



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2022 – 03:53 AM EST

PDB ID : 6UTA
Title : Crystal structure of Z004 iGL Fab in complex with ZIKV EDIII
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Deposited on : 2019-10-29
Resolution : 3.10 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 ⓘ](#)) were used in the production of this report:

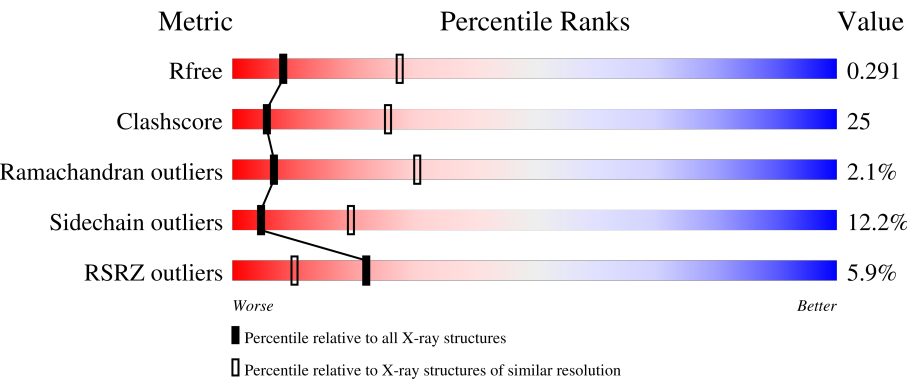
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	234	
1	H	234	
2	B	214	
2	L	214	
3	C	110	

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Mol	Chain	Length	Quality of chain
3	E	110	<div><div></div><div>12%</div><div>39%</div><div>38%</div><div>12%</div><div>•</div><div>10%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8038 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 Z004 iGL Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	221	Total	C	N	O	S	0	0	0
			1636	1029	278	323	6			
1	A	218	Total	C	N	O	S	0	0	0
			1622	1022	275	319	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	221	HIS	-	expression tag	UNP S6C4S0
H	222	HIS	-	expression tag	UNP S6C4S0
H	223	HIS	-	expression tag	UNP S6C4S0
H	224	HIS	-	expression tag	UNP S6C4S0
H	225	HIS	-	expression tag	UNP S6C4S0
A	221	HIS	-	expression tag	UNP S6C4S0
A	222	HIS	-	expression tag	UNP S6C4S0
A	223	HIS	-	expression tag	UNP S6C4S0
A	224	HIS	-	expression tag	UNP S6C4S0
A	225	HIS	-	expression tag	UNP S6C4S0

- Molecule 2 is a protein called Z004 iGL Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1638	1029	273	331	5			
2	B	212	Total	C	N	O	S	0	0	0
			1638	1029	273	331	5			

- Molecule 3 is a protein called Env.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	99	Total	C	N	O	S	0	0	0
			751	477	124	144	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	99	Total	C	N	O	S	0	0	0
			753	479	124	144	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	298	MET	-	initiating methionine	UNP A0A1X9PPI0
C	298	MET	-	initiating methionine	UNP A0A1X9PPI0

