WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:02 PM GMT

PDB ID	:	3VVJ
Title	:	Structure of Ovalbumin from Emu (Dromaius novaehollandiae)
Authors	:	Yasutake, Y.; Maehashi, K.; Matano, M.; Takeuchi, J.
Deposited on	:	2012-07-25
Resolution	:	3.30 Å(reported)

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

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	Percentile Ranks	Value
Rfree		0.224
Clashscore		25
Ramachandran outliers		3.3%
Sidechain outliers		19.7%
RSRZ outliers		0.8%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
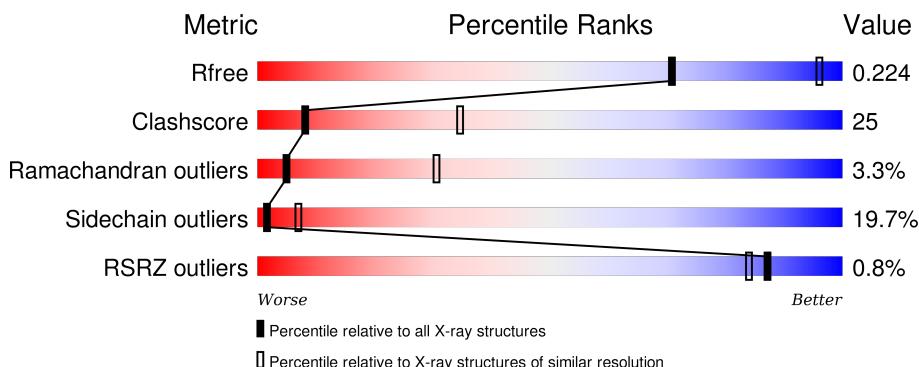
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	A	392	48% 39% 10% ••
1	B	392	% 53% 34% 11% •
1	C	392	2% 46% 40% 10% ••
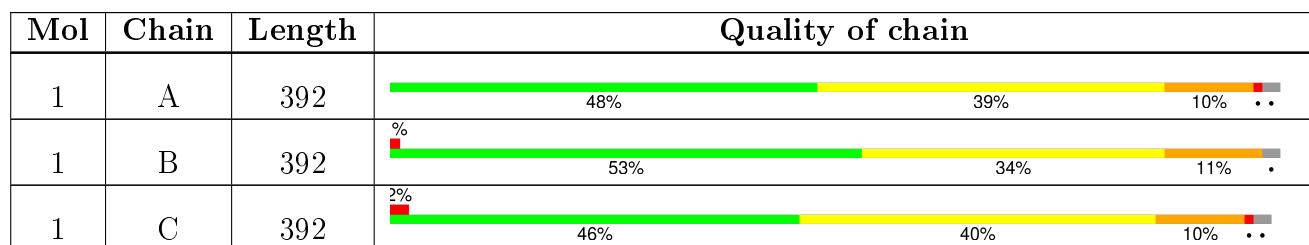
2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9027 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 Ovalbumin.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total 3009	C 1924	N 476	O 590	S 19	0	0	0
1	B	384	Total 3009	C 1924	N 476	O 590	S 19	0	0	0
1	C	384	Total 3009	C 1924	N 476	O 590	S 19	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	387	HIS	-	EXPRESSION TAG	UNP E2RVI8
A	388	HIS	-	EXPRESSION TAG	UNP E2RVI8
A	389	HIS	-	EXPRESSION TAG	UNP E2RVI8
A	390	HIS	-	EXPRESSION TAG	UNP E2RVI8
A	391	HIS	-	EXPRESSION TAG	UNP E2RVI8
A	392	HIS	-	EXPRESSION TAG	UNP E2RVI8
B	387	HIS	-	EXPRESSION TAG	UNP E2RVI8
B	388	HIS	-	EXPRESSION TAG	UNP E2RVI8
B	389	HIS	-	EXPRESSION TAG	UNP E2RVI8
B	390	HIS	-	EXPRESSION TAG	UNP E2RVI8
B	391	HIS	-	EXPRESSION TAG	UNP E2RVI8
B	392	HIS	-	EXPRESSION TAG	UNP E2RVI8
C	387	HIS	-	EXPRESSION TAG	UNP E2RVI8
C	388	HIS	-	EXPRESSION TAG	UNP E2RVI8
C	389	HIS	-	EXPRESSION TAG	UNP E2RVI8
C	390	HIS	-	EXPRESSION TAG	UNP E2RVI8
C	391	HIS	-	EXPRESSION TAG	UNP E2RVI8
C	392	HIS	-	EXPRESSION TAG	UNP E2RVI8

