



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 02:50 PM EDT

PDB ID : 3MLT  
Title : Crystal structure of anti-HIV-1 V3 Fab 2557 in complex with a UG1033 V3 peptide  
Authors : Kong, X.-P.  
Deposited on : unknown  
Resolution : 2.49 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

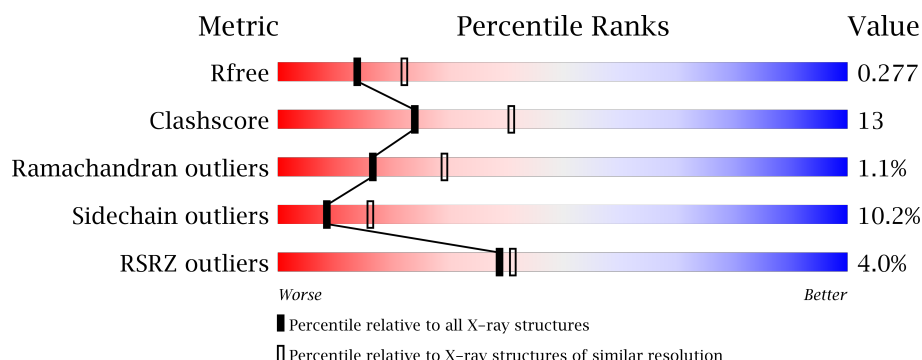
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	219	<div> <div>10%</div> <div>64%</div> <div>31%</div> <div>..</div> </div>
1	D	219	<div> <div>2%</div> <div>65%</div> <div>28%</div> <div>..</div> </div>
1	G	219	<div> <div>2%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
1	L	219	<div> <div>2%</div> <div>72%</div> <div>24%</div> <div>..</div> </div>
2	B	226	<div> <div>2%</div> <div>73%</div> <div>19%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	226	<div><div></div><div>7%</div><div>69%</div><div>23%</div><div>5%</div><div></div></div>
2	H	226	<div><div></div><div>2%</div><div>73%</div><div>19%</div><div>• 5%</div><div></div></div>
2	I	226	<div><div></div><div>4%</div><div>78%</div><div>16%</div><div>• •</div><div></div></div>
3	C	23	<div><div></div><div>13%</div><div>39%</div><div>22%</div><div>39%</div><div></div></div>
3	P	23	<div><div></div><div>30%</div><div>22%</div><div>9%</div><div>39%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13628 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 Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1623	1019	266	333	5			
1	A	215	Total	C	N	O	S	0	0	0
			1619	1017	265	332	5			
1	D	213	Total	C	N	O	S	0	0	0
			1608	1011	263	329	5			
1	G	213	Total	C	N	O	S	0	1	0
			1614	1015	263	331	5			

- Molecule 2 is a protein called Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1633	1044	263	320	6			
2	B	219	Total	C	N	O	S	0	0	0
			1659	1059	267	327	6			
2	E	219	Total	C	N	O	S	0	0	0
			1659	1059	267	327	6			
2	I	219	Total	C	N	O	S	0	0	0
			1659	1059	267	327	6			

- Molecule 3 is a protein called HIV-1 gp120 third variable region (V3) crown.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	14	Total	C	N	O	0	0	0
			113	73	23	17			
3	C	14	Total	C	N	O	0	0	0
			113	73	23	17			

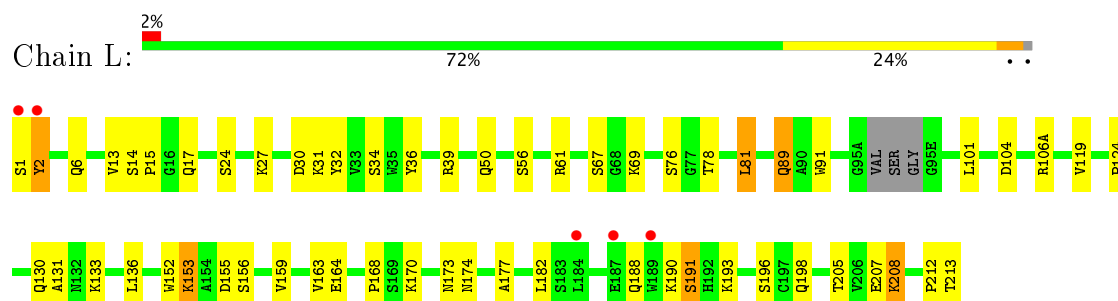
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	55	Total 55	O 55	0	0
4	H	44	Total 44	O 44	0	0
4	P	3	Total 3	O 3	0	0
4	A	12	Total 12	O 12	0	0
4	B	30	Total 30	O 30	0	0
4	C	1	Total 1	O 1	0	0
4	D	31	Total 31	O 31	0	0
4	E	49	Total 49	O 49	0	0
4	G	48	Total 48	O 48	0	0
4	I	55	Total 55	O 55	0	0

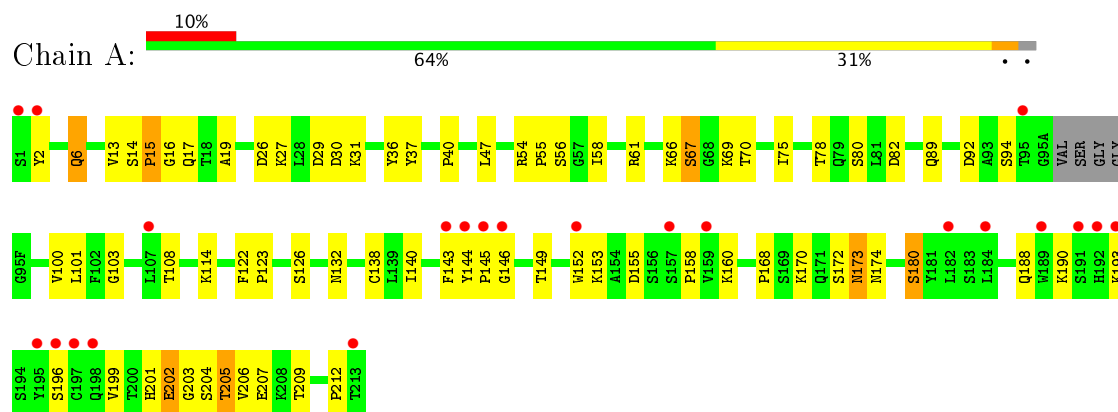
### 3 Residue-property plots

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

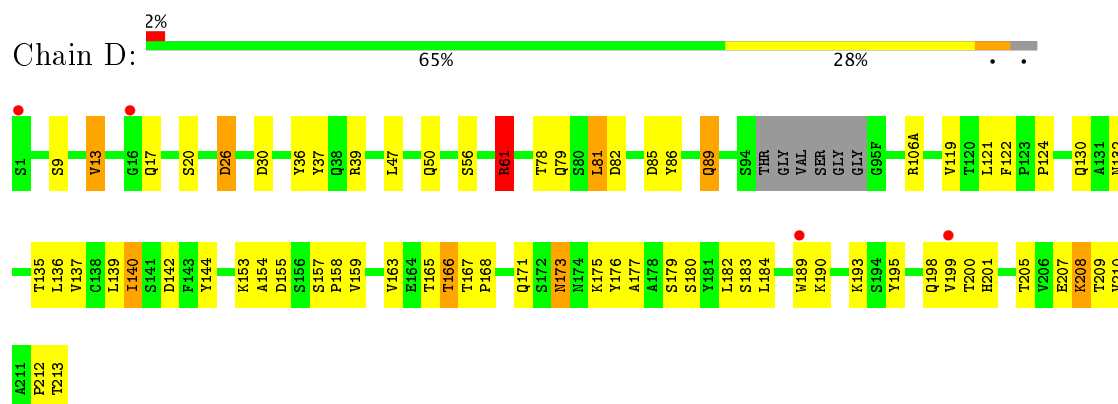
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain