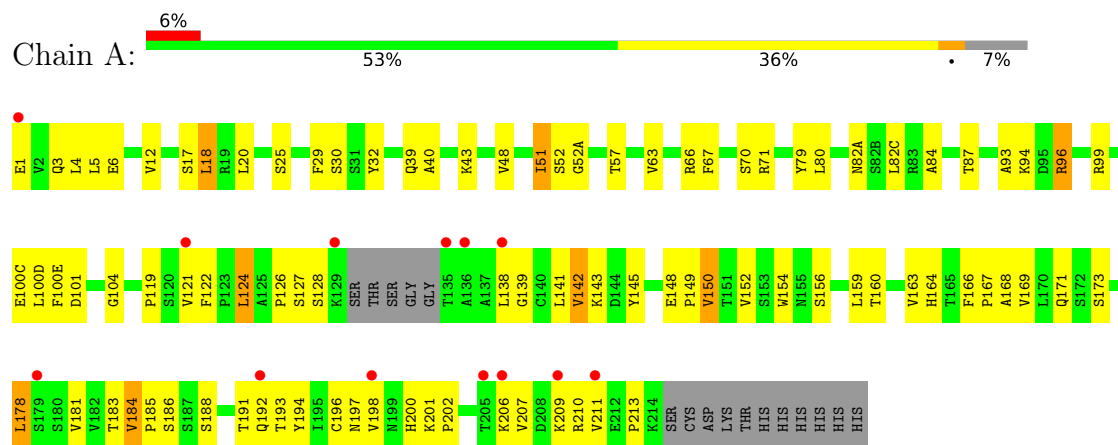
3 Residue-property plots

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

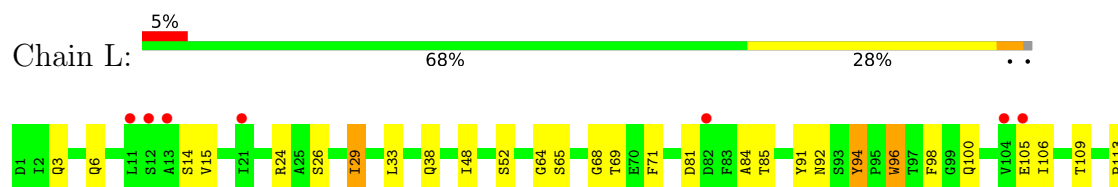
• Molecule 1: Z004 iGL Fab heavy chain

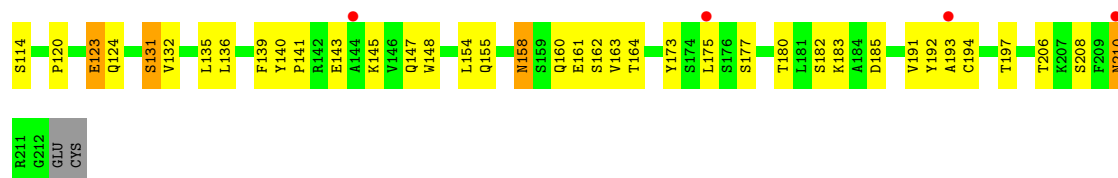


• Molecule 1: Z004 iGL Fab heavy chain

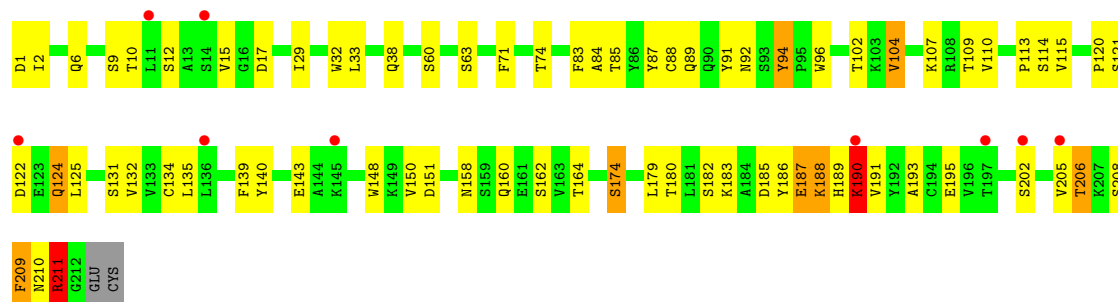


• Molecule 2: Z004 iGL Fab light chain

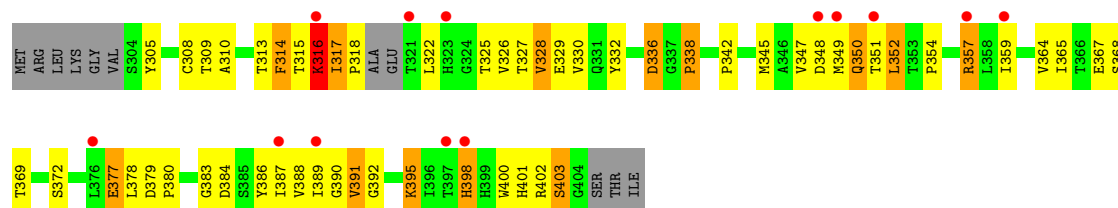




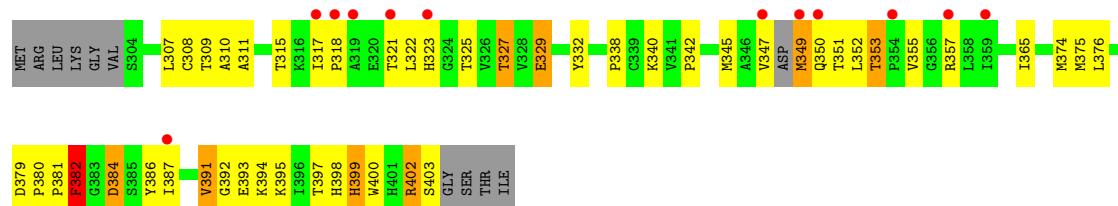
• Molecule 2: Z004 iGL Fab light chain



• Molecule 3: Env



• Molecule 3: Env



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.91Å 85.91Å 327.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.42 – 3.10 38.42 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.7 (38.42-3.10) 93.7 (38.42-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.274 , 0.291 0.274 , 0.291	Depositor DCC
R_{free} test set	1071 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 17.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8038	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	A	0.68	0/1659	0.78	0/2255
1	H	0.73	0/1673	0.81	0/2273
2	B	0.60	0/1676	0.72	0/2277
2	L	0.67	0/1676	0.72	0/2277
3	C	0.63	0/770	0.84	0/1049
3	E	0.79	0/768	0.93	0/1046
All	All	0.68	0/8222	0.78	0/11177

