Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:08 pm BST

PDB ID	:	1BQL
Title	:	STRUCTURE OF AN ANTI-HEL FAB FRAGMENT COMPLEXED WITH BOBWHITE QUAIL LYSOZYME
Authors	:	Chacko, S.; Davies, D.R.
Deposited on	:	1995-02-03
Resolution	:	2.60 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 ⓘ symbol.

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

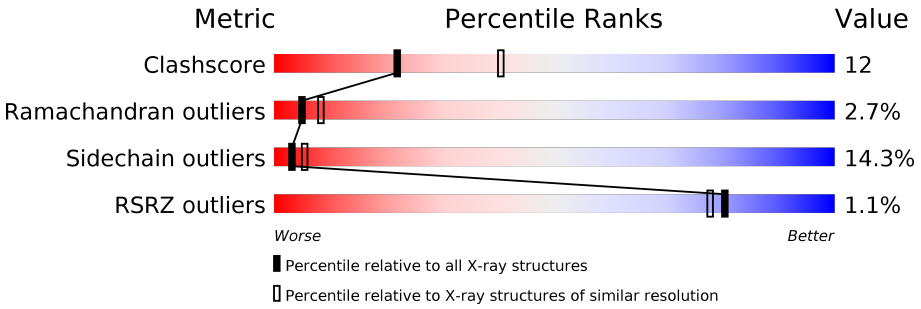
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

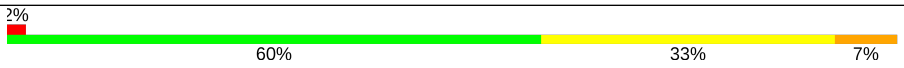
The reported resolution of this entry is 2.60 Å.

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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	212	
2	H	215	
3	Y	129	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4326 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-5 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	212	Total	C	N	O	S	0	0	0
			1635	1014	273	338	10			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	18	LYS	ARG	CONFLICT	GB 1042224
L	26	SER	ASN	CONFLICT	GB 1042224
L	30	ASN	SER	CONFLICT	GB 1042224
L	33	TYR	HIS	CONFLICT	GB 1042224
L	59	VAL	ALA	CONFLICT	GB 1042224
L	79	THR	ALA	CONFLICT	GB 1042224
L	91	GLY	SER	CONFLICT	GB 1042224
L	92	ARG	SER	CONFLICT	GB 1042224
L	93	ASN	HIS	CONFLICT	GB 1042224
L	?	-	TYR	DELETION	GB 1042224
L	111	PRO	GLN	CONFLICT	GB 1042224

- Molecule 2 is a protein called HYHEL-5 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1607	1015	263	322	7			

- Molecule 3 is a protein called BOBWHITE QUAIL LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	129	Total	C	N	O	S	0	0	0
			998	612	191	185	10			

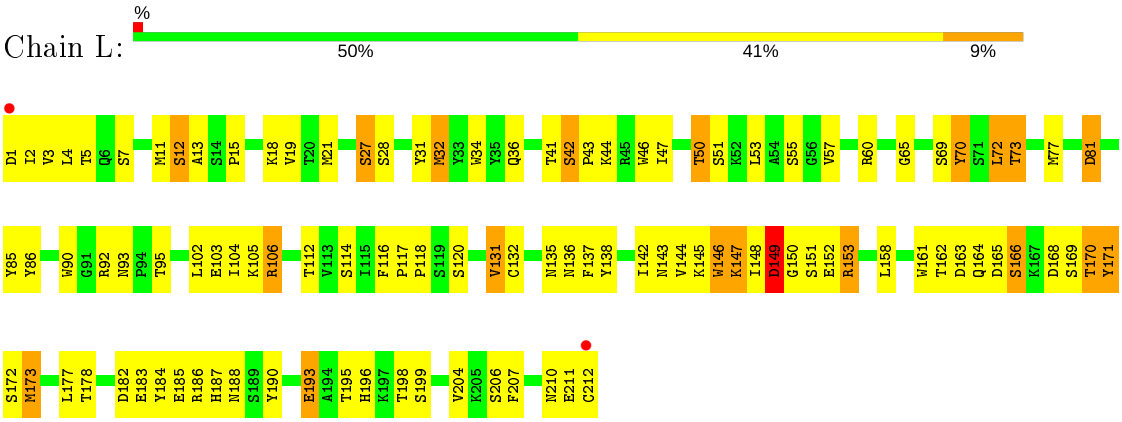
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	28	Total O 28 28	0	0
4	H	38	Total O 38 38	0	0
4	Y	20	Total O 20 20	0	0

