



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2022 – 10:24 AM JST

PDB ID : 7E5Y
Title : Molecular basis for neutralizing antibody 2B11 targeting SARS-CoV-2 RBD
Authors : Wu, H.; Yu, F.; Wang, Q.S.; Zhou, H.; Wang, W.W.; Zhao, T.; Pan, Y.B.;
Yang, X.M.
Deposited on : 2021-02-21
Resolution : 3.59 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 types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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	:	2.29
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)	:	2.29

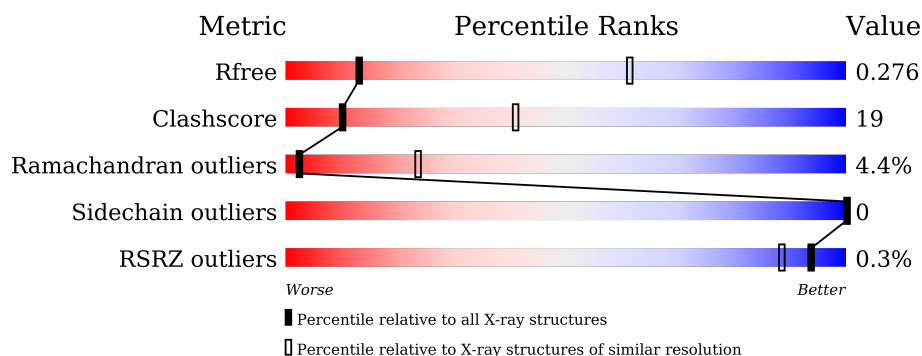
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 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	223	<div> <div>57%</div> <div>25%</div> <div>15%</div> </div>
1	R	223	<div> <div>62%</div> <div>22%</div> <div>15%</div> </div>
2	B	218	<div> <div>49%</div> <div>43%</div> <div>6%</div> </div>
2	L	218	<div> <div>53%</div> <div>35%</div> <div>7%</div> </div>
3	C	221	<div> <div>62%</div> <div>29%</div> <div>5%</div> </div>
3	H	221	<div> <div>64%</div> <div>27%</div> <div>7%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9297 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	189	Total	C	N	O	S	0	0	0
			1498	958	249	283	8			
1	A	189	Total	C	N	O	S	0	0	0
			1498	958	249	283	8			

- Molecule 2 is a protein called 2B11 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	209	Total	C	N	O	S	0	0	0
			1585	987	266	328	4			
2	B	213	Total	C	N	O	S	0	0	0
			1619	1009	272	334	4			

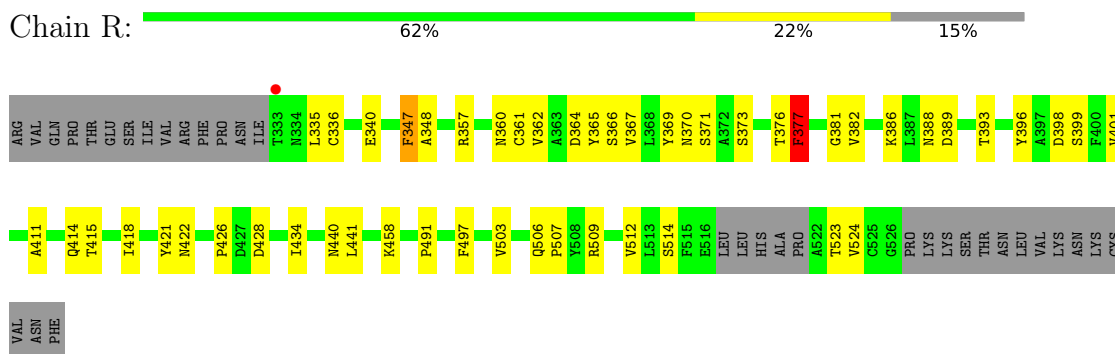
- Molecule 3 is a protein called 2B11 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	206	Total	C	N	O	S	0	0	0
			1539	968	256	307	8			
3	C	209	Total	C	N	O	S	0	0	0
			1558	980	260	310	8			

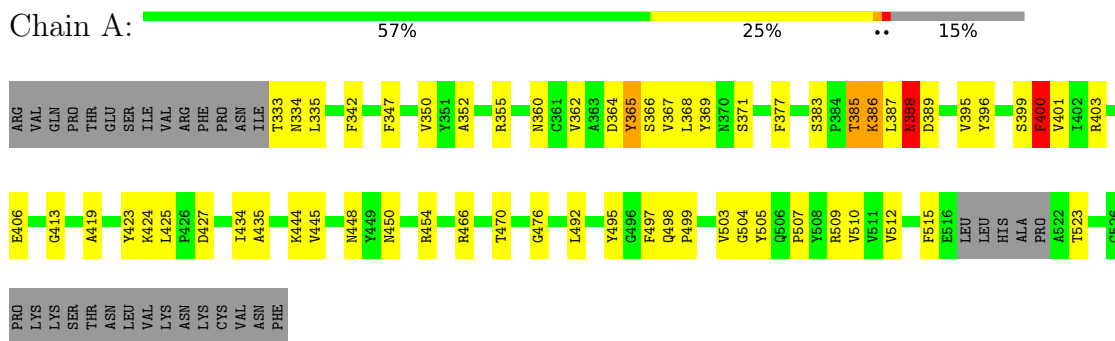
3 Residue-property plots [i](#)

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.