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1622	0	1593	103	0
1	H	1636	0	1604	71	0
2	B	1638	0	1591	98	0
2	L	1638	0	1591	64	0
3	C	753	0	748	58	0
3	E	751	0	744	62	0
All	All	8038	0	7871	405	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 (405) 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:H:90:TYR:HE2	1:H:109:VAL:CG2	1.38	1.36
1:H:90:TYR:CE2	1:H:109:VAL:HG21	1.64	1.31
2:B:185:ASP:CA	2:B:188:LYS:HD2	1.58	1.30
1:A:122:PHE:CZ	2:B:124:GLN:HG3	1.66	1.28
2:B:150:VAL:HG12	2:B:189:HIS:CD2	1.72	1.25
1:A:166:PHE:CD2	2:B:164:THR:HG23	1.73	1.22
2:B:185:ASP:CB	2:B:188:LYS:HD2	1.70	1.20
2:B:185:ASP:HA	2:B:188:LYS:CD	1.72	1.19
1:H:90:TYR:CE2	1:H:109:VAL:CG2	2.24	1.18
3:C:329:GLU:HG3	3:C:375:MET:SD	1.82	1.18
3:E:317:ILE:HD12	3:E:318:PRO:CD	1.73	1.17
1:H:100(D):LEU:HD21	2:L:91:TYR:CE2	1.86	1.11
1:A:184:VAL:HG11	1:A:194:TYR:CZ	1.88	1.08
2:B:150:VAL:CG1	2:B:189:HIS:CD2	2.36	1.08
3:E:317:ILE:HD12	3:E:318:PRO:HD2	1.14	1.07
2:B:185:ASP:HA	2:B:188:LYS:HD2	1.12	1.07
1:A:122:PHE:CZ	2:B:124:GLN:CG	2.39	1.05
3:C:317:ILE:HG21	3:C:398:HIS:CE1	1.91	1.05
3:C:349:MET:CG	3:C:353:THR:HB	1.86	1.05
1:A:122:PHE:CE1	2:B:124:GLN:HG3	1.91	1.04
3:C:349:MET:HG2	3:C:353:THR:HB	1.10	1.03
1:A:166:PHE:HD2	2:B:164:THR:HG23	1.07	1.02
3:C:347:VAL:HG23	3:C:384:ASP:O	1.60	1.02
1:A:171:GLN:HA	2:B:160:GLN:HE22	1.25	1.01
3:C:317:ILE:HG21	3:C:398:HIS:HE1	1.23	1.00
3:C:317:ILE:HD13	3:C:398:HIS:ND1	1.78	0.99
2:B:185:ASP:HB3	2:B:188:LYS:HD2	1.42	0.97
3:C:349:MET:HG2	3:C:353:THR:CB	1.93	0.96
1:H:166:PHE:CD2	2:L:164:THR:HG23	2.00	0.95
3:E:325:THR:HG21	3:E:377:GLU:OE2	1.67	0.95
3:E:317:ILE:CD1	3:E:318:PRO:HD2	1.96	0.95
1:H:90:TYR:HE2	1:H:109:VAL:HG21	0.78	0.95
2:B:193:ALA:HB2	2:B:208:SER:HB3	1.50	0.94
2:B:185:ASP:O	2:B:188:LYS:HG2	1.67	0.93
1:A:150:VAL:HG23	1:A:200:HIS:CD2	2.05	0.92
1:A:138:LEU:O	1:A:181:VAL:HG22	1.70	0.91
2:L:148:TRP:HE1	2:L:177:SER:HG	1.13	0.91
3:C:382:PHE:HA	3:C:402:ARG:HB3	1.53	0.91
1:A:166:PHE:CD2	2:B:164:THR:CG2	2.54	0.90
1:H:166:PHE:HD2	2:L:164:THR:HG23	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PHE:HB2	1:A:141:LEU:HB3	1.52	0.89
2:B:195:GLU:HB3	2:B:206:THR:HG23	1.52	0.89
1:H:51:ILE:HG13	1:H:57:THR:HG22	1.54	0.88
1:H:181:VAL:HG21	2:L:135:LEU:HD22	1.55	0.87
1:A:168:ALA:HB2	1:A:178:LEU:HD12	1.57	0.86
1:A:184:VAL:HG11	1:A:194:TYR:CE1	2.09	0.86
1:A:138:LEU:HD22	1:A:184:VAL:HG21	1.57	0.86
1:A:138:LEU:O	1:A:181:VAL:CG2	2.25	0.84
1:H:100(A):VAL:HG11	3:E:309:THR:HG22	1.58	0.84
2:B:150:VAL:CG1	2:B:189:HIS:CG	2.60	0.84
2:B:185:ASP:C	2:B:188:LYS:HG2	1.97	0.83
1:A:138:LEU:CD2	1:A:184:VAL:CG2	2.57	0.83
1:A:138:LEU:HD23	1:A:184:VAL:HG22	1.62	0.82
1:A:122:PHE:CE2	2:B:124:GLN:HG3	2.15	0.81
1:A:150:VAL:HG23	1:A:200:HIS:HD2	1.45	0.81
3:C:347:VAL:HG12	3:C:349:MET:HE1	1.59	0.81
1:H:90:TYR:CE2	1:H:109:VAL:HG22	2.15	0.81
1:H:32:TYR:CZ	1:H:98:PRO:HG3	2.14	0.81
1:H:126:PRO:HD2	1:H:213:PRO:HA	1.63	0.80
1:A:138:LEU:CD2	1:A:184:VAL:HG22	2.12	0.79
2:B:132:VAL:HG12	2:B:148:TRP:CH2	2.18	0.79
3:E:330:VAL:HG11	3:E:389:ILE:HD13	1.63	0.79
1:A:122:PHE:CE1	2:B:124:GLN:CG	2.66	0.78
2:B:150:VAL:HG11	2:B:189:HIS:CG	2.19	0.78
2:B:113:PRO:HB3	2:B:139:PHE:HB3	1.66	0.78
2:L:131:SER:HB3	2:L:180:THR:HG22	1.66	0.77
2:B:187:GLU:HA	2:B:211:ARG:NH2	1.99	0.77
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.65	0.77
2:B:185:ASP:HB3	2:B:188:LYS:CD	2.13	0.77
2:L:163:VAL:HG22	2:L:175:LEU:HB3	1.65	0.76
1:A:51:ILE:HG13	1:A:57:THR:HG22	1.66	0.76
2:B:185:ASP:O	2:B:188:LYS:CG	2.34	0.76
1:A:154:TRP:HD1	1:A:163:VAL:HG11	1.51	0.76
3:C:355:VAL:HG13	3:C:381:PRO:HG3	1.66	0.75
2:B:150:VAL:HG11	2:B:189:HIS:CD2	2.22	0.75
3:C:349:MET:HE2	3:C:353:THR:HG22	1.70	0.74
2:B:12:SER:HB3	2:B:107:LYS:HE3	1.68	0.74
1:A:32:TYR:O	1:A:71:ARG:NH2	2.20	0.74
1:A:152:VAL:HG23	1:A:198:VAL:HA	1.67	0.73
1:H:82:MET:HB3	1:H:82(C):LEU:HD21	1.71	0.73
2:L:33:LEU:HD13	2:L:71:PHE:CD2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:317:ILE:HD12	3:E:318:PRO:HD3	1.68	0.72
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.24	0.72
1:H:138:LEU:H	1:H:138:LEU:HD23	1.54	0.72
3:C:355:VAL:CG1	3:C:381:PRO:HG3	2.20	0.72
1:A:138:LEU:CD2	1:A:184:VAL:HG21	2.19	0.72
1:A:93:ALA:HB1	1:A:100(E):PHE:HB3	1.71	0.71
2:L:94:TYR:HE2	3:E:336:ASP:HB3	1.54	0.71
1:A:100(D):LEU:HD11	3:C:393:GLU:HG3	1.73	0.71
3:E:325:THR:OG1	3:E:359:ILE:HD12	1.90	0.71
3:C:349:MET:HG2	3:C:353:THR:H	1.55	0.71
2:L:105:GLU:HG3	2:L:173:TYR:OH	1.91	0.70
2:B:185:ASP:CA	2:B:188:LYS:CD	2.43	0.70
1:H:100(D):LEU:HD21	2:L:91:TYR:CD2	2.26	0.70
1:H:181:VAL:HG21	2:L:135:LEU:CD2	2.22	0.70
2:B:195:GLU:HB3	2:B:206:THR:CG2	2.21	0.70