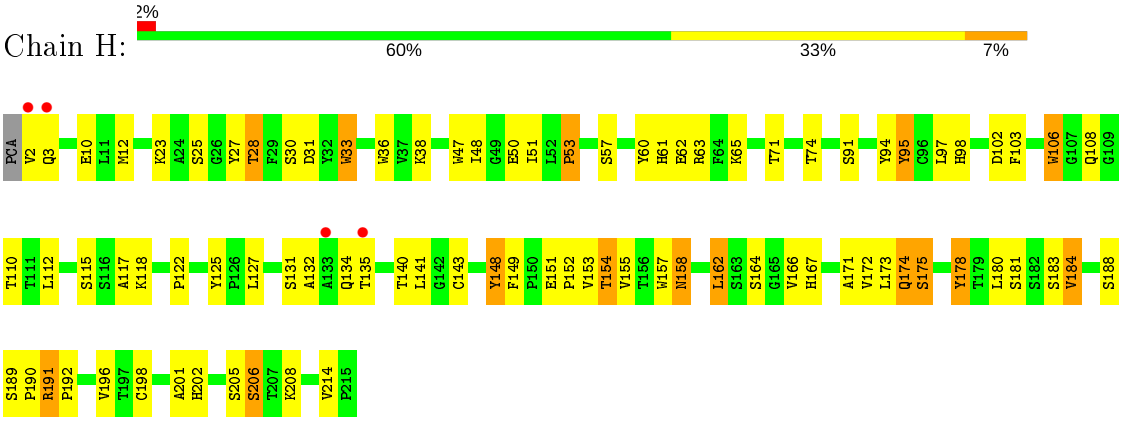
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

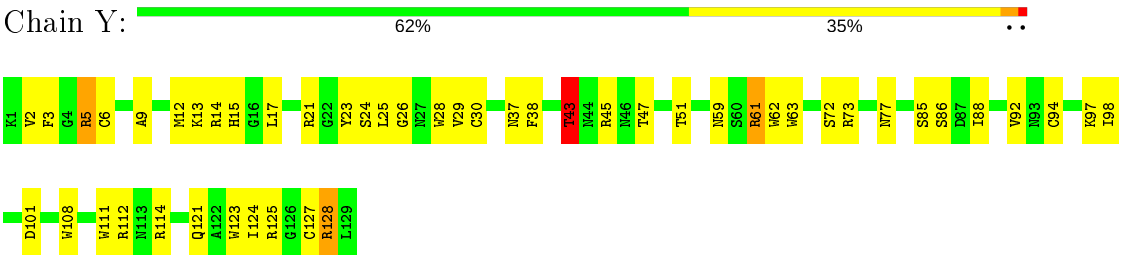
- Molecule 1: HYHEL-5 FAB (LIGHT CHAIN)



- Molecule 2: HYHEL-5 FAB (HEAVY CHAIN)



- Molecule 3: BOBWHITE QUAIL LYSOZYME



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.80Å 74.80Å 79.00Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 37.40 – 2.58	Depositor EDS
% Data completeness (in resolution range)	55.0 (8.00-2.60) 83.0 (37.40-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.191 , 0.291 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 98.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4326	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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