3 Residue-property plots ⓘ

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

- Molecule 1: Ovalbumin

- Molecule 1: Ovalbumin

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Chain C:
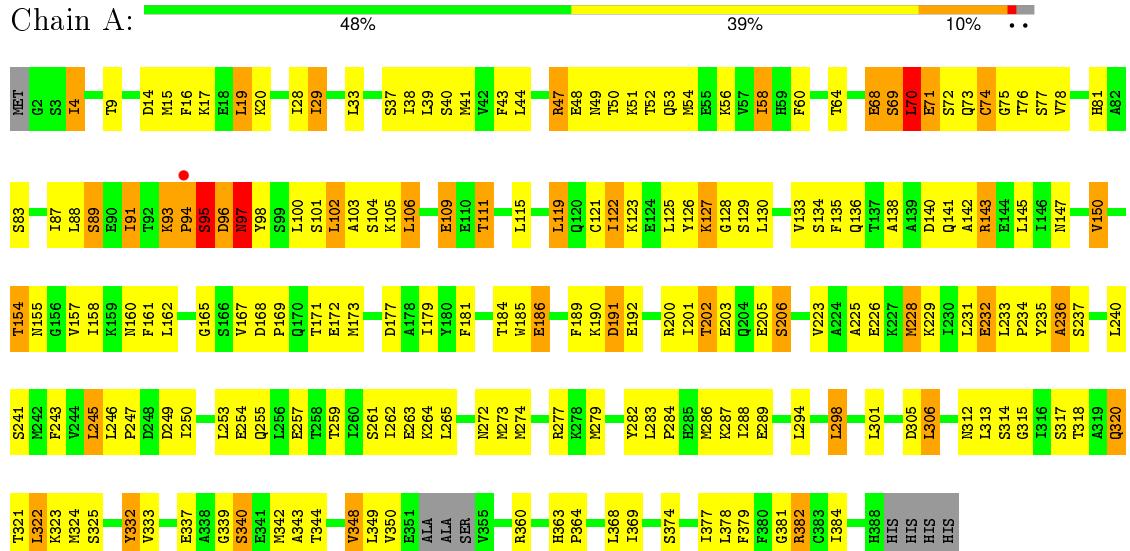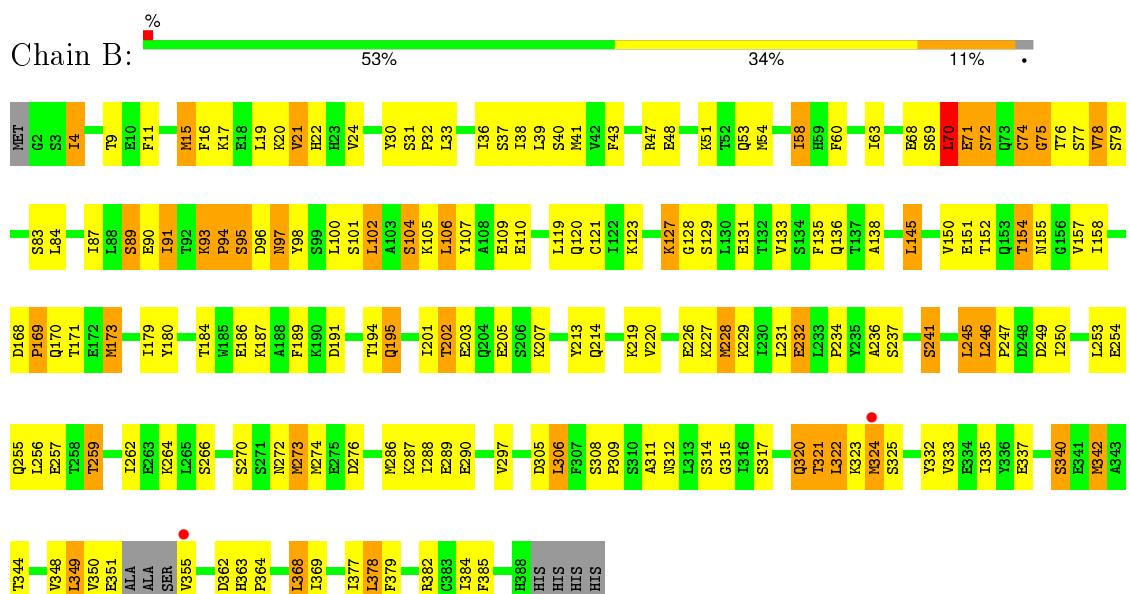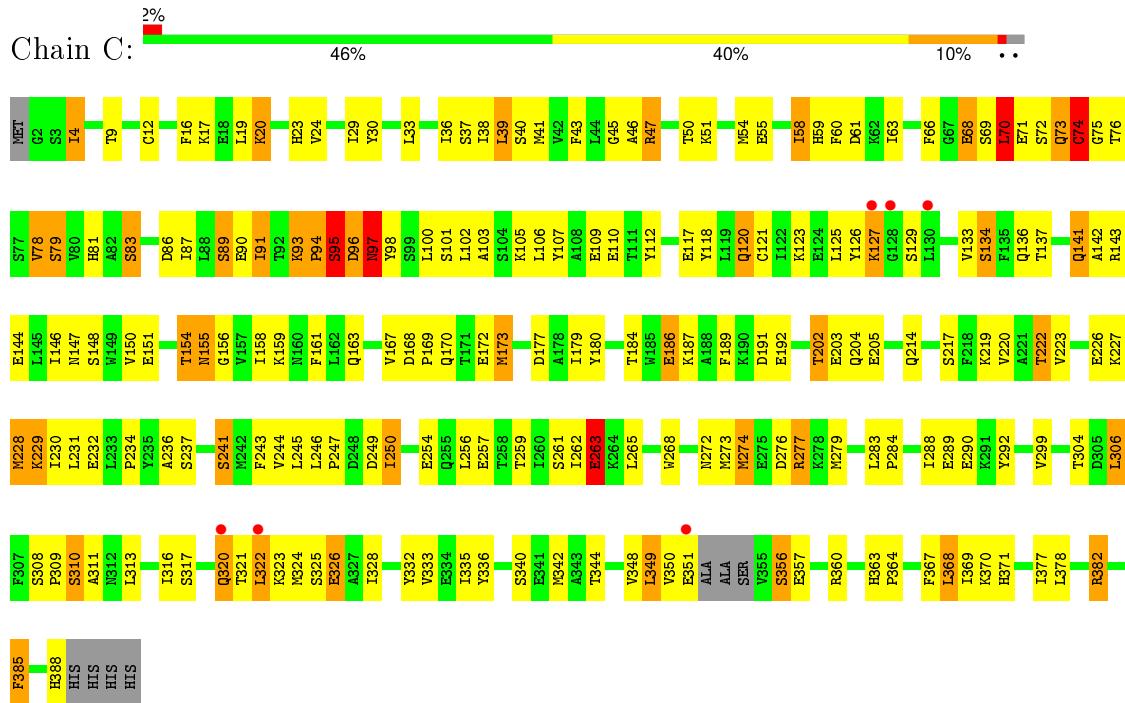
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	152.69Å 171.82Å 175.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.88 – 3.30 48.88 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.88-3.30) 100.0 (48.88-3.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.176 , 0.226 0.175 , 0.224	Depositor DCC
R_{free} test set	1751 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	80.3	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.5	EDS
Estimated twinning fraction	0.028 for -h,-l,-k	Xtriage
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Outliers	0 of 34971 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9027	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]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 (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	A	0.70	1/3070 (0.0%)	0.96	5/4152 (0.1%)
1	B	0.74	0/3070	0.99	5/4152 (0.1%)
1	C	0.70	1/3070 (0.0%)	0.94	8/4152 (0.2%)
All	All	0.71	2/9210 (0.0%)	0.96	18/12456 (0.1%)

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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	TRP	CD2-CE2	5.53	1.48	1.41
1	C	268	TRP	CD2-CE2	5.05	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	70	LEU	CA-CB-CG	12.24	143.46	115.30
1	C	70	LEU	CA-CB-CG	12.16	143.28	115.30
1	A	70	LEU	CA-CB-CG	10.28	138.94	115.30
1	C	74	CYS	CA-CB-SG	-7.09	101.23	114.00
1	B	368	LEU	CA-CB-CG	7.07	131.56	115.30
1	C	368	LEU	CA-CB-CG	6.79	130.91	115.30
1	A	102	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	362	ASP	CB-CG-OD1	5.95	123.66	118.30
1	C	66	PHE	CB-CG-CD2	5.84	124.89	120.80
1	C	70	LEU	CB-CG-CD2	5.65	120.60	111.00
1	C	360	ARG	NE-CZ-NH2	-5.54	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	246	LEU	CB-CG-CD1	-5.23	102.10	111.00
1	C	263	GLU	N-CA-CB	-5.20	101.24	110.60
1	C	277	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	145	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	102	LEU	CA-CB-CG	5.15	127.14	115.30
1	B	145	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	143	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	356	SER	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	A	3009	0	2975	153	0
1	B	3009	0	2975	138	0
1	C	3009	0	2975	153	0
All	All	9027	0	8925	440	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 25.