1:H:138:LEU:HD23	1:H:138:LEU:N	2.06	0.69
3:E:326:VAL:HG21	3:E:400:TRP:CZ2	2.26	0.69
2:B:151:ASP:OD1	2:B:191:VAL:HG23	1.90	0.69
3:E:305:TYR:CE2	3:E:338:PRO:HG2	2.27	0.69
1:A:184:VAL:CG1	1:A:194:TYR:CZ	2.73	0.69
2:B:150:VAL:HG12	2:B:189:HIS:HD2	1.52	0.69
2:L:94:TYR:CE2	3:E:336:ASP:HB3	2.27	0.69
3:E:388:VAL:CG1	3:E:395:LYS:HG3	2.23	0.69
1:A:171:GLN:HA	2:B:160:GLN:NE2	2.03	0.69
3:E:386:TYR:HD1	3:E:398:HIS:O	1.77	0.68
3:C:347:VAL:CG2	3:C:384:ASP:O	2.40	0.68
3:C:307:LEU:HD23	3:C:340:LYS:HB2	1.76	0.68
2:L:24:ARG:HG2	2:L:24:ARG:HH11	1.60	0.67
1:A:167:PRO:HG2	2:B:162:SER:OG	1.95	0.67
2:B:185:ASP:HA	2:B:188:LYS:CG	2.25	0.66
1:A:184:VAL:CG1	1:A:194:TYR:CE1	2.78	0.66
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.78	0.66
1:A:154:TRP:HD1	1:A:163:VAL:CG1	2.08	0.66
1:H:66:ARG:NH2	1:H:86:ASP:OD2	2.29	0.66
2:L:136:LEU:HD22	2:L:175:LEU:HD21	1.77	0.66
1:A:138:LEU:HD22	1:A:184:VAL:CG2	2.23	0.66
2:B:193:ALA:CB	2:B:208:SER:HB3	2.25	0.65
3:E:326:VAL:CG2	3:E:400:TRP:CZ2	2.80	0.65
3:E:330:VAL:CG1	3:E:389:ILE:HD13	2.26	0.65
1:H:199:ASN:HA	1:H:206:LYS:HA	1.79	0.65
2:B:125:LEU:O	2:B:183:LYS:NZ	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:350:GLN:O	3:E:350:GLN:HG2	1.96	0.64
3:C:317:ILE:HD13	3:C:398:HIS:CE1	2.32	0.64
3:E:308:CYS:HB3	3:E:332:TYR:OH	1.98	0.64
1:A:96:ARG:HG2	1:A:101:ASP:CG	2.18	0.63
3:C:322:LEU:HD12	3:C:322:LEU:N	2.13	0.63
3:E:325:THR:CG2	3:E:377:GLU:OE2	2.45	0.63
1:H:12:VAL:HG11	1:H:82(C):LEU:HD12	1.80	0.63
1:A:150:VAL:CG2	1:A:200:HIS:CD2	2.79	0.63
3:E:338:PRO:HA	3:E:365:ILE:O	1.99	0.63
1:A:128:SER:O	1:A:128:SER:OG	2.13	0.63
2:L:175:LEU:C	2:L:175:LEU:HD12	2.19	0.62
3:E:345:MET:HE2	3:E:378:LEU:HD22	1.81	0.62
2:B:94:TYR:HD2	3:C:309:THR:HG1	1.47	0.62
3:C:349:MET:CE	3:C:353:THR:HG22	2.29	0.62
3:C:345:MET:HE3	3:C:380:PRO:HA	1.81	0.62
1:H:51:ILE:HG13	1:H:57:THR:CG2	2.29	0.62
3:E:347:VAL:HG12	3:E:347:VAL:O	1.98	0.62
3:C:317:ILE:CD1	3:C:398:HIS:ND1	2.58	0.62
3:C:329:GLU:CG	3:C:375:MET:SD	2.74	0.62
2:B:187:GLU:HA	2:B:211:ARG:HH21	1.62	0.62
2:B:185:ASP:HA	2:B:188:LYS:CE	2.30	0.62
1:H:171:GLN:HA	2:L:160:GLN:NE2	2.15	0.61
3:E:308:CYS:HB3	3:E:332:TYR:CZ	2.35	0.61
2:L:136:LEU:HD13	2:L:175:LEU:HD11	1.81	0.61
2:B:33:LEU:CD2	2:B:71:PHE:CG	2.84	0.61
2:B:83:PHE:HA	2:B:104:VAL:HG22	1.83	0.61
3:E:357:ARG:HB2	3:E:379:ASP:HB3	1.82	0.61
2:B:29:ILE:HG13	2:B:29:ILE:O	2.01	0.60
2:L:136:LEU:HD22	2:L:175:LEU:HD11	1.82	0.60
2:L:193:ALA:HB2	2:L:208:SER:HB3	1.83	0.60
3:C:349:MET:HG2	3:C:353:THR:N	2.16	0.60
1:A:154:TRP:CD1	1:A:163:VAL:CG1	2.84	0.60
3:E:403:SER:O	3:E:403:SER:OG	2.13	0.60
1:A:122:PHE:CZ	2:B:124:GLN:HG2	2.32	0.60
2:B:33:LEU:HD12	2:B:89:GLN:O	2.02	0.60
3:C:347:VAL:HG13	3:C:347:VAL:O	2.02	0.60
3:E:310:ALA:HB3	3:E:332:TYR:CE1	2.37	0.60
1:H:100(D):LEU:CD2	2:L:91:TYR:CD2	2.85	0.60
3:E:336:ASP:OD1	3:E:336:ASP:N	2.35	0.59
1:A:29:PHE:O	1:A:71:ARG:NH2	2.34	0.59
3:E:351:THR:HG22	3:E:351:THR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:166:PHE:CD2	2:L:164:THR:CG2	2.82	0.59
1:H:96:ARG:O	1:H:96:ARG:HG3	2.03	0.59
3:C:342:PRO:HG2	3:C:391:VAL:HG22	1.84	0.58
2:L:148:TRP:HZ2	2:L:177:SER:O	1.86	0.58
1:A:139:GLY:HA3	1:A:181:VAL:HG23	1.85	0.58
1:H:90:TYR:CD2	1:H:109:VAL:HG22	2.39	0.58
1:A:152:VAL:CG2	1:A:198:VAL:HG22	2.33	0.58
1:A:181:VAL:HG11	2:B:135:LEU:HD22	1.85	0.58
1:A:185:PRO:HD2	1:A:188:SER:OG	2.04	0.58
2:B:134:CYS:HB2	2:B:148:TRP:CZ2	2.39	0.57
3:C:318:PRO:HG2	3:C:400:TRP:CZ3	2.39	0.57
3:C:322:LEU:HD12	3:C:322:LEU:H	1.69	0.57
1:A:160:THR:HG23	1:A:160:THR:O	2.04	0.57
2:B:33:LEU:HD11	2:B:88:CYS:SG	2.44	0.57
2:B:131:SER:HB3	2:B:180:THR:HG22	1.86	0.57
3:C:321:THR:HG22	3:C:321:THR:O	2.03	0.57
1:A:152:VAL:HG23	1:A:198:VAL:CA	2.34	0.57
1:H:188:SER:O	1:H:188:SER:OG	2.22	0.56
1:A:63:VAL:HG13	1:A:67:PHE:HB2	1.87	0.56
1:H:199:ASN:ND2	1:H:206:LYS:HG2	2.20	0.56
2:B:92:ASN:O	3:C:394:LYS:HE2	2.05	0.56
1:H:205:THR:O	1:H:205:THR:HG22	2.05	0.56
3:C:352:LEU:HD21	3:C:395:LYS:HE2	1.88	0.56
1:H:87:THR:HG23	1:H:110:THR:HA	1.87	0.56
3:E:384:ASP:HA	3:E:400:TRP:O	2.05	0.56
2:B:120:PRO:HB2	2:B:125:LEU:HD11	1.88	0.56
3:E:395:LYS:O	3:E:395:LYS:HG2	2.05	0.56
1:H:100(C):GLU:OE1	3:E:392:GLY:HA3	2.06	0.55
3:E:357:ARG:HB2	3:E:379:ASP:CB	2.36	0.55
3:C:347:VAL:N	3:C:349:MET:SD	2.78	0.55
1:A:138:LEU:O	1:A:181:VAL:HG23	2.04	0.55
3:E:386:TYR:CD1	3:E:398:HIS:O	2.59	0.55
1:A:100(C):GLU:HG2	2:B:96:TRP:CH2	2.42	0.55
1:A:96:ARG:HG2	1:A:101:ASP:HB2	1.89	0.55
3:E:380:PRO:HG2	3:E:402:ARG:HD2	1.88	0.54
2:B:132:VAL:HG11	2:B:148:TRP:CZ3	2.41	0.54
1:A:121:VAL:CG2	1:A:207:VAL:HG11	2.37	0.54
1:H:17:SER:HB2	1:H:82(A):ASN:HA	1.89	0.54
