



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2021 – 07:26 PM JST

PDB ID : 7CHE
Title : Crystal structure of the SARS-CoV-2 RBD in complex with BD-236 Fab and BD-368-2 Fab
Authors : Xiao, J.; Zhu, Q.
Deposited on : 2020-07-05
Resolution : 3.42 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	:	2.18
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)	:	2.18

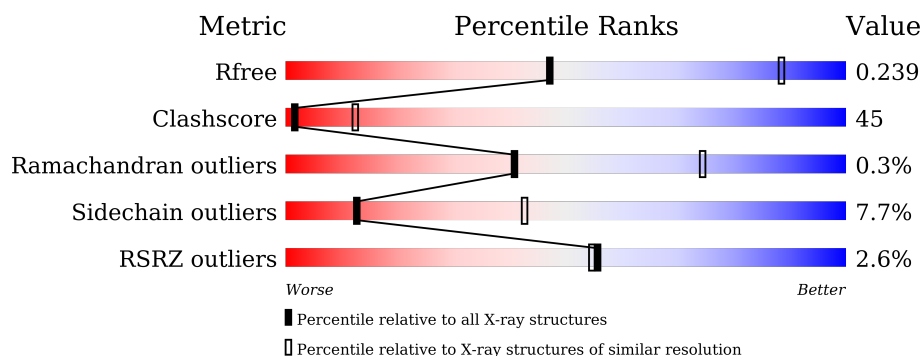
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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	H	223	<div> <div>7%</div> <div>43% 44% 8% 5%</div> </div>
2	L	214	<div> <div>51% 40% 7%</div> </div>
3	R	223	<div> <div>7%</div> <div>38% 39% 7% 15%</div> </div>
4	A	230	<div> <div>41% 42% 11% 5%</div> </div>
5	B	219	<div> <div>4%</div> <div>42% 49% 7%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7956 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 BD-236 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	212	Total	C	N	O	S	0	0	0
			1559	977	262	313	7			

- Molecule 2 is a protein called BD-236 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1604	1007	269	324	4			

- Molecule 3 is a protein called Spike protein S1.

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

- Molecule 4 is a protein called BD-368-2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	219	Total	C	N	O	S	0	0	0
			1636	1034	278	318	6			

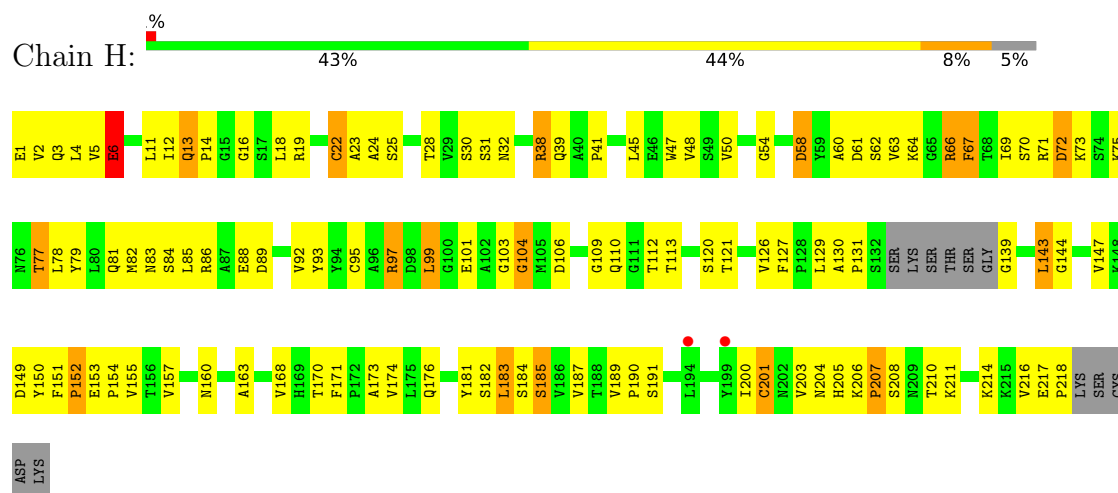
- Molecule 5 is a protein called BD-368-2 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	216	Total	C	N	O	S	0	0	0
			1659	1038	281	334	6			

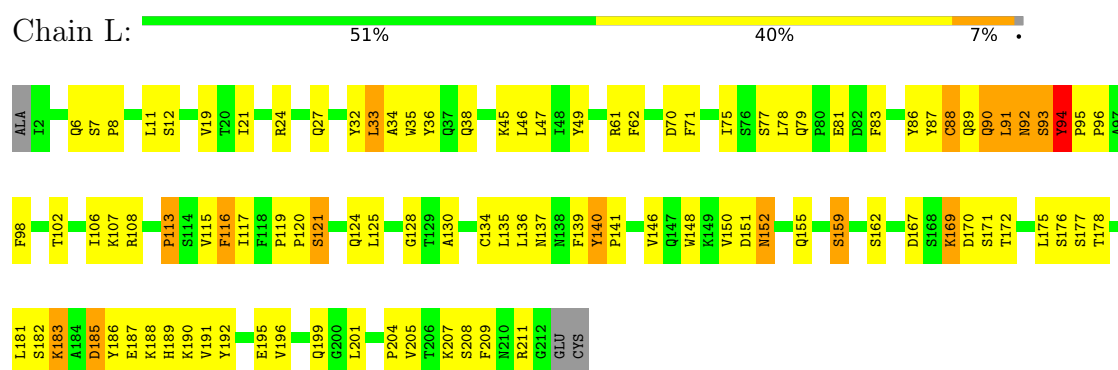
3 Residue-property plots

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.

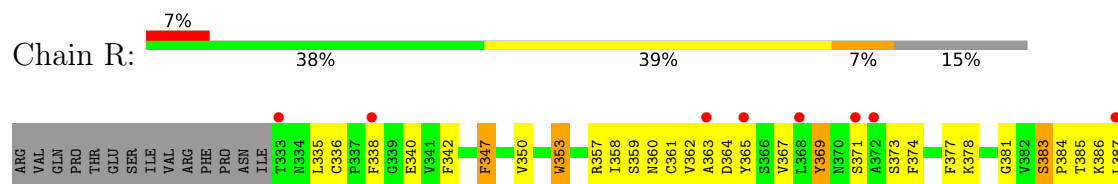
• Molecule 1: BD-236 Fab heavy chain

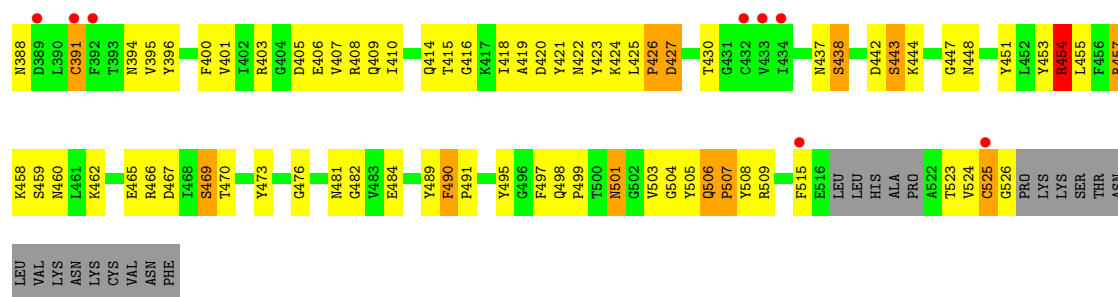


• Molecule 2: BD-236 Fab light chain



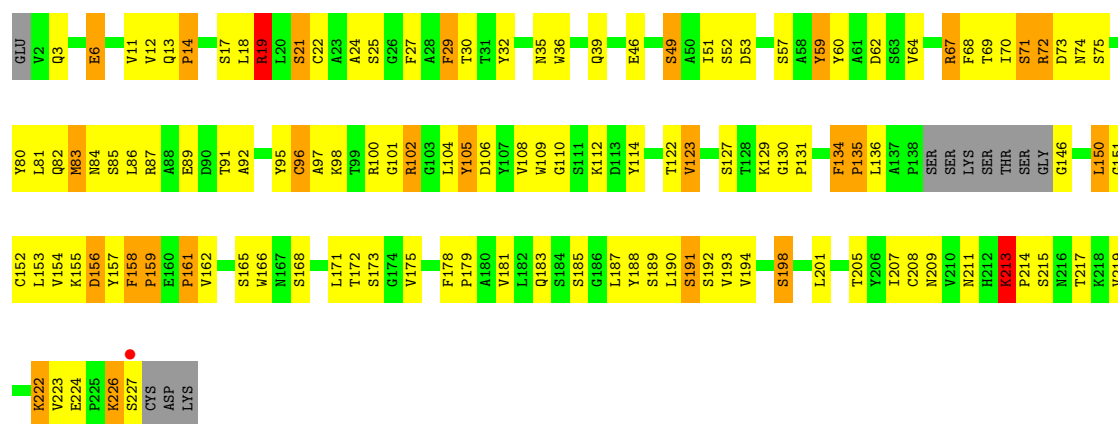
• Molecule 3: Spike protein S1





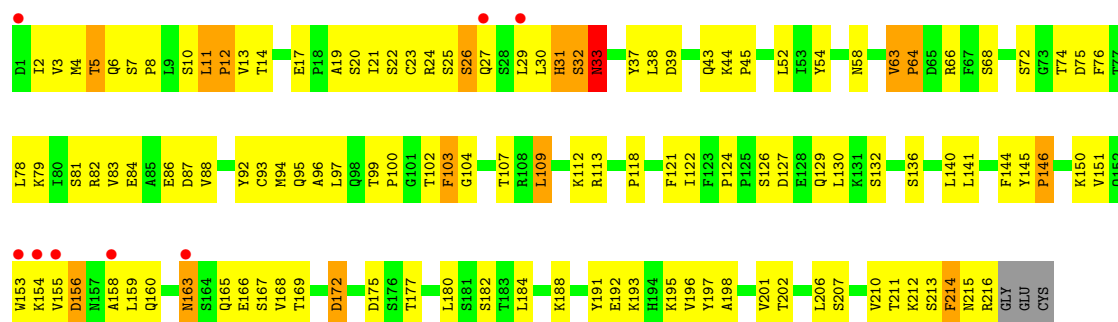
• Molecule 4: BD-368-2 Fab heavy chain

Chain A: 41% 42% 11% 5%



• Molecule 5: BD-368-2 Fab light chain

Chain B: 4% 42% 49% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.02Å 114.30Å 116.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 3.42 49.62 – 3.42	Depositor EDS
% Data completeness (in resolution range)	94.6 (49.62-3.42) 94.6 (49.62-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.225 , 0.239 0.225 , 0.239	Depositor DCC
R_{free} test set	1771 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7956	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	H	1.37	11/1591 (0.7%)	1.36	15/2166 (0.7%)
2	L	1.53	12/1639 (0.7%)	1.38	21/2227 (0.9%)
3	R	1.39	13/1538 (0.8%)	1.32	12/2090 (0.6%)
4	A	1.65	17/1675 (1.0%)	1.42	20/2280 (0.9%)
5	B	1.61	14/1695 (0.8%)	1.36	15/2303 (0.7%)
All	All	1.52	67/8138 (0.8%)	1.37	83/11066 (0.8%)

