



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:06 PM UTC

PDB ID : 7CHE / pdb_00007che
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 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 : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

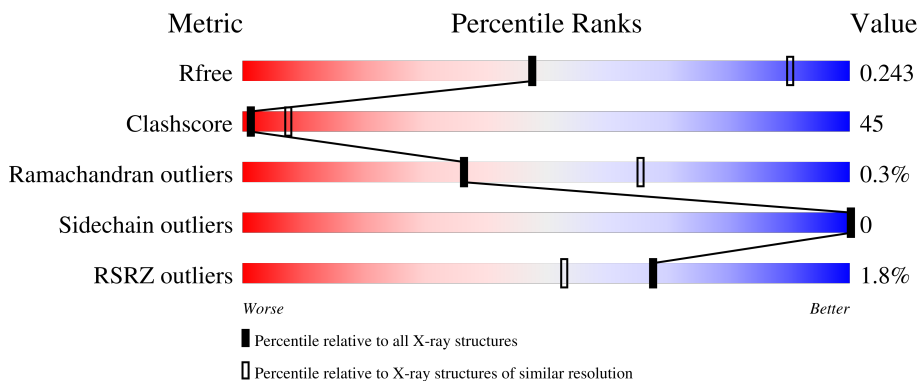
1 Overall quality at a glance

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}	180053	1210 (3.48-3.36)
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)
RSRZ outliers	180081	1210 (3.48-3.36)

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	
2	L	214	
3	R	223	
4	A	230	
5	B	219	

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	H	212	1559	977	262	313	7	0	0	0

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

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

- Molecule 3 is a protein called Spike protein S1.

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

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

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

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

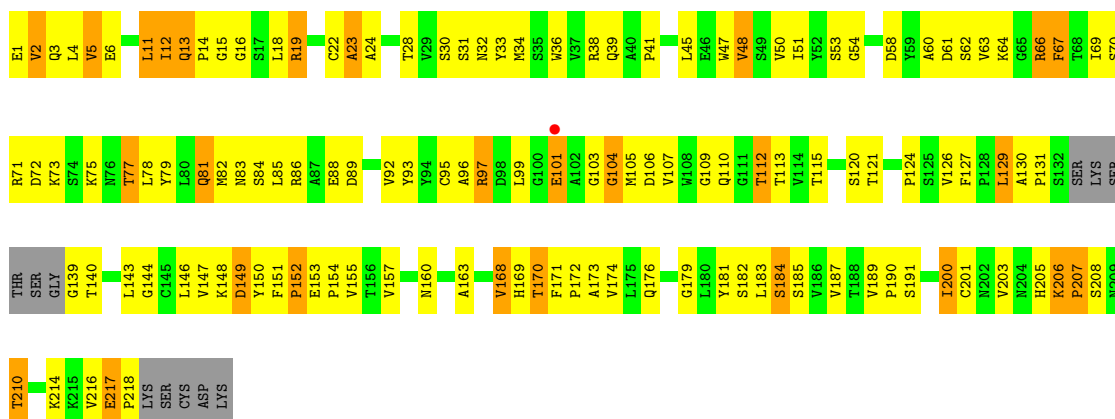
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	216	1659	1038	281	334	6	0	0	0

3 Residue-property plots

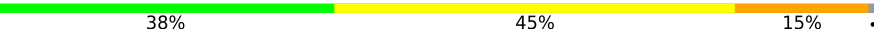
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

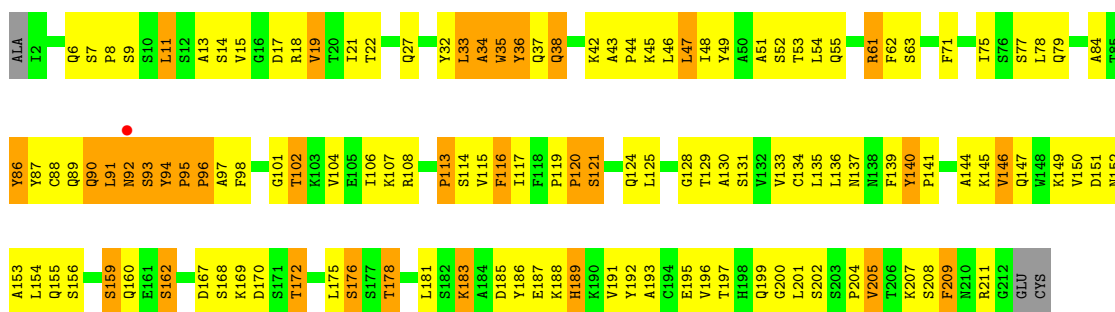
- Molecule 1: BD-236 Fab heavy chain

Chain H: 