1:H:139:GLY:HA2	1:H:154:TRP:CZ2	2.42	0.54
3:C:349:MET:HG2	3:C:353:THR:CA	2.38	0.54
3:E:315:THR:OG1	3:E:329:GLU:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.90	0.54
2:B:185:ASP:CA	2:B:188:LYS:HG2	2.38	0.54
1:A:154:TRP:CD1	1:A:163:VAL:HG13	2.42	0.54
2:B:29:ILE:HB	2:B:92:ASN:HB2	1.89	0.54
1:H:135:THR:O	1:H:184:VAL:O	2.26	0.54
1:A:4:LEU:C	1:A:5:LEU:HD12	2.28	0.54
3:C:352:LEU:HD21	3:C:395:LYS:CE	2.39	0.53
3:E:383:GLY:O	3:E:401:HIS:HA	2.07	0.53
1:A:121:VAL:HG21	1:A:207:VAL:CG1	2.37	0.53
3:E:367:GLU:HG3	3:E:369:THR:HG22	1.90	0.53
1:H:82:MET:CB	1:H:82(C):LEU:HD21	2.39	0.53
1:A:48:VAL:HG13	1:A:63:VAL:HG21	1.90	0.53
2:B:32:TRP:HB3	2:B:91:TYR:CD1	2.43	0.53
2:B:185:ASP:CA	2:B:188:LYS:CG	2.86	0.53
1:H:35:SER:HA	1:H:50:ALA:HA	1.91	0.53
3:E:310:ALA:HB3	3:E:332:TYR:CZ	2.44	0.53
1:H:12:VAL:HG11	1:H:82(C):LEU:CD1	2.38	0.52
3:C:382:PHE:N	3:C:382:PHE:CD2	2.77	0.52
1:H:100(A):VAL:HG12	2:L:96:TRP:HZ2	1.75	0.52
1:A:152:VAL:HG21	1:A:198:VAL:HG22	1.91	0.52
3:C:322:LEU:N	3:C:322:LEU:CD1	2.72	0.52
1:A:139:GLY:HA2	1:A:154:TRP:HZ2	1.75	0.52
3:C:317:ILE:CD1	3:C:398:HIS:CE1	2.92	0.52
3:C:349:MET:CG	3:C:353:THR:H	2.22	0.52
2:L:105:GLU:HG2	2:L:106:ILE:N	2.25	0.52
1:A:52:SER:O	1:A:71:ARG:NH1	2.42	0.52
1:A:96:ARG:HG2	1:A:101:ASP:CB	2.39	0.52
2:B:33:LEU:HD22	2:B:71:PHE:CD2	2.45	0.51
1:H:122:PHE:CD1	2:L:123:GLU:HG3	2.45	0.51
1:H:166:PHE:HA	2:L:164:THR:HG22	1.92	0.51
3:C:386:TYR:CZ	3:C:399:HIS:CE1	2.98	0.51
1:H:198:VAL:O	1:H:207:VAL:N	2.37	0.51
2:L:33:LEU:HD13	2:L:71:PHE:CG	2.45	0.51
1:H:121:VAL:HG11	1:H:198:VAL:HG21	1.92	0.51
2:B:63:SER:HB3	2:B:74:THR:HB	1.92	0.51
3:E:305:TYR:HE2	3:E:338:PRO:HG2	1.73	0.51
1:A:121:VAL:HG21	1:A:207:VAL:HG11	1.93	0.51
2:L:155:GLN:HB3	2:L:158:ASN:OD1	2.11	0.51
1:H:138:LEU:N	1:H:138:LEU:CD2	2.73	0.51
3:E:330:VAL:HG11	3:E:389:ILE:HG21	1.93	0.51
1:A:164:HIS:CG	2:B:174:SER:HG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:VAL:CG1	2:B:148:TRP:CH2	2.92	0.51
2:L:3:GLN:HB2	2:L:26:SER:HB3	1.93	0.51
1:A:184:VAL:HG11	1:A:194:TYR:OH	2.09	0.50
2:B:132:VAL:CG1	2:B:148:TRP:CZ3	2.94	0.50
2:L:6:GLN:N	2:L:100:GLN:HE22	2.10	0.50
2:L:182:SER:OG	2:L:185:ASP:HB3	2.12	0.50
1:A:166:PHE:HA	2:B:164:THR:HG22	1.92	0.50
3:C:308:CYS:HB3	3:C:332:TYR:CZ	2.46	0.50
2:B:209:PHE:CD1	2:B:209:PHE:C	2.85	0.50
2:L:29:ILE:HB	2:L:92:ASN:HB2	1.94	0.50
1:A:51:ILE:CD1	1:A:71:ARG:HB2	2.41	0.50
2:B:189:HIS:O	2:B:211:ARG:NH1	2.45	0.50
1:A:121:VAL:HG11	1:A:209:LYS:HB2	1.93	0.50
1:A:154:TRP:HB3	1:A:159:LEU:HB3	1.95	0.49
2:B:182:SER:OG	2:B:185:ASP:OD2	2.29	0.49
2:B:211:ARG:HH11	2:B:211:ARG:CG	2.26	0.49
1:A:39:GLN:OE1	2:B:38:GLN:NE2	2.42	0.49
1:A:149:PRO:O	1:A:149:PRO:HG2	2.12	0.49
3:C:345:MET:CE	3:C:380:PRO:HA	2.43	0.49
1:A:122:PHE:CE1	2:B:124:GLN:HA	2.47	0.48
1:A:164:HIS:CE1	2:B:174:SER:HG	2.30	0.48
1:H:74:SER:HB2	1:H:75:LYS:HD2	1.95	0.48
1:A:20:LEU:HD12	1:A:80:LEU:HD23	1.95	0.48
1:A:184:VAL:CG1	1:A:194:TYR:OH	2.62	0.48
3:E:326:VAL:HG23	3:E:400:TRP:CZ2	2.49	0.48
1:H:138:LEU:HD23	1:H:182:VAL:O	2.13	0.48
3:E:348:ASP:OD2	3:E:386:TYR:CG	2.67	0.48
1:H:199:ASN:CG	1:H:206:LYS:HG2	2.34	0.48
3:E:368:SER:O	2:B:60:SER:HB3	2.14	0.48
3:E:400:TRP:HA	3:E:400:TRP:CE3	2.49	0.47
1:A:51:ILE:CG1	1:A:57:THR:HG22	2.40	0.47
2:B:187:GLU:CA	2:B:211:ARG:NH2	2.73	0.47
1:H:164:HIS:HB2	1:H:181:VAL:HG12	1.97	0.47
1:A:183:THR:O	1:A:183:THR:OG1	2.32	0.47
2:L:6:GLN:H	2:L:100:GLN:NE2	2.13	0.47
2:B:113:PRO:CB	2:B:139:PHE:HB3	2.42	0.47
2:L:124:GLN:NE2	2:L:131:SER:OG	2.28	0.47
2:L:145:LYS:HB3	2:L:197:THR:HB	1.96	0.47
1:A:164:HIS:CE1	2:B:174:SER:OG	2.67	0.47
3:C:338:PRO:HA	3:C:365:ILE:O	2.15	0.47
3:E:342:PRO:O	3:E:390:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PRO:HB2	1:A:142:VAL:HG12	1.96	0.47
1:H:154:TRP:HB3	1:H:159:LEU:HB3	1.96	0.47
3:E:314:PHE:CZ	3:E:389:ILE:HD12	2.50	0.46
1:H:122:PHE:HD1	2:L:123:GLU:HG3	1.80	0.46
2:L:191:VAL:HA	2:L:210:ASN:HA	1.97	0.46
3:E:326:VAL:HG21	3:E:400:TRP:CE2	2.50	0.46
3:E:314:PHE:HE2	3:E:328:VAL:HG21	1.79	0.46
1:H:169:VAL:HG11	2:L:161:GLU:O	2.15	0.46
2:B:121:SER:OG	2:B:124:GLN:HB2	2.16	0.46
1:H:121:VAL:HG13	1:H:142:VAL:HG22	1.98	0.46
2:L:141:PRO:HB2	2:L:143:GLU:OE1	2.15	0.46
3:E:395:LYS:HB3	3:E:395:LYS:HE2	1.58	0.46
1:A:124:LEU:HB2	1:A:139:GLY:O	2.15	0.46
1:H:99:ARG:CZ	3:E:351:THR:HG23	2.46	0.46
1:H:100(D):LEU:HD21	2:L:91:TYR:HE2	1.65	0.46
1:A:148:GLU:O	1:A:148:GLU:HG3	2.15	0.46
1:A:154:TRP:CH2	1:A:196:CYS:HB3	2.50	0.46
2:B:148:TRP:HB3	2:B:179:LEU:HD22	1.98	0.45
3:E:388:VAL:HG13	3:E:395:LYS:HG3	1.95	0.45
1:A:152:VAL:HG23	1:A:198:VAL:HG22	1.97	0.45
2:L:6:GLN:H	2:L:100:GLN:HE22	1.63	0.45