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
2	L	0	1
3	R	0	1
4	A	0	1
5	B	0	1
All	All	0	4

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	64	PRO	N-CD	-31.65	1.03	1.47
4	A	159	PRO	N-CD	-28.88	1.07	1.47
2	L	113	PRO	N-CD	-27.76	1.08	1.47
4	A	161	PRO	N-CD	-20.10	1.19	1.47
5	B	146	PRO	N-CA	13.56	1.70	1.47
1	H	154	PRO	N-CD	-13.30	1.29	1.47
1	H	207	PRO	N-CA	13.11	1.69	1.47
4	A	14	PRO	N-CA	13.06	1.69	1.47
1	H	152	PRO	N-CA	12.46	1.68	1.47
3	R	426	PRO	N-CA	12.36	1.68	1.47
3	R	507	PRO	N-CA	12.10	1.67	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	159	PRO	N-CA	12.05	1.67	1.47
5	B	12	PRO	N-CA	11.93	1.67	1.47
5	B	64	PRO	N-CA	11.61	1.67	1.47
4	A	161	PRO	N-CA	11.29	1.66	1.47
4	A	135	PRO	N-CA	10.95	1.65	1.47
2	L	204	PRO	N-CD	-9.48	1.34	1.47
1	H	41	PRO	N-CD	-9.31	1.34	1.47
3	R	484	GLU	CD-OE2	-8.46	1.16	1.25
4	A	130	GLY	C-N	8.11	1.49	1.34
3	R	462	LYS	C-N	8.04	1.49	1.34
3	R	383	SER	C-N	7.96	1.49	1.34
1	H	127	PHE	C-N	7.95	1.49	1.34
3	R	490	PHE	C-N	7.88	1.49	1.34
4	A	213	LYS	C-N	7.84	1.49	1.34
2	L	79	GLN	C-N	7.54	1.48	1.34
3	R	465	GLU	CD-OE1	-7.36	1.17	1.25
2	L	81	GLU	CD-OE1	-6.56	1.18	1.25
4	A	71	SER	CA-CB	-6.49	1.43	1.52
1	H	182	SER	CA-CB	-6.35	1.43	1.52
2	L	7	SER	CA-CB	-6.04	1.43	1.52
5	B	32	SER	CA-CB	-6.02	1.44	1.52
4	A	191	SER	CA-CB	-5.97	1.44	1.52
5	B	126	SER	CA-CB	-5.93	1.44	1.52
2	L	208	SER	CA-CB	-5.83	1.44	1.52
5	B	20	SER	CA-CB	-5.80	1.44	1.52
4	A	134	PHE	C-N	5.77	1.45	1.34
4	A	165	SER	CA-CB	-5.74	1.44	1.52
5	B	11	LEU	C-N	5.72	1.45	1.34
2	L	159	SER	CA-CB	-5.69	1.44	1.52
3	R	459	SER	CA-CB	-5.63	1.44	1.52
4	A	13	GLN	C-N	5.58	1.44	1.34
5	B	63	VAL	C-N	5.56	1.44	1.34
1	H	120	SER	CA-CB	-5.51	1.44	1.52
4	A	25	SER	CA-CB	-5.46	1.44	1.52
2	L	121	SER	CA-CB	-5.41	1.44	1.52
5	B	64	PRO	C-O	-5.39	1.12	1.23
3	R	506	GLN	C-N	5.38	1.44	1.34
5	B	145	TYR	C-N	5.34	1.44	1.34
2	L	141	PRO	N-CD	-5.31	1.40	1.47
2	L	81	GLU	CD-OE2	-5.30	1.19	1.25
5	B	10	SER	CA-CB	-5.29	1.45	1.52
3	R	425	LEU	C-N	5.24	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	465	GLU	CD-OE2	-5.24	1.19	1.25
3	R	443	SER	CA-CB	-5.21	1.45	1.52
1	H	151	PHE	C-N	5.20	1.44	1.34
3	R	484	GLU	CD-OE1	-5.18	1.20	1.25
1	H	6	GLU	CD-OE1	-5.16	1.20	1.25
4	A	158	PHE	C-N	5.11	1.44	1.34
1	H	70	SER	CA-CB	-5.11	1.45	1.52
2	L	141	PRO	C-O	-5.09	1.13	1.23
2	L	171	SER	CA-CB	-5.08	1.45	1.52
5	B	22	SER	CA-CB	-5.08	1.45	1.52
1	H	104	GLY	C-O	-5.08	1.15	1.23
4	A	135	PRO	C-O	-5.08	1.13	1.23
4	A	6	GLU	CD-OE1	-5.07	1.20	1.25
5	B	182	SER	CA-CB	-5.02	1.45	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	39	ASP	CB-CA-C	-13.10	84.21	110.40
1	H	154	PRO	CA-N-CD	11.89	128.34	111.70
1	H	153	GLU	C-N-CD	-10.30	97.94	120.60
5	B	12	PRO	CA-N-CD	-10.29	97.10	111.50
2	L	91	LEU	CB-CA-C	9.71	128.66	110.20
2	L	151	ASP	CB-CA-C	9.08	128.56	110.40
4	A	159	PRO	N-CD-CG	9.05	116.78	103.20
3	R	391	CYS	CA-CB-SG	9.01	130.22	114.00
5	B	64	PRO	N-CD-CG	8.86	116.49	103.20
4	A	14	PRO	CA-N-CD	-8.80	99.19	111.50
2	L	93	SER	N-CA-CB	8.77	123.65	110.50
2	L	93	SER	N-CA-C	-8.66	87.62	111.00
1	H	79	TYR	CB-CA-C	-8.64	93.12	110.40
5	B	146	PRO	CA-N-CD	-8.61	99.45	111.50
4	A	19	ARG	CG-CD-NE	-8.41	94.14	111.80
1	H	154	PRO	N-CA-CB	-8.30	93.34	103.30
1	H	67	PHE	CB-CA-C	-8.22	93.97	110.40
3	R	507	PRO	CA-N-CD	-8.14	100.10	111.50
3	R	501	ASN	CB-CA-C	-7.92	94.57	110.40
1	H	97	ARG	CB-CG-CD	-7.73	91.50	111.60
2	L	91	LEU	N-CA-C	-7.70	90.22	111.00
3	R	426	PRO	CA-N-CD	-7.61	100.84	111.50
4	A	161	PRO	N-CA-CB	-7.44	94.37	103.30
1	H	154	PRO	N-CD-CG	-7.27	92.29	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	92	ASN	N-CA-C	7.19	130.41	111.00
4	A	3	GLN	CB-CA-C	-6.92	96.57	110.40
4	A	161	PRO	CA-N-CD	-6.91	101.82	111.50
2	L	116	PHE	CB-CA-C	-6.73	96.94	110.40
1	H	154	PRO	N-CA-C	6.63	129.34	112.10
4	A	102	ARG	CG-CD-NE	-6.49	98.18	111.80
1	H	207	PRO	CA-N-CD	-6.44	102.48	111.50
5	B	172	ASP	CB-CA-C	-6.41	97.58	110.40
2	L	113	PRO	N-CA-CB	-6.37	95.60	102.60
2	L	45	LYS	CB-CA-C	-6.35	97.70	110.40
1	H	13	GLN	CB-CA-C	-6.23	97.93	110.40
2	L	137	ASN	CB-CA-C	-6.21	97.97	110.40
2	L	98	PHE	CB-CA-C	-6.21	97.98	110.40
2	L	141	PRO	N-CD-CG	-6.13	94.00	103.20
3	R	342	PHE	CB-CA-C	-6.13	98.14	110.40
4	A	159	PRO	CA-N-CD	-6.12	102.93	111.50
3	R	374	PHE	CB-CA-C	-6.09	98.23	110.40
2	L	199	GLN	CB-CA-C	-6.08	98.24	110.40
3	R	454	ARG	CG-CD-NE	-6.07	99.05	111.80
4	A	226	LYS	CB-CA-C	6.01	122.41	110.40
1	H	152	PRO	CA-N-CD	-6.00	103.10	111.50
3	R	442	ASP	CB-CA-C	5.89	122.18	110.40
4	A	72	ARG	NE-CZ-NH1	-5.81	117.39	120.30
5	B	103	PHE	CB-CA-C	-5.78	98.84	110.40
1	H	32	ASN	CB-CA-C	-5.69	99.01	110.40
4	A	14	PRO	N-CA-C	-5.67	97.37	112.10
2	L	94	TYR	N-CA-CB	5.62	120.72	110.60
3	R	415	THR	CB-CA-C	-5.61	96.46	111.60
2	L	108	ARG	CG-CD-NE	-5.61	100.02	111.80
3	R	391	CYS	N-CA-CB	5.61	120.69	110.60
3	R	451	TYR	CA-CB-CG	-5.57	102.82	113.40
2	L	204	PRO	CB-CA-C	-5.55	98.12	112.00
3	R	457	ARG	NE-CZ-NH1	-5.54	117.53	120.30
4	A	135	PRO	CA-N-CD	-5.50	103.79	111.50
2	L	119	PRO	N-CD-CG	-5.47	95.00	103.20
4	A	123	VAL	CA-CB-CG1	5.46	119.09	110.90
4	A	95	TYR	CB-CA-C	-5.46	99.48	110.40
5	B	211	THR	CB-CA-C	-5.46	96.87	111.60
5	B	5	THR	CB-CA-C	-5.43	96.93	111.60
2	L	90	GLN	CB-CA-C	-5.36	99.68	110.40
1	H	77	THR	N-CA-CB	5.36	120.48	110.30
4	A	46	GLU	CB-CA-C	-5.32	99.76	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	177	THR	CB-CA-C	-5.32	97.24	111.60
5	B	30	LEU	O-C-N	5.31	131.20	122.70
2	L	92	ASN	CB-CA-C	-5.29	99.81	110.40
4	A	105	TYR	CB-CA-C	5.29	120.98	110.40
4	A	60	TYR	CB-CA-C	-5.28	99.83	110.40
2	L	87	TYR	CB-CA-C	-5.28	99.84	110.40
5	B	79	LYS	CB-CA-C	-5.27	99.85	110.40
1	H	97	ARG	CG-CD-NE	5.27	122.87	111.80
1	H	66	ARG	CG-CD-NE	-5.27	100.74	111.80
5	B	33	ASN	CB-CA-C	-5.20	100.00	110.40
2	L	113	PRO	N-CD-CG	5.19	110.98	103.20
4	A	152	CYS	CA-CB-SG	-5.13	104.77	114.00
5	B	169	THR	CB-CA-C	-5.11	97.81	111.60
4	A	82	GLN	CB-CA-C	-5.09	100.22	110.40
5	B	64	PRO	CA-N-CD	-5.09	104.38	111.50
5	B	156	ASP	CB-CA-C	5.07	120.53	110.40
4	A	172	THR	CB-CA-C	-5.04	97.99	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	62	ASP	Mainchain
5	B	32	SER	Mainchain
2	L	140	TYR	Peptide
3	R	501	ASN	Mainchain

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	H	1559	0	1534	158	0
2	L	1604	0	1569	125	1
3	R	1498	0	1408	138	0
4	A	1636	0	1597	172	1
5	B	1659	0	1616	160	0
All	All	7956	0	7724	703	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 45.