All (440) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LYS:HB3	1:A:94:PRO:CD	1.50	1.39
1:A:93:LYS:CB	1:A:94:PRO:HD3	1.58	1.32
1:B:342:MET:HE1	1:B:369:ILE:HD13	1.19	1.15
1:C:93:LYS:HB3	1:C:94:PRO:CD	1.77	1.10
1:C:93:LYS:HB3	1:C:94:PRO:HD3	1.12	1.08
1:A:245:LEU:H	1:A:245:LEU:HD12	1.19	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:MET:CE	1:B:369:ILE:HD13	1.86	1.04
1:B:93:LYS:CB	1:B:94:PRO:HD3	1.90	1.01
1:C:91:ILE:HD11	1:C:102:LEU:HB2	1.41	1.00
1:B:91:ILE:HD11	1:B:102:LEU:HB2	1.42	0.99
1:C:20:LYS:HE3	1:C:257:GLU:OE1	1.63	0.98
1:C:47:ARG:HH21	1:C:47:ARG:HB3	1.28	0.98
1:C:262:ILE:HG23	1:C:263:GLU:H	1.30	0.96
1:A:333:VAL:HG22	1:A:342:MET:HG2	1.46	0.95
1:C:154:THR:CG2	1:C:158:ILE:H	1.82	0.93
1:A:89:SER:O	1:A:93:LYS:HG2	1.69	0.93
1:C:326:GLU:HB3	1:C:349:LEU:HG	1.51	0.91
1:A:324:MET:SD	1:A:348:VAL:HG13	2.11	0.90
1:B:255:GLN:O	1:B:259:THR:HG22	1.72	0.90
1:B:93:LYS:HB3	1:B:94:PRO:HD3	1.54	0.89
1:B:342:MET:HE1	1:B:369:ILE:HG21	1.54	0.88
1:C:70:LEU:HD13	1:C:71:GLU:HB2	1.56	0.87
1:C:37:SER:O	1:C:40:SER:HB3	1.74	0.87
1:B:4:ILE:HG22	1:B:83:SER:HB3	1.55	0.86
1:A:4:ILE:HG22	1:A:83:SER:HB3	1.55	0.86
1:A:342:MET:HE1	1:A:369:ILE:HD13	1.54	0.86
1:C:168:ASP:HB2	1:C:169:PRO:HD2	1.57	0.86
1:C:324:MET:SD	1:C:348:VAL:HG13	2.16	0.86
1:B:37:SER:O	1:B:40:SER:HB3	1.74	0.86
1:A:342:MET:CE	1:A:369:ILE:HD13	2.05	0.85
1:B:342:MET:HE1	1:B:369:ILE:CD1	2.05	0.83
1:A:202:THR:CG2	1:A:205:GLU:HB2	2.11	0.81
1:C:93:LYS:CB	1:C:94:PRO:HD3	2.05	0.81
1:B:127:LYS:HG2	1:B:127:LYS:O	1.79	0.81
1:C:333:VAL:HG22	1:C:342:MET:HG2	1.64	0.80
1:B:93:LYS:HB3	1:B:94:PRO:CD	2.09	0.80
1:C:109:GLU:OE2	1:C:136:GLN:HG2	1.82	0.80
1:A:115:LEU:HD21	1:A:318:THR:CB	2.11	0.80
1:B:102:LEU:HD23	1:B:179:ILE:HG12	1.65	0.79
1:A:294:LEU:O	1:A:298:LEU:HD12	1.85	0.77
1:B:93:LYS:HB2	1:B:94:PRO:HD3	1.65	0.77
1:C:154:THR:HG23	1:C:158:ILE:H	1.49	0.77
1:C:261:SER:OG	1:C:263:GLU:HB3	1.85	0.76
1:B:342:MET:CE	1:B:369:ILE:HG21	2.16	0.75
1:A:70:LEU:HD13	1:A:71:GLU:H	1.52	0.75
1:C:363:HIS:HB2	1:C:364:PRO:HD2	1.69	0.75
1:B:333:VAL:HG22	1:B:342:MET:HG2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:MET:HE1	1:C:369:ILE:HG21	1.70	0.74
1:B:231:LEU:HD12	1:B:232:GLU:N	2.03	0.74
1:C:47:ARG:CB	1:C:47:ARG:HH21	2.00	0.74
1:A:133:VAL:HG11	1:A:142:ALA:HB2	1.70	0.73
1:C:89:SER:O	1:C:93:LYS:HG2	1.89	0.73
1:A:200:ARG:HA	1:A:206:SER:HB3	1.69	0.73
1:C:154:THR:HG21	1:C:158:ILE:H	1.54	0.73
1:C:72:SER:HB2	1:C:78:VAL:H	1.54	0.72
1:C:29:ILE:HG22	1:C:290:GLU:HB2	1.69	0.72
1:B:245:LEU:H	1:B:245:LEU:HD12	1.54	0.72
1:A:37:SER:O	1:A:40:SER:HB3	1.88	0.72
1:B:364:PRO:HB3	1:B:384:ILE:HA	1.72	0.72
1:C:277:ARG:HD3	1:C:279:MET:HE2	1.71	0.71
1:A:223:VAL:HB	1:A:228:MET:CE	2.20	0.71
1:A:234:PRO:HA	1:A:241:SER:HB3	1.73	0.71
1:B:151:GLU:O	1:B:154:THR:HG22	1.91	0.71
1:C:371:HIS:HB2	1:C:378:LEU:HD13	1.72	0.70
1:A:9:THR:HG23	1:A:377:ILE:HD11	1.73	0.70
1:C:342:MET:HE1	1:C:369:ILE:HD13	1.74	0.70
1:A:126:TYR:O	1:A:127:LYS:HE3	1.92	0.70
1:A:41:MET:CE	1:A:104:SER:HB3	2.22	0.70
1:C:96:ASP:OD1	1:C:96:ASP:N	2.25	0.69
1:C:179:ILE:HB	1:C:344:THR:HG22	1.75	0.69
1:C:4:ILE:HG22	1:C:83:SER:HB3	1.73	0.69
1:C:81:HIS:CE1	1:C:125:LEU:HD21	2.28	0.69
1:C:342:MET:CE	1:C:369:ILE:HD13	2.23	0.69
1:A:9:THR:HA	1:A:377:ILE:HD12	1.74	0.69
1:A:91:ILE:HD11	1:A:102:LEU:HB2	1.75	0.68
1:C:277:ARG:HD3	1:C:279:MET:CE	2.24	0.68
1:C:86:ASP:O	1:C:90:GLU:HG3	1.93	0.68
1:A:245:LEU:N	1:A:245:LEU:HD12	2.02	0.68
1:C:105:LYS:HD3	1:C:107:TYR:CE1	2.29	0.68
1:A:160:ASN:HD22	1:B:195:GLN:NE2	1.91	0.68
1:A:154:THR:CG2	1:A:158:ILE:H	2.07	0.67
1:A:93:LYS:CB	1:A:94:PRO:CD	2.33	0.67
1:B:109:GLU:OE2	1:B:136:GLN:HG2	1.95	0.67
1:A:231:LEU:HD21	1:A:233:LEU:HD21	1.76	0.67
1:C:127:LYS:O	1:C:127:LYS:HG2	1.92	0.67
1:C:9:THR:HA	1:C:377:ILE:HD13	1.76	0.67
1:A:168:ASP:HB2	1:A:169:PRO:HD2	1.75	0.67
1:A:363:HIS:HB2	1:A:364:PRO:CD	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:THR:HG21	1:A:158:ILE:H	1.59	0.66
1:A:168:ASP:OD1	1:A:171:THR:HG23	1.96	0.66
1:C:154:THR:HG21	1:C:158:ILE:HB	1.78	0.65
1:C:250:ILE:C	1:C:250:ILE:HD12	2.16	0.65
1:C:155:ASN:HB2	1:C:180:TYR:CE1	2.32	0.65
1:B:207:LYS:HZ1	1:B:385:PHE:HA	1.62	0.65
1:A:4:ILE:HG13	1:A:4:ILE:O	1.96	0.64
1:B:4:ILE:CG2	1:B:83:SER:HB3	2.27	0.64
1:B:97:ASN:HD22	1:B:97:ASN:N	1.95	0.64
1:A:223:VAL:HB	1:A:228:MET:HE1	1.79	0.64
1:B:168:ASP:O	1:B:170:GLN:N	2.30	0.64
1:C:74:CYS:O	1:C:76:THR:N	2.27	0.64
1:B:91:ILE:HD11	1:B:102:LEU:CB	2.24	0.63
1:B:189:PHE:CE2	1:B:214:GLN:HG2	2.32	0.63
1:A:277:ARG:HG3	1:A:279:MET:HG2	1.80	0.63
1:B:74:CYS:O	1:B:76:THR:N	2.21	0.63
1:B:289:GLU:O	1:B:290:GLU:HG2	1.99	0.63
1:C:283:LEU:HD12	1:C:284:PRO:HD2	1.81	0.63
1:C:250:ILE:O	1:C:250:ILE:HD12	1.99	0.63
1:A:324:MET:SD	1:A:348:VAL:CG1	2.86	0.63
1:C:189:PHE:CE2	1:C:214:GLN:HG2	2.34	0.63
1:C:226:GLU:HB2	1:C:228:MET:HE2	1.80	0.63