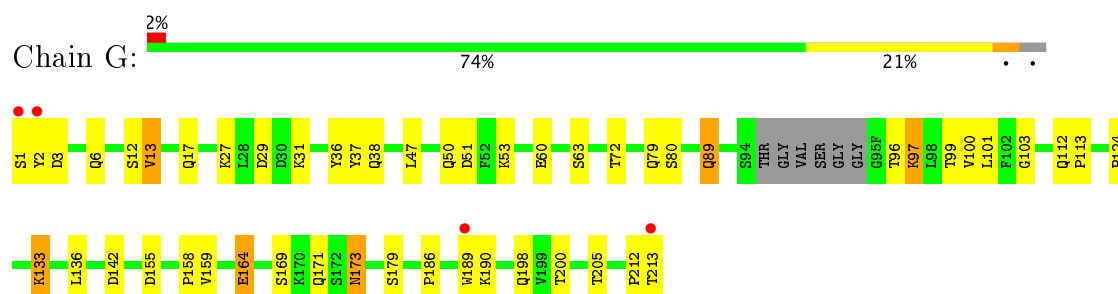
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain



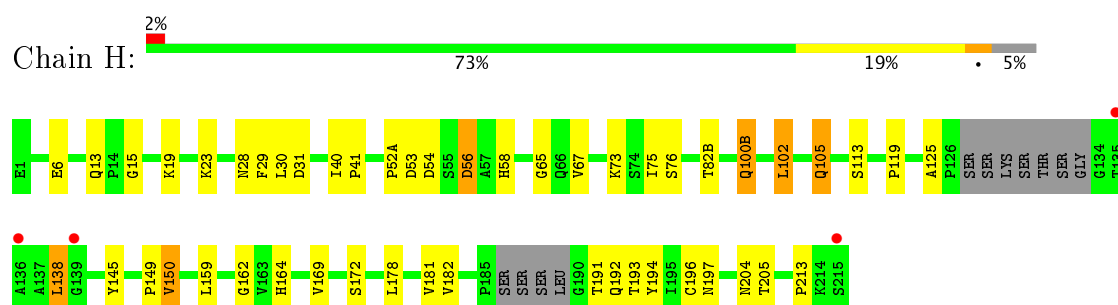
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain



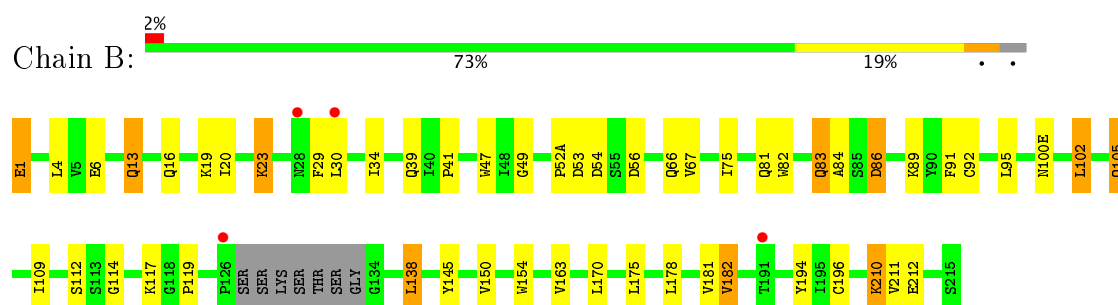
- Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab light chain



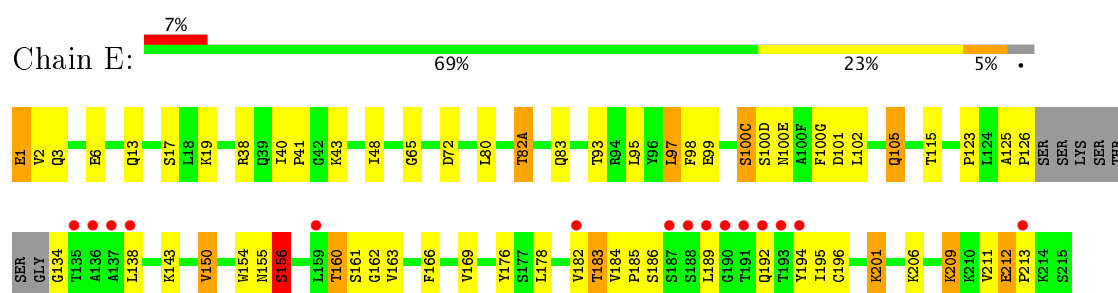
- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain



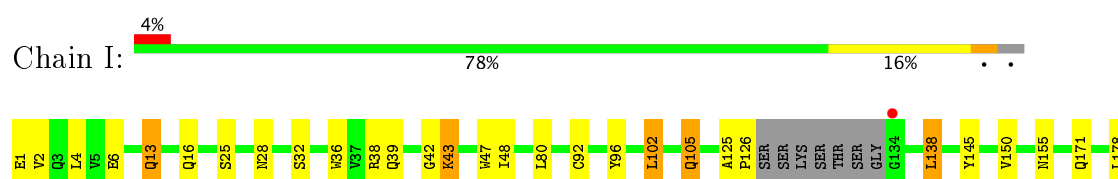
- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain

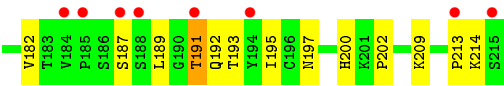


- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain

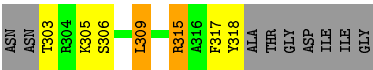
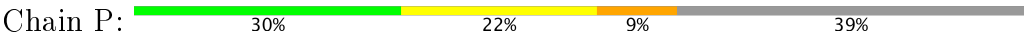


- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 2557 Fab heavy chain

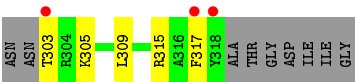




- Molecule 3: HIV-1 gp120 third variable region (V3) crown



- Molecule 3: HIV-1 gp120 third variable region (V3) crown





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.68 Å 142.93 Å 85.01 Å 90.00° 95.00° 90.00°	Depositor
Resolution (Å)	35.74 – 2.49 35.73 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.3 (35.74-2.49) 99.3 (35.73-2.49)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 2.48 Å)	Xtriage
Refinement program	CNS, REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.280 0.204 , 0.277	Depositor DCC
$R_{free}$ test set	3177 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.69	0/1658	0.75	0/2261
1	D	0.76	0/1647	0.80	1/2246 (0.0%)
1	G	0.79	0/1656	0.83	0/2258
1	L	0.79	0/1662	0.82	0/2266
2	B	0.76	1/1702 (0.1%)	0.76	0/2319
2	E	0.83	0/1702	0.84	3/2319 (0.1%)
2	H	0.81	0/1675	0.83	1/2281 (0.0%)
2	I	0.83	1/1702 (0.1%)	0.81	0/2319
3	C	0.85	0/116	0.88	0/154
3	P	0.81	0/116	0.95	0/154
All	All	0.79	2/13636 (0.0%)	0.81	5/18577 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	92	CYS	CB-SG	-5.57	1.72	1.81
2	B	92	CYS	CB-SG	-5.17	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	101	ASP	CB-CG-OD1	6.09	123.78	118.30
2	E	101	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	D	61	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	H	102	LEU	CA-CB-CG	5.09	127.00	115.30
2	E	72	ASP	CB-CG-OD2	5.06	122.86	118.30

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	1619	0	1578	56	0
1	D	1608	0	1568	48	0
1	G	1614	0	1574	37	0
1	L	1623	0	1581	38	0
2	B	1659	0	1618	36	0
2	E	1659	0	1618	52	0
2	H	1633	0	1591	38	0
2	I	1659	0	1618	30	0
3	C	113	0	115	6	0
3	P	113	0	115	8	0
4	A	12	0	0	0	0
4	B	30	0	0	0	0
4	C	1	0	0	0	0
4	D	31	0	0	1	0
4	E	49	0	0	1	0
4	G	48	0	0	2	0
4	H	44	0	0	0	0
4	I	55	0	0	1	0
4	L	55	0	0	4	0
4	P	3	0	0	0	0
All	All	13628	0	12976	329	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 13.