All (703) 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)
4:A:68:PHE:CD1	4:A:83:MET:HB2	1.44	1.51
4:A:68:PHE:CE1	4:A:83:MET:HB2	1.43	1.51
5:B:153:TRP:CG	5:B:184:LEU:HD11	1.48	1.48
1:H:207:PRO:CA	1:H:207:PRO:N	1.69	1.43
3:R:507:PRO:N	3:R:507:PRO:CA	1.67	1.43
5:B:146:PRO:N	5:B:146:PRO:CA	1.70	1.43
4:A:159:PRO:N	4:A:159:PRO:CA	1.67	1.43
3:R:426:PRO:N	3:R:426:PRO:CA	1.68	1.42
5:B:153:TRP:CD2	5:B:184:LEU:HD13	1.54	1.42
4:A:14:PRO:CA	4:A:14:PRO:N	1.69	1.39
1:H:152:PRO:CA	1:H:152:PRO:N	1.68	1.39
5:B:153:TRP:CD2	5:B:184:LEU:CD1	2.06	1.39
4:A:68:PHE:CD1	4:A:83:MET:CB	2.08	1.37
5:B:12:PRO:N	5:B:12:PRO:CA	1.67	1.36
5:B:129:GLN:NE2	5:B:136:SER:OG	1.57	1.36
4:A:222:LYS:NZ	4:A:224:GLU:CG	1.92	1.32
3:R:357:ARG:HD2	3:R:396:TYR:CE1	1.66	1.31
3:R:369:TYR:CE2	3:R:384:PRO:HG3	1.64	1.31
4:A:68:PHE:CG	4:A:83:MET:HB3	1.65	1.30
4:A:222:LYS:NZ	4:A:224:GLU:CD	1.86	1.29
3:R:437:ASN:ND2	3:R:508:TYR:OH	1.61	1.28
5:B:153:TRP:CG	5:B:184:LEU:CD1	2.16	1.26
1:H:86:ARG:HD3	1:H:88:GLU:OE1	1.33	1.26
1:H:86:ARG:CD	1:H:88:GLU:OE1	1.83	1.25
4:A:67:ARG:CZ	4:A:87:ARG:NH1	2.01	1.22
4:A:68:PHE:CE2	4:A:83:MET:SD	2.36	1.18
3:R:361:CYS:O	3:R:524:VAL:HA	1.43	1.17
4:A:101:GLY:HA3	4:A:106:ASP:OD2	1.02	1.16
4:A:222:LYS:HZ2	4:A:224:GLU:CD	1.43	1.15
4:A:68:PHE:CE1	4:A:83:MET:CB	2.25	1.14
4:A:101:GLY:CA	4:A:106:ASP:OD2	1.96	1.13
4:A:222:LYS:HZ1	4:A:224:GLU:CG	1.53	1.10
4:A:222:LYS:HZ1	4:A:224:GLU:HG3	1.02	1.09
4:A:68:PHE:CD2	4:A:83:MET:HB3	1.86	1.08
1:H:6:GLU:OE2	1:H:109:GLY:HA3	1.53	1.08
5:B:129:GLN:O	5:B:132:SER:HB2	1.54	1.07
4:A:67:ARG:HG2	4:A:85:SER:OG	1.52	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:150:VAL:CG1	2:L:189:HIS:HD2	1.68	1.06
4:A:183:GLN:O	4:A:185:SER:O	1.73	1.05
4:A:222:LYS:NZ	4:A:224:GLU:HG3	1.56	1.05
3:R:357:ARG:HD2	3:R:396:TYR:HE1	0.94	1.04
1:H:86:ARG:CB	1:H:88:GLU:OE1	2.06	1.04
4:A:30:THR:HG22	4:A:74:ASN:HB3	1.37	1.03
4:A:68:PHE:CG	4:A:83:MET:CB	2.32	1.03
5:B:191:TYR:CD1	5:B:197:TYR:CE2	2.46	1.03
3:R:437:ASN:ND2	3:R:508:TYR:CZ	2.26	1.02
5:B:153:TRP:CE3	5:B:184:LEU:HD13	1.95	1.01
4:A:156:ASP:OD1	4:A:183:GLN:NE2	1.94	1.01
1:H:139:GLY:C	1:H:191:SER:HG	1.64	1.01
3:R:369:TYR:CE2	3:R:384:PRO:CG	2.44	1.01
3:R:362:VAL:HB	3:R:525:CYS:H	1.25	1.01
1:H:139:GLY:O	1:H:191:SER:OG	1.81	0.99
5:B:168:VAL:HG22	5:B:180:LEU:HD13	1.40	0.99
2:L:93:SER:OG	3:R:505:TYR:OH	1.80	0.98
5:B:191:TYR:HA	5:B:197:TYR:OH	1.63	0.97
5:B:153:TRP:CE2	5:B:184:LEU:HD13	1.99	0.96
5:B:130:LEU:O	5:B:188:LYS:HD2	1.65	0.96
4:A:68:PHE:CZ	4:A:83:MET:SD	2.59	0.96
5:B:153:TRP:CB	5:B:184:LEU:HD11	1.97	0.95
3:R:482:GLY:O	4:A:104:LEU:O	1.85	0.95
2:L:120:PRO:HG2	2:L:186:TYR:CE2	2.01	0.94
2:L:93:SER:HG	3:R:505:TYR:HH	1.13	0.94
5:B:150:LYS:O	5:B:202:THR:HG22	1.65	0.94
2:L:150:VAL:HG11	2:L:189:HIS:HD2	1.31	0.93
5:B:197:TYR:HB2	5:B:214:PHE:CE1	2.03	0.93
1:H:19:ARG:HD3	1:H:81:GLN:NE2	1.84	0.93
3:R:357:ARG:CD	3:R:396:TYR:HE1	1.82	0.93
2:L:33:LEU:HD12	2:L:71:PHE:CG	2.04	0.92
1:H:95:CYS:O	1:H:95:CYS:SG	2.28	0.92
3:R:444:LYS:O	3:R:499:PRO:HD3	1.69	0.92
2:L:33:LEU:HD23	2:L:89:GLN:O	1.70	0.91
5:B:198:ALA:HB2	5:B:213:SER:HB2	1.48	0.91
4:A:136:LEU:HB2	4:A:151:GLY:O	1.68	0.91
3:R:369:TYR:HD2	3:R:384:PRO:CB	1.83	0.91
5:B:191:TYR:HD1	5:B:197:TYR:CZ	1.89	0.91
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.53	0.91
1:H:86:ARG:HB2	1:H:88:GLU:HG2	1.53	0.90
3:R:357:ARG:CZ	3:R:394:ASN:ND2	2.34	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:CYS:O	1:H:201:CYS:SG	2.30	0.90
3:R:357:ARG:NH2	3:R:394:ASN:ND2	2.19	0.89
3:R:361:CYS:O	3:R:524:VAL:CA	2.20	0.89
5:B:191:TYR:HD1	5:B:197:TYR:CE2	1.87	0.89
2:L:150:VAL:CG1	2:L:189:HIS:CD2	2.56	0.88
4:A:67:ARG:NH1	4:A:87:ARG:CZ	2.35	0.88
5:B:13:VAL:HG12	5:B:14:THR:H	1.36	0.88
5:B:191:TYR:CE1	5:B:197:TYR:HE2	1.91	0.88
3:R:369:TYR:HD2	3:R:384:PRO:HB2	1.38	0.88
4:A:91:THR:OG1	4:A:122:THR:HA	1.73	0.88
3:R:388:ASN:O	3:R:526:GLY:C	2.13	0.88
3:R:357:ARG:CD	3:R:396:TYR:CE1	2.55	0.87
5:B:84:GLU:O	5:B:87:ASP:OD1	1.93	0.87
5:B:11:LEU:HD21	5:B:19:ALA:HB1	1.55	0.87
5:B:153:TRP:CE2	5:B:184:LEU:CD1	2.58	0.87
1:H:19:ARG:HD3	1:H:81:GLN:HE21	1.39	0.87
4:A:67:ARG:NH1	4:A:87:ARG:NH1	2.23	0.87
4:A:104:LEU:H	4:A:104:LEU:HD23	1.38	0.87
3:R:395:VAL:HG23	3:R:515:PHE:CD1	2.10	0.87
3:R:369:TYR:HE2	3:R:384:PRO:HG3	1.02	0.86
4:A:222:LYS:CE	4:A:224:GLU:HG3	2.05	0.86
5:B:141:LEU:HD11	5:B:201:VAL:HG11	1.58	0.86
2:L:183:LYS:HE3	2:L:187:GLU:OE2	1.75	0.86
3:R:369:TYR:HE2	3:R:384:PRO:CG	1.83	0.86
3:R:369:TYR:CD2	3:R:384:PRO:CG	2.57	0.86
2:L:150:VAL:HG13	2:L:192:TYR:CE1	2.11	0.85
5:B:191:TYR:CE1	5:B:197:TYR:CE2	2.65	0.85
4:A:68:PHE:CZ	4:A:83:MET:CB	2.59	0.84
3:R:503:VAL:HA	3:R:506:GLN:OE1	1.76	0.84
4:A:157:TYR:CE1	4:A:162:VAL:CG2	2.59	0.84
1:H:217:GLU:HG2	1:H:218:PRO:HD2	1.56	0.84
1:H:86:ARG:HB3	1:H:88:GLU:OE1	1.74	0.84
4:A:131:PRO:HB3	4:A:157:TYR:HB3	1.60	0.84
3:R:369:TYR:CD2	3:R:384:PRO:HG3	2.13	0.83
4:A:222:LYS:HZ2	4:A:224:GLU:CG	1.74	0.83
4:A:161:PRO:HD2	4:A:161:PRO:O	1.79	0.83
2:L:34:ALA:HB2	2:L:91:LEU:HD11	1.61	0.82
2:L:21:ILE:HD13	2:L:102:THR:HG21	1.61	0.82
1:H:150:TYR:OH	1:H:183:LEU:CD2	2.26	0.82
2:L:150:VAL:HG12	2:L:189:HIS:CD2	2.14	0.82
3:R:335:LEU:HD12	3:R:335:LEU:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:191:TYR:CD1	5:B:197:TYR:HE2	1.94	0.82
5:B:197:TYR:HB2	5:B:214:PHE:HE1	1.42	0.82
1:H:62:SER:O	1:H:66:ARG:NH2	2.13	0.81
1:H:205:HIS:CD2	1:H:207:PRO:HD2	2.15	0.81
5:B:8:PRO:O	5:B:107:THR:HG23	1.80	0.81
4:A:157:TYR:CZ	4:A:162:VAL:CG2	2.63	0.81
5:B:198:ALA:HB2	5:B:213:SER:CB	2.10	0.81
5:B:153:TRP:CD2	5:B:184:LEU:HD11	1.91	0.81
4:A:68:PHE:CZ	4:A:83:MET:CG	2.63	0.81
5:B:151:VAL:HG12	5:B:201:VAL:HG22	1.61	0.81
2:L:33:LEU:HD12	2:L:71:PHE:CD2	2.16	0.80
3:R:405:ASP:HB3	3:R:504:GLY:O	1.82	0.80
3:R:405:ASP:CB	3:R:504:GLY:O	2.30	0.79
5:B:155:VAL:HG13	5:B:197:TYR:CD1	2.17	0.79
3:R:369:TYR:CD2	3:R:384:PRO:CB	2.66	0.79
4:A:12:VAL:HG21	4:A:86:LEU:HD12	1.64	0.79
3:R:362:VAL:CB	3:R:525:CYS:H	1.95	0.79
1:H:139:GLY:C	1:H:191:SER:OG	2.17	0.79
1:H:86:ARG:CD	1:H:88:GLU:CD	2.52	0.78
1:H:66:ARG:O	1:H:83:ASN:HB2	1.82	0.78