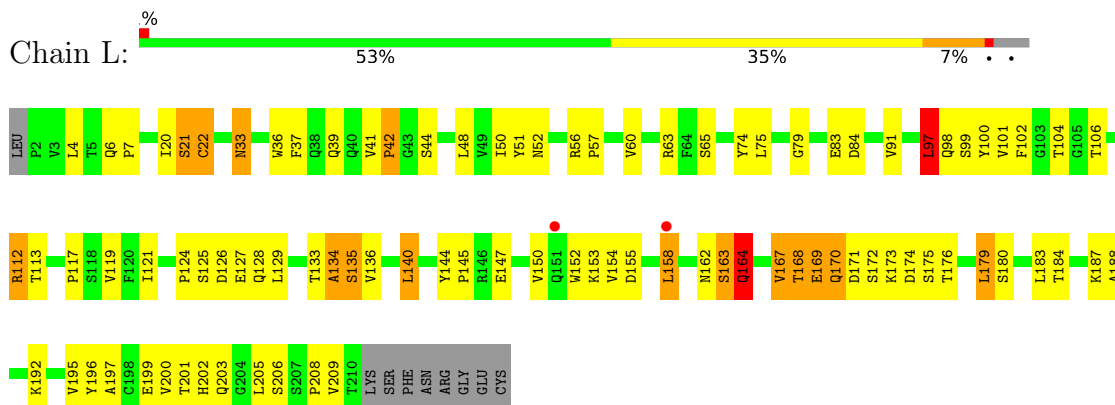
- Molecule 1: Spike protein S1



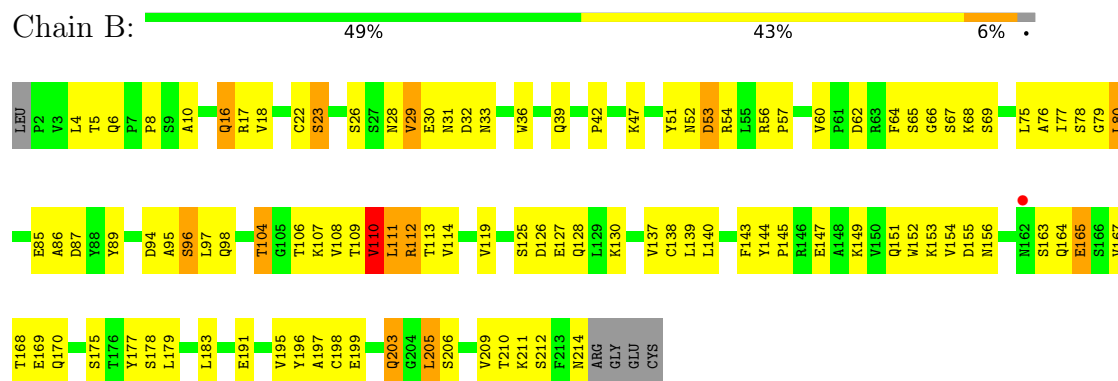
- Molecule 1: Spike protein S1



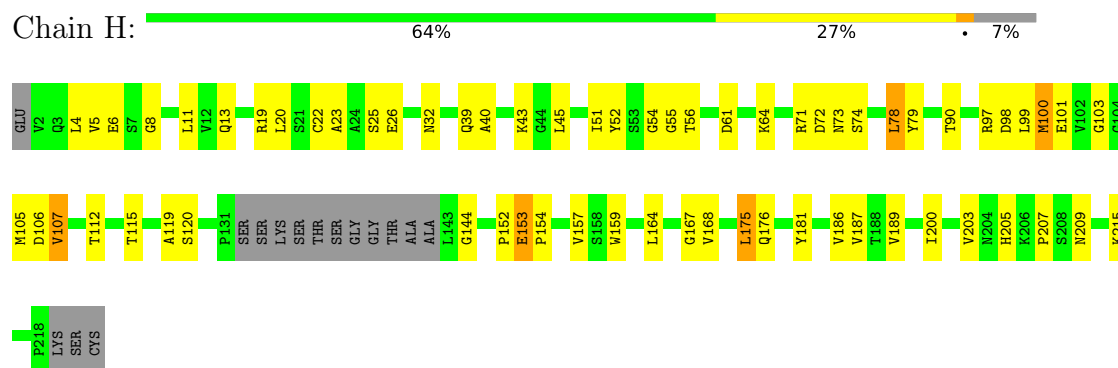
- Molecule 2: 2B11 Fab Light chain



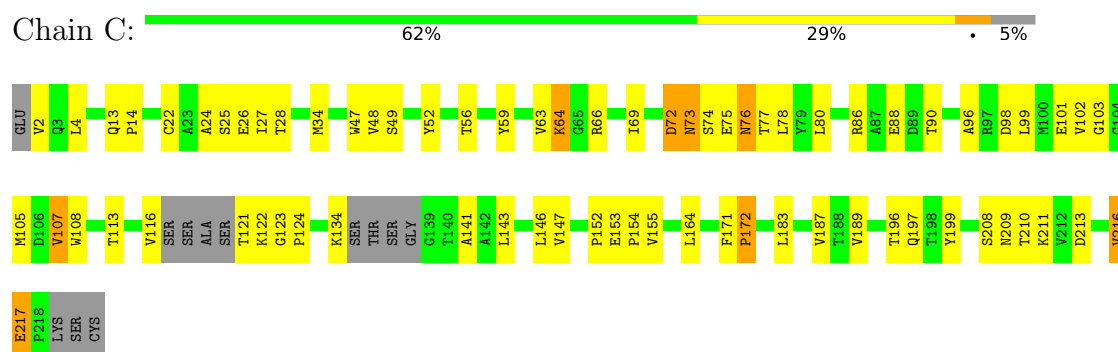
- Molecule 2: 2B11 Fab Light chain



- Molecule 3: 2B11 Fab Heavy chain



- Molecule 3: 2B11 Fab Heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	150.76Å 152.60Å 177.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.68 – 3.59 18.68 – 3.59	Depositor EDS
% Data completeness (in resolution range)	99.9 (18.68-3.59) 99.9 (18.68-3.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.232 , 0.277 0.232 , 0.276	Depositor DCC
R_{free} test set	1137 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	129.9	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 87.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.027 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9297	wwPDB-VP
Average B, all atoms (Å ²)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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 [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	0.38	1/1538 (0.1%)	0.77	1/2090 (0.0%)
1	R	0.54	3/1538 (0.2%)	1.42	6/2090 (0.3%)
2	B	0.35	0/1655	0.76	2/2256 (0.1%)
2	L	0.39	2/1620 (0.1%)	0.75	5/2210 (0.2%)
3	C	0.38	1/1590 (0.1%)	0.72	2/2166 (0.1%)
3	H	0.32	0/1572	0.68	3/2144 (0.1%)
All	All	0.40	7/9513 (0.1%)	0.88	19/12956 (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	A	0	4
1	R	0	1
2	L	0	1
3	C	0	1
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	377	PHE	CG-CD2	10.39	1.54	1.38
1	R	340	GLU	CD-OE2	-6.42	1.18	1.25
2	L	164	GLN	CB-CG	5.22	1.66	1.52
1	A	388	ASN	CG-ND2	5.22	1.46	1.32
3	C	73	ASN	CG-OD1	5.14	1.35	1.24
1	R	377	PHE	CE1-CZ	5.13	1.47	1.37
2	L	164	GLN	CG-CD	5.08	1.62	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	340	GLU	OE1-CD-OE2	-40.32	74.91	123.30
1	R	377	PHE	CB-CG-CD2	-26.85	102.01	120.80
1	R	340	GLU	CG-CD-OE1	19.31	156.92	118.30
1	R	340	GLU	CG-CD-OE2	-17.98	82.34	118.30
1	R	377	PHE	CB-CG-CD1	17.15	132.81	120.80
3	C	73	ASN	CB-CA-C	-10.76	88.87	110.40
1	A	400	PHE	CB-CG-CD2	-10.19	113.67	120.80
1	R	377	PHE	CD1-CG-CD2	-7.39	108.69	118.30
2	L	97	LEU	CB-CG-CD2	-7.28	98.62	111.00
3	H	175	LEU	CB-CG-CD2	-6.89	99.28	111.00
2	B	205	LEU	CA-CB-CG	6.89	131.14	115.30
3	H	153	GLU	C-N-CD	-5.99	107.42	120.60
2	B	110	VAL	CG1-CB-CG2	-5.81	101.60	110.90
2	L	164	GLN	N-CA-CB	-5.61	100.51	110.60
2	L	158	LEU	CA-CB-CG	5.48	127.91	115.30
3	C	72	ASP	C-N-CA	-5.47	108.02	121.70
3	H	78	LEU	CA-CB-CG	5.20	127.25	115.30
2	L	179	LEU	CA-CB-CG	5.12	127.08	115.30
2	L	140	LEU	CB-CG-CD2	5.01	119.52	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	369	TYR	Peptide
1	A	385	THR	Peptide
1	A	388	ASN	Sidechain
1	A	400	PHE	Sidechain
3	C	73	ASN	Sidechain
2	L	163	SER	Peptide
1	R	377	PHE	Sidechain

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	1498	0	1411	46	0
1	R	1498	0	1411	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1619	0	1557	92	0
2	L	1585	0	1524	79	0
3	C	1558	0	1527	58	0
3	H	1539	0	1505	50	1
All	All	9297	0	8935	344	1

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 19.