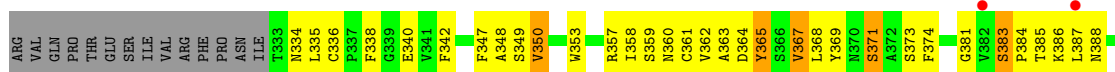
- Molecule 2: BD-236 Fab light chain

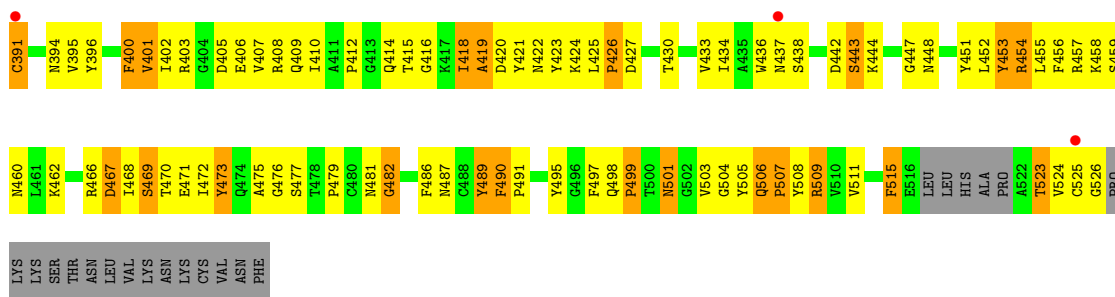
Chain L: 



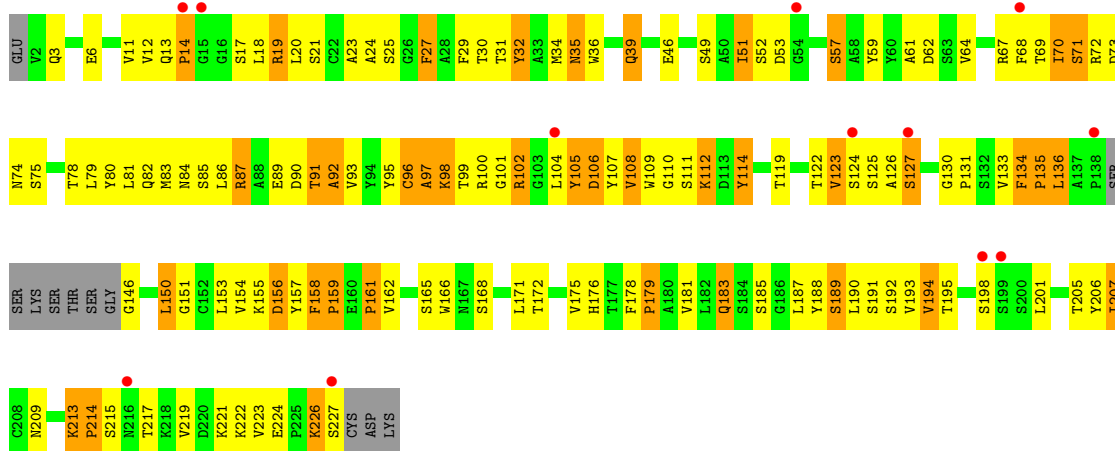
- Molecule 3: Spike protein S1

Chain R: 