3:C:310:ALA:HB3	3:C:332:TYR:CE1	2.51	0.45
1:H:96:ARG:HA	1:H:101:ASP:HB2	1.99	0.45
2:L:3:GLN:H	2:L:26:SER:HB3	1.81	0.45
2:L:113:PRO:HB3	2:L:139:PHE:CB	2.41	0.45
3:E:345:MET:HE1	3:E:387:ILE:HG12	1.98	0.45
3:C:357:ARG:H	3:C:379:ASP:HB3	1.80	0.45
1:H:93:ALA:HB1	1:H:100(E):PHE:HB3	1.99	0.45
2:B:121:SER:O	2:B:124:GLN:N	2.48	0.45
1:H:198:VAL:O	1:H:206:LYS:HA	2.17	0.45
2:L:193:ALA:CB	2:L:208:SER:HB3	2.47	0.45
1:A:122:PHE:CD2	1:A:141:LEU:HD23	2.52	0.45
1:H:63:VAL:HG13	1:H:67:PHE:HB2	1.98	0.44
1:H:100(E):PHE:HE2	2:L:98:PHE:CZ	2.35	0.44
1:A:12:VAL:HG11	1:A:82(C):LEU:HD13	1.99	0.44
3:E:359:ILE:HB	3:E:377:GLU:HG3	1.99	0.44
2:B:115:VAL:HG21	2:B:205:VAL:HG11	1.99	0.44
1:A:3:GLN:HB2	1:A:25:SER:OG	2.17	0.44
1:A:66:ARG:O	1:A:82(A):ASN:HB2	2.17	0.44
2:L:81:ASP:OD2	2:L:81:ASP:N	2.48	0.44
1:H:99:ARG:NH2	3:E:351:THR:HG23	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:PHE:HD1	2:L:123:GLU:CG	2.31	0.44
2:L:38:GLN:O	2:L:84:ALA:HB1	2.18	0.44
1:H:201:LYS:HB2	1:H:201:LYS:HE2	1.45	0.44
1:A:6:GLU:OE2	1:A:104:GLY:HA3	2.18	0.44
1:A:39:GLN:CD	2:B:38:GLN:HE22	2.19	0.43
2:L:24:ARG:HH11	2:L:24:ARG:CG	2.27	0.43
3:E:316:LYS:HD2	3:E:329:GLU:OE1	2.18	0.43
2:B:132:VAL:HB	2:B:179:LEU:HB3	2.00	0.43
3:C:311:ALA:HB2	3:C:394:LYS:HD2	2.01	0.43
3:C:318:PRO:HG2	3:C:400:TRP:CH2	2.53	0.43
1:H:167:PRO:HD2	2:L:162:SER:OG	2.18	0.43
2:L:91:TYR:HA	2:L:96:TRP:HE3	1.82	0.43
2:L:140:TYR:CG	2:L:141:PRO:HA	2.52	0.43
3:E:348:ASP:O	3:E:350:GLN:N	2.52	0.43
1:H:11:LEU:HD12	1:H:110:THR:O	2.17	0.43
1:H:121:VAL:CG1	1:H:198:VAL:HG21	2.49	0.43
2:L:192:TYR:O	2:L:208:SER:HB2	2.18	0.43
1:A:52(A):GLY:HA2	1:A:71:ARG:CZ	2.49	0.43
2:B:38:GLN:O	2:B:84:ALA:HB1	2.19	0.43
2:B:120:PRO:HG2	2:B:186:TYR:CZ	2.53	0.43
2:B:185:ASP:HA	2:B:188:LYS:HG2	2.00	0.43
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.54	0.43
2:L:113:PRO:CB	2:L:139:PHE:HB3	2.41	0.43
2:L:140:TYR:CD2	2:L:141:PRO:HA	2.54	0.43
3:E:388:VAL:HG11	3:E:395:LYS:HD3	2.01	0.43
2:B:6:GLN:OE1	2:B:87:TYR:HA	2.18	0.43
3:C:340:LYS:O	3:C:342:PRO:HD3	2.18	0.43
2:B:190:LYS:O	2:B:210:ASN:HA	2.19	0.42
2:L:210:ASN:N	2:L:210:ASN:OD1	2.52	0.42
1:A:211:VAL:HG12	1:A:211:VAL:O	2.17	0.42
2:B:91:TYR:O	3:C:394:LYS:HE3	2.18	0.42
1:A:51:ILE:HD12	1:A:71:ARG:HB2	2.01	0.42
1:A:191:THR:OG1	1:A:192:GLN:N	2.52	0.42
2:B:33:LEU:CD2	2:B:71:PHE:CB	2.97	0.42
1:A:51:ILE:HG13	1:A:57:THR:CG2	2.45	0.42
1:A:124:LEU:HB2	1:A:139:GLY:C	2.40	0.42
2:B:186:TYR:C	2:B:188:LYS:H	2.23	0.42
3:C:386:TYR:CZ	3:C:399:HIS:HE1	2.38	0.42
3:C:392:GLY:H	3:C:395:LYS:HZ2	1.67	0.42
1:H:29:PHE:C	1:H:31:SER:H	2.23	0.42
1:A:122:PHE:HE1	2:B:124:GLN:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:310:ALA:HB3	3:C:332:TYR:CZ	2.55	0.42
1:A:70:SER:OG	1:A:79:TYR:HB2	2.20	0.42
3:C:347:VAL:O	3:C:347:VAL:CG1	2.67	0.42
3:E:391:VAL:O	3:E:391:VAL:CG1	2.68	0.41
1:A:12:VAL:HB	1:A:18:LEU:HD22	2.02	0.41
3:C:392:GLY:H	3:C:395:LYS:NZ	2.18	0.41
1:H:58:TYR:CD2	1:H:58:TYR:N	2.88	0.41
2:L:163:VAL:HG22	2:L:175:LEU:CB	2.44	0.41
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.56	0.41
2:B:211:ARG:NH1	2:B:211:ARG:CG	2.82	0.41
2:L:24:ARG:CG	2:L:24:ARG:NH1	2.83	0.41
3:E:380:PRO:HG2	3:E:402:ARG:CD	2.49	0.41
2:B:150:VAL:HG12	2:B:189:HIS:CG	2.30	0.41
1:H:75:LYS:O	1:H:77:THR:HG23	2.20	0.41
2:L:147:GLN:O	2:L:194:CYS:HA	2.20	0.41
1:A:40:ALA:HB3	1:A:43:LYS:HD2	2.01	0.41
3:C:321:THR:O	3:C:321:THR:CG2	2.69	0.41
2:B:85:THR:HA	2:B:102:THR:O	2.20	0.41
2:B:185:ASP:HA	2:B:188:LYS:HE3	2.02	0.41
1:H:31:SER:O	1:H:99:ARG:N	2.50	0.41
1:A:119:PRO:CB	1:A:145:TYR:HB3	2.49	0.41
1:A:6:GLU:OE1	1:A:6:GLU:N	2.50	0.41
1:A:84:ALA:O	1:A:87:THR:HG22	2.21	0.41
2:B:211:ARG:NH1	2:B:211:ARG:HG2	2.34	0.41
1:H:129:LYS:H	1:H:129:LYS:HG2	1.56	0.41
3:E:388:VAL:HG12	3:E:395:LYS:HG3	2.01	0.41
3:C:327:THR:HA	3:C:376:LEU:O	2.21	0.41
3:E:326:VAL:O	3:E:377:GLU:HA	2.21	0.41
2:B:107:LYS:HA	2:B:140:TYR:OH	2.20	0.41
1:H:86:ASP:O	1:H:90:TYR:OH	2.27	0.40
2:L:154:LEU:HD23	2:L:155:GLN:O	2.21	0.40
1:A:154:TRP:CZ3	1:A:196:CYS:HB3	2.56	0.40
2:L:52:SER:HB3	2:L:64:GLY:O	2.21	0.40
3:E:316:LYS:CD	3:E:329:GLU:OE1	2.69	0.40
1:A:126:PRO:HD2	1:A:213:PRO:HA	2.03	0.40
3:C:387:ILE:O	3:C:397:THR:HA	2.20	0.40
3:C:315:THR:OG1	3:C:329:GLU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	214/234 (92%)	196 (92%)	17 (8%)	1 (0%)	29	64
1	H	217/234 (93%)	193 (89%)	20 (9%)	4 (2%)	8	34
2	B	210/214 (98%)	195 (93%)	11 (5%)	4 (2%)	8	33
2	L	210/214 (98%)	200 (95%)	8 (4%)	2 (1%)	15	49
3	C	95/110 (86%)	81 (85%)	10 (10%)	4 (4%)	3	16
3	E	95/110 (86%)	79 (83%)	9 (10%)	7 (7%)	1	6
All	All	1041/1116 (93%)	944 (91%)	75 (7%)	22 (2%)	7	30