All (329) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:42:GLY:O	2:I:43:LYS:HE3	1.43	1.15
1:A:31:LYS:NZ	3:C:309:LEU:HD13	1.61	1.13
3:P:315:ARG:HH11	3:P:315:ARG:HG3	1.14	1.12
2:E:212:GLU:HB3	2:E:213:PRO:CD	1.79	1.11
2:E:212:GLU:HB3	2:E:213:PRO:HD3	1.12	1.05
2:H:192:GLN:NE2	2:H:193:THR:H	1.57	1.02
3:C:309:LEU:HD11	3:C:315:ARG:HD3	1.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:105:GLN:HE21	2:I:105:GLN:H	1.02	1.00
1:A:2:TYR:CD1	1:A:2:TYR:O	2.16	0.98
2:B:13:GLN:H	2:B:16:GLN:HE21	1.03	0.97
1:L:36:TYR:HE1	1:L:89:GLN:HG2	1.28	0.95
2:I:43:LYS:CE	2:I:43:LYS:HA	1.96	0.95
1:A:2:TYR:OH	1:A:31:LYS:HD2	1.67	0.95
2:H:192:GLN:HE21	2:H:193:THR:H	1.14	0.94
1:G:198:GLN:HG3	1:G:205:THR:CG2	1.98	0.93
2:I:13:GLN:HG2	2:I:16:GLN:NE2	1.84	0.92
1:D:166:THR:CG2	1:D:179:SER:H	1.82	0.92
2:H:149:PRO:HG3	2:E:201:LYS:HG3	1.51	0.91
2:H:105:GLN:HE21	2:H:105:GLN:H	0.99	0.91
1:A:205:THR:HG23	1:A:206:VAL:N	1.84	0.90
2:E:105:GLN:HE21	2:E:105:GLN:H	0.94	0.90
1:L:17:GLN:O	1:L:78:THR:HG23	1.72	0.89
2:I:13:GLN:H	2:I:16:GLN:HE21	1.17	0.89
2:E:105:GLN:H	2:E:105:GLN:NE2	1.70	0.88
2:H:105:GLN:NE2	2:H:105:GLN:H	1.73	0.87
1:L:2:TYR:HE2	1:L:31:LYS:HZ2	1.16	0.87
2:B:23:LYS:NZ	2:B:75:ILE:O	2.08	0.87
2:B:6:GLU:H	2:B:105:GLN:HE22	1.18	0.86
2:B:105:GLN:H	2:B:105:GLN:HE21	1.24	0.85
2:H:192:GLN:HE21	2:H:193:THR:N	1.75	0.85
1:A:31:LYS:HZ2	3:C:309:LEU:HD13	1.39	0.85
1:G:198:GLN:HG3	1:G:205:THR:HG21	1.56	0.84
1:D:171:GLN:HE21	1:D:177:ALA:HB2	1.43	0.83
1:G:171:GLN:HE21	1:G:173:ASN:HD21	1.26	0.83
2:H:105:GLN:HE21	2:H:105:GLN:N	1.76	0.83
1:G:37:TYR:HB2	1:G:47:LEU:HD11	1.61	0.83
1:G:36:TYR:HE1	1:G:89:GLN:HG2	1.43	0.82
1:L:36:TYR:CE1	1:L:89:GLN:HG2	2.13	0.82
2:E:105:GLN:HE21	2:E:105:GLN:N	1.76	0.82
2:H:40:ILE:HG23	2:H:41:PRO:HD2	1.61	0.82
1:D:36:TYR:HE1	1:D:89:GLN:HG2	1.45	0.82
2:E:1:GLU:OE2	2:E:1:GLU:N	2.12	0.81
2:I:43:LYS:HE2	2:I:43:LYS:HA	1.62	0.80
2:B:13:GLN:H	2:B:16:GLN:NE2	1.82	0.78
2:I:6:GLU:H	2:I:105:GLN:HE22	1.31	0.78
2:H:6:GLU:H	2:H:105:GLN:HE22	1.32	0.77
2:I:105:GLN:NE2	2:I:105:GLN:H	1.79	0.77
1:A:2:TYR:CG	1:A:2:TYR:O	2.38	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:315:ARG:HG3	3:P:315:ARG:NH1	1.95	0.76
2:I:105:GLN:HE21	2:I:105:GLN:N	1.83	0.75
2:B:105:GLN:H	2:B:105:GLN:NE2	1.83	0.75
1:A:153:LYS:HA	1:A:158:PRO:HA	1.68	0.74
2:H:149:PRO:HG3	2:E:201:LYS:CG	2.16	0.74
1:D:37:TYR:HB2	1:D:47:LEU:HD11	1.70	0.74
1:G:38:GLN:OE1	2:I:39:GLN:NE2	2.16	0.73
2:B:82:TRP:NE1	2:B:86:ASP:OD1	2.21	0.73
1:A:36:TYR:HE1	1:A:89:GLN:HG2	1.53	0.73
1:L:153:LYS:HD2	1:L:198:GLN:HE22	1.52	0.73
1:L:188:GLN:HA	1:L:191:SER:HB3	1.72	0.72
1:D:142:ASP:H	1:D:171:GLN:HE22	1.36	0.71
2:E:212:GLU:CB	2:E:213:PRO:CD	2.65	0.71
1:A:31:LYS:HZ3	3:C:309:LEU:HD13	1.55	0.70
1:A:170:LYS:HE3	1:A:174:ASN:ND2	2.07	0.70
1:G:173:ASN:N	1:G:173:ASN:HD22	1.88	0.70
1:L:163:VAL:HG22	1:L:182:LEU:CD1	2.21	0.69
2:E:163:VAL:HG22	2:E:182:VAL:HG22	1.73	0.69
1:G:164:GLU:HG2	2:I:171:GLN:HA	1.73	0.69
2:B:13:GLN:HG2	2:B:16:GLN:NE2	2.07	0.69
2:E:126:PRO:HD3	2:E:212:GLU:O	1.92	0.69
1:G:36:TYR:CE1	1:G:89:GLN:HG2	2.27	0.69
1:D:166:THR:HG22	1:D:179:SER:O	1.93	0.68
1:D:39:ARG:NH2	1:D:81:LEU:HD22	2.09	0.68
1:A:114:LYS:HE3	1:A:202:GLU:OE2	1.94	0.68
2:E:98:PHE:H	2:E:100(E):ASN:ND2	1.91	0.68
1:A:13:VAL:HG22	1:A:14:SER:N	2.09	0.68
1:G:173:ASN:H	1:G:173:ASN:HD22	1.42	0.68
1:D:171:GLN:NE2	1:D:177:ALA:HB2	2.09	0.67
2:E:150:VAL:HG22	2:E:178:LEU:HD21	1.77	0.67
1:D:163:VAL:HG23	1:D:182:LEU:HD13	1.77	0.67
1:D:119:VAL:O	1:D:208:LYS:HE3	1.95	0.66
3:C:309:LEU:HD11	3:C:315:ARG:CD	2.23	0.66
1:A:14:SER:O	1:A:15:PRO:O	2.14	0.66
1:A:173:ASN:HD22	1:A:173:ASN:C	1.99	0.66
2:I:13:GLN:H	2:I:16:GLN:NE2	1.93	0.66
2:I:43:LYS:HE3	2:I:43:LYS:HA	1.75	0.66
2:H:192:GLN:NE2	2:H:193:THR:N	2.35	0.65
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.78	0.65
2:H:192:GLN:NE2	2:H:193:THR:OG1	2.30	0.65
1:A:201:HIS:O	1:A:202:GLU:CB	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:104:ASP:HB2	4:L:238:HOH:O	1.98	0.64
2:E:186:SER:HA	2:E:189:LEU:HD13	1.79	0.63
2:B:54:ASP:OD2	2:B:56:ASP:HB2	1.98	0.63
2:E:154:TRP:O	2:E:155:ASN:HB2	1.99	0.62
2:E:195:ILE:HA	2:E:209:LYS:O	2.00	0.62
1:A:36:TYR:CE1	1:A:89:GLN:HG2	2.33	0.62
1:A:201:HIS:C	1:A:202:GLU:HG3	2.20	0.61
1:A:67:SER:O	1:A:70:THR:HG22	1.99	0.61
1:L:173:ASN:O	1:L:174:ASN:HB2	2.00	0.61
2:B:6:GLU:H	2:B:105:GLN:NE2	1.95	0.61
1:G:124:PRO:HD3	1:G:136:LEU:HD23	1.83	0.60
2:E:201:LYS:HZ2	2:E:201:LYS:H	1.49	0.60
1:L:50:GLN:NE2	4:L:216:HOH:O	2.20	0.60
1:D:200:THR:OG1	1:D:205:THR:HG22	2.01	0.60
1:A:55:PRO:HD2	1:A:58:ILE:HG13	1.83	0.59
2:B:6:GLU:N	2:B:105:GLN:HE22	1.96	0.59
2:E:100(C):SER:HB3	2:E:100(E):ASN:ND2	2.18	0.59
1:L:106(A):ARG:NH1	4:L:247:HOH:O	2.20	0.59
1:A:201:HIS:O	1:A:202:GLU:HG3	2.02	0.58
3:P:305:LYS:HE2	3:P:318:TYR:CD2	2.38	0.58
1:G:96:THR:HG23	1:G:97:LYS:N	2.18	0.58
1:A:37:TYR:HB2	1:A:47:LEU:HD11	1.84	0.58
1:D:61:ARG:NH2	1:D:82:ASP:OD1	2.34	0.58
1:L:164:GLU:HB3	2:H:169:VAL:HG11	1.85	0.58