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	0.90	2/1673 (0.1%)	1.78	40/2270 (1.8%)
2	H	0.92	0/1652	1.76	33/2257 (1.5%)
3	Y	0.89	0/1018	1.95	44/1375 (3.2%)
All	All	0.90	2/4343 (0.0%)	1.81	117/5902 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	150	GLY	N-CA	5.65	1.54	1.46
1	L	27	SER	CA-CB	-5.23	1.45	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	63	TRP	CD1-CG-CD2	10.21	114.47	106.30
1	L	169	SER	N-CA-CB	-10.06	95.41	110.50
3	Y	62	TRP	CD1-CG-CD2	9.96	114.27	106.30
3	Y	125	ARG	NE-CZ-NH1	9.45	125.02	120.30
2	H	33	TRP	CD1-CG-CD2	9.22	113.68	106.30
1	L	146	TRP	CD1-CG-CD2	9.22	113.68	106.30
3	Y	21	ARG	NE-CZ-NH1	9.02	124.81	120.30
3	Y	62	TRP	CE2-CD2-CG	-8.94	100.14	107.30
3	Y	108	TRP	CD1-CG-CD2	8.87	113.39	106.30
2	H	157	TRP	CD1-CG-CD2	8.84	113.37	106.30
2	H	36	TRP	CG-CD2-CE3	8.83	141.85	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	90	TRP	CD1-CG-CD2	8.77	113.31	106.30
3	Y	123	TRP	CD1-CG-CD2	8.72	113.28	106.30
3	Y	111	TRP	CE2-CD2-CG	-8.54	100.47	107.30
1	L	46	TRP	CD1-CG-CD2	8.51	113.10	106.30
2	H	33	TRP	CE2-CD2-CG	-8.48	100.52	107.30
1	L	161	TRP	CD1-CG-CD2	8.46	113.07	106.30
2	H	47	TRP	CD1-CG-CD2	8.44	113.05	106.30
2	H	157	TRP	CE2-CD2-CG	-8.41	100.57	107.30
3	Y	111	TRP	CD1-CG-CD2	8.39	113.01	106.30
1	L	173	MET	CG-SD-CE	-8.35	86.84	100.20
3	Y	108	TRP	CE2-CD2-CG	-8.26	100.70	107.30
3	Y	63	TRP	CE2-CD2-CG	-8.22	100.72	107.30
2	H	36	TRP	CB-CG-CD1	-8.17	116.38	127.00
1	L	149	ASP	C-N-CA	-8.09	105.32	122.30
2	H	125	TYR	CB-CG-CD2	-8.06	116.17	121.00
2	H	36	TRP	CE2-CD2-CG	-7.84	101.03	107.30
3	Y	28	TRP	CE2-CD2-CG	-7.71	101.13	107.30
2	H	36	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	L	90	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	L	34	TRP	CD1-CG-CD2	7.58	112.36	106.30
3	Y	123	TRP	CE2-CD2-CG	-7.52	101.29	107.30
2	H	106	TRP	CD1-CG-CD2	7.49	112.29	106.30
1	L	46	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	L	146	TRP	CE2-CD2-CG	-7.46	101.33	107.30
3	Y	73	ARG	NE-CZ-NH2	-7.44	116.58	120.30
2	H	106	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	L	153	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	L	161	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	L	171	TYR	CB-CG-CD1	-7.29	116.63	121.00
2	H	148	TYR	CB-CG-CD2	-7.27	116.64	121.00
3	Y	45	ARG	NE-CZ-NH2	-7.15	116.73	120.30
3	Y	28	TRP	CD1-CG-CD2	7.02	111.92	106.30
2	H	47	TRP	CE2-CD2-CG	-6.95	101.74	107.30
3	Y	112	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	H	60	TYR	CB-CG-CD2	-6.89	116.87	121.00
3	Y	111	TRP	CB-CG-CD1	-6.88	118.06	127.00
3	Y	28	TRP	CG-CD2-CE3	6.83	140.05	133.90
3	Y	111	TRP	CG-CD2-CE3	6.79	140.01	133.90
3	Y	43	THR	CA-CB-CG2	-6.79	102.90	112.40
1	L	199	SER	CA-C-N	-6.78	102.29	117.20
3	Y	63	TRP	CG-CD1-NE1	-6.77	103.33	110.10
3	Y	23	TYR	CB-CG-CD1	-6.59	117.05	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	34	TRP	CE2-CD2-CG	-6.57	102.05	107.30