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



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) 94.5 (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)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.225 , 0.239 0.225 , 0.243	Depositor DCC
R_{free} test set	1772 reflections (9.45%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtrriage
Anisotropy	0.172	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.026 for -h,l,k	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7956	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage'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 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	H	1.82	35/1591 (2.2%)	1.96	46/2166 (2.1%)
2	L	2.01	67/1639 (4.1%)	1.99	53/2227 (2.4%)
3	R	1.90	42/1538 (2.7%)	2.08	39/2090 (1.9%)
4	A	2.11	49/1675 (2.9%)	2.13	65/2280 (2.9%)
5	B	2.09	52/1695 (3.1%)	2.06	52/2303 (2.3%)
All	All	1.99	245/8138 (3.0%)	2.05	255/11066 (2.3%)

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 (245) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	64	PRO	N-CD	-31.58	1.03	1.47
4	A	159	PRO	N-CD	-28.88	1.07	1.47
2	L	113	PRO	N-CD	-27.69	1.08	1.47
4	A	161	PRO	N-CD	-20.10	1.19	1.47
4	A	14	PRO	N-CA	18.51	1.69	1.47
3	R	426	PRO	N-CA	17.03	1.68	1.47
1	H	207	PRO	N-CA	16.67	1.69	1.47
5	B	64	PRO	N-CA	16.20	1.67	1.47
3	R	507	PRO	N-CA	16.01	1.67	1.47
5	B	12	PRO	N-CA	15.79	1.67	1.47
4	A	135	PRO	N-CA	15.15	1.65	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	490	PHE	C-N	14.26	1.49	1.34
3	R	383	SER	C-N	14.20	1.49	1.34
5	B	146	PRO	N-CA	13.56	1.70	1.47
3	R	462	LYS	C-N	13.49	1.49	1.33
1	H	154	PRO	N-CD	-13.30	1.29	1.47
1	H	127	PHE	C-N	13.01	1.49	1.33
4	A	130	GLY	C-N	12.99	1.49	1.33
1	H	152	PRO	N-CA	12.46	1.68	1.47
2	L	79	GLN	C-N	12.32	1.48	1.33
4	A	159	PRO	N-CA	12.05	1.67	1.47
4	A	161	PRO	N-CA	11.29	1.66	1.47
4	A	134	PHE	C-N	9.83	1.45	1.33
4	A	135	PRO	C-O	-9.43	1.13	1.23
2	L	204	PRO	N-CD	-9.41	1.34	1.47
4	A	13	GLN	C-N	9.40	1.44	1.33
1	H	41	PRO	N-CD	-9.24	1.34	1.47
5	B	64	PRO	C-O	-9.16	1.12	1.23
3	R	425	LEU	C-N	8.78	1.44	1.33
2	L	87	TYR	C-O	-8.64	1.14	1.24
3	R	511	VAL	C-O	-8.64	1.15	1.24
5	B	63	VAL	C-N	8.42	1.44	1.33
5	B	118	PRO	C-O	-8.39	1.14	1.23
3	R	489	TYR	C-O	-8.35	1.14	1.24
5	B	92	TYR	C-O	-8.22	1.13	1.23
4	A	111	SER	C-O	-7.95	1.14	1.23