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	30	SER
1	H	135	THR
1	H	188	SER
3	E	349	MET
3	E	352	LEU
3	E	403	SER
3	E	350	GLN
3	C	323	HIS
3	C	351	THR
3	C	382	PHE
1	H	187	SER
2	B	187	GLU
2	B	211	ARG
3	C	384	ASP
1	A	127	SER
2	B	190	LYS
2	L	96	TRP
3	E	316	LYS
2	B	158	ASN
2	L	68	GLY

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Mol	Chain	Res	Type
3	E	354	PRO
3	E	338	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/194 (93%)	157 (87%)	23 (13%)	4	18
1	H	181/194 (93%)	159 (88%)	22 (12%)	5	19
2	B	187/189 (99%)	166 (89%)	21 (11%)	6	24
2	L	187/189 (99%)	171 (91%)	16 (9%)	10	37
3	C	85/94 (90%)	73 (86%)	12 (14%)	3	15
3	E	85/94 (90%)	69 (81%)	16 (19%)	1	6
All	All	905/954 (95%)	795 (88%)	110 (12%)	5	19

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	GLU
1	H	3	GLN
1	H	17	SER
1	H	35	SER
1	H	89	VAL
1	H	94	LYS
1	H	96	ARG
1	H	100(A)	VAL
1	H	120	SER
1	H	121	VAL
1	H	124	LEU
1	H	129	LYS
1	H	132	SER
1	H	138	LEU
1	H	152	VAL
1	H	161	SER