2	H	63	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	L	60	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	L	92	ARG	NE-CZ-NH1	6.34	123.47	120.30
3	Y	123	TRP	CA-CB-CG	-6.34	101.66	113.70
2	H	178	TYR	CB-CG-CD2	-6.27	117.24	121.00
2	H	23	LYS	CA-C-N	-6.26	103.42	117.20
3	Y	63	TRP	CG-CD2-CE3	6.25	139.53	133.90
1	L	207	PHE	CB-CG-CD2	-6.23	116.44	120.80
3	Y	21	ARG	CA-C-N	6.12	128.44	116.20
3	Y	108	TRP	CG-CD2-CE3	6.10	139.39	133.90
1	L	70	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	L	60	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	H	117	ALA	N-CA-CB	-6.06	101.61	110.10
3	Y	61	ARG	NE-CZ-NH2	-6.04	117.28	120.30
3	Y	125	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	L	46	TRP	CG-CD2-CE3	5.96	139.26	133.90
3	Y	28	TRP	CB-CG-CD1	-5.85	119.39	127.00
3	Y	123	TRP	CG-CD1-NE1	-5.82	104.28	110.10
3	Y	112	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	L	46	TRP	CG-CD1-NE1	-5.75	104.35	110.10
1	L	136	ASN	N-CA-C	5.72	126.46	111.00
1	L	146	TRP	CB-CG-CD1	-5.72	119.56	127.00
3	Y	63	TRP	CB-CG-CD1	-5.70	119.59	127.00
1	L	86	TYR	CB-CG-CD1	-5.69	117.59	121.00
3	Y	62	TRP	CB-CG-CD1	-5.67	119.63	127.00
1	L	34	TRP	CG-CD2-CE3	5.65	138.99	133.90
1	L	146	TRP	CG-CD1-NE1	-5.62	104.48	110.10
3	Y	123	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	L	34	TRP	CB-CG-CD1	-5.61	119.71	127.00
3	Y	21	ARG	O-C-N	-5.54	113.78	123.20
3	Y	62	TRP	CG-CD1-NE1	-5.53	104.57	110.10
2	H	63	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	L	193	GLU	CA-CB-CG	5.52	125.54	113.40
2	H	33	TRP	CB-CG-CD1	-5.51	119.84	127.00
2	H	206	SER	N-CA-CB	-5.50	102.25	110.50
1	L	146	TRP	CG-CD2-CE3	5.45	138.81	133.90
2	H	47	TRP	CG-CD1-NE1	-5.45	104.66	110.10
1	L	178	THR	CA-C-N	-5.43	105.26	117.20
3	Y	62	TRP	CG-CD2-CE3	5.40	138.76	133.90
2	H	106	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	L	90	TRP	CG-CD2-CE3	5.37	138.73	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	95	TYR	CB-CG-CD2	-5.36	117.79	121.00
3	Y	108	TRP	CB-CG-CD1	-5.35	120.04	127.00
3	Y	114	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	H	33	TRP	CG-CD2-CE3	5.33	138.69	133.90
1	L	81	ASP	CB-CG-OD1	5.28	123.05	118.30
3	Y	2	VAL	N-CA-C	-5.28	96.75	111.00
2	H	47	TRP	CB-CG-CD1	-5.27	120.14	127.00
2	H	134	GLN	CA-C-N	-5.25	105.65	117.20
3	Y	112	ARG	CA-CB-CG	5.24	124.93	113.40
2	H	175	SER	N-CA-CB	-5.22	102.66	110.50
1	L	90	TRP	CG-CD1-NE1	-5.20	104.90	110.10
2	H	47	TRP	CG-CD2-CE3	5.19	138.57	133.90
3	Y	123	TRP	CB-CG-CD1	-5.18	120.26	127.00
2	H	3	GLN	CA-CB-CG	5.15	124.73	113.40
3	Y	21	ARG	N-CA-C	-5.14	97.13	111.00
1	L	46	TRP	CB-CG-CD1	-5.11	120.36	127.00
2	H	33	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	L	90	TRP	CB-CG-CD1	-5.08	120.40	127.00
1	L	161	TRP	CB-CG-CD1	-5.06	120.42	127.00
2	H	118	LYS	CA-CB-CG	5.04	124.48	113.40
1	L	3	VAL	CA-CB-CG2	-5.01	103.39	110.90
1	L	131	VAL	CA-CB-CG2	-5.01	103.39	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	104	ILE	Mainchain
1	L	171	TYR	Sidechain

