47
2:H:114:ALA:HB3	2:H:146:PHE:CE1	2.49	0.47
3:Y:61:ARG:HG2	3:Y:62:TRP:CD1	2.48	0.47
2:H:184:PRO:O	2:H:187:PRO:HB2	2.14	0.47
2:H:132:THR:O	2:H:133:ASN:CB	2.52	0.47
2:H:184:PRO:HB2	2:H:187:PRO:HB2	1.97	0.47
2:H:197:VAL:HG22	2:H:198:ALA:N	2.29	0.47
2:H:166:PHE:N	2:H:166:PHE:CD2	2.79	0.47
3:Y:46:ASN:HB2	3:Y:50:SER:OG	2.14	0.47
1:L:133:VAL:HG22	1:L:178:THR:HG23	1.96	0.47
1:L:14:THR:HA	1:L:15:PRO:HD2	1.84	0.47
3:Y:52:ASP:HB3	3:Y:57:GLN:HB3	1.96	0.47
1:L:144:ILE:HG23	1:L:144:ILE:O	2.14	0.47
1:L:142:LYS:O	1:L:163:TRP:CZ3	2.66	0.47
2:H:35:SER:O	2:H:78:TYR:OH	2.26	0.47
3:Y:61:ARG:HD3	3:Y:62:TRP:CZ2	2.49	0.47
3:Y:120:VAL:O	3:Y:121:GLN:C	2.54	0.46
2:H:124:LEU:HB2	2:H:139:GLY:C	2.36	0.46
1:L:140:TYR:O	1:L:198:HIS:HE1	1.98	0.46
2:H:155:ASN:O	2:H:156:SER:C	2.53	0.46
1:L:192:TYR:HB2	1:L:209:PHE:CE2	2.51	0.46
3:Y:120:VAL:C	3:Y:122:ALA:N	2.68	0.46
3:Y:109:VAL:O	3:Y:113:ASN:N	2.39	0.46
2:H:52:SER:HB2	3:Y:101:ASP:HB2	1.97	0.46
2:H:42:GLY:O	2:H:43:ASN:OD1	2.34	0.46
1:L:50:TYR:CE1	3:Y:96:LYS:HD3	2.50	0.46
3:Y:51:THR:H	3:Y:60:SER:HB2	1.81	0.46
2:H:134:SER:C	2:H:185:SER:HB2	2.36	0.46
2:H:18:LEU:CD1	2:H:109:VAL:HG11	2.45	0.46
1:L:173:TYR:O	1:L:174:SER:CB	2.64	0.46
2:H:29:ILE:CG2	2:H:76:ASN:OD1	2.64	0.46
1:L:190:ASN:O	1:L:211:ARG:N	2.46	0.46
3:Y:95:ALA:C	3:Y:97:LYS:N	2.69	0.45
2:H:5:GLN:NE2	2:H:25:THR:CG2	2.78	0.45
1:L:117:ILE:C	1:L:118:PHE:CD2	2.90	0.45
1:L:173:TYR:HB3	1:L:174:SER:H	1.52	0.45
3:Y:4:GLY:O	3:Y:6:CYS:N	2.49	0.45
1:L:120:PRO:HG2	1:L:186:TYR:CZ	2.51	0.45
2:H:146:PHE:CD2	2:H:147:PRO:CA	2.81	0.45
3:Y:109:VAL:HG13	3:Y:110:ALA:N	2.31	0.45
1:L:160:LEU:HD12	1:L:160:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:151:ASP:OD1	1:L:189:HIS:ND1	2.43	0.45
1:L:30:GLY:O	1:L:31:ASN:CB	2.39	0.45
3:Y:125:ARG:HG2	3:Y:125:ARG:HH21	1.82	0.45
1:L:139:PHE:CE1	1:L:144:ILE:HG21	2.52	0.45
3:Y:78:ILE:HG13	3:Y:82:ALA:HB3	1.99	0.45
2:H:67:ILE:HG12	2:H:68:SER:N	2.32	0.45
3:Y:109:VAL:HG13	3:Y:110:ALA:H	1.81	0.45