1:A:13:VAL:CG2	1:A:14:SER:N	2.66	0.58
1:G:72:THR:OG1	4:G:276:HOH:O	2.17	0.58
2:B:1:GLU:CD	2:B:1:GLU:N	2.56	0.58
1:L:153:LYS:HB3	1:L:196:SER:HB2	1.83	0.58
1:L:32:TYR:OH	2:H:100(B):GLN:HG3	2.04	0.58
1:G:50:GLN:HE21	1:G:53:LYS:NZ	2.02	0.58
2:E:160:THR:O	2:E:160:THR:OG1	2.22	0.57
1:A:201:HIS:O	1:A:202:GLU:HB2	2.02	0.57
1:G:173:ASN:H	1:G:173:ASN:ND2	2.00	0.57
2:E:123:PRO:HD3	2:E:209:LYS:HE2	1.87	0.57
1:G:50:GLN:HE21	1:G:53:LYS:HZ2	1.53	0.57
2:B:210:LYS:HD2	2:B:212:GLU:HG3	1.86	0.56
2:E:2:VAL:HG13	2:E:102:LEU:HD11	1.87	0.56
1:D:173:ASN:HD21	1:D:175:LYS:HB2	1.70	0.56
2:I:150:VAL:CG2	2:I:178:LEU:HD21	2.36	0.56
1:D:130:GLN:C	1:D:132:ASN:H	2.09	0.56
1:L:2:TYR:OH	1:L:31:LYS:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:163:VAL:HG22	1:L:182:LEU:HD11	1.88	0.55
1:L:36:TYR:HE1	1:L:89:GLN:CG	2.10	0.55
1:D:13:VAL:HG22	1:D:17:GLN:HB2	1.88	0.55
2:B:105:GLN:N	2:B:105:GLN:HE21	1.98	0.55
1:D:166:THR:HG23	1:D:179:SER:H	1.66	0.55
1:A:152:TRP:HE1	1:A:180:SER:HB3	1.70	0.55
2:E:134:GLY:O	2:E:185:PRO:HA	2.07	0.55
1:G:36:TYR:HE1	1:G:89:GLN:CG	2.16	0.55
1:A:143:PHE:HE2	1:A:146:GLY:HA2	1.72	0.54
2:E:100(D):SER:OG	2:E:100(D):SER:O	2.23	0.54
2:I:13:GLN:HG2	2:I:16:GLN:HE21	1.65	0.54
1:G:171:GLN:NE2	1:G:173:ASN:HD21	2.01	0.54
2:H:19:LYS:NZ	1:A:203:GLY:HA3	2.22	0.54
1:A:173:ASN:ND2	1:A:173:ASN:C	2.61	0.54
1:A:153:LYS:HB2	1:A:196:SER:HB3	1.90	0.54
2:E:138:LEU:HD23	2:E:182:VAL:O	2.08	0.54
1:A:144:TYR:O	1:A:201:HIS:CE1	2.61	0.53
2:E:201:LYS:NZ	2:E:201:LYS:H	2.06	0.53
1:G:142:ASP:OD1	1:G:171:GLN:NE2	2.40	0.53
2:E:138:LEU:H	2:E:138:LEU:HD23	1.73	0.53
1:L:2:TYR:HE2	1:L:31:LYS:NZ	1.98	0.53
1:D:140:ILE:HD12	1:D:199:VAL:HG21	1.90	0.52
2:B:1:GLU:CD	2:B:1:GLU:H3	2.12	0.52
1:L:39:ARG:NH2	1:L:81:LEU:HD22	2.24	0.52
2:H:193:THR:O	2:H:194:TYR:HB2	2.08	0.52
1:A:114:LYS:CE	1:A:202:GLU:OE2	2.56	0.52
1:D:173:ASN:ND2	1:D:175:LYS:H	2.08	0.52
2:H:28:ASN:HD21	2:H:31:ASP:CG	2.12	0.52
2:H:149:PRO:CG	2:E:201:LYS:HG3	2.32	0.52
2:H:162:GLY:O	2:H:182:VAL:HA	2.10	0.52
1:A:2:TYR:OH	1:A:31:LYS:CD	2.48	0.51
1:A:201:HIS:C	1:A:202:GLU:CG	2.77	0.51
1:G:171:GLN:HE21	1:G:173:ASN:ND2	2.02	0.51
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.37	0.51
1:D:163:VAL:HG23	1:D:182:LEU:CD1	2.40	0.51
2:I:126:PRO:HG3	2:I:138:LEU:HD23	1.93	0.51
1:D:184:LEU:HD11	1:D:195:TYR:CZ	2.46	0.51
2:E:138:LEU:HD12	2:E:211:VAL:HB	1.92	0.51
1:G:171:GLN:HB2	1:G:173:ASN:HD21	1.76	0.51
1:A:17:GLN:O	1:A:78:THR:HG23	2.11	0.51
1:G:171:GLN:HB2	1:G:173:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:TYR:CZ	1:G:27:LYS:HB2	2.46	0.51
2:B:89:LYS:HD3	2:B:91:PHE:CZ	2.45	0.50
1:A:13:VAL:CG2	1:A:14:SER:H	2.23	0.50
1:D:140:ILE:HD12	1:D:199:VAL:CG2	2.42	0.50
1:D:153:LYS:HE2	1:D:198:GLN:NE2	2.27	0.50
2:I:4:LEU:HG	2:I:102:LEU:HD13	1.92	0.50
1:L:119:VAL:O	1:L:208:LYS:NZ	2.45	0.50
1:L:2:TYR:HB2	4:L:226:HOH:O	2.12	0.50
1:D:130:GLN:C	1:D:132:ASN:N	2.65	0.49
1:L:124:PRO:HD3	1:L:136:LEU:HD23	1.94	0.49
2:I:214:LYS:NZ	4:I:230:HOH:O	2.44	0.49
1:D:144:TYR:O	1:D:201:HIS:HE1	1.95	0.49
2:H:28:ASN:ND2	2:H:31:ASP:CG	2.65	0.49
2:B:4:LEU:HG	2:B:102:LEU:HD13	1.94	0.49
1:D:36:TYR:CE1	1:D:89:GLN:HG2	2.36	0.49
2:H:138:LEU:O	2:H:181:VAL:HG23	2.12	0.49
1:D:198:GLN:HG2	1:D:207:GLU:HB2	1.94	0.49
1:D:85:ASP:OD1	1:D:106(A):ARG:HD3	2.13	0.49
2:I:1:GLU:HG2	2:I:2:VAL:N	2.28	0.49
1:G:112:GLN:HB2	1:G:113:PRO:HD2	1.95	0.49
1:L:168:PRO:HA	1:L:177:ALA:O	2.13	0.49
2:E:38:ARG:HB2	2:E:48:ILE:HD11	1.93	0.49
1:L:153:LYS:HG2	1:L:156:SER:HA	1.95	0.49
2:E:184:VAL:HG11	2:E:194:TYR:CE1	2.49	0.48
2:H:119:PRO:HD2	2:H:205:THR:HG21	1.94	0.48
2:B:210:LYS:CD	2:B:212:GLU:HG3	2.42	0.48
2:H:40:ILE:CG2	2:H:41:PRO:HD2	2.40	0.48
2:H:54:ASP:OD2	2:H:56:ASP:HB2	2.13	0.48
2:B:154:TRP:CH2	2:B:196:CYS:HB3	2.49	0.48
1:G:50:GLN:O	1:G:51:ASP:HB2	2.13	0.48
1:L:152:TRP:CD2	1:L:182:LEU:HD13	2.49	0.48
1:A:14:SER:O	1:A:15:PRO:C	2.52	0.48
1:D:163:VAL:CG2	1:D:182:LEU:HD13	2.43	0.48
1:G:99:THR:HG22	1:G:101:LEU:HD23	1.95	0.48
2:H:28:ASN:ND2	2:H:31:ASP:HB2	2.28	0.48
3:C:305:LYS:O	3:C:305:LYS:HG2	2.12	0.47
2:I:145:TYR:CE1	2:I:150:VAL:HG13	2.48	0.47
2:E:17:SER:HB3	2:E:82(A):THR:O	2.14	0.47
1:D:166:THR:HG21	1:D:179:SER:H	1.74	0.47
2:B:30:LEU:HD13	2:B:53:ASP:OD1	2.14	0.47
1:A:26:ASP:OD2	1:A:69:LYS:NZ	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:PRO:HD3	1:D:136:LEU:HD23	1.96	0.47
1:G:13:VAL:HG22	1:G:17:GLN:HB2	1.97	0.47
3:P:315:ARG:CG	3:P:315:ARG:HH11	2.01	0.47
2:B:29:PHE:CE2	2:B:52(A):PRO:HB3	2.49	0.47
2:E:95:LEU:HD21	2:E:97:LEU:HG	1.97	0.47
2:B:83:GLN:HG2	2:B:84:ALA:N	2.30	0.47
2:E:2:VAL:O	2:E:3:GLN:HB3	2.15	0.47
1:D:122:PHE:HE1	2:E:125:ALA:O	1.97	0.46
1:G:186:PRO:O	1:G:190:LYS:HG3	2.15	0.46
1:A:201:HIS:O	1:A:202:GLU:CG	2.62	0.46
2:B:210:LYS:NZ	2:B:211:VAL:O	2.43	0.46
2:B:163:VAL:HG22	2:B:182:VAL:HG13	1.97	0.46
1:D:26:ASP:N	1:D:26:ASP:OD1	2.41	0.46
1:A:54:ARG:NH1	1:A:58:ILE:O	2.44	0.46
2:I:191:THR:HG22	2:I:192:GLN:N	2.31	0.46