5	B	50	GLN	C-O	-7.91	1.14	1.23
2	L	153	ALA	C-O	-7.38	1.15	1.24
2	L	44	PRO	C-O	-7.36	1.14	1.23
3	R	412	PRO	C-O	-7.35	1.15	1.23
2	L	96	PRO	C-O	-7.34	1.18	1.24
5	B	12	PRO	C-O	-7.33	1.14	1.24
2	L	53	THR	C-O	-7.33	1.15	1.24
5	B	124	PRO	C-O	-7.30	1.16	1.24
1	H	97	ARG	C-O	-7.30	1.15	1.24
3	R	459	SER	C-O	-7.25	1.14	1.23
5	B	58	ASN	C-O	-7.23	1.15	1.24
4	A	98	LYS	C-O	-7.21	1.15	1.24
3	R	426	PRO	C-O	-7.19	1.14	1.23
4	A	51	ILE	C-O	-7.16	1.17	1.24
5	B	94	MET	C-O	-7.13	1.15	1.23
5	B	53	ILE	C-O	-7.12	1.16	1.24
2	L	37	GLN	C-O	-7.11	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	19	VAL	C-O	-7.10	1.16	1.24
3	R	486	PHE	C-O	-7.07	1.15	1.23
3	R	473	TYR	C-O	-7.03	1.15	1.24
2	L	84	ALA	C-O	-7.02	1.17	1.24
3	R	348	ALA	C-O	-7.01	1.14	1.23
4	A	176	HIS	C-O	-6.97	1.15	1.23
4	A	25	SER	C-O	-6.93	1.14	1.23
2	L	102	THR	C-O	-6.92	1.16	1.23
1	H	214	LYS	C-O	-6.88	1.16	1.24
4	A	194	VAL	C-O	-6.83	1.16	1.23
2	L	119	PRO	C-O	-6.81	1.16	1.24
5	B	43	GLN	C-O	-6.79	1.16	1.24
4	A	78	THR	C-O	-6.77	1.16	1.23
3	R	453	TYR	C-O	-6.75	1.15	1.23
5	B	180	LEU	C-O	-6.75	1.15	1.23
1	H	206	LYS	C-N	6.75	1.43	1.33
1	H	107	VAL	C-O	-6.73	1.16	1.24
3	R	400	PHE	C-O	-6.71	1.15	1.23
3	R	469	SER	C-O	-6.69	1.14	1.23
4	A	71	SER	CA-CB	-6.66	1.43	1.53
5	B	15	PRO	C-O	-6.62	1.15	1.23
4	A	31	THR	C-O	-6.59	1.15	1.24
4	A	213	LYS	C-N	6.54	1.49	1.33
3	R	401	VAL	C-O	-6.50	1.17	1.24
5	B	40	TRP	C-O	-6.47	1.16	1.24
2	L	9	SER	C-O	-6.47	1.16	1.24
5	B	45	PRO	C-O	-6.45	1.16	1.23
1	H	51	ILE	C-O	-6.45	1.17	1.24
2	L	91	LEU	C-O	-6.43	1.15	1.23
3	R	456	PHE	C-O	-6.43	1.16	1.24
5	B	141	LEU	C-O	-6.43	1.16	1.24
5	B	107	THR	C-O	-6.42	1.16	1.23
5	B	82	ARG	C-O	-6.42	1.16	1.24
4	A	92	ALA	C-O	-6.41	1.16	1.23
1	H	124	PRO	C-O	-6.39	1.16	1.23
2	L	131	SER	C-O	-6.38	1.16	1.23
5	B	171	GLN	C-O	-6.38	1.16	1.23
5	B	32	SER	CA-CB	-6.37	1.44	1.53
4	A	179	PRO	C-O	-6.36	1.17	1.23
2	L	36	TYR	C-O	-6.36	1.15	1.23
5	B	125	PRO	C-O	-6.34	1.16	1.23
1	H	33	TYR	C-O	-6.33	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	182	SER	CA-CB	-6.33	1.43	1.53
5	B	90	VAL	C-O	-6.33	1.17	1.24
4	A	87	ARG	C-O	-6.33	1.16	1.24
5	B	7	SER	C-O	-6.31	1.17	1.24
3	R	350	VAL	C-O	-6.27	1.17	1.24
3	R	479	PRO	C-O	-6.26	1.16	1.23
2	L	162	SER	C-O	-6.25	1.17	1.23
1	H	104	GLY	C-O	-6.22	1.15	1.23
5	B	59	ARG	C-O	-6.22	1.16	1.23
3	R	451	TYR	C-O	-6.22	1.16	1.23
5	B	167	SER	C-O	-6.20	1.16	1.23