1:C:289:GLU:HG3	1:C:332:TYR:HD2	1.64	0.63
1:B:228:MET:HG2	1:B:229:LYS:N	2.14	0.62
1:A:257:GLU:OE2	1:A:382:ARG:HG3	1.99	0.62
1:A:47:ARG:HH21	1:A:47:ARG:HB3	1.62	0.62
1:A:202:THR:OG1	1:A:203:GLU:N	2.32	0.62
1:C:150:VAL:O	1:C:154:THR:HB	1.99	0.62
1:A:282:TYR:HB2	1:A:360:ARG:HA	1.82	0.62
1:C:70:LEU:CD1	1:C:71:GLU:H	2.13	0.62
1:B:47:ARG:HD3	1:B:315:GLY:HA3	1.81	0.62
1:B:93:LYS:CB	1:B:94:PRO:CD	2.61	0.62
1:C:97:ASN:N	1:C:97:ASN:HD22	1.96	0.62
1:A:150:VAL:O	1:A:154:THR:HB	1.99	0.61
1:B:305:ASP:O	1:B:311:ALA:HB2	2.01	0.61
1:A:332:TYR:C	1:A:332:TYR:CD1	2.72	0.61
1:C:40:SER:O	1:C:43:PHE:HB3	2.00	0.61
1:A:41:MET:HE1	1:A:104:SER:HB3	1.83	0.61
1:C:112:TYR:CB	1:C:172:GLU:HG3	2.31	0.61
1:A:236:ALA:O	1:A:237:SER:CB	2.48	0.61
1:B:69:SER:OG	1:B:70:LEU:N	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG11	1:A:161:PHE:HB3	1.82	0.60
1:C:4:ILE:HG22	1:C:83:SER:CB	2.31	0.60
1:A:9:THR:HG23	1:A:377:ILE:CD1	2.31	0.59
1:B:97:ASN:N	1:B:97:ASN:ND2	2.49	0.59
1:C:38:ILE:HD13	1:C:41:MET:CE	2.33	0.59
1:B:150:VAL:O	1:B:154:THR:HB	2.02	0.59
1:C:4:ILE:HG23	1:C:87:ILE:HD13	1.84	0.59
1:A:93:LYS:HB3	1:A:94:PRO:HD3	0.69	0.59
1:C:151:GLU:O	1:C:154:THR:HG22	2.03	0.59
1:C:97:ASN:ND2	1:C:97:ASN:N	2.51	0.59
1:A:342:MET:HE1	1:A:369:ILE:HG21	1.83	0.59
1:B:40:SER:O	1:B:43:PHE:HB3	2.02	0.59
1:C:9:THR:HG23	1:C:377:ILE:HD11	1.84	0.59
1:A:143:ARG:HB2	1:A:167:VAL:CG2	2.32	0.59
1:A:382:ARG:HG3	1:A:382:ARG:HH21	1.68	0.59
1:A:14:ASP:HB3	1:A:301:LEU:HD21	1.83	0.59
1:B:335:ILE:HA	1:B:340:SER:HB3	1.83	0.59
1:C:262:ILE:CG2	1:C:263:GLU:H	2.09	0.58
1:A:102:LEU:HD23	1:A:179:ILE:HG12	1.85	0.58
1:B:31:SER:CB	1:B:344:THR:HG21	2.33	0.58
1:B:320:GLN:NE2	1:B:321:THR:O	2.37	0.58
1:A:228:MET:HG2	1:A:229:LYS:N	2.18	0.58
1:C:322:LEU:HD13	1:C:350:VAL:HG11	1.85	0.58
1:A:202:THR:HG23	1:A:205:GLU:H	1.69	0.58
1:B:154:THR:CG2	1:B:158:ILE:H	2.17	0.58
1:B:270:SER:HB3	1:B:273:MET:HB2	1.86	0.58
1:C:172:GLU:OE1	1:C:322:LEU:HD23	2.03	0.58
1:B:363:HIS:HB2	1:B:364:PRO:HD3	1.86	0.58
1:A:363:HIS:HB2	1:A:364:PRO:HD3	1.85	0.58
1:A:283:LEU:HD12	1:A:284:PRO:HD2	1.86	0.58
1:A:289:GLU:HG2	1:A:332:TYR:CD2	2.39	0.57
1:C:103:ALA:O	1:C:177:ASP:HB2	2.03	0.57
1:C:70:LEU:HD13	1:C:71:GLU:H	1.69	0.57
1:A:133:VAL:HG11	1:A:142:ALA:CB	2.35	0.57
1:C:262:ILE:HG23	1:C:263:GLU:N	2.12	0.57
1:A:181:PHE:CE2	1:A:240:LEU:HD22	2.39	0.57
1:B:16:PHE:HB2	1:B:30:TYR:OH	2.05	0.57
1:C:117:GLU:HA	1:C:120:GLN:HB3	1.85	0.57
1:A:154:THR:O	1:A:157:VAL:HG23	2.04	0.57
1:B:342:MET:HB3	1:B:379:PHE:CZ	2.40	0.57
1:C:363:HIS:HB2	1:C:364:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HG2	1:A:127:LYS:O	2.04	0.57
1:A:41:MET:HE2	1:A:104:SER:HB3	1.87	0.57
1:A:223:VAL:HB	1:A:228:MET:HE3	1.85	0.57
1:B:194:THR:HG21	1:B:337:GLU:OE2	2.05	0.57
1:A:255:GLN:O	1:A:259:THR:HG22	2.04	0.56
1:A:342:MET:HE1	1:A:369:ILE:CD1	2.31	0.56
1:B:289:GLU:HG2	1:B:332:TYR:HD2	1.69	0.56
1:C:236:ALA:O	1:C:237:SER:CB	2.53	0.56
1:B:38:ILE:HD13	1:B:41:MET:CE	2.35	0.56
1:C:151:GLU:HG3	1:C:159:LYS:HA	1.87	0.56
1:A:70:LEU:CD1	1:A:71:GLU:H	2.16	0.56
1:A:289:GLU:HG2	1:A:332:TYR:HD2	1.71	0.56
1:B:171:THR:HA	1:B:351:GLU:HG2	1.87	0.56
1:B:89:SER:O	1:B:93:LYS:HG2	2.06	0.56
1:C:187:LYS:HE3	1:C:217:SER:O	2.06	0.56
1:A:69:SER:HA	1:A:77:SER:HB3	1.87	0.56
1:C:228:MET:HG2	1:C:229:LYS:N	2.20	0.56
1:A:184:THR:HA	1:A:339:GLY:HA3	1.86	0.56
1:B:154:THR:O	1:B:154:THR:HG23	2.04	0.56
1:B:31:SER:HB2	1:B:344:THR:HG21	1.87	0.56
1:A:306:LEU:HD22	1:A:324:MET:HB3	1.87	0.56
1:A:378:LEU:HB3	1:A:379:PHE:HD2	1.71	0.56
1:B:286:MET:HE2	1:B:288:ILE:CD1	2.36	0.56
1:A:147:ASN:O	1:A:150:VAL:HG12	2.06	0.55
1:C:38:ILE:HD13	1:C:41:MET:HE1	1.88	0.55
1:B:9:THR:HG23	1:B:377:ILE:HD11	1.86	0.55
1:C:168:ASP:HB2	1:C:169:PRO:CD	2.34	0.55
1:B:154:THR:HG21	1:B:158:ILE:H	1.72	0.55
1:C:234:PRO:HA	1:C:241:SER:HB3	1.88	0.55
1:C:73:GLN:HE21	1:C:81:HIS:CD2	2.25	0.55
1:B:202:THR:HG23	1:B:205:GLU:H	1.71	0.55
1:B:4:ILE:HD13	1:B:84:LEU:HD23	1.88	0.54
1:B:9:THR:HG23	1:B:377:ILE:CD1	2.37	0.54
1:A:97:ASN:N	1:A:97:ASN:HD22	2.06	0.54
1:C:46:ALA:HA	1:C:313:LEU:HD23	1.90	0.54
1:C:154:THR:HG21	1:C:158:ILE:N	2.22	0.54
1:C:91:ILE:HD11	1:C:102:LEU:CB	2.27	0.54
1:B:247:PRO:HG3	1:B:253:LEU:HB2	1.90	0.54
1:A:28:ILE:O	1:A:381:GLY:HA3	2.08	0.54
1:A:200:ARG:HA	1:A:206:SER:CB	2.37	0.54
1:A:157:VAL:HG11	1:A:343:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:LYS:O	1:C:351:GLU:N	2.36	0.53
1:C:256:LEU:HA	1:C:259:THR:HG22	1.91	0.53
1:C:223:VAL:O	1:C:223:VAL:HG12	2.07	0.53
1:C:324:MET:HA	1:C:350:VAL:HA	1.90	0.53
1:B:70:LEU:HD13	1:B:71:GLU:H	1.72	0.53
1:B:378:LEU:HB3	1:B:379:PHE:HD2	1.74	0.53
1:B:202:THR:OG1	1:B:203:GLU:N	2.41	0.53
1:B:245:LEU:N	1:B:245:LEU:HD12	2.21	0.53
1:B:105:LYS:HD3	1:B:107:TYR:CE1	2.44	0.53
1:C:41:MET:HG2	1:C:126:TYR:CE2	2.43	0.53
1:A:4:ILE:CG2	1:A:83:SER:HB3	2.36	0.52