2:B:150:VAL:CG2	2:B:178:LEU:HD21	2.46	0.46
2:E:2:VAL:CG1	2:E:102:LEU:HD11	2.46	0.46
2:H:75:ILE:O	2:H:76:SER:HB2	2.15	0.46
1:L:27:LYS:HB2	1:L:31:LYS:HE3	1.98	0.46
2:B:82:TRP:CD1	2:B:86:ASP:OD1	2.69	0.46
1:A:205:THR:O	1:A:206:VAL:HG23	2.16	0.46
1:A:2:TYR:CZ	1:A:31:LYS:HD2	2.48	0.46
2:B:20:ILE:HG21	2:B:109:ILE:HD11	1.98	0.46
1:D:171:GLN:NE2	1:D:176:TYR:O	2.49	0.46
4:D:222:HOH:O	2:E:143:LYS:HG2	2.16	0.46
1:G:189:TRP:CZ2	1:G:212:PRO:HA	2.51	0.46
1:A:100:VAL:HB	2:B:47:TRP:CG	2.51	0.45
1:A:140:ILE:HG12	1:A:199:VAL:HG21	1.97	0.45
1:D:189:TRP:CZ2	1:D:212:PRO:HA	2.51	0.45
1:L:17:GLN:O	1:L:78:THR:CG2	2.54	0.45
1:A:19:ALA:N	1:A:75:ILE:O	2.40	0.45
2:I:200:HIS:CD2	2:I:202:PRO:HD2	2.50	0.45
2:E:82(A):THR:N	4:E:227:HOH:O	2.49	0.45
1:G:89:GLN:HA	1:G:101:LEU:O	2.17	0.45
1:A:144:TYR:CG	1:A:145:PRO:HA	2.51	0.45
2:E:19:LYS:HA	2:E:80:LEU:O	2.17	0.45
2:E:154:TRP:O	2:E:156:SER:N	2.50	0.45
1:D:166:THR:CG2	1:D:179:SER:N	2.66	0.45
1:G:133:LYS:HA	1:G:133:LYS:HE3	1.99	0.45
1:G:96:THR:CG2	1:G:97:LYS:N	2.79	0.45
2:I:38:ARG:HB2	2:I:48:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:LEU:HD11	2:B:100(E):ASN:HB3	1.99	0.45
1:D:165:THR:HG1	1:D:180:SER:HG	1.65	0.45
2:H:15:GLY:HA2	2:H:82(B):THR:HG23	1.99	0.44
1:L:152:TRP:CG	1:L:182:LEU:HD13	2.52	0.44
2:H:178:LEU:C	2:H:178:LEU:HD12	2.38	0.44
2:I:43:LYS:CA	2:I:43:LYS:CE	2.82	0.44
2:E:40:ILE:HG23	2:E:41:PRO:HD2	1.99	0.44
1:D:79:GLN:NE2	1:D:82:ASP:OD2	2.51	0.44
2:E:138:LEU:CD2	2:E:184:VAL:HG22	2.47	0.44
2:E:155:ASN:N	2:E:195:ILE:O	2.34	0.44
1:G:169:SER:HB3	4:G:245:HOH:O	2.18	0.44
1:A:144:TYR:CD1	1:A:145:PRO:HA	2.53	0.43
1:L:14:SER:O	1:L:15:PRO:C	2.55	0.43
2:B:178:LEU:C	2:B:178:LEU:HD12	2.38	0.43
1:D:13:VAL:HG11	1:D:78:THR:HG21	2.00	0.43
1:L:198:GLN:HG3	1:L:207:GLU:HG3	2.00	0.43
1:D:39:ARG:HH21	1:D:81:LEU:HD22	1.77	0.43
1:L:177:ALA:HB3	2:H:164:HIS:CE1	2.54	0.43
1:D:139:LEU:HD22	2:E:166:PHE:CE1	2.53	0.43
2:E:212:GLU:CB	2:E:213:PRO:HD3	2.07	0.43
2:H:19:LYS:HZ2	1:A:203:GLY:HA3	1.83	0.43
2:I:36:TRP:CE3	2:I:80:LEU:HD22	2.54	0.43
2:H:54:ASP:OD1	3:P:305:LYS:NZ	2.50	0.43
1:A:190:LYS:HA	1:A:212:PRO:HG3	2.00	0.43
1:D:154:ALA:HB2	1:D:195:TYR:CE2	2.53	0.43
2:E:93:THR:HG23	2:E:100(G):PHE:CD1	2.54	0.43
1:A:92:ASP:HB2	1:A:101:LEU:HD11	2.01	0.43
1:D:155:ASP:OD1	1:D:193:LYS:HB2	2.19	0.42
2:H:125:ALA:HB1	2:H:213:PRO:HA	1.99	0.42
1:A:31:LYS:O	1:A:66:LYS:NZ	2.51	0.42
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.55	0.42
2:E:154:TRP:CZ3	2:E:196:CYS:HB3	2.54	0.42
2:I:209:LYS:HD2	2:I:209:LYS:HA	1.85	0.42
1:A:14:SER:O	1:A:17:GLN:HB3	2.19	0.42
2:E:100(C):SER:HB3	2:E:100(E):ASN:HD21	1.84	0.42
1:G:31:LYS:HA	1:G:31:LYS:HD2	1.84	0.42
1:L:2:TYR:OH	1:L:31:LYS:CD	2.67	0.42
2:H:30:LEU:HA	2:H:52(A):PRO:HB2	2.01	0.42
2:E:162:GLY:O	2:E:183:THR:N	2.41	0.42
2:H:145:TYR:CZ	2:H:150:VAL:HG13	2.55	0.42
1:L:61:ARG:HD2	1:L:76:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:309:LEU:N	3:P:309:LEU:HD23	2.34	0.42
1:D:157:SER:HA	1:D:158:PRO:HD3	1.94	0.42
2:I:150:VAL:HG22	2:I:178:LEU:HD21	2.01	0.42
1:D:36:TYR:O	1:D:86:TYR:HA	2.19	0.42
3:P:309:LEU:HG	3:P:317:PHE:HE1	1.84	0.42
1:G:100:VAL:HB	2:I:47:TRP:CD2	2.54	0.42
1:L:193:LYS:O	1:L:212:PRO:HD2	2.20	0.41
1:L:31:LYS:HD3	1:L:91:TRP:O	2.20	0.41
2:H:29:PHE:CE2	2:H:52(A):PRO:HB3	2.54	0.41
2:H:58:HIS:NE2	3:P:318:TYR:OH	2.45	0.41
1:A:122:PHE:HA	1:A:123:PRO:HD3	1.90	0.41
1:A:138:CYS:HB2	1:A:152:TRP:CZ2	2.56	0.41
1:A:61:ARG:HH22	1:A:82:ASP:CG	2.20	0.41
2:I:125:ALA:HA	2:I:126:PRO:HD3	1.87	0.41
2:B:138:LEU:O	2:B:181:VAL:HA	2.20	0.41
2:B:194:TYR:H	2:B:210:LYS:HZ1	1.66	0.41
1:L:89:GLN:HA	1:L:101:LEU:O	2.21	0.41
1:G:89:GLN:HB2	1:G:101:LEU:O	2.20	0.41
1:A:6:GLN:OE1	1:A:103:GLY:HA3	2.21	0.41
2:E:169:VAL:O	2:E:176:TYR:HA	2.21	0.41
1:D:144:TYR:O	1:D:201:HIS:CE1	2.72	0.41
1:D:167:THR:O	1:D:168:PRO:C	2.59	0.41
2:E:6:GLU:H	2:E:105:GLN:HE22	1.69	0.41
1:L:212:PRO:HA	1:L:213:THR:HA	1.61	0.41
1:D:135:THR:OG1	2:E:143:LYS:HE2	2.20	0.40
1:G:6:GLN:OE1	1:G:103:GLY:HA3	2.21	0.40
2:I:32:SER:HB3	2:I:96:TYR:CE2	2.56	0.40
2:E:209:LYS:HD3	2:E:209:LYS:HA	1.85	0.40
1:D:121:LEU:HD12	1:D:137:VAL:O	2.20	0.40
1:A:89:GLN:HA	1:A:101:LEU:O	2.20	0.40
2:B:83:GLN:HG2	2:B:84:ALA:H	1.86	0.40
2:H:53:ASP:O	2:H:73:LYS:NZ	2.47	0.40
1:L:34:SER:HB2	1:L:89:GLN:HG3	2.03	0.40
2:B:154:TRP:CZ3	2:B:196:CYS:HB3	2.56	0.40
2:H:40:ILE:HG23	2:H:41:PRO:CD	2.40	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	211/219 (96%)	187 (89%)	19 (9%)	5 (2%)	7	11
1	D	209/219 (95%)	196 (94%)	13 (6%)	0	100	100
1	G	210/219 (96%)	199 (95%)	9 (4%)	2 (1%)	18	32
1	L	212/219 (97%)	198 (93%)	10 (5%)	4 (2%)	9	15
2	B	215/226 (95%)	202 (94%)	11 (5%)	2 (1%)	20	36
2	E	215/226 (95%)	196 (91%)	16 (7%)	3 (1%)	13	23
2	H	209/226 (92%)	194 (93%)	13 (6%)	2 (1%)	18	32
2	I	215/226 (95%)	203 (94%)	11 (5%)	1 (0%)	32	53
3	C	12/23 (52%)	12 (100%)	0	0	100	100
3	P	12/23 (52%)	12 (100%)	0	0	100	100
All	All	1720/1826 (94%)	1599 (93%)	102 (6%)	19 (1%)	17	29