2	L	48	ILE	C-O	-6.18	1.16	1.23
2	L	145	LYS	C-O	-6.18	1.16	1.23
1	H	105	MET	C-O	-6.16	1.16	1.24
5	B	60	ALA	C-O	-6.15	1.15	1.23
4	A	70	ILE	C-O	-6.11	1.16	1.24
2	L	86	TYR	C-O	-6.07	1.16	1.24
4	A	114	TYR	C-O	-6.07	1.17	1.23
4	A	192	SER	C-O	-6.05	1.16	1.24
4	A	46	GLU	C-O	-6.04	1.16	1.23
2	L	7	SER	CA-CB	-6.04	1.43	1.53
5	B	119	SER	C-O	-6.03	1.16	1.24
2	L	38	GLN	C-O	-6.03	1.17	1.24
3	R	472	ILE	C-O	-6.03	1.17	1.24
5	B	41	TYR	C-O	-6.00	1.16	1.23
5	B	126	SER	CA-CB	-5.99	1.44	1.53
3	R	407	VAL	C-O	-5.96	1.16	1.24
3	R	499	PRO	C-O	-5.95	1.16	1.24
2	L	104	VAL	C-O	-5.93	1.17	1.24
5	B	139	CYS	C-O	-5.92	1.17	1.23
4	A	32	TYR	C-O	-5.91	1.17	1.23
2	L	133	VAL	C-O	-5.90	1.18	1.24
4	A	108	VAL	C-O	-5.86	1.16	1.24
3	R	402	ILE	C-O	-5.85	1.17	1.24
4	A	221	LYS	C-O	-5.83	1.17	1.24
2	L	35	TRP	C-O	-5.83	1.17	1.24
2	L	149	LYS	C-O	-5.83	1.17	1.24
5	B	14	THR	C-O	-5.82	1.16	1.24
5	B	81	SER	C-O	-5.82	1.17	1.24
5	B	79	LYS	C-O	-5.81	1.16	1.23
2	L	54	LEU	C-O	-5.80	1.16	1.23
2	L	33	LEU	C-O	-5.79	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	31	HIS	C-O	-5.77	1.16	1.24
1	H	120	SER	CA-CB	-5.76	1.44	1.53
4	A	96	CYS	C-O	-5.73	1.16	1.23
2	L	205	VAL	C-O	-5.73	1.17	1.24
2	L	47	LEU	C-O	-5.73	1.16	1.23
4	A	112	LYS	C-O	-5.73	1.17	1.24
1	H	48	VAL	C-O	-5.71	1.17	1.24
2	L	154	LEU	C-O	-5.71	1.17	1.23
3	R	475	ALA	C-O	-5.70	1.16	1.24
1	H	172	PRO	C-O	-5.68	1.17	1.23
3	R	459	SER	CA-CB	-5.68	1.44	1.53
2	L	121	SER	CA-CB	-5.67	1.44	1.53
5	B	11	LEU	C-O	-5.67	1.19	1.25
5	B	61	SER	C-O	-5.67	1.17	1.24
5	B	86	GLU	C-O	-5.66	1.15	1.24
4	A	57	SER	C-O	-5.66	1.17	1.23
2	L	42	LYS	C-O	-5.65	1.16	1.23
2	L	34	ALA	C-O	-5.64	1.17	1.23
2	L	43	ALA	C-O	-5.63	1.16	1.23
2	L	63	SER	C-O	-5.63	1.16	1.23
5	B	114	THR	C-O	-5.63	1.17	1.23
2	L	97	ALA	C-O	-5.62	1.17	1.23
4	A	39	GLN	C-O	-5.62	1.17	1.23
2	L	172	THR	C-O	-5.60	1.16	1.23
2	L	193	ALA	C-O	-5.59	1.16	1.23
3	R	477	SER	CA-CB	-5.57	1.46	1.54
4	A	93	VAL	C-O	-5.57	1.17	1.24
2	L	101	GLY	C-O	-5.56	1.17	1.24
3	R	434	ILE	C-O	-5.55	1.18	1.24
5	B	123	PHE	C-O	-5.55	1.18	1.24
2	L	208	SER	CA-CB	-5.53	1.44	1.53
5	B	91	TYR	C-O	-5.53	1.17	1.24
1	H	184	SER	C-O	-5.52	1.17	1.23
4	A	25	SER	CA-CB	-5.52	1.44	1.53
5	B	63	VAL	C-O	-5.52	1.18	1.25
3	R	471	GLU	C-O	-5.51	1.17	1.23
4	A	100	ARG	C-O	-5.51	1.17	1.24
1	H	36	TRP	C-O	-5.50	1.17	1.24
1	H	207	PRO	C-O	-5.49	1.17	1.24