1:H:38:ARG:HG2	1:H:48:VAL:CG2	2.13	0.78
1:H:39:GLN:NE2	2:L:38:GLN:OE1	2.16	0.78
1:H:77:THR:HG22	1:H:78:LEU:H	1.47	0.78
1:H:101:GLU:OE1	3:R:453:TYR:OH	2.01	0.78
4:A:67:ARG:CZ	4:A:87:ARG:HH12	1.96	0.77
1:H:23:ALA:N	1:H:77:THR:HG23	1.99	0.77
5:B:99:THR:HG23	5:B:100:PRO:HD3	1.65	0.77
2:L:32:TYR:HD2	2:L:92:ASN:ND2	1.81	0.77
5:B:172:ASP:OD2	5:B:175:ASP:OD1	2.03	0.76
1:H:208:SER:HG	1:H:210:THR:HG1	1.24	0.76
1:H:86:ARG:CG	1:H:88:GLU:OE1	2.33	0.76
2:L:169:LYS:HA	2:L:169:LYS:HE2	1.67	0.76
5:B:206:LEU:HD13	5:B:210:VAL:HG23	1.65	0.76
3:R:444:LYS:O	3:R:499:PRO:CD	2.32	0.76
1:H:61:ASP:HA	1:H:64:LYS:HD2	1.67	0.75
2:L:150:VAL:HG12	2:L:189:HIS:HD2	1.48	0.75
1:H:77:THR:HG22	1:H:78:LEU:N	2.01	0.75
1:H:149:ASP:OD1	1:H:176:GLN:NE2	2.20	0.75
1:H:82:MET:HE1	1:H:93:TYR:CZ	2.22	0.74
5:B:153:TRP:CD1	5:B:184:LEU:CD1	2.69	0.74
1:H:86:ARG:HD2	1:H:88:GLU:CD	2.08	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:191:TYR:CA	5:B:197:TYR:OH	2.35	0.74
1:H:71:ARG:HE	1:H:73:LYS:HE2	1.52	0.74
1:H:170:THR:OG1	1:H:185:SER:HB2	1.87	0.74
1:H:47:TRP:CB	2:L:96:PRO:CG	2.66	0.74
2:L:90:GLN:OE1	2:L:93:SER:HB2	1.87	0.74
1:H:6:GLU:H	1:H:110:GLN:HE21	1.36	0.73
5:B:38:LEU:HD22	5:B:94:MET:O	1.87	0.73
3:R:503:VAL:HG12	3:R:506:GLN:OE1	1.89	0.73
5:B:52:LEU:HA	5:B:63:VAL:HG21	1.68	0.73
4:A:157:TYR:CZ	4:A:162:VAL:HG23	2.22	0.73
3:R:357:ARG:NH2	3:R:394:ASN:HD22	1.86	0.73
5:B:24:ARG:HD3	5:B:75:ASP:OD1	1.88	0.73
4:A:14:PRO:N	4:A:14:PRO:C	2.41	0.72
4:A:67:ARG:HG2	4:A:67:ARG:HH11	1.53	0.71
3:R:361:CYS:O	3:R:524:VAL:CB	2.38	0.71
3:R:490:PHE:CD1	3:R:491:PRO:HD2	2.26	0.71
4:A:157:TYR:CE1	4:A:162:VAL:HG23	2.25	0.71
1:H:86:ARG:HB2	1:H:88:GLU:CG	2.20	0.71
3:R:403:ARG:HG2	3:R:505:TYR:HA	1.73	0.71
4:A:51:ILE:HG21	4:A:72:ARG:HD2	1.71	0.71
1:H:6:GLU:H	1:H:110:GLN:NE2	1.88	0.71
5:B:38:LEU:CD2	5:B:94:MET:O	2.39	0.70
3:R:385:THR:HG23	3:R:386:LYS:H	1.56	0.70
2:L:186:TYR:HE1	2:L:211:ARG:HG2	1.57	0.70
3:R:457:ARG:HG2	3:R:457:ARG:HH11	1.55	0.70
2:L:185:ASP:HA	2:L:188:LYS:HG3	1.73	0.70
4:A:222:LYS:CE	4:A:224:GLU:CG	2.68	0.70
5:B:159:LEU:HD23	5:B:160:GLN:O	1.92	0.70
5:B:118:PRO:CB	5:B:141:LEU:HD12	2.22	0.70
2:L:148:TRP:HE1	2:L:177:SER:HG	1.38	0.69
1:H:72:ASP:OD1	1:H:75:LYS:HG3	1.91	0.69
3:R:357:ARG:CZ	3:R:394:ASN:HD22	2.04	0.69
1:H:13:GLN:CD	1:H:13:GLN:H	1.95	0.69
5:B:118:PRO:HG3	5:B:141:LEU:HD12	1.74	0.69
3:R:350:VAL:HG22	3:R:422:ASN:HB3	1.74	0.69
3:R:395:VAL:CG2	3:R:515:PHE:CE1	2.75	0.69
4:A:207:ILE:HG22	4:A:209:ASN:ND2	2.07	0.69
1:H:50:VAL:HG21	2:L:94:TYR:OH	1.92	0.69
1:H:143:LEU:HD12	1:H:216:VAL:HG11	1.73	0.69
5:B:12:PRO:N	5:B:12:PRO:C	2.47	0.68
1:H:22:CYS:C	1:H:77:THR:HG23	2.14	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:67:ARG:HG2	4:A:85:SER:HG	1.58	0.68
4:A:68:PHE:CD2	4:A:83:MET:CB	2.68	0.68
2:L:150:VAL:HG11	2:L:189:HIS:CD2	2.21	0.68
5:B:84:GLU:N	5:B:87:ASP:OD1	2.23	0.68
2:L:116:PHE:HD2	2:L:135:LEU:HD23	1.57	0.68
1:H:150:TYR:CE2	1:H:155:VAL:HG21	2.28	0.68
4:A:97:ALA:HB1	4:A:112:LYS:HB3	1.75	0.68
2:L:152:ASN:O	2:L:152:ASN:ND2	2.26	0.68
4:A:193:VAL:HG11	5:B:140:LEU:HD13	1.74	0.68
4:A:157:TYR:CZ	4:A:162:VAL:HG21	2.29	0.67
4:A:193:VAL:HG21	5:B:140:LEU:HD11	1.75	0.67
5:B:13:VAL:HG12	5:B:14:THR:N	2.09	0.67
2:L:181:LEU:HD12	2:L:181:LEU:O	1.93	0.67
4:A:190:LEU:HD12	4:A:190:LEU:C	2.14	0.67
3:R:457:ARG:NE	3:R:467:ASP:OD2	2.24	0.67
4:A:35:ASN:HB3	4:A:49:SER:O	1.95	0.67
4:A:183:GLN:HA	5:B:165:GLN:HE22	1.58	0.67
4:A:67:ARG:CZ	4:A:87:ARG:CZ	2.70	0.67
4:A:105:TYR:O	5:B:37:TYR:OH	2.08	0.67
1:H:92:VAL:HG22	1:H:113:THR:HG22	1.77	0.67
4:A:205:THR:HG23	4:A:205:THR:O	1.94	0.67
3:R:406:GLU:OE1	3:R:495:TYR:OH	2.05	0.67
4:A:67:ARG:NH1	4:A:87:ARG:NH2	2.42	0.67
2:L:120:PRO:CG	2:L:186:TYR:CE2	2.78	0.66
5:B:24:ARG:HG2	5:B:75:ASP:HA	1.77	0.66
3:R:357:ARG:CZ	3:R:394:ASN:HD21	2.08	0.66
3:R:362:VAL:HB	3:R:525:CYS:N	2.06	0.66
4:A:222:LYS:HZ1	4:A:224:GLU:CD	1.72	0.66
1:H:6:GLU:OE2	1:H:109:GLY:CA	2.39	0.66
5:B:17:GLU:O	5:B:83:VAL:HG23	1.95	0.66
4:A:67:ARG:NH2	4:A:87:ARG:NH1	2.42	0.66
1:H:11:LEU:HD22	1:H:152:PRO:HD3	1.78	0.66
5:B:4:MET:HE3	5:B:23:CYS:SG	2.36	0.66
1:H:1:GLU:HG3	1:H:2:VAL:HG23	1.78	0.65
3:R:409:GLN:OE1	3:R:416:GLY:HA3	1.96	0.65
3:R:405:ASP:HB2	3:R:504:GLY:O	1.96	0.65
4:A:68:PHE:CE2	4:A:83:MET:CB	2.79	0.65
4:A:146:GLY:O	4:A:198:SER:N	2.25	0.65
4:A:68:PHE:CE2	4:A:83:MET:HB3	2.32	0.65
5:B:153:TRP:O	5:B:160:GLN:N	2.25	0.65
4:A:222:LYS:NZ	4:A:224:GLU:OE1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:TRP:HB2	2:L:96:PRO:HG3	1.79	0.65
1:H:217:GLU:HG2	1:H:218:PRO:CD	2.25	0.65
2:L:116:PHE:CD2	2:L:135:LEU:HD23	2.31	0.64
1:H:6:GLU:N	1:H:110:GLN:NE2	2.44	0.64
1:H:47:TRP:CD2	2:L:96:PRO:HD3	2.33	0.64
1:H:47:TRP:HB2	2:L:96:PRO:CG	2.26	0.64
3:R:395:VAL:HG21	3:R:515:PHE:CE1	2.32	0.64
1:H:22:CYS:H	1:H:77:THR:CG2	2.10	0.64
2:L:170:ASP:OD1	2:L:170:ASP:N	2.25	0.64
3:R:457:ARG:HG2	3:R:457:ARG:NH1	2.13	0.64
5:B:160:GLN:HA	5:B:160:GLN:OE1	1.98	0.64
4:A:68:PHE:CD2	4:A:81:LEU:HD21	2.33	0.64
5:B:191:TYR:CD1	5:B:197:TYR:CZ	2.76	0.63
2:L:32:TYR:CD2	2:L:92:ASN:ND2	2.66	0.63
3:R:391:CYS:HA	3:R:525:CYS:HB3	1.80	0.63
5:B:150:LYS:O	5:B:202:THR:CG2	2.44	0.63
1:H:14:PRO:C	1:H:16:GLY:H	2.01	0.63
1:H:22:CYS:O	1:H:22:CYS:SG	2.57	0.63
1:H:82:MET:CE	1:H:93:TYR:CZ	2.82	0.63
3:R:336:CYS:H	3:R:363:ALA:HB2	1.63	0.63
3:R:369:TYR:HD1	3:R:369:TYR:O	1.81	0.63
4:A:98:LYS:HE3	4:A:114:TYR:HD1	1.64	0.63
1:H:47:TRP:HB3	2:L:96:PRO:HD2	1.80	0.63
4:A:159:PRO:N	4:A:159:PRO:C	2.47	0.62
3:R:371:SER:OG	3:R:373:SER:OG	2.15	0.62
1:H:82:MET:CE	1:H:93:TYR:CE2	2.82	0.62
4:A:89:GLU:OE1	4:A:89:GLU:N	2.30	0.62
5:B:118:PRO:CG	5:B:141:LEU:HD12	2.28	0.62
1:H:19:ARG:CD	1:H:81:GLN:HE21	2.11	0.62
1:H:173:ALA:HB2	1:H:183:LEU:HD22	1.79	0.62
3:R:438:SER:HB3	3:R:507:PRO:O	1.98	0.62
4:A:127:SER:O	4:A:158:PHE:HD1	1.83	0.62
1:H:12:ILE:HG23	1:H:12:ILE:O	1.99	0.62
1:H:19:ARG:HB2	1:H:81:GLN:NE2	2.15	0.62
1:H:103:GLY:HA2	2:L:49:TYR:CG	2.35	0.62
3:R:481:ASN:HB3	5:B:33:ASN:HB2	1.81	0.62
4:A:12:VAL:HG11	4:A:18:LEU:HB2	1.81	0.62
1:H:47:TRP:CE3	2:L:96:PRO:HD3	2.35	0.62
1:H:61:ASP:HA	1:H:64:LYS:CD	2.30	0.62