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	2	TYR
2	E	156	SER
2	E	212	GLU
1	L	131	ALA
1	A	15	PRO
1	A	16	GLY
1	A	168	PRO
2	B	114	GLY
2	H	65	GLY
1	A	67	SER
2	B	41	PRO
1	G	155	ASP
2	I	213	PRO
1	L	155	ASP

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Mol	Chain	Res	Type
1	A	202	GLU
1	L	191	SER
2	H	172	SER
2	E	65	GLY
1	G	158	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	184/186 (99%)	161 (88%)	23 (12%)	5	10
1	D	183/186 (98%)	163 (89%)	20 (11%)	7	14
1	G	184/186 (99%)	166 (90%)	18 (10%)	9	18
1	L	184/186 (99%)	166 (90%)	18 (10%)	9	18
2	B	188/194 (97%)	168 (89%)	20 (11%)	8	15
2	E	188/194 (97%)	169 (90%)	19 (10%)	9	17
2	H	184/194 (95%)	169 (92%)	15 (8%)	13	25
2	I	188/194 (97%)	173 (92%)	15 (8%)	14	27
3	C	11/17 (65%)	9 (82%)	2 (18%)	2	3
3	P	11/17 (65%)	7 (64%)	4 (36%)	0	0
All	All	1505/1554 (97%)	1351 (90%)	154 (10%)	8	16