All (344) 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)
3:C:2:VAL:N	3:C:25:SER:HG	1.58	1.02
3:H:153:GLU:HG2	3:H:154:PRO:HA	1.39	1.00
3:C:107:VAL:HG12	3:C:108:TRP:H	1.30	0.96
2:B:87:ASP:OD2	2:B:107:LYS:HG2	1.66	0.95
2:B:94:ASP:OD2	2:B:98:GLN:NE2	2.00	0.93
2:L:195:VAL:HG23	2:L:209:VAL:HG22	1.52	0.91
2:B:168:THR:OG1	2:B:178:SER:O	1.88	0.90
2:L:155:ASP:H	2:L:196:TYR:HA	1.35	0.90
2:L:65:SER:HB2	1:A:470:THR:HG21	1.57	0.85
2:L:37:PHE:HZ	3:H:105:MET:HB2	1.44	0.82
2:B:140:LEU:HD12	2:B:179:LEU:HB2	1.62	0.81
2:B:170:GLN:OE1	2:B:175:SER:N	2.14	0.80
2:B:205:LEU:HD23	2:B:206:SER:H	1.47	0.79
2:L:140:LEU:HD11	2:L:150:VAL:HG11	1.65	0.79
2:B:143:PHE:HZ	2:B:179:LEU:HG	1.48	0.78
1:R:393:THR:O	1:R:523:THR:OG1	2.01	0.77
1:R:360:ASN:H	1:R:523:THR:HB	1.50	0.77
2:B:56:ARG:HD2	2:B:57:PRO:HD2	1.65	0.77
2:B:199:GLU:HG2	2:B:209:VAL:HG22	1.66	0.77
2:B:151:GLN:HB2	2:B:199:GLU:HB2	1.65	0.76
2:L:150:VAL:HG12	2:L:200:VAL:HA	1.68	0.76
1:A:333:THR:HG23	1:A:334:ASN:H	1.51	0.76
2:B:52:ASN:HB2	2:B:67:SER:HB2	1.68	0.74
1:R:396:TYR:HB2	1:R:514:SER:HB3	1.68	0.74
3:H:200:ILE:HG12	3:H:215:LYS:HG2	1.69	0.73
1:A:366:SER:H	1:A:388:ASN:HD22	1.35	0.73
3:C:24:ALA:O	3:C:76:ASN:ND2	2.21	0.73
3:C:216:VAL:HG23	3:C:217:GLU:H	1.52	0.73
1:R:367:VAL:HA	1:R:370:ASN:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:GLN:NE2	2:L:42:PRO:O	2.22	0.73
3:C:98:ASP:HA	3:C:103:GLY:HA2	1.70	0.73
2:B:113:THR:HG22	2:B:114:VAL:H	1.54	0.73
2:B:96:SER:HB2	2:B:98:GLN:HE22	1.55	0.72
2:B:167:VAL:HA	2:B:179:LEU:HD22	1.71	0.71
1:A:365:TYR:HB2	1:A:388:ASN:HB2	1.70	0.71
2:L:124:PRO:HD3	2:L:136:VAL:HG22	1.73	0.71
2:L:37:PHE:CZ	3:H:105:MET:HB2	2.26	0.70
2:L:33:ASN:HB3	2:L:52:ASN:HA	1.73	0.70
1:A:498:GLN:OE1	1:A:499:PRO:HD2	1.91	0.69
2:L:121:ILE:HD13	2:L:208:PRO:HB2	1.75	0.69
2:B:53:ASP:HA	2:B:65:SER:HB3	1.73	0.69
2:B:53:ASP:HB3	2:B:54:ARG:NH1	2.08	0.69
1:A:364:ASP:O	1:A:388:ASN:ND2	2.26	0.68
2:L:56:ARG:HB3	2:L:60:VAL:HG11	1.75	0.68
3:C:153:GLU:HG2	3:C:154:PRO:HA	1.76	0.67
2:B:26:SER:HB2	2:B:29:VAL:HG22	1.76	0.67
1:R:415:THR:OG1	3:H:56:THR:HB	1.94	0.67
1:R:364:ASP:OD1	1:R:366:SER:OG	2.13	0.67
3:H:51:ILE:HD13	3:H:71:ARG:HG3	1.77	0.66
2:L:128:GLN:NE2	2:L:135:SER:OG	2.28	0.66
2:B:125:SER:HB3	2:B:128:GLN:HG3	1.77	0.66
2:L:164:GLN:NE2	3:H:176:GLN:HA	2.10	0.66
1:A:399:SER:O	1:A:400:PHE:HB3	1.94	0.66
2:B:68:LYS:HG3	2:B:69:SER:N	2.11	0.66
2:B:191:GLU:HA	2:B:214:ASN:HD22	1.61	0.65
2:L:7:PRO:HD3	2:L:21:SER:OG	1.97	0.65
3:H:52:TYR:HB2	3:H:55:GLY:O	1.96	0.65
2:L:170:GLN:HG3	2:L:171:ASP:H	1.61	0.65
2:B:56:ARG:CD	2:B:57:PRO:HD2	2.26	0.65
2:B:147:GLU:HB3	2:B:203:GLN:HE21	1.61	0.65
2:B:96:SER:HB2	2:B:98:GLN:NE2	2.13	0.64
1:A:364:ASP:HB3	1:A:367:VAL:HG22	1.79	0.64
3:C:143:LEU:HD13	3:C:216:VAL:HG21	1.80	0.64
3:H:32:ASN:ND2	3:H:97:ARG:HD2	2.13	0.64
3:C:75:GLU:O	3:C:77:THR:N	2.30	0.64
3:C:4:LEU:HG	3:C:24:ALA:HB1	1.78	0.64
3:C:211:LYS:NZ	3:C:213:ASP:OD2	2.31	0.64
3:C:107:VAL:CG1	3:C:108:TRP:H	2.07	0.63
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.81	0.63
3:H:205:HIS:CD2	3:H:207:PRO:HD2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:GLU:CG	3:C:154:PRO:HA	2.29	0.62
2:L:155:ASP:N	2:L:196:TYR:HA	2.12	0.62
2:L:155:ASP:OD2	2:L:192:LYS:NZ	2.32	0.62
3:C:164:LEU:HD11	3:C:199:TYR:HD1	1.64	0.62
3:H:175:LEU:HD21	3:H:181:TYR:CZ	2.35	0.61
3:C:107:VAL:HG12	3:C:108:TRP:N	2.11	0.61
3:H:11:LEU:HB2	3:H:152:PRO:HG3	1.80	0.61
2:L:153:LYS:HD3	2:L:199:GLU:OE2	2.01	0.60
2:B:109:THR:O	2:B:110:VAL:HG23	2.00	0.60
2:B:155:ASP:HA	2:B:195:VAL:HG23	1.83	0.60
2:L:162:ASN:HB2	2:L:183:LEU:HD12	1.84	0.60
3:C:52:TYR:HB2	3:C:56:THR:HB	1.84	0.60
1:A:425:LEU:HD21	1:A:512:VAL:HG11	1.84	0.59
3:C:2:VAL:N	3:C:25:SER:OG	2.32	0.59
1:R:377:PHE:CD1	1:R:434:ILE:HG12	2.38	0.58