1:B:11:PHE:O	1:B:15:MET:HB3	2.09	0.52
1:A:119:LEU:HD11	1:A:130:LEU:HD22	1.90	0.52
1:A:109:GLU:HG2	1:A:135:PHE:HB2	1.91	0.52
1:B:72:SER:HB2	1:B:77:SER:HA	1.91	0.52
1:C:173:MET:HB3	1:C:350:VAL:HB	1.92	0.52
1:B:154:THR:O	1:B:157:VAL:HG23	2.09	0.52
1:A:143:ARG:HB2	1:A:167:VAL:HG21	1.91	0.52
1:B:21:VAL:CG1	1:B:22:HIS:CD2	2.92	0.52
1:B:95:SER:O	1:B:95:SER:OG	2.27	0.52
1:B:256:LEU:HA	1:B:259:THR:HG23	1.92	0.52
1:B:363:HIS:HB2	1:B:364:PRO:CD	2.40	0.52
1:A:122:ILE:HG22	1:A:128:GLY:HA3	1.92	0.52
1:B:168:ASP:C	1:B:170:GLN:H	2.12	0.52
1:A:324:MET:HG3	1:A:325:SER:N	2.24	0.52
1:B:201:ILE:HG23	1:B:384:ILE:HG22	1.91	0.52
1:C:105:LYS:HD3	1:C:107:TYR:CZ	2.45	0.52
1:B:38:ILE:HD13	1:B:41:MET:HE1	1.90	0.52
1:A:123:LYS:HA	1:A:128:GLY:H	1.74	0.52
1:A:165:GLY:HA2	1:B:213:TYR:CZ	2.46	0.51
1:A:226:GLU:HB2	1:A:228:MET:HE2	1.93	0.51
1:A:158:ILE:HG22	1:A:161:PHE:HB2	1.91	0.51
1:A:378:LEU:HB3	1:A:379:PHE:CD2	2.45	0.51
1:A:277:ARG:HG3	1:A:279:MET:CG	2.40	0.51
1:B:24:VAL:CG2	1:C:204:GLN:HB3	2.41	0.51
1:B:71:GLU:HG2	1:B:75:GLY:N	2.25	0.51
1:A:52:THR:O	1:A:56:LYS:HG2	2.10	0.51
1:C:95:SER:O	1:C:95:SER:OG	2.28	0.51
1:C:69:SER:OG	1:C:70:LEU:N	2.44	0.51
1:A:95:SER:OG	1:A:95:SER:O	2.26	0.51
1:A:96:ASP:N	1:A:96:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:PRO:HB3	1:A:384:ILE:HA	1.92	0.51
1:B:257:GLU:OE2	1:B:382:ARG:NH2	2.38	0.51
1:B:171:THR:HG21	1:B:349:LEU:HD12	1.93	0.51
1:B:78:VAL:HG13	1:B:79:SER:N	2.25	0.51
1:B:106:LEU:HD13	1:B:173:MET:CE	2.41	0.51
1:A:16:PHE:O	1:A:20:LYS:HG2	2.11	0.51
1:A:232:GLU:HG3	1:A:232:GLU:O	2.09	0.51
1:C:261:SER:HG	1:C:263:GLU:HB3	1.73	0.50
1:C:16:PHE:HB2	1:C:30:TYR:OH	2.11	0.50
1:A:29:ILE:HG21	1:A:288:ILE:HG22	1.92	0.50
1:C:54:MET:O	1:C:58:ILE:HB	2.11	0.50
1:B:4:ILE:CD1	1:B:84:LEU:HD23	2.41	0.50
1:C:202:THR:OG1	1:C:203:GLU:N	2.45	0.50
1:C:324:MET:HG3	1:C:325:SER:N	2.25	0.50
1:A:97:ASN:N	1:A:97:ASN:ND2	2.60	0.50
1:B:105:LYS:HE3	1:B:131:GLU:HG3	1.92	0.50
1:C:50:THR:O	1:C:54:MET:HG3	2.12	0.50
1:A:262:ILE:HG23	1:A:263:GLU:N	2.27	0.50
1:A:69:SER:OG	1:A:70:LEU:N	2.44	0.50
1:B:105:LYS:CE	1:B:131:GLU:HG3	2.42	0.50
1:A:228:MET:HB2	1:A:247:PRO:HA	1.93	0.49
1:A:332:TYR:O	1:A:332:TYR:HD1	1.95	0.49
1:A:253:LEU:O	1:A:257:GLU:HG3	2.13	0.49
1:A:58:ILE:HG22	1:A:60:PHE:CD1	2.47	0.49
1:A:324:MET:HA	1:A:350:VAL:HA	1.93	0.49
1:A:103:ALA:HA	1:A:127:LYS:NZ	2.27	0.49
1:B:97:ASN:HD22	1:B:97:ASN:H	1.61	0.49
1:B:226:GLU:O	1:B:227:LYS:C	2.51	0.49
1:B:21:VAL:HG13	1:B:22:HIS:CD2	2.47	0.49
1:C:299:VAL:HG13	1:C:304:THR:HG22	1.93	0.49
1:B:109:GLU:HG2	1:B:135:PHE:HB2	1.95	0.49
1:C:228:MET:HB2	1:C:247:PRO:HA	1.95	0.49
1:B:70:LEU:CD1	1:B:71:GLU:H	2.25	0.49
1:C:23:HIS:O	1:C:382:ARG:NH1	2.46	0.49
1:A:320:GLN:O	1:A:320:GLN:HG3	2.12	0.49
1:B:342:MET:CE	1:B:369:ILE:CD1	2.75	0.49
1:C:147:ASN:HA	1:C:150:VAL:HG12	1.95	0.49
1:C:220:VAL:HG12	1:C:222:THR:HG22	1.93	0.49
1:B:173:MET:HB3	1:B:350:VAL:HB	1.95	0.49
1:B:231:LEU:HD12	1:B:232:GLU:H	1.75	0.48
1:B:256:LEU:HA	1:B:259:THR:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ILE:HG13	1:C:30:TYR:N	2.28	0.48
1:C:71:GLU:O	1:C:72:SER:C	2.51	0.48
1:C:78:VAL:HG13	1:C:79:SER:N	2.28	0.48
1:C:123:LYS:O	1:C:127:LYS:HA	2.13	0.48
1:A:184:THR:O	1:A:236:ALA:N	2.26	0.48
1:C:184:THR:O	1:C:236:ALA:N	2.47	0.48
1:A:235:TYR:CE1	1:A:340:SER:OG	2.67	0.48
1:C:349:LEU:HD23	1:C:349:LEU:N	2.28	0.48
1:A:48:GLU:HB3	1:A:49:ASN:H	1.50	0.48
1:B:104:SER:O	1:B:128:GLY:HA2	2.13	0.48
1:B:207:LYS:NZ	1:B:385:PHE:HA	2.28	0.47
1:B:168:ASP:C	1:B:170:GLN:N	2.68	0.47
1:A:235:TYR:HE1	1:A:340:SER:OG	1.97	0.47
1:B:58:ILE:CG2	1:B:60:PHE:CD1	2.98	0.47
1:A:202:THR:HG23	1:A:205:GLU:HB2	1.93	0.47
1:B:286:MET:HE2	1:B:288:ILE:HD12	1.96	0.47
1:C:101:SER:O	1:C:179:ILE:HA	2.15	0.47
1:C:308:SER:C	1:C:310:SER:H	2.18	0.47
1:C:289:GLU:HG3	1:C:332:TYR:CD2	2.49	0.47
1:C:256:LEU:HA	1:C:259:THR:CG2	2.45	0.47
1:C:47:ARG:CG	1:C:47:ARG:HH21	2.28	0.46
1:B:189:PHE:HB2	1:B:337:GLU:HA	1.96	0.46
1:C:58:ILE:HD12	1:C:58:ILE:HA	1.66	0.46
1:C:143:ARG:HB2	1:C:167:VAL:HG21	1.97	0.46
1:B:201:ILE:HD11	1:B:207:LYS:HG2	1.97	0.46
1:C:377:ILE:N	1:C:377:ILE:HD12	2.30	0.46
1:C:29:ILE:O	1:C:292:TYR:HE2	1.99	0.46
1:C:41:MET:HG2	1:C:126:TYR:CZ	2.51	0.46
1:A:243:PHE:HB2	1:A:368:LEU:HB3	1.97	0.46
1:B:342:MET:HE1	1:B:369:ILE:CG2	2.34	0.46
1:A:186:GLU:HB2	1:A:234:PRO:HB2	1.98	0.46
1:C:45:GLY:O	1:C:47:ARG:HG2	2.17	0.45
1:C:168:ASP:C	1:C:170:GLN:H	2.19	0.45
1:B:24:VAL:HG22	1:C:204:GLN:HB3	1.97	0.45
1:A:72:SER:HB2	1:A:77:SER:HA	1.97	0.45
1:B:152:THR:C	1:B:154:THR:H	2.20	0.45
1:A:179:ILE:HB	1:A:344:THR:HG22	1.99	0.45
1:C:60:PHE:CD1	1:C:63:ILE:HD12	2.51	0.45
1:C:322:LEU:HD13	1:C:350:VAL:CG1	2.47	0.45
1:B:127:LYS:CG	1:B:127:LYS:O	2.56	0.45
1:B:32:PRO:HD2	1:B:377:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LEU:HD13	1:B:324:MET:HE3	1.97	0.45