3	R	443	SER	C-O	-5.46	1.17	1.23
2	L	168	SER	C-O	-5.44	1.16	1.24
3	R	452	LEU	C-O	-5.43	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	13	ALA	C-O	-5.42	1.17	1.23
5	B	21	ILE	C-O	-5.41	1.18	1.24
2	L	61	ARG	C-O	-5.41	1.16	1.24
2	L	160	GLN	C-O	-5.40	1.17	1.23
5	B	10	SER	CA-CB	-5.40	1.45	1.52
3	R	467	ASP	C-O	-5.40	1.17	1.24
2	L	159	SER	CA-CB	-5.39	1.44	1.53
5	B	102	THR	C-O	-5.38	1.17	1.23
4	A	3	GLN	C-O	-5.38	1.17	1.23
3	R	509	ARG	C-O	-5.36	1.17	1.23
1	H	112	THR	C-O	-5.36	1.17	1.23
5	B	177	THR	C-O	-5.36	1.16	1.23
5	B	145	TYR	C-N	5.34	1.44	1.34
1	H	70	SER	CA-CB	-5.33	1.45	1.53
1	H	129	LEU	C-O	-5.32	1.17	1.24
4	A	165	SER	CA-CB	-5.32	1.44	1.53
2	L	141	PRO	N-CD	-5.31	1.40	1.47
1	H	200	ILE	C-O	-5.30	1.18	1.24
1	H	120	SER	C-O	-5.29	1.17	1.23
3	R	443	SER	CA-CB	-5.29	1.45	1.53
3	R	419	ALA	C-O	-5.28	1.17	1.24
1	H	179	GLY	C-O	-5.26	1.17	1.24
3	R	418	ILE	C-O	-5.24	1.17	1.24
2	L	11	LEU	C-O	-5.24	1.17	1.23
4	A	20	LEU	C-O	-5.20	1.17	1.23
1	H	5	VAL	C-O	-5.20	1.18	1.24
1	H	151	PHE	C-N	5.20	1.44	1.34
4	A	153	LEU	C-O	-5.20	1.17	1.23
1	H	169	HIS	C-O	-5.19	1.17	1.23
4	A	27	PHE	C-O	-5.19	1.17	1.23
2	L	147	GLN	C-O	-5.19	1.17	1.24
1	H	146	LEU	C-O	-5.18	1.18	1.24
2	L	51	ALA	C-O	-5.17	1.17	1.24
2	L	52	SER	C-O	-5.17	1.17	1.24
4	A	97	ALA	C-O	-5.17	1.17	1.23
4	A	150	LEU	C-O	-5.17	1.17	1.23
4	A	95	TYR	C-O	-5.16	1.17	1.24
3	R	349	SER	C-O	-5.14	1.17	1.23
2	L	146	VAL	C-O	-5.14	1.18	1.24
2	L	120	PRO	C-O	-5.14	1.18	1.23
4	A	176	HIS	CG-ND1	-5.14	1.32	1.38
3	R	436	TRP	C-O	-5.12	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	158	PHE	C-N	5.11	1.44	1.34
1	H	12	ILE	C-O	-5.09	1.18	1.24
2	L	141	PRO	C-O	-5.09	1.13	1.23
2	L	17	ASP	C-O	-5.09	1.17	1.23
1	H	96	ALA	C-O	-5.08	1.17	1.23
2	L	96	PRO	N-CA	-5.08	1.42	1.47
2	L	114	SER	C-O	-5.08	1.17	1.24
3	R	433	VAL	C-O	-5.08	1.17	1.24
1	H	168	VAL	C-O	-5.07	1.19	1.24
2	L	18	ARG	C-O	-5.07	1.17	1.24
2	L	14	SER	C-O	-5.07	1.17	1.23
2	L	63	SER	CA-CB	-5.06	1.45	1.53
2	L	195	GLU	C-O	-5.05	1.17	1.24
2	L	156	SER	C-O	-5.05	1.17	1.23
1	H	23	ALA	C-O	-5.05	1.17	1.24
4	A	23	ALA	C-O	-5.04	1.18	1.24
2	L	55	GLN	C-O	-5.04	1.17	1.23
3	R	482	GLY	C-O	-5.04	1.17	1.24
5	B	165	GLN	C-O	-5.04	1.17	1.23
4	A	99	THR	C-O	-5.04	1.17	1.23
2	L	200	GLY	C-O	-5.02	1.18	1.23
5	B	140	LEU	C-O	-5.01	1.17	1.24
2	L	209	PHE	C-O	-5.01	1.17	1.23
2	L	15	VAL	C-O	-5.01	1.18	1.24