4:A:207:ILE:CG2	4:A:209:ASN:ND2	2.62	0.62
5:B:155:VAL:HG11	5:B:197:TYR:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:ARG:HD3	1:H:84:SER:O	1.99	0.62
5:B:130:LEU:O	5:B:188:LYS:CD	2.45	0.62
3:R:357:ARG:NE	3:R:394:ASN:HD22	1.97	0.61
2:L:113:PRO:HB3	2:L:139:PHE:CD2	2.35	0.61
1:H:72:ASP:OD1	1:H:75:LYS:N	2.33	0.61
3:R:357:ARG:NE	3:R:394:ASN:ND2	2.48	0.61
3:R:361:CYS:O	3:R:524:VAL:HB	1.99	0.61
4:A:135:PRO:O	4:A:135:PRO:HG2	2.00	0.61
2:L:6:GLN:HG2	2:L:88:CYS:SG	2.40	0.61
2:L:78:LEU:HD21	2:L:106:ILE:CD1	2.30	0.61
4:A:64:VAL:HG12	4:A:64:VAL:O	2.00	0.61
1:H:67:PHE:HD1	1:H:82:MET:HA	1.66	0.61
5:B:141:LEU:HD11	5:B:201:VAL:CG1	2.30	0.61
5:B:155:VAL:CG1	5:B:197:TYR:CD1	2.84	0.61
2:L:146:VAL:HG22	2:L:196:VAL:HG22	1.83	0.61
3:R:357:ARG:HD2	3:R:396:TYR:CZ	2.29	0.61
4:A:32:TYR:CE1	4:A:102:ARG:HD3	2.35	0.61
4:A:134:PHE:CE2	5:B:129:GLN:HG3	2.36	0.61
4:A:215:SER:OG	4:A:217:THR:OG1	2.14	0.60
1:H:61:ASP:OD1	1:H:64:LYS:NZ	2.31	0.60
3:R:437:ASN:CG	3:R:508:TYR:CZ	2.74	0.60
4:A:104:LEU:HD23	4:A:104:LEU:N	2.14	0.60
1:H:72:ASP:CG	1:H:75:LYS:HG3	2.20	0.60
5:B:118:PRO:HG3	5:B:141:LEU:CD1	2.31	0.60
5:B:191:TYR:CD1	5:B:197:TYR:OH	2.55	0.60
1:H:47:TRP:CE3	2:L:96:PRO:CD	2.85	0.60
2:L:152:ASN:HD22	2:L:152:ASN:C	2.03	0.60
3:R:395:VAL:HG21	3:R:515:PHE:HE1	1.66	0.60
5:B:141:LEU:HD21	5:B:201:VAL:HG21	1.82	0.60
2:L:150:VAL:HG23	2:L:155:GLN:HG3	1.84	0.60
4:A:193:VAL:HG11	5:B:140:LEU:CD1	2.31	0.60
3:R:408:ARG:NH1	3:R:414:GLN:HE22	2.00	0.60
4:A:24:ALA:HB1	4:A:27:PHE:CE1	2.36	0.60
1:H:47:TRP:CB	2:L:96:PRO:HG3	2.31	0.59
1:H:157:VAL:HG22	1:H:203:VAL:HG22	1.84	0.59
2:L:120:PRO:CG	2:L:186:TYR:HE2	2.15	0.59
1:H:112:THR:O	1:H:112:THR:HG23	2.03	0.59
4:A:157:TYR:CE2	4:A:162:VAL:HG21	2.38	0.59
3:R:395:VAL:HG23	3:R:515:PHE:CE1	2.38	0.59
4:A:104:LEU:H	4:A:104:LEU:CD2	2.13	0.59
5:B:24:ARG:HG2	5:B:74:THR:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:191:TYR:HD1	5:B:197:TYR:OH	1.85	0.59
4:A:11:VAL:CG1	4:A:159:PRO:HB3	2.33	0.58
4:A:161:PRO:O	4:A:161:PRO:CD	2.48	0.58
5:B:3:VAL:HG12	5:B:26:SER:HB2	1.85	0.58
5:B:153:TRP:CE3	5:B:184:LEU:CD1	2.68	0.58
5:B:196:VAL:HG13	5:B:196:VAL:O	2.02	0.58
4:A:30:THR:HG22	4:A:74:ASN:CB	2.23	0.58
2:L:120:PRO:HG2	2:L:186:TYR:HE2	1.62	0.58
5:B:122:ILE:HG23	5:B:122:ILE:O	2.02	0.58
3:R:458:LYS:HD2	3:R:473:TYR:CE1	2.39	0.58
2:L:78:LEU:CD2	2:L:106:ILE:CD1	2.82	0.58
2:L:167:ASP:OD1	2:L:170:ASP:OD1	2.22	0.58
3:R:357:ARG:NH2	3:R:394:ASN:HD21	2.02	0.58
1:H:47:TRP:HB3	2:L:96:PRO:CD	2.34	0.57
1:H:86:ARG:HB2	1:H:88:GLU:OE1	1.97	0.57
3:R:470:THR:HB	3:R:490:PHE:HE1	1.69	0.57
5:B:4:MET:CE	5:B:23:CYS:SG	2.92	0.57
4:A:67:ARG:HG2	4:A:67:ARG:NH1	2.17	0.57
5:B:168:VAL:CG2	5:B:180:LEU:HD13	2.26	0.57
2:L:36:TYR:CE1	2:L:89:GLN:OE1	2.58	0.57
3:R:458:LYS:HD2	3:R:473:TYR:HE1	1.69	0.57
1:H:106:ASP:OD1	1:H:106:ASP:N	2.34	0.57
2:L:201:LEU:HD13	2:L:205:VAL:HG13	1.86	0.57
3:R:353:TRP:O	3:R:466:ARG:NH1	2.38	0.57
4:A:178:PHE:HB3	4:A:179:PRO:CD	2.34	0.57
5:B:27:GLN:HA	5:B:27:GLN:OE1	2.04	0.57
1:H:67:PHE:CD1	1:H:82:MET:HA	2.40	0.57
1:H:200:ILE:HG22	1:H:200:ILE:O	2.03	0.57
2:L:113:PRO:HB3	2:L:139:PHE:CB	2.33	0.57
4:A:73:ASP:OD2	4:A:75:SER:OG	2.22	0.57
4:A:168:SER:HA	4:A:209:ASN:OD1	2.05	0.57
5:B:197:TYR:CB	5:B:214:PHE:HE1	2.14	0.57
2:L:107:LYS:HG3	2:L:140:TYR:OH	2.05	0.56
5:B:202:THR:HG23	5:B:202:THR:O	2.04	0.56
1:H:38:ARG:HG2	1:H:48:VAL:HG23	1.86	0.56
1:H:77:THR:CG2	1:H:78:LEU:H	2.19	0.56
4:A:29:PHE:CE1	4:A:72:ARG:NH2	2.74	0.56
4:A:83:MET:HG3	4:A:86:LEU:HD21	1.86	0.56
5:B:129:GLN:NE2	5:B:136:SER:CB	2.63	0.56
4:A:219:VAL:HG12	4:A:219:VAL:O	2.06	0.56
4:A:29:PHE:C	4:A:29:PHE:HD1	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:217:THR:O	4:A:219:VAL:HG23	2.05	0.56
1:H:23:ALA:CA	1:H:77:THR:HG23	2.36	0.56
1:H:152:PRO:N	1:H:152:PRO:C	2.52	0.56
5:B:154:LYS:HA	5:B:158:ALA:O	2.06	0.56
2:L:169:LYS:HA	2:L:169:LYS:CE	2.27	0.55
1:H:147:VAL:HG12	1:H:147:VAL:O	2.06	0.55
3:R:438:SER:HB2	3:R:509:ARG:HG3	1.88	0.55
5:B:66:ARG:HD2	5:B:82:ARG:NH2	2.22	0.55
5:B:118:PRO:CG	5:B:141:LEU:CD1	2.84	0.55
4:A:32:TYR:CZ	4:A:102:ARG:HD3	2.42	0.55
4:A:158:PHE:HB2	4:A:187:LEU:HD13	1.87	0.55
5:B:6:GLN:HE21	5:B:104:GLY:HA3	1.70	0.55
5:B:21:ILE:HD12	5:B:78:LEU:HD23	1.87	0.55
5:B:118:PRO:CB	5:B:141:LEU:CD1	2.84	0.55
5:B:130:LEU:N	5:B:130:LEU:HD23	2.21	0.55
1:H:190:PRO:O	1:H:190:PRO:HG2	2.06	0.55
4:A:39:GLN:C	4:A:92:ALA:HB1	2.28	0.55
4:A:112:LYS:HZ3	5:B:94:MET:HE1	1.72	0.55
2:L:181:LEU:CD1	2:L:186:TYR:HB2	2.37	0.55
2:L:176:SER:O	2:L:176:SER:OG	2.25	0.55
4:A:67:ARG:CG	4:A:85:SER:OG	2.40	0.55
4:A:193:VAL:HG21	5:B:140:LEU:CD1	2.35	0.55
1:H:30:SER:HB3	1:H:73:LYS:HD3	1.88	0.54
3:R:381:GLY:HA3	3:R:430:THR:HG23	1.88	0.54
4:A:127:SER:O	4:A:158:PHE:CD1	2.60	0.54
3:R:490:PHE:HB3	4:A:102:ARG:NH2	2.22	0.54
4:A:146:GLY:C	4:A:198:SER:HB2	2.27	0.54
1:H:19:ARG:CD	1:H:81:GLN:NE2	2.67	0.54
1:H:82:MET:HE3	1:H:93:TYR:CE2	2.42	0.54
1:H:150:TYR:OH	1:H:183:LEU:HD23	2.07	0.54
5:B:191:TYR:CA	5:B:197:TYR:HH	2.20	0.54
1:H:86:ARG:HD2	1:H:88:GLU:OE1	1.90	0.54
2:L:94:TYR:O	2:L:94:TYR:CD1	2.60	0.54
3:R:347:PHE:HB3	3:R:401:VAL:HG23	1.90	0.54
4:A:68:PHE:CE1	4:A:83:MET:CG	2.88	0.54
5:B:124:PRO:O	5:B:124:PRO:HG2	2.07	0.54
5:B:195:LYS:HG3	5:B:196:VAL:HG12	1.89	0.54
3:R:408:ARG:HH12	3:R:414:GLN:HE22	1.54	0.54
4:A:51:ILE:CD1	4:A:71:SER:HA	2.38	0.54
1:H:189:VAL:HB	1:H:190:PRO:HD2	1.89	0.53
2:L:113:PRO:CB	2:L:139:PHE:HB3	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:13:VAL:O	5:B:112:LYS:HB2	2.08	0.53
3:R:427:ASP:N	3:R:427:ASP:OD1	2.40	0.53
4:A:29:PHE:C	4:A:29:PHE:CD1	2.82	0.53
5:B:198:ALA:CB	5:B:213:SER:CB	2.85	0.53
1:H:126:VAL:HG12	1:H:126:VAL:O	2.07	0.53
2:L:78:LEU:HD21	2:L:106:ILE:HD13	1.90	0.53
4:A:190:LEU:HD12	4:A:190:LEU:O	2.08	0.53
1:H:130:ALA:HB1	1:H:131:PRO:CD	2.38	0.53
1:H:174:VAL:HG13	2:L:162:SER:HB3	1.90	0.53
2:L:140:TYR:CD1	2:L:140:TYR:C	2.81	0.53
4:A:136:LEU:CB	4:A:151:GLY:O	2.51	0.53
4:A:159:PRO:HD2	4:A:159:PRO:O	2.07	0.53
4:A:222:LYS:HE3	4:A:224:GLU:HG3	1.88	0.53
3:R:490:PHE:CB	4:A:102:ARG:NH2	2.72	0.53