3:C:121:THR:HG23	3:C:152:PRO:HD3	1.86	0.58
3:C:48:VAL:HG11	3:C:80:LEU:HD21	1.86	0.58
2:L:167:VAL:O	2:L:168:THR:HG23	2.03	0.58
3:H:32:ASN:HD21	3:H:97:ARG:HD2	1.68	0.58
3:H:90:THR:HG23	3:H:115:THR:HA	1.84	0.58
2:L:153:LYS:HB2	2:L:199:GLU:HG3	1.84	0.58
3:H:11:LEU:HD22	3:H:152:PRO:HD3	1.86	0.58
3:H:97:ARG:HH21	3:H:106:ASP:HB3	1.69	0.58
2:L:144:TYR:HB3	2:L:145:PRO:HD3	1.85	0.58
3:H:19:ARG:HB3	3:H:19:ARG:NH1	2.19	0.57
1:A:366:SER:H	1:A:388:ASN:ND2	2.02	0.57
2:L:125:SER:OG	2:L:128:GLN:HB2	2.04	0.57
1:A:364:ASP:HB3	1:A:367:VAL:CG2	2.35	0.57
2:B:85:GLU:HB3	2:B:109:THR:HG22	1.86	0.57
2:L:41:VAL:HG13	2:L:42:PRO:HD2	1.84	0.57
2:L:41:VAL:HB	2:L:44:SER:OG	2.05	0.57
1:A:350:VAL:HG23	1:A:400:PHE:CD2	2.39	0.57
2:L:56:ARG:HB3	2:L:60:VAL:CG1	2.35	0.56
2:L:119:VAL:HG22	2:L:140:LEU:HD22	1.85	0.56
3:H:72:ASP:HB2	3:H:79:TYR:CE2	2.41	0.56
3:H:72:ASP:HB2	3:H:79:TYR:HE2	1.70	0.56
3:H:61:ASP:HA	3:H:64:LYS:HD3	1.87	0.56
1:A:454:ARG:HA	1:A:492:LEU:HD23	1.87	0.56
3:C:4:LEU:HG	3:C:24:ALA:CB	2.34	0.56
2:B:111:LEU:HD22	2:B:112:ARG:NH1	2.21	0.56
2:B:111:LEU:HD22	2:B:112:ARG:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:PHE:CZ	2:B:179:LEU:HG	2.37	0.56
1:A:383:SER:HB2	1:A:386:LYS:HD3	1.87	0.55
3:H:4:LEU:HD13	3:H:107:VAL:HG12	1.88	0.55
3:C:99:LEU:HD21	3:C:102:VAL:HB	1.89	0.55
1:A:403:ARG:HD2	1:A:505:TYR:HA	1.89	0.55
2:L:201:THR:HG22	2:L:205:LEU:HG	1.88	0.55
2:B:197:ALA:HA	2:B:211:LYS:HA	1.88	0.55
2:B:54:ARG:NE	2:B:54:ARG:HA	2.22	0.55
2:B:6:GLN:HE21	2:B:104:THR:C	2.10	0.55
2:B:53:ASP:HB3	2:B:54:ARG:HH12	1.70	0.54
2:B:168:THR:CG2	3:C:172:PRO:HD2	2.37	0.54
3:H:159:TRP:HB3	3:H:164:LEU:HD12	1.89	0.54
1:R:365:TYR:HD2	1:R:388:ASN:HA	1.73	0.53
2:L:112:ARG:NH2	2:L:113:THR:OG1	2.41	0.53
2:L:200:VAL:HG13	2:L:206:SER:HB3	1.90	0.53
1:A:352:ALA:HA	1:A:466:ARG:HD3	1.90	0.53
1:R:440:ASN:OD1	1:R:441:LEU:N	2.41	0.53
1:R:369:TYR:HA	1:R:377:PHE:HE2	1.74	0.53
2:L:135:SER:HA	2:L:184:THR:HA	1.91	0.53
2:B:138:CYS:HB2	2:B:152:TRP:CH2	2.44	0.53
3:C:124:PRO:HB3	3:C:147:VAL:HG13	1.91	0.53
1:R:364:ASP:O	1:R:367:VAL:HG22	2.08	0.53
2:B:144:TYR:HB3	2:B:145:PRO:HD3	1.91	0.53
2:B:62:ASP:HB2	2:B:79:GLY:H	1.73	0.53
2:B:137:VAL:HG12	2:B:139:LEU:HG	1.90	0.52
3:C:4:LEU:HB2	3:C:107:VAL:HG22	1.91	0.52
1:R:369:TYR:HB2	1:R:377:PHE:CE2	2.44	0.52
1:A:403:ARG:HG2	1:A:504:GLY:O	2.09	0.52
2:B:112:ARG:HH21	2:B:175:SER:HB3	1.73	0.52
3:H:157:VAL:HG13	3:H:203:VAL:HG22	1.92	0.52
1:A:444:LYS:HD3	1:A:445:VAL:N	2.25	0.52
2:B:64:PHE:HB3	2:B:76:ALA:HB3	1.91	0.52
3:C:86:ARG:HB3	3:C:88:GLU:OE1	2.09	0.52
2:L:6:GLN:HG2	2:L:106:THR:OG1	2.10	0.52
2:L:174:ASP:O	2:L:176:THR:N	2.40	0.52
2:B:5:THR:OG1	2:B:23:SER:HB3	2.09	0.52
2:B:8:PRO:HA	2:B:106:THR:HA	1.90	0.52
2:B:66:GLY:C	2:B:68:LYS:H	2.14	0.52
1:A:413:GLY:H	1:A:424:LYS:HZ1	1.59	0.51
1:R:347:PHE:CE1	1:R:399:SER:HB2	2.45	0.51
3:C:90:THR:HG23	3:C:113:THR:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:VAL:HG13	2:B:80:LEU:HD11	1.92	0.51
2:B:113:THR:HG22	2:B:114:VAL:N	2.25	0.51
3:H:19:ARG:HB3	3:H:19:ARG:HH11	1.76	0.51
2:L:41:VAL:CG1	2:L:42:PRO:HD2	2.40	0.51
3:C:216:VAL:HG23	3:C:217:GLU:N	2.23	0.51
2:L:153:LYS:O	2:L:158:LEU:HA	2.11	0.51
1:R:426:PRO:HB2	1:R:428:ASP:OD1	2.12	0.50
2:L:20:ILE:HD12	2:L:75:LEU:HD23	1.93	0.50
3:H:168:VAL:HA	3:H:187:VAL:HG12	1.94	0.50
3:H:187:VAL:HG23	3:H:189:VAL:HG13	1.94	0.50
3:C:13:GLN:HG2	3:C:116:VAL:HG12	1.94	0.50
2:L:134:ALA:O	2:L:135:SER:OG	2.27	0.50
2:L:127:GLU:OE1	2:L:127:GLU:N	2.44	0.49
2:L:153:LYS:HE3	2:L:158:LEU:HD22	1.92	0.49
2:L:21:SER:HA	2:L:74:TYR:HD1	1.77	0.49
2:L:171:ASP:O	2:L:173:LYS:N	2.45	0.49
1:A:366:SER:OG	1:A:388:ASN:ND2	2.45	0.49
2:B:6:GLN:HE22	2:B:89:TYR:HA	1.77	0.49
2:L:164:GLN:HE21	3:H:176:GLN:HA	1.75	0.49