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	1635	0	1557	52	0
2	H	1607	0	1547	38	0
3	Y	998	0	957	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	38	0	0	2	0
4	L	28	0	0	6	0
4	Y	20	0	0	2	0
All	All	4326	0	4061	98	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 12.

All (98) 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:1:ASP:HB2	1:L:2:ILE:HD12	1.66	0.77
2:H:191:ARG:HD2	2:H:192:PRO:HA	1.68	0.76
1:L:2:ILE:HG12	1:L:27:SER:HB2	1.68	0.75
3:Y:59:ASN:OD1	3:Y:61:ARG:HB3	1.89	0.72
2:H:2:VAL:N	2:H:25:SER:HG	1.89	0.70
1:L:4:LEU:HG	4:L:235:HOH:O	1.92	0.69
1:L:182:ASP:HA	1:L:185:GLU:HG2	1.76	0.68
1:L:12:SER:HB3	1:L:103:GLU:HG3	1.78	0.66
2:H:10:GLU:HB2	2:H:112:LEU:HD13	1.81	0.61
3:Y:15:HIS:HA	4:Y:144:HOH:O	2.02	0.60
1:L:148:ILE:HD11	1:L:177:LEU:HD21	1.84	0.59
2:H:91:SER:HA	2:H:112:LEU:O	2.03	0.59
1:L:147:LYS:HG3	1:L:151:SER:HA	1.84	0.59
1:L:81:ASP:O	1:L:102:LEU:HD23	2.03	0.58
1:L:15:PRO:HA	1:L:77:MET:O	2.03	0.58
1:L:187:HIS:H	1:L:210:ASN:HD21	1.51	0.58
2:H:108:GLN:HB3	4:H:235:HOH:O	2.04	0.58
2:H:191:ARG:HH11	2:H:191:ARG:HB3	1.68	0.57
1:L:142:ILE:HG13	4:L:226:HOH:O	2.02	0.57
2:H:57:SER:HB3	3:Y:43:THR:OG1	2.04	0.57
1:L:53:LEU:HB3	1:L:57:VAL:HB	1.85	0.57
3:Y:9:ALA:HB2	3:Y:29:VAL:HG21	1.86	0.57
1:L:142:ILE:HD13	1:L:196:HIS:CD2	2.40	0.56
2:H:166:VAL:HA	2:H:183:SER:O	2.06	0.56
1:L:138:TYR:O	1:L:196:HIS:HE1	1.89	0.56
1:L:144:VAL:HG21	1:L:173:MET:CE	2.37	0.55
2:H:122:PRO:HB3	2:H:148:TYR:HB3	1.88	0.55
2:H:110:THR:HG21	4:H:245:HOH:O	2.07	0.53
3:Y:13:LYS:HB2	3:Y:25:LEU:HD11	1.90	0.53
1:L:158:LEU:HD11	2:H:174:GLN:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:131:VAL:HG11	2:H:127:LEU:HD13	1.90	0.52
1:L:135:ASN:OD1	2:H:167:HIS:HD2	1.94	0.50
3:Y:15:HIS:HB3	3:Y:92:VAL:HG11	1.93	0.50
3:Y:94:CYS:O	3:Y:98:ILE:HG13	2.11	0.50
1:L:47:ILE:HD12	1:L:72:LEU:HD12	1.94	0.50
2:H:171:ALA:HB1	2:H:178:TYR:HB3	1.94	0.49
1:L:31:TYR:HA	1:L:50:THR:HG23	1.94	0.49
1:L:44:LYS:HA	4:L:229:HOH:O	2.11	0.49
1:L:184:TYR:O	1:L:210:ASN:ND2	2.44	0.49
2:H:51:ILE:O	2:H:53:PRO:HD3	2.12	0.49
1:L:65:GLY:HA3	1:L:70:TYR:HA	1.94	0.49
3:Y:17:LEU:HD11	3:Y:92:VAL:HG22	1.95	0.49
2:H:140:THR:HA	2:H:184:VAL:O	2.14	0.48
1:L:146:TRP:HE3	4:L:231:HOH:O	1.96	0.48
3:Y:26:GLY:O	3:Y:30:CYS:HB2	2.14	0.48
2:H:158:ASN:ND2	2:H:196:VAL:HA	2.28	0.48
2:H:173:LEU:HD13	2:H:178:TYR:CE1	2.49	0.48
1:L:11:MET:HE1	1:L:19:VAL:HG13	1.96	0.47