4:A:207:ILE:CG2	4:A:209:ASN:HD21	2.22	0.53
4:A:81:LEU:O	4:A:81:LEU:HD23	2.09	0.53
2:L:115:VAL:HG21	2:L:205:VAL:CG2	2.39	0.53
4:A:112:LYS:HZ1	5:B:94:MET:HE3	1.74	0.53
4:A:178:PHE:HD1	4:A:191:SER:O	1.92	0.53
3:R:362:VAL:CG2	3:R:525:CYS:H	2.20	0.53
3:R:419:ALA:O	3:R:424:LYS:HB2	2.09	0.52
4:A:166:TRP:HB2	4:A:171:LEU:HB3	1.91	0.52
2:L:33:LEU:CD1	2:L:71:PHE:CD2	2.90	0.52
2:L:186:TYR:HE1	2:L:211:ARG:CG	2.22	0.52
1:H:147:VAL:HG22	1:H:203:VAL:HG21	1.92	0.52
2:L:167:ASP:CG	2:L:170:ASP:OD1	2.48	0.52
3:R:408:ARG:HG3	3:R:408:ARG:HH21	1.74	0.52
1:H:47:TRP:HB3	2:L:96:PRO:CG	2.40	0.52
2:L:61:ARG:HD2	2:L:77:SER:O	2.10	0.52
4:A:68:PHE:HA	4:A:83:MET:HA	1.92	0.52
5:B:155:VAL:CG1	5:B:197:TYR:CE1	2.93	0.52
5:B:191:TYR:HE1	5:B:197:TYR:CE2	2.26	0.52
1:H:5:VAL:HG12	1:H:5:VAL:O	2.10	0.52
1:H:23:ALA:HA	1:H:77:THR:HG23	1.92	0.52
2:L:92:ASN:O	3:R:403:ARG:NH1	2.41	0.52
2:L:209:PHE:CD1	2:L:209:PHE:C	2.83	0.51
3:R:357:ARG:HH21	3:R:394:ASN:HD22	1.56	0.51
4:A:67:ARG:HB3	4:A:84:ASN:O	2.11	0.51
4:A:159:PRO:C	4:A:159:PRO:CD	2.70	0.51
2:L:150:VAL:HG13	2:L:192:TYR:CD1	2.44	0.51
3:R:365:TYR:HD2	3:R:388:ASN:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:17:SER:O	4:A:17:SER:OG	2.28	0.51
1:H:47:TRP:CE3	2:L:96:PRO:HD2	2.45	0.51
4:A:109:TRP:CD1	4:A:109:TRP:C	2.84	0.51
2:L:61:ARG:O	2:L:61:ARG:HG3	2.11	0.51
2:L:121:SER:O	2:L:121:SER:OG	2.27	0.51
5:B:11:LEU:O	5:B:109:LEU:HA	2.11	0.51
3:R:358:ILE:HB	3:R:395:VAL:HG12	1.91	0.51
4:A:68:PHE:CE2	4:A:83:MET:CG	2.90	0.51
1:H:4:LEU:HD23	1:H:4:LEU:N	2.26	0.51
5:B:33:ASN:N	5:B:33:ASN:OD1	2.41	0.51
5:B:118:PRO:HB2	5:B:141:LEU:CD1	2.41	0.51
5:B:43:GLN:O	5:B:43:GLN:HG2	2.11	0.51
4:A:52:SER:HB3	4:A:57:SER:HB2	1.92	0.50
2:L:128:GLY:O	2:L:183:LYS:N	2.44	0.50
3:R:338:PHE:C	3:R:340:GLU:H	2.14	0.50
3:R:438:SER:N	3:R:507:PRO:O	2.42	0.50
4:A:68:PHE:HE2	4:A:83:MET:SD	2.20	0.50
1:H:18:LEU:O	1:H:82:MET:HB2	2.12	0.50
4:A:112:LYS:NZ	5:B:94:MET:HE1	2.26	0.50
5:B:29:LEU:HD21	5:B:95:GLN:HB3	1.94	0.50
2:L:181:LEU:HD12	2:L:181:LEU:C	2.32	0.50
4:A:112:LYS:NZ	5:B:94:MET:CE	2.75	0.50
5:B:6:GLN:HE22	5:B:92:TYR:HA	1.77	0.50
1:H:28:THR:OG1	1:H:31:SER:HB2	2.12	0.50
2:L:11:LEU:HD21	2:L:19:VAL:HG13	1.94	0.50
1:H:82:MET:HE1	1:H:93:TYR:CE2	2.46	0.50
3:R:438:SER:O	3:R:438:SER:OG	2.26	0.50
1:H:129:LEU:HB2	1:H:144:GLY:O	2.12	0.49
3:R:447:GLY:HA2	3:R:498:GLN:HG2	1.93	0.49
2:L:33:LEU:CD2	2:L:89:GLN:O	2.51	0.49
3:R:419:ALA:HA	3:R:423:TYR:O	2.12	0.49
5:B:153:TRP:HB3	5:B:184:LEU:HD11	1.87	0.49
3:R:383:SER:OG	3:R:385:THR:HG22	2.12	0.49
3:R:422:ASN:OD1	3:R:454:ARG:N	2.37	0.49
3:R:418:ILE:HG22	3:R:418:ILE:O	2.10	0.49
5:B:102:THR:O	5:B:102:THR:OG1	2.30	0.49
5:B:24:ARG:CG	5:B:75:ASP:HA	2.43	0.49
5:B:153:TRP:CD1	5:B:184:LEU:HD12	2.46	0.49
1:H:54:GLY:HA3	3:R:421:TYR:OH	2.13	0.49
2:L:8:PRO:O	2:L:8:PRO:HG2	2.12	0.49
4:A:19:ARG:O	4:A:19:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:5:THR:O	5:B:5:THR:OG1	2.28	0.49
5:B:29:LEU:HD13	5:B:76:PHE:HE2	1.78	0.49
5:B:191:TYR:C	5:B:197:TYR:HH	2.16	0.49
1:H:77:THR:CG2	1:H:78:LEU:N	2.71	0.49
1:H:150:TYR:CE1	1:H:181:TYR:HB2	2.48	0.49
3:R:358:ILE:HB	3:R:395:VAL:CG1	2.43	0.49
4:A:67:ARG:HH12	4:A:87:ARG:CZ	2.21	0.49
4:A:98:LYS:HE3	4:A:114:TYR:CD1	2.46	0.49
1:H:85:LEU:HD23	1:H:89:ASP:OD2	2.12	0.48
1:H:104:GLY:H	2:L:46:LEU:CD2	2.25	0.48
2:L:150:VAL:HG23	2:L:155:GLN:CG	2.43	0.48
1:H:47:TRP:CD2	2:L:96:PRO:CD	2.96	0.48
3:R:454:ARG:NH2	3:R:469:SER:O	2.47	0.48
1:H:47:TRP:CG	2:L:96:PRO:HG3	2.48	0.48
1:H:82:MET:HE1	1:H:93:TYR:OH	2.13	0.48
3:R:385:THR:HG23	3:R:386:LYS:N	2.27	0.48
4:A:213:LYS:HG2	4:A:214:PRO:HD3	1.95	0.48
2:L:35:TRP:O	2:L:47:LEU:HB2	2.13	0.48
2:L:125:LEU:HD21	2:L:130:ALA:HB2	1.95	0.48
4:A:104:LEU:C	4:A:106:ASP:H	2.15	0.48
2:L:150:VAL:CG1	2:L:192:TYR:CE1	2.91	0.48
2:L:90:GLN:CD	2:L:93:SER:HB2	2.34	0.48
4:A:159:PRO:O	4:A:159:PRO:CD	2.62	0.48
5:B:118:PRO:HB2	5:B:141:LEU:HD13	1.96	0.48
1:H:47:TRP:CB	2:L:96:PRO:CD	2.92	0.48
2:L:159:SER:HA	2:L:178:THR:O	2.14	0.48
5:B:97:LEU:O	5:B:97:LEU:HD23	2.13	0.48
5:B:188:LYS:O	5:B:192:GLU:HG3	2.14	0.48
4:A:222:LYS:HD2	4:A:224:GLU:HG2	1.95	0.48
5:B:12:PRO:HD2	5:B:12:PRO:O	2.14	0.48
5:B:163:ASN:OD1	5:B:163:ASN:N	2.47	0.48
3:R:410:ILE:HD12	3:R:423:TYR:HD2	1.78	0.48
1:H:69:ILE:HG23	1:H:69:ILE:O	2.13	0.47
2:L:125:LEU:HD23	2:L:125:LEU:HA	1.64	0.47
3:R:358:ILE:HG22	3:R:524:VAL:HG11	1.96	0.47
3:R:410:ILE:O	3:R:410:ILE:HG22	2.14	0.47
4:A:49:SER:OG	4:A:70:ILE:HD12	2.14	0.47
4:A:53:ASP:OD1	4:A:53:ASP:N	2.46	0.47
4:A:6:GLU:OE2	4:A:96:CYS:SG	2.73	0.47
4:A:150:LEU:HG	4:A:194:VAL:HG12	1.95	0.47
5:B:3:VAL:O	5:B:3:VAL:CG1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:TYR:OH	1:H:183:LEU:HD22	2.10	0.47
4:A:67:ARG:NE	4:A:87:ARG:NH1	2.54	0.47
5:B:6:GLN:HG2	5:B:93:CYS:SG	2.54	0.47
1:H:207:PRO:N	1:H:207:PRO:C	2.61	0.47
2:L:6:GLN:CG	2:L:88:CYS:SG	3.01	0.47
3:R:406:GLU:O	3:R:409:GLN:HG3	2.14	0.47
5:B:66:ARG:NH2	5:B:87:ASP:OD2	2.47	0.47
5:B:103:PHE:N	5:B:103:PHE:CD1	2.82	0.47
1:H:72:ASP:OD1	1:H:75:LYS:CG	2.61	0.47
3:R:357:ARG:HH21	3:R:394:ASN:ND2	2.09	0.47
3:R:359:SER:HB2	3:R:523:THR:HG21	1.96	0.47
3:R:420:ASP:HB3	3:R:460:ASN:HB3	1.97	0.47
4:A:175:VAL:O	4:A:175:VAL:CG1	2.62	0.47
5:B:2:ILE:O	5:B:102:THR:HG21	2.15	0.47
2:L:170:ASP:O	2:L:172:THR:HG23	2.15	0.47
3:R:454:ARG:NH1	3:R:454:ARG:CG	2.73	0.47
1:H:39:GLN:HE22	2:L:38:GLN:CD	2.16	0.47
3:R:408:ARG:NH1	3:R:414:GLN:NE2	2.63	0.47
3:R:444:LYS:O	3:R:499:PRO:HD2	2.15	0.47
5:B:129:GLN:NE2	5:B:136:SER:N	2.63	0.47
3:R:457:ARG:NH1	3:R:457:ARG:CG	2.72	0.46
4:A:110:GLY:HA2	5:B:96:ALA:HB1	1.97	0.46
1:H:14:PRO:C	1:H:16:GLY:N	2.66	0.46
3:R:387:LEU:HD21	3:R:515:PHE:CE2	2.51	0.46
5:B:54:TYR:O	5:B:58:ASN:HB2	2.16	0.46
1:H:99:LEU:HD11	3:R:489:TYR:OH	2.16	0.46
2:L:121:SER:O	2:L:124:GLN:HB3	2.16	0.46
5:B:129:GLN:NE2	5:B:136:SER:H	2.14	0.46
3:R:503:VAL:CG1	3:R:506:GLN:OE1	2.63	0.46
5:B:63:VAL:HA	5:B:64:PRO:HD3	1.74	0.46
4:A:67:ARG:NE	4:A:87:ARG:HH12	2.14	0.46
1:H:6:GLU:N	1:H:110:GLN:HE21	2.05	0.46
1:H:121:THR:HG21	1:H:207:PRO:O	2.15	0.46
4:A:105:TYR:N	4:A:105:TYR:CD1	2.84	0.46
1:H:39:GLN:HG3	1:H:45:LEU:HD23	1.97	0.45