1:C:78:VAL:HG13	1:C:79:SER:H	1.82	0.45
1:C:308:SER:OG	1:C:310:SER:HB2	2.17	0.45
1:A:191:ASP:HA	1:A:337:GLU:HG2	1.98	0.45
1:B:155:ASN:HB2	1:B:180:TYR:CE1	2.52	0.45
1:C:356:SER:OG	1:C:357:GLU:N	2.46	0.45
1:A:245:LEU:CD1	1:A:245:LEU:H	1.99	0.45
1:B:136:GLN:HA	1:B:169:PRO:HA	1.99	0.45
1:B:337:GLU:N	1:B:337:GLU:OE1	2.50	0.45
1:B:226:GLU:HB2	1:B:228:MET:HE3	1.98	0.45
1:B:16:PHE:O	1:B:20:LYS:HG2	2.16	0.45
1:A:286:MET:HE3	1:A:288:ILE:HD12	1.99	0.45
1:C:202:THR:HG23	1:C:205:GLU:H	1.82	0.45
1:B:308:SER:O	1:B:323:LYS:HG3	2.17	0.45
1:C:154:THR:HG23	1:C:154:THR:O	2.17	0.44
1:A:101:SER:O	1:A:179:ILE:HA	2.17	0.44
1:C:186:GLU:HG3	1:C:187:LYS:HG3	1.99	0.44
1:A:189:PHE:HB2	1:A:337:GLU:HA	1.98	0.44
1:A:38:ILE:HG12	1:A:177:ASP:OD2	2.16	0.44
1:C:335:ILE:HA	1:C:340:SER:HB3	1.99	0.44
1:B:289:GLU:HG2	1:B:332:TYR:CD2	2.52	0.44
1:C:226:GLU:O	1:C:227:LYS:C	2.56	0.44
1:B:324:MET:HG3	1:B:325:SER:N	2.32	0.44
1:A:74:CYS:O	1:A:76:THR:N	2.46	0.44
1:A:322:LEU:HD13	1:A:350:VAL:HG11	1.99	0.44
1:A:53:GLN:OE1	1:A:305:ASP:HB2	2.17	0.44
1:C:142:ALA:O	1:C:146:ILE:HG13	2.18	0.44
1:C:154:THR:HG21	1:C:158:ILE:CB	2.46	0.44
1:C:306:LEU:HD22	1:C:324:MET:HB3	2.00	0.44
1:A:64:THR:HG21	1:A:69:SER:HB2	1.98	0.44
1:C:97:ASN:O	1:C:98:TYR:HB3	2.18	0.44
1:A:109:GLU:OE1	1:A:111:THR:HG23	2.17	0.44
1:B:78:VAL:HG13	1:B:79:SER:H	1.83	0.44
1:A:44:LEU:HD23	1:A:76:THR:HG23	2.00	0.44
1:B:236:ALA:O	1:B:237:SER:CB	2.65	0.43
1:B:332:TYR:C	1:B:332:TYR:CD1	2.92	0.43
1:B:38:ILE:HD12	1:B:38:ILE:HG23	1.73	0.43
1:A:19:LEU:HA	1:A:19:LEU:HD23	1.82	0.43
1:C:39:LEU:HD12	1:C:39:LEU:HA	1.83	0.43
1:C:47:ARG:NH2	1:C:47:ARG:CG	2.82	0.43
1:C:147:ASN:O	1:C:151:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:MET:CE	1:A:288:ILE:HD12	2.48	0.43
1:A:81:HIS:CE1	1:A:125:LEU:HD21	2.53	0.43
1:C:274:MET:HB3	1:C:274:MET:HE2	1.88	0.43
1:A:49:ASN:O	1:A:53:GLN:HB2	2.18	0.43
1:B:324:MET:SD	1:B:348:VAL:HG13	2.59	0.43
1:A:119:LEU:HD21	1:A:130:LEU:HB2	2.01	0.43
1:B:58:ILE:HA	1:B:58:ILE:HD12	1.54	0.43
1:B:306:LEU:HD22	1:B:324:MET:HB3	2.00	0.43
1:C:336:TYR:CZ	1:C:340:SER:HA	2.53	0.43
1:C:150:VAL:HG11	1:C:161:PHE:HB3	2.00	0.43
1:A:40:SER:O	1:A:43:PHE:HB3	2.18	0.43
1:A:87:ILE:HG13	1:A:374:SER:HB2	2.01	0.43
1:C:71:GLU:HA	1:C:73:GLN:O	2.19	0.43
1:A:87:ILE:O	1:A:91:ILE:HG23	2.19	0.42
1:A:98:TYR:HB2	1:A:181:PHE:HE1	1.84	0.42
1:C:230:ILE:HA	1:C:244:VAL:O	2.19	0.42
1:C:243:PHE:O	1:C:367:PHE:HA	2.19	0.42
1:C:141:GLN:O	1:C:144:GLU:HB3	2.18	0.42
1:A:133:VAL:CG1	1:A:142:ALA:HB2	2.45	0.42
1:A:102:LEU:CD2	1:A:179:ILE:HG12	2.48	0.42
1:A:236:ALA:O	1:A:237:SER:OG	2.36	0.42
1:B:220:VAL:O	1:B:220:VAL:HG12	2.19	0.42
1:A:261:SER:OG	1:A:264:LYS:HB2	2.20	0.42
1:C:168:ASP:CB	1:C:169:PRO:HD2	2.39	0.42
1:C:226:GLU:HB2	1:C:228:MET:CE	2.48	0.42
1:B:58:ILE:HG23	1:B:60:PHE:CD1	2.55	0.42
1:B:246:LEU:HA	1:B:247:PRO:HD2	1.91	0.42
1:B:287:LYS:HE2	1:B:332:TYR:OH	2.19	0.42
1:A:236:ALA:O	1:A:237:SER:HB3	2.20	0.42
1:B:322:LEU:HD13	1:B:350:VAL:HG11	2.02	0.42
1:C:151:GLU:HG2	1:C:156:GLY:HA2	2.02	0.42
1:C:55:GLU:OE2	1:C:61:ASP:HA	2.20	0.42
1:C:236:ALA:O	1:C:237:SER:OG	2.33	0.42
1:A:29:ILE:CG2	1:A:288:ILE:HG22	2.50	0.42
1:C:163:GLN:HB3	1:C:163:GLN:HE21	1.68	0.42
1:B:101:SER:O	1:B:179:ILE:HA	2.20	0.41
1:C:58:ILE:O	1:C:59:HIS:HB2	2.19	0.41
1:C:230:ILE:HG23	1:C:245:LEU:HG	2.03	0.41
1:A:105:LYS:HG2	1:A:106:LEU:N	2.35	0.41
1:C:385:PHE:CD2	1:C:388:HIS:CE1	3.08	0.41
1:B:87:ILE:HA	1:B:90:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:VAL:H	1:B:297:VAL:HG23	1.57	0.41
1:A:313:LEU:C	1:A:315:GLY:H	2.23	0.41
1:B:53:GLN:OE1	1:B:305:ASP:HB2	2.21	0.41
1:A:332:TYR:O	1:A:332:TYR:CD1	2.74	0.41
1:B:322:LEU:HD13	1:B:350:VAL:CG1	2.50	0.41
1:A:202:THR:HG22	1:A:205:GLU:HB2	1.95	0.41
1:B:60:PHE:HA	1:B:63:ILE:HG13	2.02	0.41
1:A:123:LYS:O	1:A:127:LYS:HA	2.21	0.41
1:C:9:THR:O	1:C:12:CYS:HB3	2.20	0.41
1:B:97:ASN:O	1:B:98:TYR:HB3	2.20	0.41
1:B:234:PRO:HA	1:B:241:SER:HB3	2.02	0.41
1:A:173:MET:HB3	1:A:350:VAL:HB	2.03	0.41
1:A:69:SER:O	1:A:70:LEU:HB3	2.21	0.41
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.63	0.41
1:C:110:GLU:CG	1:C:134:SER:HB2	2.51	0.41
1:C:118:TYR:CE1	1:C:316:ILE:HG12	2.56	0.41
1:C:222:THR:HA	1:C:229:LYS:HB3	2.02	0.40
1:B:105:LYS:HD3	1:B:107:TYR:CZ	2.55	0.40
1:A:265:LEU:HA	1:A:265:LEU:HD12	1.85	0.40
1:A:133:VAL:HG12	1:A:134:SER:N	2.37	0.40
1:A:201:ILE:HG23	1:A:384:ILE:CG2	2.51	0.40
1:B:286:MET:CE	1:B:288:ILE:HD11	2.52	0.40
1:B:54:MET:O	1:B:58:ILE:HB	2.21	0.40
1:A:50:THR:O	1:A:54:MET:HG3	2.21	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	A	380/392 (97%)	325 (86%)	42 (11%)	13 (3%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	380/392 (97%)	338 (89%)	31 (8%)	11 (3%)	6	34
1	C	380/392 (97%)	327 (86%)	39 (10%)	14 (4%)	4	27
All	All	1140/1176 (97%)	990 (87%)	112 (10%)	38 (3%)	5	30