3:Y:45:ARG:HA	3:Y:51:THR:HA	1.99	0.44
3:Y:30:CYS:HB2	3:Y:123:TRP:CD1	2.52	0.44
1:L:144:ILE:CG2	1:L:144:ILE:O	2.65	0.44
1:L:6:GLN:HE21	1:L:35:TRP:HZ3	1.65	0.44
2:H:197:VAL:CG2	2:H:198:ALA:N	2.81	0.44
1:L:76:ASN:O	1:L:77:SER:HB3	2.17	0.44
2:H:16:GLN:H	2:H:85:VAL:CG2	2.30	0.44
3:Y:98:ILE:C	3:Y:100:SER:H	2.21	0.44
1:L:154:GLU:O	1:L:155:ARG:NE	2.50	0.44
3:Y:88:ILE:O	3:Y:89:THR:C	2.55	0.44
1:L:123:GLU:H	1:L:123:GLU:CD	2.21	0.44
3:Y:3:PHE:HB3	3:Y:8:LEU:HB2	2.00	0.44
2:H:197:VAL:CG2	2:H:198:ALA:H	2.31	0.44
2:H:188:ARG:HG2	2:H:212:PRO:CG	2.47	0.43
2:H:97:ASN:O	2:H:99:ASP:N	2.50	0.43
1:L:81:GLU:HG3	1:L:81:GLU:O	2.17	0.43
1:L:186:TYR:CE2	1:L:192:TYR:CE2	3.06	0.43
1:L:8:PRO:HG2	1:L:11:LEU:HG	2.00	0.43
3:Y:41:GLN:O	3:Y:42:ALA:C	2.57	0.43
1:L:96:TYR:HH	2:H:98:TRP:HH2	1.63	0.43
1:L:61:ARG:HG2	1:L:76:ASN:O	2.18	0.43
1:L:150:ILE:HD11	1:L:155:ARG:NH1	2.09	0.43
1:L:1:ASP:HB2	1:L:95:PRO:HD2	2.00	0.43
1:L:166:GLN:HG2	1:L:171:SER:HA	2.00	0.43
2:H:16:GLN:N	2:H:85:VAL:HG22	2.33	0.43
3:Y:58:ILE:HG23	3:Y:63:TRP:CB	2.49	0.43
2:H:67:ILE:CG1	2:H:68:SER:H	2.31	0.43
2:H:88:GLU:C	2:H:90:THR:H	2.22	0.43
3:Y:74:ASN:CG	3:Y:77:ASN:HA	2.38	0.43
2:H:188:ARG:HE	2:H:212:PRO:HB2	1.82	0.43
1:L:155:ARG:HA	1:L:155:ARG:NE	2.09	0.42
1:L:2:ILE:CD1	1:L:29:ILE:HG21	2.49	0.42
1:L:115:VAL:HB	1:L:207:LYS:HG2	2.00	0.42
2:H:150:VAL:HG23	2:H:151:THR:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:ILE:HD12	1:L:54:SER:HA	2.01	0.42
1:L:89:GLN:HB2	1:L:98:PHE:CE2	2.55	0.42
2:H:211:VAL:O	2:H:213:ARG:HB3	2.18	0.42
2:H:166:PHE:H	2:H:166:PHE:HD2	1.63	0.42
2:H:186:SER:HA	2:H:187:PRO:C	2.38	0.42
2:H:41:PRO:C	2:H:43:ASN:H	2.22	0.42
2:H:210:ILE:C	2:H:210:ILE:HD12	2.40	0.42
2:H:208:LYS:HE3	2:H:209:LYS:HZ1	1.85	0.42
2:H:29:ILE:C	2:H:31:SER:N	2.73	0.42
3:Y:31:ALA:O	3:Y:35:GLU:HB3	2.20	0.42
2:H:2:VAL:HG13	2:H:27:ASP:HB3	2.01	0.42
3:Y:63:TRP:CZ2	3:Y:98:ILE:HG12	2.55	0.42
2:H:78:TYR:OH	2:H:95:CYS:HB2	2.20	0.42
2:H:86:THR:C	2:H:111:VAL:HG11	2.40	0.42