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Mol	Chain	Res	Type
1	H	166	PHE
1	H	189	LEU
1	H	201	LYS
1	H	206	LYS
1	H	207	VAL
1	H	209	LYS
2	L	14	SER
2	L	15	VAL
2	L	29	ILE
2	L	48	ILE
2	L	65	SER
2	L	69	THR
2	L	85	THR
2	L	94	TYR
2	L	109	THR
2	L	114	SER
2	L	123	GLU
2	L	131	SER
2	L	158	ASN
2	L	183	LYS
2	L	206	THR
2	L	210	ASN
3	E	313	THR
3	E	314	PHE
3	E	316	LYS
3	E	317	ILE
3	E	322	LEU
3	E	327	THR
3	E	328	VAL
3	E	336	ASP
3	E	352	LEU
3	E	357	ARG
3	E	364	VAL
3	E	372	SER
3	E	377	GLU
3	E	391	VAL
3	E	395	LYS
3	E	398	HIS
1	A	1	GLU
1	A	17	SER
1	A	18	LEU
1	A	30	SER

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Mol	Chain	Res	Type
1	A	51	ILE
1	A	94	LYS
1	A	96	ARG
1	A	99	ARG
1	A	124	LEU
1	A	142	VAL
1	A	143	LYS
1	A	150	VAL
1	A	156	SER
1	A	169	VAL
1	A	173	SER
1	A	178	LEU
1	A	184	VAL
1	A	186	SER
1	A	193	THR
1	A	197	ASN
1	A	201	LYS
1	A	206	LYS
1	A	210	ARG
2	B	1	ASP
2	B	2	ILE
2	B	9	SER
2	B	10	THR
2	B	15	VAL
2	B	17	ASP
2	B	94	TYR
2	B	104	VAL
2	B	109	THR
2	B	110	VAL
2	B	114	SER
2	B	122	ASP
2	B	124	GLN
2	B	143	GLU
2	B	174	SER
2	B	188	LYS
2	B	190	LYS
2	B	202	SER
2	B	206	THR
2	B	209	PHE
2	B	211	ARG
3	C	325	THR
3	C	327	THR

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Mol	Chain	Res	Type
3	C	329	GLU
3	C	349	MET
3	C	350	GLN
3	C	353	THR
3	C	374	MET
3	C	382	PHE
3	C	391	VAL
3	C	399	HIS
3	C	402	ARG
3	C	403	SER

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

Mol	Chain	Res	Type
1	H	76	ASN
1	H	204	ASN
2	L	92	ASN
2	L	147	GLN
2	L	160	GLN
3	E	399	HIS
1	A	39	GLN
1	A	164	HIS
1	A	171	GLN
2	B	38	GLN
2	B	124	GLN
2	B	137	ASN
2	B	160	GLN
2	B	189	HIS
3	C	398	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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/234 (93%)	0.50	13 (5%) 21 10	45, 58, 90, 101	0
1	H	221/234 (94%)	0.42	5 (2%) 60 39	47, 56, 70, 93	0
2	B	212/214 (99%)	0.47	9 (4%) 36 18	46, 63, 81, 86	0
2	L	212/214 (99%)	0.53	11 (5%) 27 12	45, 61, 73, 77	0
3	C	99/110 (90%)	0.72	12 (12%) 4 1	50, 61, 85, 93	0
3	E	99/110 (90%)	0.84	13 (13%) 3 1	52, 68, 86, 103	0
All	All	1061/1116 (95%)	0.53	63 (5%) 22 10	45, 60, 83, 103	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	316	LYS	3.6
3	C	350	GLN	3.5
3	E	348	ASP	3.5
3	C	347	VAL	3.5
3	C	318	PRO	3.4
2	L	105	GLU	3.3
1	A	198	VAL	3.2
1	A	192	GLN	3.2
1	A	206	LYS	3.1
1	A	135	THR	3.1
3	C	354	PRO	3.1
1	H	132	SER	3.1
3	C	319	ALA	3.1
1	A	129	LYS	3.0
2	B	197	THR	3.0
1	A	138	LEU	2.9
2	B	190	LYS	2.9
3	E	323	HIS	2.9
3	E	321	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	L	12	SER	2.8
2	L	11	LEU	2.7
3	E	351	THR	2.7
3	E	359	ILE	2.7
2	B	136	LEU	2.7
1	H	13	GLN	2.6
3	E	389	ILE	2.6
1	A	209	LYS	2.6
3	E	357	ARG	2.6
2	L	144	ALA	2.5
1	A	121	VAL	2.5
2	L	210	ASN	2.4
1	A	1	GLU	2.4
1	A	179	SER	2.4
1	A	205	THR	2.4
3	C	357	ARG	2.4
1	A	136	ALA	2.3
1	H	128	SER	2.3
2	L	193	ALA	2.3
3	E	387	ILE	2.3
2	B	122	ASP	2.3
3	C	387	ILE	2.3
1	A	211	VAL	2.3
1	H	127	SER	2.3
2	B	14	SER	2.3
3	E	397	THR	2.3
2	B	11	LEU	2.2
2	L	21	ILE	2.2
3	E	349	MET	2.2
2	L	13	ALA	2.2
2	B	202	SER	2.1
3	C	321	THR	2.1
3	C	359	ILE	2.1
3	E	398	HIS	2.1
2	B	145	LYS	2.1
3	C	349	MET	2.1
2	L	82	ASP	2.1
2	L	175	LEU	2.1
1	H	214	LYS	2.1
2	B	205	VAL	2.1
3	C	317	ILE	2.0
3	C	323	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	L	104	VAL	2.0
3	E	376	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.