1:H:47:TRP:CZ3	2:L:95:PRO:HA	2.51	0.45
1:H:97:ARG:O	1:H:97:ARG:HG2	2.16	0.45
5:B:11:LEU:HD23	5:B:109:LEU:HD12	1.98	0.45
3:R:338:PHE:C	3:R:340:GLU:N	2.69	0.45
4:A:87:ARG:O	4:A:123:VAL:HG11	2.16	0.45
1:H:86:ARG:HB2	1:H:88:GLU:CD	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:VAL:HG22	1:H:187:VAL:HB	1.97	0.45
3:R:347:PHE:CE2	3:R:509:ARG:HB3	2.51	0.45
1:H:71:ARG:O	1:H:71:ARG:HG3	2.17	0.45
3:R:443:SER:OG	3:R:498:GLN:C	2.54	0.45
3:R:448:ASN:N	3:R:497:PHE:O	2.46	0.45
5:B:188:LYS:O	5:B:192:GLU:CG	2.65	0.45
1:H:22:CYS:H	1:H:77:THR:HG22	1.80	0.45
1:H:216:VAL:HG12	1:H:216:VAL:O	2.16	0.45
4:A:29:PHE:HE1	4:A:72:ARG:CZ	2.28	0.45
5:B:156:ASP:OD1	5:B:195:LYS:HG2	2.16	0.45
1:H:47:TRP:CE3	2:L:95:PRO:HA	2.52	0.45
1:H:130:ALA:HB1	1:H:131:PRO:HD2	1.98	0.45
2:L:209:PHE:CD1	2:L:209:PHE:O	2.69	0.45
2:L:136:LEU:HB3	2:L:139:PHE:CE2	2.50	0.45
5:B:216:ARG:HH11	5:B:216:ARG:HG2	1.81	0.45
4:A:11:VAL:HG13	4:A:159:PRO:HG3	1.99	0.45
5:B:86:GLU:O	5:B:86:GLU:HG3	2.16	0.45
3:R:403:ARG:CB	3:R:406:GLU:HG3	2.47	0.45
3:R:437:ASN:CG	3:R:508:TYR:CE1	2.90	0.45
4:A:190:LEU:C	4:A:190:LEU:CD1	2.84	0.45
5:B:38:LEU:HD13	5:B:38:LEU:C	2.37	0.44
3:R:385:THR:HG23	3:R:386:LYS:HG2	1.99	0.44
4:A:36:TRP:HD1	4:A:70:ILE:HD12	1.82	0.44
4:A:59:TYR:HE1	4:A:108:VAL:HG21	1.82	0.44
5:B:129:GLN:O	5:B:132:SER:CB	2.45	0.44
5:B:166:GLU:HB3	5:B:180:LEU:HD11	1.99	0.44
3:R:360:ASN:HD22	3:R:523:THR:CG2	2.30	0.44
4:A:39:GLN:O	4:A:92:ALA:HB1	2.18	0.44
5:B:141:LEU:HD21	5:B:201:VAL:CG2	2.45	0.44
5:B:195:LYS:O	5:B:215:ASN:HA	2.17	0.44
2:L:36:TYR:HE1	2:L:89:GLN:OE1	1.98	0.44
3:R:364:ASP:OD2	3:R:367:VAL:N	2.51	0.44
4:A:181:VAL:CG1	5:B:167:SER:HB3	2.47	0.44
5:B:113:ARG:NH1	5:B:113:ARG:HG3	2.32	0.44
1:H:47:TRP:CG	2:L:96:PRO:CD	3.00	0.44
2:L:186:TYR:CE1	2:L:211:ARG:CG	3.01	0.44
2:L:196:VAL:O	2:L:196:VAL:HG12	2.17	0.44
4:A:104:LEU:C	4:A:106:ASP:N	2.71	0.44
1:H:3:GLN:HG2	1:H:3:GLN:O	2.18	0.44
1:H:160:ASN:HB3	1:H:163:ALA:HB3	2.00	0.44
4:A:226:LYS:HB3	4:A:226:LYS:HE2	1.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:136:LEU:HD11	2:L:196:VAL:HG21	2.00	0.44
5:B:21:ILE:CD1	5:B:78:LEU:HD23	2.47	0.44
5:B:88:VAL:HG23	5:B:109:LEU:O	2.16	0.44
2:L:172:THR:O	2:L:172:THR:OG1	2.33	0.44
3:R:408:ARG:HG3	3:R:408:ARG:NH2	2.31	0.44
5:B:84:GLU:CA	5:B:87:ASP:OD1	2.65	0.44
2:L:93:SER:OG	3:R:505:TYR:CZ	2.69	0.43
3:R:357:ARG:CG	3:R:396:TYR:CE1	3.01	0.43
4:A:67:ARG:CZ	4:A:87:ARG:HH11	2.18	0.43
1:H:150:TYR:CZ	1:H:155:VAL:CG2	3.01	0.43
1:H:206:LYS:N	1:H:207:PRO:HD3	2.33	0.43
4:A:51:ILE:O	4:A:51:ILE:CG2	2.66	0.43
1:H:38:ARG:HG2	1:H:48:VAL:HG21	1.98	0.43
1:H:171:PHE:HD1	1:H:184:SER:O	2.01	0.43
5:B:72:SER:HA	5:B:76:PHE:HE1	1.83	0.43
1:H:150:TYR:CE2	1:H:183:LEU:HD23	2.54	0.43
3:R:443:SER:OG	3:R:499:PRO:N	2.52	0.43
5:B:31:HIS:ND1	5:B:31:HIS:C	2.71	0.43
5:B:118:PRO:HB3	5:B:144:PHE:HB3	2.00	0.43
2:L:186:TYR:CE1	2:L:211:ARG:HG2	2.46	0.43
3:R:455:LEU:O	3:R:455:LEU:HD12	2.19	0.43
1:H:50:VAL:HG12	1:H:58:ASP:HB2	2.01	0.43
2:L:175:LEU:HD23	2:L:176:SER:N	2.34	0.43
1:H:86:ARG:HD3	1:H:88:GLU:CD	2.19	0.43
2:L:62:PHE:CE1	2:L:75:ILE:HG12	2.54	0.43
5:B:198:ALA:HB1	5:B:212:LYS:O	2.18	0.43
2:L:90:GLN:HG2	2:L:91:LEU:O	2.19	0.43
2:L:90:GLN:NE2	2:L:92:ASN:OD1	2.52	0.42
3:R:426:PRO:N	3:R:426:PRO:C	2.57	0.42
4:A:207:ILE:HG21	4:A:209:ASN:HD21	1.83	0.42
4:A:155:LYS:HA	4:A:189:SER:HB2	2.01	0.42
2:L:186:TYR:CD1	2:L:186:TYR:C	2.92	0.42
2:L:96:PRO:O	2:L:96:PRO:HG2	2.20	0.42
4:A:85:SER:OG	4:A:85:SER:O	2.34	0.42
1:H:139:GLY:O	1:H:191:SER:CB	2.67	0.42
4:A:223:VAL:O	4:A:223:VAL:HG12	2.17	0.42
1:H:50:VAL:HG21	2:L:94:TYR:CZ	2.54	0.42
3:R:357:ARG:HE	3:R:394:ASN:HD22	1.67	0.42
5:B:121:PHE:O	5:B:140:LEU:N	2.44	0.42
4:A:194:VAL:O	4:A:194:VAL:CG1	2.68	0.42
4:A:201:LEU:HD23	4:A:201:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:13:VAL:CG1	5:B:14:THR:H	2.19	0.42
5:B:66:ARG:HD2	5:B:82:ARG:CZ	2.49	0.42
1:H:12:ILE:O	1:H:12:ILE:CG2	2.67	0.42
4:A:156:ASP:HA	4:A:188:TYR:O	2.20	0.42
4:A:168:SER:CA	4:A:209:ASN:OD1	2.68	0.42
5:B:6:GLN:HA	5:B:23:CYS:HA	2.02	0.42
1:H:104:GLY:H	2:L:46:LEU:HD21	1.85	0.42
2:L:32:TYR:CD2	2:L:92:ASN:HB3	2.54	0.42
4:A:68:PHE:CD1	4:A:83:MET:CA	2.96	0.42
2:L:113:PRO:O	2:L:113:PRO:CD	2.65	0.41
3:R:437:ASN:OD1	3:R:508:TYR:CE1	2.73	0.41
5:B:130:LEU:C	5:B:132:SER:H	2.24	0.41
3:R:454:ARG:HD3	3:R:457:ARG:HD2	2.02	0.41
4:A:11:VAL:HG11	4:A:159:PRO:HB3	2.02	0.41
2:L:62:PHE:CD1	2:L:75:ILE:HG12	2.55	0.41
1:H:4:LEU:HD22	1:H:24:ALA:HB2	2.02	0.41
5:B:44:LYS:HB3	5:B:45:PRO:CD	2.51	0.41
5:B:97:LEU:HD23	5:B:97:LEU:C	2.40	0.41
4:A:64:VAL:O	4:A:64:VAL:CG1	2.68	0.41
5:B:88:VAL:O	5:B:88:VAL:HG13	2.19	0.41
2:L:134:CYS:O	2:L:176:SER:HA	2.20	0.41
3:R:383:SER:HB2	3:R:384:PRO:HD2	2.03	0.41
4:A:154:VAL:HG11	4:A:162:VAL:HG11	2.02	0.41
5:B:156:ASP:OD1	5:B:195:LYS:CG	2.69	0.41
1:H:206:LYS:N	1:H:207:PRO:CD	2.84	0.41
2:L:191:VAL:O	2:L:191:VAL:HG12	2.20	0.41
3:R:400:PHE:CD1	3:R:400:PHE:N	2.88	0.41
1:H:131:PRO:HG3	1:H:143:LEU:HB3	2.03	0.41
5:B:25:SER:OG	5:B:26:SER:N	2.53	0.41
1:H:28:THR:CG2	3:R:476:GLY:O	2.69	0.41
1:H:77:THR:HG22	1:H:78:LEU:O	2.21	0.41
2:L:102:THR:O	2:L:102:THR:HG22	2.21	0.41
2:L:117:ILE:O	2:L:117:ILE:HG23	2.19	0.41
3:R:454:ARG:CG	3:R:454:ARG:HH11	2.33	0.41
3:R:523:THR:CG2	3:R:523:THR:O	2.69	0.41
4:A:69:THR:O	4:A:69:THR:OG1	2.36	0.41
4:A:189:SER:O	4:A:189:SER:OG	2.39	0.41
1:H:60:ALA:O	1:H:63:VAL:HG12	2.21	0.41
3:R:407:VAL:O	3:R:407:VAL:HG12	2.21	0.41
4:A:21:SER:HB2	4:A:80:TYR:CE1	2.56	0.41
5:B:27:GLN:OE1	5:B:27:GLN:CA	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187:VAL:O	1:H:187:VAL:HG13	2.20	0.40
2:L:86:TYR:CD1	2:L:86:TYR:N	2.90	0.40
4:A:21:SER:HB2	4:A:80:TYR:CD1	2.56	0.40
1:H:150:TYR:CZ	1:H:155:VAL:HG21	2.57	0.40
2:L:207:LYS:HD3	2:L:207:LYS:HA	1.57	0.40
4:A:171:LEU:HD12	4:A:171:LEU:HA	1.65	0.40
3:R:338:PHE:O	3:R:340:GLU:N	2.55	0.40
1:H:19:ARG:HB2	1:H:81:GLN:HE22	1.84	0.40
1:H:71:ARG:NE	1:H:73:LYS:HE2	2.29	0.40
3:R:395:VAL:HG23	3:R:515:PHE:HD1	1.73	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)
2:L:27:GLN:O	4:A:227:SER:OG[3_645]	1.89	0.31