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	LYS
1	A	94	PRO
1	A	186	GLU
1	B	93	LYS
1	C	93	LYS
1	A	68	GLU
1	A	74	CYS
1	A	75	GLY
1	A	97	ASN
1	A	138	ALA
1	B	75	GLY
1	B	94	PRO
1	B	138	ALA
1	B	169	PRO
1	C	68	GLU
1	C	74	CYS
1	C	75	GLY
1	C	78	VAL
1	C	94	PRO
1	C	263	GLU
1	C	311	ALA
1	C	320	GLN
1	A	70	LEU
1	A	95	SER
1	A	225	ALA
1	A	236	ALA
1	A	314	SER
1	B	314	SER
1	C	70	LEU
1	C	186	GLU
1	B	110	GLU
1	B	186	GLU
1	B	320	GLN
1	C	97	ASN

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Mol	Chain	Res	Type
1	C	309	PRO
1	C	95	SER
1	B	78	VAL
1	B	309	PRO

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	A	340/348 (98%)	275 (81%)	65 (19%)	2	8
1	B	340/348 (98%)	272 (80%)	68 (20%)	1	6
1	C	340/348 (98%)	272 (80%)	68 (20%)	1	6
All	All	1020/1044 (98%)	819 (80%)	201 (20%)	1	7