1:L:13:ALA:HB3	1:L:77:MET:HE2	1.95	0.47
3:Y:124:ILE:O	3:Y:127:CYS:HB2	2.15	0.47
2:H:154:THR:OG1	2:H:201:ALA:HB3	2.15	0.47
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.97	0.47
2:H:158:ASN:HB2	2:H:162:LEU:HB2	1.97	0.46
3:Y:128:ARG:HB2	4:Y:149:HOH:O	2.15	0.46
1:L:166:SER:C	1:L:168:ASP:H	2.16	0.46
2:H:191:ARG:NH1	2:H:192:PRO:HG3	2.32	0.45
1:L:118:PRO:HD2	1:L:184:TYR:OH	2.16	0.45
1:L:193:GLU:HB3	1:L:204:VAL:HG12	1.98	0.45
3:Y:3:PHE:HB2	3:Y:38:PHE:HB3	1.98	0.45
1:L:93:ASN:HB2	2:H:61:HIS:CD2	2.52	0.45
1:L:164:GLN:HA	1:L:170:THR:O	2.17	0.44
2:H:115:SER:HG	2:H:149:PHE:HZ	1.64	0.44
1:L:187:HIS:N	1:L:210:ASN:HD21	2.14	0.44
1:L:18:LYS:HB3	1:L:18:LYS:HE2	1.58	0.44
1:L:148:ILE:HG12	1:L:190:TYR:CE2	2.53	0.44
1:L:31:TYR:HA	1:L:50:THR:CG2	2.47	0.44
1:L:32:MET:H	1:L:50:THR:HG22	1.81	0.44
1:L:12:SER:HB2	1:L:105:LYS:HG3	1.99	0.44
1:L:182:ASP:O	1:L:186:ARG:HB2	2.18	0.44
3:Y:43:THR:HG22	3:Y:51:THR:HG22	1.98	0.44
2:H:191:ARG:NH1	2:H:191:ARG:HB3	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:VAL:O	1:L:73:THR:HA	2.18	0.43
2:H:162:LEU:O	2:H:166:VAL:HG21	2.17	0.43
1:L:137:PHE:CE1	1:L:172:SER:HA	2.53	0.43
1:L:183:GLU:O	1:L:187:HIS:HD2	2.01	0.43
2:H:27:TYR:OH	2:H:98:HIS:CE1	2.72	0.43
3:Y:12:MET:HB3	3:Y:17:LEU:HD12	2.00	0.42
2:H:38:LYS:HD2	2:H:94:TYR:OH	2.20	0.42
1:L:114:SER:O	1:L:132:CYS:HA	2.20	0.42
1:L:21:MET:SD	1:L:85:TYR:HB2	2.59	0.42
3:Y:6:CYS:HB3	3:Y:128:ARG:NH1	2.35	0.42
1:L:44:LYS:HD2	4:L:229:HOH:O	2.19	0.42
1:L:12:SER:HB3	4:L:218:HOH:O	2.19	0.42
1:L:106:ARG:HH11	1:L:106:ARG:HD3	1.65	0.41
1:L:43:PRO:HD2	2:H:106:TRP:CE3	2.55	0.41
3:Y:121:GLN:O	3:Y:124:ILE:HD12	2.20	0.41
2:H:202:HIS:ND1	2:H:205:SER:OG	2.50	0.41
2:H:27:TYR:HH	2:H:98:HIS:CE1	2.38	0.41
2:H:33:TRP:CE3	2:H:50:GLU:HG3	2.55	0.41
1:L:158:LEU:HD22	2:H:172:VAL:HG11	2.02	0.41
1:L:65:GLY:HA3	1:L:69:SER:O	2.20	0.41
2:H:51:ILE:HA	2:H:57:SER:O	2.21	0.41
1:L:42:SER:HB3	2:H:95:TYR:CE1	2.56	0.41
1:L:116:PHE:HA	1:L:117:PRO:HD2	1.90	0.40
2:H:62:GLU:O	2:H:65:LYS:HE2	2.21	0.40
2:H:28:THR:O	2:H:31:ASP:HB2	2.21	0.40
2:H:143:CYS:O	2:H:181:SER:HA	2.22	0.40
1:L:118:PRO:HG2	1:L:184:TYR:CZ	2.56	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	210/212 (99%)	181 (86%)	21 (10%)	8 (4%)	3 4
2	H	212/215 (99%)	186 (88%)	21 (10%)	5 (2%)	6 10
3	Y	127/129 (98%)	113 (89%)	12 (9%)	2 (2%)	9 19
All	All	549/556 (99%)	480 (87%)	54 (10%)	15 (3%)	5 8