3:H:8:GLY:HA3	3:H:20:LEU:HD22	1.94	0.49
2:B:68:LYS:HG3	2:B:69:SER:H	1.78	0.49
1:R:421:TYR:HH	3:H:54:GLY:H	1.60	0.49
1:R:369:TYR:CA	1:R:377:PHE:HE2	2.24	0.49
2:L:100:TYR:OH	3:H:100:MET:SD	2.69	0.49
2:B:154:VAL:HG22	2:B:196:TYR:CE1	2.47	0.49
3:H:119:ALA:O	3:H:120:SER:OG	2.29	0.49
3:C:164:LEU:HD11	3:C:199:TYR:CD1	2.47	0.49
2:L:6:GLN:O	2:L:104:THR:OG1	2.29	0.48
1:A:448:ASN:C	1:A:450:ASN:H	2.17	0.48
2:L:126:ASP:HB2	2:L:127:GLU:OE1	2.13	0.48
2:B:137:VAL:HG21	3:C:146:LEU:HD13	1.95	0.48
1:A:497:PHE:CG	1:A:507:PRO:HG3	2.49	0.48
2:B:169:GLU:HA	2:B:177:TYR:HD1	1.78	0.48
2:B:191:GLU:HA	2:B:214:ASN:ND2	2.27	0.48
2:L:36:TRP:HB2	2:L:50:ILE:HB	1.94	0.48
1:R:357:ARG:HG3	1:R:357:ARG:O	2.14	0.48
3:H:144:GLY:HA3	3:H:186:VAL:HG12	1.95	0.48
3:C:66:ARG:NH2	3:C:86:ARG:HH21	2.12	0.48
2:L:150:VAL:HA	2:L:199:GLU:O	2.13	0.47
3:H:4:LEU:HD13	3:H:107:VAL:CG1	2.44	0.47
2:L:117:PRO:O	2:L:119:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:LEU:HD23	2:B:139:LEU:HA	1.67	0.47
2:L:179:LEU:HD23	2:L:180:SER:N	2.30	0.47
1:A:476:GLY:HA2	3:C:28:THR:HG23	1.95	0.47
2:L:97:LEU:HD13	3:H:61:ASP:OD2	2.14	0.47
2:L:21:SER:OG	2:L:22:CYS:N	2.45	0.47
2:L:97:LEU:O	2:L:99:SER:N	2.48	0.47
3:C:171:PHE:O	3:C:183:LEU:HG	2.15	0.47
1:R:401:VAL:HG22	1:R:509:ARG:HG2	1.96	0.47
2:L:197:ALA:HB2	2:L:209:VAL:HG23	1.97	0.47
1:A:360:ASN:HA	1:A:523:THR:O	2.14	0.47
2:L:192:LYS:HD2	2:L:192:LYS:O	2.14	0.47
3:C:47:TRP:CH2	3:C:49:SER:HA	2.50	0.47
3:H:11:LEU:HA	3:H:115:THR:O	2.15	0.46
2:B:119:VAL:HG22	2:B:140:LEU:HD22	1.97	0.46
1:R:386:LYS:O	1:R:389:ASP:HB2	2.16	0.46
3:C:78:LEU:HD23	3:C:78:LEU:H	1.80	0.46
2:L:147:GLU:OE2	2:L:203:GLN:NE2	2.49	0.46
1:A:444:LYS:HD3	1:A:445:VAL:O	2.15	0.46
1:R:364:ASP:OD1	1:R:367:VAL:HG13	2.16	0.46
2:L:197:ALA:HB2	2:L:209:VAL:CG2	2.45	0.46
3:C:98:ASP:CA	3:C:103:GLY:HA2	2.43	0.46
1:R:411:ALA:HB3	1:R:414:GLN:HG3	1.97	0.46
2:L:63:ARG:NH2	2:L:79:GLY:O	2.49	0.46
1:A:395:VAL:HG22	1:A:515:PHE:HD1	1.81	0.46
1:A:406:GLU:OE1	1:A:495:TYR:OH	2.16	0.46
3:H:97:ARG:NH1	3:H:99:LEU:HB2	2.30	0.46
2:B:4:LEU:HD23	2:B:22:CYS:SG	2.55	0.46
3:C:59:TYR:HE1	3:C:69:ILE:H	1.62	0.46
1:R:398:ASP:HB2	1:R:512:VAL:HB	1.98	0.45
2:B:60:VAL:HG23	2:B:62:ASP:OD1	2.16	0.45
3:C:208:SER:HB3	3:C:210:THR:HG23	1.98	0.45
2:B:147:GLU:HB3	2:B:203:GLN:NE2	2.30	0.45
2:B:51:TYR:CZ	3:C:101:GLU:HA	2.51	0.45
2:B:108:VAL:O	2:B:109:THR:HG23	2.16	0.45
2:B:112:ARG:NH2	2:B:175:SER:HB3	2.32	0.45
3:C:187:VAL:HG13	3:C:189:VAL:HG13	1.97	0.45
2:B:29:VAL:HG13	2:B:94:ASP:OD1	2.17	0.45
1:R:360:ASN:N	1:R:523:THR:HB	2.27	0.45
2:B:140:LEU:O	2:B:178:SER:HB2	2.16	0.45
2:B:198:CYS:N	2:B:210:THR:O	2.36	0.45
3:C:99:LEU:CD2	3:C:102:VAL:HB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:5:VAL:CG1	3:H:23:ALA:HB3	2.47	0.45
3:H:167:GLY:O	3:H:187:VAL:HA	2.17	0.45
3:H:99:LEU:HD23	3:H:103:GLY:HA3	1.98	0.45
1:A:387:LEU:HD21	1:A:515:PHE:CE2	2.51	0.45
2:B:10:ALA:HB3	2:B:107:LYS:O	2.16	0.45
3:C:122:LYS:HG2	3:C:123:GLY:N	2.31	0.45
1:R:369:TYR:HA	1:R:377:PHE:CE2	2.51	0.45
1:A:366:SER:N	1:A:388:ASN:HD22	2.08	0.45
2:B:16:GLN:HB3	2:B:17:ARG:H	1.64	0.45
1:A:355:ARG:HD3	1:A:396:TYR:HB3	1.99	0.44
2:B:62:ASP:HA	2:B:78:SER:HB2	2.00	0.44
3:H:6:GLU:HB3	3:H:112:THR:OG1	2.17	0.44
3:C:72:ASP:OD2	3:C:74:SER:HB2	2.17	0.44
3:H:40:ALA:HB3	3:H:43:LYS:HG3	1.99	0.44
2:B:39:GLN:O	2:B:86:ALA:HB1	2.17	0.44
3:C:122:LYS:HG2	3:C:123:GLY:H	1.83	0.44
1:R:369:TYR:CA	1:R:377:PHE:CE2	3.00	0.44
1:A:435:ALA:HB2	1:A:510:VAL:HG22	1.99	0.44
2:L:21:SER:HA	2:L:74:TYR:CD1	2.53	0.44
2:L:33:ASN:ND2	3:H:101:GLU:HG2	2.33	0.44
2:L:129:LEU:HA	2:L:133:THR:O	2.18	0.44
2:L:195:VAL:CG2	2:L:209:VAL:HG22	2.36	0.44
1:R:497:PHE:CG	1:R:507:PRO:HG3	2.53	0.44
2:L:119:VAL:HG13	2:L:140:LEU:HD23	1.99	0.44