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	15	MET
1	A	17	LYS
1	A	19	LEU
1	A	29	ILE
1	A	33	LEU
1	A	39	LEU
1	A	47	ARG
1	A	51	LYS
1	A	58	ILE
1	A	68	GLU
1	A	69	SER
1	A	71	GLU
1	A	73	GLN
1	A	78	VAL
1	A	88	LEU
1	A	89	SER
1	A	91	ILE

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Mol	Chain	Res	Type
1	A	95	SER
1	A	96	ASP
1	A	97	ASN
1	A	100	LEU
1	A	106	LEU
1	A	109	GLU
1	A	111	THR
1	A	119	LEU
1	A	121	CYS
1	A	122	ILE
1	A	127	LYS
1	A	129	SER
1	A	136	GLN
1	A	140	ASP
1	A	141	GLN
1	A	150	VAL
1	A	154	THR
1	A	155	ASN
1	A	172	GLU
1	A	190	LYS
1	A	191	ASP
1	A	192	GLU
1	A	202	THR
1	A	206	SER
1	A	228	MET
1	A	232	GLU
1	A	245	LEU
1	A	249	ASP
1	A	250	ILE
1	A	254	GLU
1	A	272	ASN
1	A	273	MET
1	A	274	MET
1	A	287	LYS
1	A	298	LEU
1	A	306	LEU
1	A	312	ASN
1	A	317	SER
1	A	320	GLN
1	A	321	THR
1	A	322	LEU
1	A	323	LYS

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Mol	Chain	Res	Type
1	A	332	TYR
1	A	340	SER
1	A	348	VAL
1	A	349	LEU
1	A	382	ARG
1	B	4	ILE
1	B	15	MET
1	B	17	LYS
1	B	19	LEU
1	B	21	VAL
1	B	33	LEU
1	B	36	ILE
1	B	39	LEU
1	B	48	GLU
1	B	51	LYS
1	B	58	ILE
1	B	68	GLU
1	B	70	LEU
1	B	71	GLU
1	B	72	SER
1	B	74	CYS
1	B	89	SER
1	B	91	ILE
1	B	95	SER
1	B	96	ASP
1	B	97	ASN
1	B	100	LEU
1	B	104	SER
1	B	106	LEU
1	B	119	LEU
1	B	120	GLN
1	B	121	CYS
1	B	123	LYS
1	B	127	LYS
1	B	129	SER
1	B	133	VAL
1	B	145	LEU
1	B	154	THR
1	B	173	MET
1	B	184	THR
1	B	187	LYS
1	B	191	ASP

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Mol	Chain	Res	Type
1	B	195	GLN
1	B	202	THR
1	B	219	LYS
1	B	228	MET
1	B	232	GLU
1	B	241	SER
1	B	245	LEU
1	B	246	LEU
1	B	249	ASP
1	B	250	ILE
1	B	254	GLU
1	B	259	THR
1	B	262	ILE
1	B	264	LYS
1	B	266	SER
1	B	272	ASN
1	B	273	MET
1	B	274	MET
1	B	276	ASP
1	B	306	LEU
1	B	312	ASN
1	B	317	SER
1	B	321	THR
1	B	322	LEU
1	B	324	MET
1	B	340	SER
1	B	342	MET
1	B	349	LEU
1	B	355	VAL
1	B	368	LEU
1	B	378	LEU
1	C	4	ILE
1	C	17	LYS
1	C	19	LEU
1	C	20	LYS
1	C	24	VAL
1	C	33	LEU
1	C	36	ILE
1	C	39	LEU
1	C	47	ARG
1	C	51	LYS
1	C	58	ILE

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Mol	Chain	Res	Type
1	C	68	GLU
1	C	73	GLN
1	C	74	CYS
1	C	79	SER
1	C	83	SER
1	C	89	SER
1	C	91	ILE
1	C	95	SER
1	C	96	ASP
1	C	97	ASN
1	C	100	LEU
1	C	106	LEU
1	C	120	GLN
1	C	121	CYS
1	C	127	LYS
1	C	129	SER
1	C	133	VAL
1	C	134	SER
1	C	137	THR
1	C	141	GLN
1	C	148	SER
1	C	154	THR
1	C	155	ASN
1	C	173	MET
1	C	191	ASP
1	C	192	GLU
1	C	202	THR
1	C	219	LYS
1	C	222	THR
1	C	228	MET
1	C	229	LYS
1	C	231	LEU
1	C	232	GLU
1	C	241	SER
1	C	246	LEU
1	C	249	ASP
1	C	250	ILE
1	C	254	GLU
1	C	265	LEU
1	C	272	ASN
1	C	273	MET
1	C	274	MET

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Mol	Chain	Res	Type
1	C	276	ASP
1	C	288	ILE
1	C	306	LEU
1	C	310	SER
1	C	317	SER
1	C	320	GLN
1	C	321	THR
1	C	322	LEU
1	C	326	GLU
1	C	328	ILE
1	C	349	LEU
1	C	368	LEU
1	C	370	LYS
1	C	382	ARG
1	C	385	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	73	GLN
1	A	81	HIS
1	A	97	ASN
1	A	136	GLN
1	A	153	GLN
1	A	170	GLN
1	A	255	GLN
1	A	388	HIS
1	B	22	HIS
1	B	49	ASN
1	B	73	GLN
1	B	97	ASN
1	B	136	GLN
1	B	141	GLN
1	B	170	GLN
1	B	195	GLN
1	B	320	GLN
1	C	81	HIS
1	C	97	ASN
1	C	163	GLN
1	C	388	HIS

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 (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(Å²)	Q<0.9
1	A	384/392 (97%)	-0.16	1 (0%)	94	94	58, 88, 124, 156	0
1	B	384/392 (97%)	-0.26	2 (0%)	91	90	55, 85, 126, 165	0
1	C	384/392 (97%)	0.00	6 (1%)	74	69	57, 93, 141, 179	0
All	All	1152/1176 (97%)	-0.14	9 (0%)	87	84	55, 88, 131, 179	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	VAL	3.1
1	C	322	LEU	2.7
1	C	351	GLU	2.3
1	A	94	PRO	2.2
1	C	320	GLN	2.1
1	C	130	LEU	2.1
1	C	128	GLY	2.1
1	B	324	MET	2.1
1	C	127	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.