1:L:120:PRO:HB3	1:L:130:ALA:CA	2.49	0.41
3:Y:84:LEU:CD1	3:Y:84:LEU:N	2.81	0.41
2:H:4:LEU:HD21	2:H:34:TRP:HZ3	1.85	0.41
1:L:1:ASP:CB	1:L:95:PRO:HD2	2.50	0.41
2:H:159:LEU:HD13	2:H:181:VAL:HG21	2.02	0.41
2:H:18:LEU:HD13	2:H:109:VAL:HG11	2.02	0.41
3:Y:45:ARG:HH12	3:Y:68:ARG:CZ	2.32	0.41
1:L:3:VAL:O	1:L:25:ALA:HA	2.20	0.41
3:Y:43:THR:C	3:Y:44:ASN:HD22	2.23	0.41
2:H:98:TRP:HB3	2:H:99:ASP:H	1.62	0.41
3:Y:12:MET:HG2	3:Y:17:LEU:CD1	2.41	0.41
1:L:50:TYR:HB2	1:L:53:GLN:HG3	2.02	0.41
1:L:198:HIS:CG	1:L:199:LYS:H	2.39	0.41
3:Y:6:CYS:O	3:Y:7:GLU:C	2.58	0.41
2:H:177:LEU:CD1	2:H:177:LEU:C	2.87	0.41
2:H:153:THR:O	2:H:196:ASN:N	2.44	0.41
2:H:48:MET:O	2:H:60:ASN:HB2	2.20	0.41
3:Y:88:ILE:HG13	3:Y:92:VAL:CG2	2.50	0.41
3:Y:79:PRO:O	3:Y:82:ALA:HB3	2.20	0.41
2:H:64:LYS:HB2	2:H:66:ARG:HG2	1.99	0.41
3:Y:121:GLN:CB	3:Y:125:ARG:HE	2.16	0.41
1:L:11:LEU:HA	1:L:11:LEU:HD23	1.70	0.41
2:H:145:TYR:CE2	2:H:175:TYR:HB3	2.55	0.41
1:L:150:ILE:O	1:L:151:ASP:HB2	2.21	0.41
2:H:102:TYR:O	2:H:103:TRP:CD1	2.74	0.41
1:L:187:GLU:H	1:L:187:GLU:HG3	1.76	0.41
2:H:6:GLU:HG2	2:H:6:GLU:H	1.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:108:ARG:NH2	1:L:109:ALA:O	2.52	0.40
3:Y:31:ALA:O	3:Y:35:GLU:CB	2.69	0.40
2:H:20:LEU:N	2:H:20:LEU:HD12	2.36	0.40
2:H:188:ARG:NE	2:H:212:PRO:HB2	2.36	0.40
2:H:18:LEU:HD22	2:H:85:VAL:HG12	2.03	0.40
2:H:59:TYR:HE1	2:H:69:ILE:CG1	2.33	0.40
1:L:82:ASP:O	1:L:104:LEU:HD22	2.22	0.40
1:L:118:PHE:CE2	1:L:135:PHE:HD1	2.40	0.40
3:Y:53:TYR:HB2	3:Y:83:LEU:HD12	2.03	0.40
2:H:155:ASN:O	2:H:156:SER:O	2.40	0.40
2:H:121:VAL:CG2	2:H:197:VAL:HG11	2.38	0.40
2:H:30:THR:C	2:H:31:SER:OG	2.59	0.40
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.92	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	212/214 (99%)	162 (76%)	33 (16%)	17 (8%)	1 5
2	H	213/215 (99%)	155 (73%)	38 (18%)	20 (9%)	1 4
3	Y	127/129 (98%)	86 (68%)	24 (19%)	17 (13%)	0 1
All	All	552/558 (99%)	403 (73%)	95 (17%)	54 (10%)	1 3