2:B:152:TRP:CE2	2:B:183:LEU:HG	2.52	0.44
3:C:49:SER:OG	3:C:69:ILE:HD11	2.17	0.44
3:C:196:THR:OG1	3:C:197:GLN:N	2.50	0.44
2:L:174:ASP:C	2:L:176:THR:H	2.20	0.43
3:H:39:GLN:HB2	3:H:45:LEU:HD23	2.00	0.43
2:L:50:ILE:HD13	2:L:56:ARG:HG2	1.99	0.43
3:H:98:ASP:HB2	3:H:105:MET:HE3	2.00	0.43
1:R:376:THR:O	1:R:434:ILE:HA	2.18	0.43
1:A:347:PHE:CD1	1:A:509:ARG:CZ	3.01	0.43
1:A:386:LYS:O	1:A:389:ASP:HB2	2.18	0.43
2:B:36:TRP:CE3	2:B:75:LEU:HD22	2.53	0.43
3:H:144:GLY:HA2	3:H:159:TRP:CZ2	2.53	0.43
1:A:335:LEU:HA	1:A:362:VAL:HB	2.01	0.43
3:C:13:GLN:HG2	3:C:14:PRO:HD2	1.99	0.43
3:C:22:CYS:O	3:C:78:LEU:HD23	2.18	0.43
3:C:27:ILE:HD12	3:C:27:ILE:H	1.83	0.43
3:C:134:LYS:HD3	3:C:141:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:458:LYS:HE2	1:R:458:LYS:HB2	1.72	0.43
2:L:4:LEU:HG	2:L:101:VAL:HG12	1.99	0.43
1:A:333:THR:HG23	1:A:334:ASN:N	2.27	0.43
1:A:386:LYS:H	1:A:386:LYS:HD2	1.83	0.43
2:B:29:VAL:O	2:B:31:ASN:N	2.50	0.43
3:C:99:LEU:O	3:C:103:GLY:N	2.52	0.43
3:C:155:VAL:CG2	3:C:183:LEU:HD13	2.49	0.43
1:R:347:PHE:CE2	1:R:509:ARG:HD3	2.54	0.42
3:H:8:GLY:C	3:H:112:THR:HG21	2.39	0.42
1:R:347:PHE:HD2	1:R:509:ARG:CZ	2.32	0.42
1:R:418:ILE:HA	1:R:422:ASN:HB2	2.01	0.42
2:B:28:ASN:HB2	2:B:94:ASP:OD1	2.20	0.42
2:B:149:LYS:HB2	2:B:149:LYS:HE2	1.76	0.42
2:L:170:GLN:HG3	2:L:171:ASP:N	2.32	0.42
2:L:187:LYS:HD2	2:L:188:ALA:N	2.34	0.42
3:H:22:CYS:HB3	3:H:78:LEU:HD23	2.00	0.42
3:C:199:TYR:O	3:C:216:VAL:HG22	2.18	0.42
1:R:347:PHE:HB3	1:R:348:ALA:H	1.52	0.42
2:L:169:GLU:HB3	2:L:170:GLN:H	1.68	0.42
1:A:368:LEU:O	1:A:371:SER:HB2	2.20	0.42
1:A:419:ALA:HA	1:A:423:TYR:O	2.18	0.42
1:A:505:TYR:CZ	2:B:31:ASN:HB2	2.54	0.42
2:L:145:PRO:HB2	2:L:202:HIS:NE2	2.35	0.42
2:B:17:ARG:HA	2:B:77:ILE:O	2.19	0.42
2:B:153:LYS:HD3	2:B:156:ASN:HA	2.01	0.42
3:H:97:ARG:HH12	3:H:99:LEU:HD22	1.85	0.42
1:A:342:PHE:HE2	1:A:434:ILE:HG21	1.84	0.42
2:B:17:ARG:NH1	2:B:78:SER:OG	2.53	0.42
2:B:112:ARG:HB3	2:B:113:THR:H	1.37	0.42
2:B:125:SER:HB3	2:B:128:GLN:CG	2.47	0.42
2:B:169:GLU:HA	2:B:177:TYR:CD1	2.53	0.42
2:L:153:LYS:CE	2:L:158:LEU:HD22	2.50	0.41
2:B:56:ARG:NE	2:B:57:PRO:HD2	2.34	0.41
2:B:127:GLU:HA	2:B:130:LYS:HD2	2.00	0.41
2:B:196:TYR:HB2	2:B:212:SER:OG	2.20	0.41
3:C:25:SER:O	3:C:27:ILE:N	2.52	0.41
1:R:382:VAL:HG12	1:R:386:LYS:HB2	2.02	0.41
1:A:403:ARG:CD	1:A:505:TYR:HA	2.50	0.41
2:B:125:SER:OG	2:B:127:GLU:OE1	2.38	0.41
2:B:168:THR:HG21	3:C:172:PRO:HD2	2.01	0.41
2:L:199:GLU:O	2:L:201:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:25:SER:O	3:H:26:GLU:HB2	2.19	0.41
1:R:336:CYS:N	1:R:361:CYS:HB2	2.35	0.41
2:B:178:SER:O	2:B:179:LEU:HD23	2.20	0.41
2:L:119:VAL:HG21	2:L:200:VAL:HG11	2.02	0.41
3:C:107:VAL:CG1	3:C:108:TRP:N	2.78	0.41
2:L:83:GLU:HG3	2:L:84:ASP:N	2.35	0.41
1:A:403:ARG:CG	1:A:505:TYR:HA	2.50	0.41
3:C:34:MET:HA	3:C:96:ALA:O	2.21	0.41
1:R:335:LEU:HD23	1:R:362:VAL:HB	2.02	0.41
2:L:48:LEU:HD21	2:L:51:TYR:HB3	2.03	0.41
2:L:112:ARG:CZ	2:L:113:THR:OG1	2.69	0.41
2:B:47:LYS:NZ	3:C:102:VAL:O	2.54	0.41
2:B:97:LEU:HD23	2:B:97:LEU:O	2.21	0.41
2:B:111:LEU:CD2	2:B:112:ARG:HD3	2.51	0.41
2:B:163:SER:HB3	2:B:183:LEU:HD23	2.01	0.41
1:A:377:PHE:CE1	1:A:434:ILE:HG12	2.56	0.41
1:A:505:TYR:HE1	2:B:32:ASP:HB2	1.86	0.40
2:B:95:ALA:O	2:B:96:SER:C	2.59	0.40
2:L:152:TRP:CD1	2:L:163:SER:HB2	2.56	0.40
3:C:63:VAL:HG23	3:C:64:LYS:N	2.36	0.40
2:B:126:ASP:O	2:B:130:LYS:HG3	2.21	0.40
1:R:371:SER:C	1:R:373:SER:H	2.25	0.40
2:L:91:VAL:HG22	2:L:102:PHE:CD1	2.56	0.40
2:L:187:LYS:HE3	2:L:187:LYS:HB3	1.91	0.40
1:A:355:ARG:CD	1:A:396:TYR:HB3	2.52	0.40
1:R:503:VAL:O	1:R:506:GLN:HB2	2.21	0.40
3:H:73:ASN:O	3:H:74:SER:OG	2.23	0.40
2:B:164:GLN:O	2:B:165:GLU:HB2	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:13:GLN:NE2	3:H:209:ASN:OD1[4_555]	2.11	0.09