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	208/223 (93%)	199 (96%)	9 (4%)	0	100	100
2	L	209/214 (98%)	198 (95%)	11 (5%)	0	100	100
3	R	185/223 (83%)	167 (90%)	18 (10%)	0	100	100
4	A	215/230 (94%)	198 (92%)	16 (7%)	1 (0%)	29	65
5	B	214/219 (98%)	198 (92%)	14 (6%)	2 (1%)	17	53
All	All	1031/1109 (93%)	960 (93%)	68 (7%)	3 (0%)	41	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	33	ASN
5	B	31	HIS
4	A	156	ASP

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	H	175/185 (95%)	161 (92%)	14 (8%)	12	41
2	L	182/184 (99%)	168 (92%)	14 (8%)	13	42
3	R	163/196 (83%)	153 (94%)	10 (6%)	18	51
4	A	178/188 (95%)	158 (89%)	20 (11%)	6	26
5	B	190/192 (99%)	180 (95%)	10 (5%)	22	55
All	All	888/945 (94%)	820 (92%)	68 (8%)	13	42

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

Mol	Chain	Res	Type
1	H	6	GLU
1	H	22	CYS
1	H	25	SER
1	H	38	ARG
1	H	58	ASP
1	H	72	ASP
1	H	99	LEU
1	H	143	LEU
1	H	183	LEU
1	H	185	SER
1	H	201	CYS
1	H	204	ASN
1	H	211	LYS
1	H	214	LYS
2	L	12	SER
2	L	24	ARG
2	L	33	LEU

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Mol	Chain	Res	Type
2	L	70	ASP
2	L	83	PHE
2	L	88	CYS
2	L	94	TYR
2	L	152	ASN
2	L	169	LYS
2	L	182	SER
2	L	183	LYS
2	L	185	ASP
2	L	190	LYS
2	L	195	GLU
3	R	347	PHE
3	R	353	TRP
3	R	369	TYR
3	R	377	PHE
3	R	378	LYS
3	R	427	ASP
3	R	438	SER
3	R	454	ARG
3	R	469	SER
3	R	525	CYS
4	A	19	ARG
4	A	21	SER
4	A	22	CYS
4	A	29	PHE
4	A	49	SER
4	A	59	TYR
4	A	67	ARG
4	A	83	MET
4	A	96	CYS
4	A	100	ARG
4	A	129	LYS
4	A	150	LEU
4	A	153	LEU
4	A	173	SER
4	A	192	SER
4	A	198	SER
4	A	208	CYS
4	A	211	ASN
4	A	213	LYS
4	A	222	LYS
5	B	7	SER

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Mol	Chain	Res	Type
5	B	26	SER
5	B	68	SER
5	B	81	SER
5	B	109	LEU
5	B	127	ASP
5	B	163	ASN
5	B	193	LYS
5	B	207	SER
5	B	214	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	81	GLN
1	H	110	GLN
2	L	37	GLN
2	L	38	GLN
2	L	79	GLN
2	L	152	ASN
2	L	189	HIS
2	L	199	GLN
2	L	210	ASN
3	R	360	ASN
3	R	394	ASN
3	R	414	GLN
3	R	439	ASN
4	A	77	ASN
4	A	211	ASN
4	A	216	ASN
5	B	165	GLN
5	B	203	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	H	212/223 (95%)	0.26	2 (0%) 84 83	26, 56, 80, 90	0
2	L	211/214 (98%)	0.03	0 100 100	26, 47, 72, 81	0
3	R	189/223 (84%)	0.43	16 (8%) 10 13	20, 50, 107, 123	0
4	A	219/230 (95%)	0.09	1 (0%) 91 90	25, 56, 85, 99	0
5	B	216/219 (98%)	0.36	8 (3%) 41 41	20, 52, 95, 135	0
All	All	1047/1109 (94%)	0.23	27 (2%) 56 54	20, 52, 91, 135	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	333	THR	5.6
4	A	227	SER	5.1
3	R	525	CYS	4.5
3	R	365	TYR	4.1
3	R	391	CYS	4.0
3	R	371	SER	3.7
3	R	387	LEU	3.7
3	R	432	CYS	3.1
1	H	194	LEU	3.1
1	H	199	TYR	3.0
3	R	368	LEU	2.6
3	R	363	ALA	2.6
5	B	154	LYS	2.5
5	B	1	ASP	2.5
3	R	434	ILE	2.4
3	R	389	ASP	2.4
3	R	392	PHE	2.3
3	R	433	VAL	2.3
5	B	158	ALA	2.3
5	B	27	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	R	515	PHE	2.3
5	B	155	VAL	2.2
3	R	338	PHE	2.2
3	R	372	ALA	2.2
5	B	163	ASN	2.2
5	B	153	TRP	2.0
5	B	29	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.