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	29	ILE
1	L	50	TYR
1	L	130	ALA
1	L	144	ILE

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Mol	Chain	Res	Type
1	L	154	GLU
1	L	156	GLN
1	L	174	SER
2	H	30	THR
2	H	54	SER
2	H	64	LYS
2	H	76	ASN
2	H	133	ASN
2	H	156	SER
2	H	157	GLY
2	H	187	PRO
2	H	192	THR
3	Y	5	ARG
3	Y	77	ASN
3	Y	82	ALA
3	Y	85	SER
1	L	40	SER
1	L	67	SER
1	L	142	LYS
2	H	68	SER
2	H	98	TRP
2	H	173	ASP
2	H	188	ARG
2	H	210	ILE
3	Y	48	ASP
3	Y	72	SER
3	Y	99	VAL
3	Y	116	LYS
1	L	44	PRO
1	L	168	SER
2	H	100	GLY
2	H	155	ASN
2	H	161	SER
2	H	212	PRO
3	Y	7	GLU
3	Y	33	LYS
3	Y	36	SER
3	Y	42	ALA
3	Y	47	THR
3	Y	96	LYS
1	L	15	PRO
1	L	162	SER

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Mol	Chain	Res	Type
2	H	31	SER
2	H	172	SER
1	L	151	ASP
1	L	177	SER
1	L	213	GLU
3	Y	57	GLN
3	Y	70	PRO
3	Y	102	GLY

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	192/192 (100%)	144 (75%)	48 (25%)	1 3
2	H	192/192 (100%)	140 (73%)	52 (27%)	0 2
3	Y	105/105 (100%)	92 (88%)	13 (12%)	6 24
All	All	489/489 (100%)	376 (77%)	113 (23%)	1 5

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	7	SER
1	L	12	SER
1	L	14	THR
1	L	17	ASN
1	L	18	SER
1	L	19	VAL
1	L	21	LEU
1	L	28	SER
1	L	32	ASN
1	L	34	HIS
1	L	41	HIS
1	L	43	SER
1	L	45	ARG

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Mol	Chain	Res	Type
1	L	56	SER
1	L	58	ILE
1	L	72	THR
1	L	73	LEU
1	L	77	SER
1	L	90	GLN
1	L	93	SER
1	L	107	LYS
1	L	110	ASP
1	L	126	THR
1	L	127	SER
1	L	132	VAL
1	L	143	ASP
1	L	145	ASN
1	L	147	LYS
1	L	155	ARG
1	L	156	GLN
1	L	165	ASP
1	L	168	SER
1	L	171	SER
1	L	172	THR
1	L	178	THR
1	L	181	LEU
1	L	184	ASP
1	L	187	GLU
1	L	191	SER
1	L	193	THR
1	L	197	THR
1	L	200	THR
1	L	202	THR
1	L	203	SER
1	L	211	ARG
1	L	212	ASN
1	L	213	GLU
2	H	5	GLN
2	H	6	GLU
2	H	7	SER
2	H	11	LEU
2	H	15	SER
2	H	16	GLN
2	H	18	LEU
2	H	19	SER

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Mol	Chain	Res	Type
2	H	28	SER
2	H	29	ILE
2	H	31	SER
2	H	33	TYR
2	H	38	ARG
2	H	43	ASN
2	H	53	TYR
2	H	54	SER
2	H	66	ARG
2	H	70	THR
2	H	80	LEU
2	H	86	THR
2	H	87	THR
2	H	94	TYR
2	H	98	TRP
2	H	110	THR
2	H	117	THR
2	H	120	SER
2	H	131	GLN
2	H	137	THR
2	H	142	VAL
2	H	146	PHE
2	H	153	THR
2	H	155	ASN
2	H	160	SER
2	H	166	PHE
2	H	170	LEU
2	H	171	GLN
2	H	173	ASP
2	H	176	THR
2	H	177	LEU
2	H	180	SER
2	H	182	THR
2	H	185	SER
2	H	187	PRO
2	H	190	SER
2	H	191	GLU
2	H	192	THR
2	H	193	VAL
2	H	207	ASP
2	H	209	LYS
2	H	210	ILE

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Mol	Chain	Res	Type
2	H	213	ARG
2	H	215	CYS
3	Y	12	MET
3	Y	45	ARG
3	Y	50	SER
3	Y	56	LEU
3	Y	68	ARG
3	Y	70	PRO
3	Y	86	SER
3	Y	88	ILE
3	Y	101	ASP
3	Y	120	VAL
3	Y	125	ARG
3	Y	128	ARG
3	Y	129	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	34	HIS
1	L	90	GLN
1	L	138	ASN
1	L	156	GLN
1	L	190	ASN
2	H	5	GLN
2	H	16	GLN
2	H	43	ASN
2	H	105	GLN
2	H	164	HIS
2	H	171	GLN
3	Y	57	GLN
3	Y	59	ASN
3	Y	74	ASN
3	Y	113	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	214/214 (100%)	-0.71	0 100 100	11, 16, 20, 26	0
2	H	215/215 (100%)	-0.49	2 (0%) 85 64	14, 18, 23, 26	0
3	Y	129/129 (100%)	-0.75	0 100 100	11, 16, 20, 21	0
All	All	558/558 (100%)	-0.63	2 (0%) 93 80	11, 17, 22, 26	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	ASN	2.7
2	H	130	ALA	2.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.