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	185/223 (83%)	156 (84%)	24 (13%)	5 (3%)	5	35
1	R	185/223 (83%)	163 (88%)	18 (10%)	4 (2%)	6	39
2	B	211/218 (97%)	157 (74%)	39 (18%)	15 (7%)	1	14
2	L	207/218 (95%)	154 (74%)	35 (17%)	18 (9%)	1	9
3	C	203/221 (92%)	182 (90%)	12 (6%)	9 (4%)	2	23
3	H	202/221 (91%)	173 (86%)	27 (13%)	2 (1%)	15	55
All	All	1193/1324 (90%)	985 (83%)	155 (13%)	53 (4%)	2	23

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	98	GLN
2	L	168	THR
2	L	169	GLU
1	A	365	TYR
1	A	386	LYS
1	A	503	VAL
2	B	42	PRO
2	B	96	SER
2	B	111	LEU
3	C	76	ASN
3	C	105	MET
1	R	347	PHE
2	L	164	GLN
2	L	167	VAL
2	L	172	SER
2	B	53	ASP
2	B	80	LEU
2	B	110	VAL
2	B	112	ARG
3	C	26	GLU

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Mol	Chain	Res	Type
3	C	209	ASN
3	C	217	GLU
1	R	491	PRO
1	R	524	VAL
2	L	22	CYS
2	L	33	ASN
2	L	97	LEU
2	L	154	VAL
1	A	427	ASP
2	B	165	GLU
3	C	64	LYS
2	L	57	PRO
2	L	134	ALA
2	L	135	SER
2	B	30	GLU
2	B	203	GLN
2	L	21	SER
2	L	170	GLN
3	H	100	MET
2	B	23	SER
2	B	33	ASN
2	B	104	THR
1	R	381	GLY
2	L	112	ARG
2	L	175	SER
1	A	385	THR
2	B	16	GLN
3	C	172	PRO
3	C	216	VAL
2	L	42	PRO
3	C	107	VAL
3	H	107	VAL
2	B	29	VAL