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	SER
1	L	6	GLN
1	L	13	VAL
1	L	24	SER
1	L	30	ASP
1	L	56	SER
1	L	67	SER
1	L	69	LYS

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Mol	Chain	Res	Type
1	L	81	LEU
1	L	89	GLN
1	L	130	GLN
1	L	133	LYS
1	L	153	LYS
1	L	159	VAL
1	L	170	LYS
1	L	190	LYS
1	L	205	THR
1	L	208	LYS
2	H	13	GLN
2	H	23	LYS
2	H	56	ASP
2	H	67	VAL
2	H	100(B)	GLN
2	H	102	LEU
2	H	105	GLN
2	H	113	SER
2	H	138	LEU
2	H	150	VAL
2	H	159	LEU
2	H	191	THR
2	H	196	CYS
2	H	197	ASN
2	H	204	ASN
3	P	303	THR
3	P	306	SER
3	P	309	LEU
3	P	315	ARG
1	A	6	GLN
1	A	27	LYS
1	A	29	ASP
1	A	30	ASP
1	A	40	PRO
1	A	56	SER
1	A	80	SER
1	A	94	SER
1	A	108	THR
1	A	126	SER
1	A	132	ASN
1	A	149	THR
1	A	155	ASP

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Mol	Chain	Res	Type
1	A	160	LYS
1	A	172	SER
1	A	173	ASN
1	A	180	SER
1	A	188	GLN
1	A	193	LYS
1	A	204	SER
1	A	205	THR
1	A	207	GLU
1	A	209	THR
2	B	1	GLU
2	B	13	GLN
2	B	19	LYS
2	B	23	LYS
2	B	34	ILE
2	B	39	GLN
2	B	66	GLN
2	B	67	VAL
2	B	81	GLN
2	B	83	GLN
2	B	86	ASP
2	B	102	LEU
2	B	105	GLN
2	B	112	SER
2	B	117	LYS
2	B	138	LEU
2	B	170	LEU
2	B	175	LEU
2	B	182	VAL
2	B	210	LYS
3	C	303	THR
3	C	317	PHE
1	D	9	SER
1	D	13	VAL
1	D	20	SER
1	D	26	ASP
1	D	30	ASP
1	D	50	GLN
1	D	56	SER
1	D	61	ARG
1	D	81	LEU
1	D	89	GLN

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Mol	Chain	Res	Type
1	D	140	ILE
1	D	159	VAL
1	D	166	THR
1	D	173	ASN
1	D	183	SER
1	D	190	LYS
1	D	208	LYS
1	D	209	THR
1	D	210	VAL
1	D	213	THR
2	E	1	GLU
2	E	13	GLN
2	E	43	LYS
2	E	82(A)	THR
2	E	83	GLN
2	E	97	LEU
2	E	99	GLU
2	E	100(C)	SER
2	E	105	GLN
2	E	115	THR
2	E	150	VAL
2	E	156	SER
2	E	160	THR
2	E	161	SER
2	E	183	THR
2	E	192	GLN
2	E	201	LYS
2	E	206	LYS
2	E	209	LYS
1	G	1	SER
1	G	3	ASP
1	G	12	SER
1	G	13	VAL
1	G	29	ASP
1	G	60	GLU
1	G	63	SER
1	G	79	GLN
1	G	80	SER
1	G	89	GLN
1	G	97	LYS
1	G	133	LYS
1	G	159	VAL

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Mol	Chain	Res	Type
1	G	164	GLU
1	G	173	ASN
1	G	179	SER
1	G	200	THR
1	G	213	THR
2	I	13	GLN
2	I	25	SER
2	I	28	ASN
2	I	43	LYS
2	I	102	LEU
2	I	105	GLN
2	I	138	LEU
2	I	155	ASN
2	I	182	VAL
2	I	187	SER
2	I	189	LEU
2	I	191	THR
2	I	193	THR
2	I	195	ILE
2	I	197	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	50	GLN
1	L	89	GLN
1	L	112	GLN
1	L	198	GLN
2	H	3	GLN
2	H	28	ASN
2	H	81	GLN
2	H	105	GLN
2	H	164	HIS
2	H	192	GLN
1	A	79	GLN
1	A	132	ASN
1	A	173	ASN
1	A	174	ASN
1	A	201	HIS
2	B	3	GLN
2	B	16	GLN
2	B	81	GLN

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Mol	Chain	Res	Type
2	B	83	GLN
2	B	105	GLN
2	B	192	GLN
2	B	204	ASN
1	D	171	GLN
1	D	173	ASN
1	D	174	ASN
1	D	192	HIS
1	D	201	HIS
2	E	3	GLN
2	E	13	GLN
2	E	16	GLN
2	E	81	GLN
2	E	100(E)	ASN
2	E	105	GLN
2	E	155	ASN
2	E	192	GLN
1	G	38	GLN
1	G	50	GLN
1	G	79	GLN
1	G	173	ASN
1	G	198	GLN
2	I	16	GLN
2	I	28	ASN
2	I	39	GLN
2	I	100(E)	ASN
2	I	105	GLN
2	I	155	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	215/219 (98%)	0.50	22 (10%) 7 7	26, 58, 87, 92	0
1	D	213/219 (97%)	0.09	4 (1%) 67 69	25, 46, 67, 74	0
1	G	213/219 (97%)	-0.18	4 (1%) 67 69	22, 41, 60, 67	0
1	L	216/219 (98%)	-0.02	5 (2%) 61 63	21, 37, 73, 76	0
2	B	219/226 (96%)	0.07	4 (1%) 69 70	25, 43, 59, 69	0
2	E	219/226 (96%)	0.07	15 (6%) 18 18	23, 37, 78, 88	0
2	H	215/226 (95%)	0.04	4 (1%) 67 69	22, 39, 71, 80	0
2	I	219/226 (96%)	0.02	9 (4%) 38 40	18, 34, 66, 80	0
3	C	14/23 (60%)	1.29	3 (21%) 1 1	64, 74, 87, 88	0
3	P	14/23 (60%)	0.33	0 100 100	43, 51, 62, 65	0
All	All	1757/1826 (96%)	0.09	70 (3%) 39 41	18, 42, 74, 92	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	1	SER	5.7
2	E	191	THR	5.4
1	A	2	TYR	5.3
3	C	318	TYR	5.0
1	A	184	LEU	4.8
2	E	137	ALA	4.6
2	E	193	THR	4.4
1	A	189	TRP	4.4
1	L	2	TYR	4.4
2	E	159	LEU	4.3
1	A	152	TRP	4.2
2	I	184	VAL	4.1
2	H	136	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
2	E	188	SER	4.0
1	D	1	SER	3.8
2	E	136	ALA	3.8
3	C	317	PHE	3.8
2	E	194	TYR	3.7
1	A	146	GLY	3.6
1	A	195	TYR	3.6
2	E	138	LEU	3.6
2	B	30	LEU	3.6
2	E	190	GLY	3.4
1	A	159	VAL	3.4
1	A	196	SER	3.3
1	A	213	THR	3.1
1	A	1	SER	3.1
3	C	303	THR	3.1
1	A	157	SER	2.9
2	I	188	SER	2.9
2	B	191	THR	2.9
2	I	213	PRO	2.7
2	E	189	LEU	2.7
1	G	2	TYR	2.7
2	I	191	THR	2.7
1	A	143	PHE	2.6
2	E	192	GLN	2.6
1	L	187	GLU	2.6
2	E	182	VAL	2.6
1	A	182	LEU	2.6
1	A	197	CYS	2.5
2	B	126	PRO	2.5
1	D	16	GLY	2.5
1	D	199	VAL	2.4
1	L	189	TRP	2.4
2	H	139	GLY	2.4
1	A	192	HIS	2.4
1	A	198	GLN	2.4
1	A	107	LEU	2.4
2	I	185	PRO	2.4
1	A	95	THR	2.4
1	G	213	THR	2.4
2	H	135	THR	2.4
2	I	187	SER	2.4
1	A	144	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	145	PRO	2.3
2	I	194	TYR	2.2
1	G	1	SER	2.2
2	E	135	THR	2.2
1	G	189	TRP	2.2
2	B	28	ASN	2.2
2	I	215	SER	2.2
2	E	187	SER	2.2
2	E	213	PRO	2.1
2	I	134	GLY	2.1
1	L	184	LEU	2.1
2	H	215	SER	2.1
1	A	191	SER	2.1
1	A	193	LYS	2.1
1	D	189	TRP	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.