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	175	SER
2	H	189	SER
2	H	206	SER
3	Y	5	ARG
3	Y	88	ILE
1	L	50	THR
1	L	165	ASP
1	L	166	SER
2	H	132	ALA
1	L	149	ASP
1	L	152	GLU
1	L	153	ARG
1	L	188	ASN
2	H	190	PRO
1	L	55	SER

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	187/187 (100%)	160 (86%)	27 (14%)	3 5
2	H	182/182 (100%)	154 (85%)	28 (15%)	2 4
3	Y	105/105 (100%)	92 (88%)	13 (12%)	4 8
All	All	474/474 (100%)	406 (86%)	68 (14%)	3 5

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	5	THR
1	L	7	SER
1	L	12	SER
1	L	28	SER
1	L	32	MET
1	L	36	GLN
1	L	41	THR
1	L	42	SER
1	L	51	SER
1	L	72	LEU
1	L	73	THR
1	L	95	THR
1	L	106	ARG
1	L	112	THR
1	L	120	SER
1	L	143	ASN
1	L	145	LYS
1	L	147	LYS
1	L	149	ASP
1	L	162	THR
1	L	163	ASP
1	L	170	THR
1	L	195	THR
1	L	198	THR
1	L	206	SER
1	L	211	GLU
1	L	212	CYS
2	H	12	MET
2	H	28	THR
2	H	30	SER
2	H	53	PRO
2	H	71	THR
2	H	74	THR
2	H	97	LEU
2	H	102	ASP
2	H	103	PHE
2	H	131	SER
2	H	135	THR
2	H	141	LEU
2	H	151	GLU
2	H	152	PRO
2	H	153	VAL
2	H	154	THR

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Mol	Chain	Res	Type
2	H	155	VAL
2	H	158	ASN
2	H	162	LEU
2	H	164	SER
2	H	174	GLN
2	H	180	LEU
2	H	184	VAL
2	H	188	SER
2	H	191	ARG
2	H	198	CYS
2	H	208	LYS
2	H	214	VAL
3	Y	5	ARG
3	Y	14	ARG
3	Y	24	SER
3	Y	37	ASN
3	Y	43	THR
3	Y	47	THR
3	Y	72	SER
3	Y	77	ASN
3	Y	85	SER
3	Y	86	SER
3	Y	97	LYS
3	Y	101	ASP
3	Y	128	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	37	GLN
1	L	187	HIS
2	H	39	GLN
2	H	134	GLN
2	H	158	ASN
3	Y	27	ASN
3	Y	37	ASN
3	Y	39	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	212/212 (100%)	-0.62	2 (0%) 84 82	5, 21, 48, 71	0
2	H	214/215 (99%)	-0.64	4 (1%) 66 62	2, 18, 45, 71	0
3	Y	129/129 (100%)	-0.60	0 100 100	5, 20, 40, 56	1 (0%)
All	All	555/556 (99%)	-0.62	6 (1%) 80 78	2, 20, 45, 71	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	2	VAL	6.3
2	H	3	GLN	4.1
2	H	135	THR	3.1
2	H	133	ALA	3.0
1	L	1	ASP	2.1
1	L	212	CYS	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.