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	163/196 (83%)	163 (100%)	0	100	100
1	R	163/196 (83%)	163 (100%)	0	100	100
2	B	187/191 (98%)	187 (100%)	0	100	100
2	L	183/191 (96%)	183 (100%)	0	100	100
3	C	176/186 (95%)	176 (100%)	0	100	100
3	H	175/186 (94%)	175 (100%)	0	100	100
All	All	1047/1146 (91%)	1047 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	40	GLN
2	L	128	GLN
2	L	164	GLN
1	A	388	ASN
2	B	6	GLN
2	B	214	ASN
3	C	76	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [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(Å ²)	Q<0.9
1	A	189/223 (84%)	-0.32	0 100 100	117, 177, 248, 312	0
1	R	189/223 (84%)	-0.38	1 (0%) 91 83	114, 158, 224, 251	0
2	B	213/218 (97%)	-0.36	1 (0%) 91 83	127, 168, 213, 288	0
2	L	209/218 (95%)	-0.35	2 (0%) 82 70	100, 157, 245, 296	0
3	C	209/221 (94%)	-0.49	0 100 100	114, 153, 200, 242	0
3	H	206/221 (93%)	-0.48	0 100 100	90, 134, 189, 252	0
All	All	1215/1324 (91%)	-0.40	4 (0%) 94 88	90, 158, 231, 312	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	333	THR	3.3
2	L	151	GLN	3.2
2	L	158	LEU	3.1
2	B	162	ASN	2.4

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.