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	383	SER	CA-C-N	17.74	137.20	119.82
3	R	383	SER	C-N-CA	17.74	137.20	119.82
3	R	425	LEU	CA-C-N	17.55	139.77	120.11
3	R	425	LEU	C-N-CA	17.55	139.77	120.11
4	A	134	PHE	CA-C-N	17.45	138.23	119.90
4	A	134	PHE	C-N-CA	17.45	138.23	119.90
5	B	63	VAL	CA-C-N	16.52	136.74	119.89
5	B	63	VAL	C-N-CA	16.52	136.74	119.89
5	B	11	LEU	CA-C-N	16.37	140.30	119.84
5	B	11	LEU	C-N-CA	16.37	140.30	119.84
4	A	13	GLN	CA-C-N	15.79	136.89	119.83
4	A	13	GLN	C-N-CA	15.79	136.89	119.83
1	H	206	LYS	CA-C-N	15.46	137.40	119.47
1	H	206	LYS	C-N-CA	15.46	137.40	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	506	GLN	CA-C-N	14.82	138.37	119.84
3	R	506	GLN	C-N-CA	14.82	138.37	119.84
5	B	39	ASP	CB-CA-C	-14.69	84.21	110.36
2	L	92	ASN	N-CA-C	14.56	130.41	113.38
4	A	130	GLY	CA-C-N	13.69	134.08	120.52
4	A	130	GLY	C-N-CA	13.69	134.08	120.52
3	R	367	VAL	N-CA-C	-13.37	99.59	112.96
2	L	91	LEU	N-CA-C	-12.99	90.22	110.36
2	L	79	GLN	CA-C-N	12.67	132.48	119.56
2	L	79	GLN	C-N-CA	12.67	132.48	119.56
1	H	154	PRO	CA-N-CD	12.03	128.34	111.50
2	L	93	SER	N-CA-C	-11.90	87.62	108.69
3	R	462	LYS	CA-C-N	11.83	132.59	119.93
3	R	462	LYS	C-N-CA	11.83	132.59	119.93
3	R	490	PHE	CA-C-N	10.93	131.85	120.04
3	R	490	PHE	C-N-CA	10.93	131.85	120.04
4	A	159	PRO	N-CD-CG	10.82	116.78	103.80
5	B	12	PRO	CA-N-CD	-10.65	97.10	112.00
5	B	32	SER	N-CA-C	-10.59	98.01	112.94
4	A	213	LYS	CA-C-N	10.37	132.80	119.84
4	A	213	LYS	C-N-CA	10.37	132.80	119.84
1	H	153	GLU	C-N-CD	-10.30	97.94	120.60
2	L	94	TYR	CA-C-O	-9.79	109.78	119.08
1	H	154	PRO	N-CD-CG	-9.59	92.29	103.80
4	A	14	PRO	CA-N-CD	-9.15	99.19	112.00
2	L	151	ASP	CB-CA-C	9.12	128.56	110.42
1	H	79	TYR	CB-CA-C	-9.11	93.12	110.24
4	A	14	PRO	N-CA-C	-8.87	97.37	111.03
5	B	64	PRO	N-CD-CG	8.86	116.49	103.20
5	B	124	PRO	CB-CA-C	-8.83	100.14	110.92
2	L	119	PRO	CB-CA-C	-8.73	100.27	110.92
1	H	127	PHE	CA-C-N	8.73	132.03	120.25
1	H	127	PHE	C-N-CA	8.73	132.03	120.25
5	B	125	PRO	CB-CA-C	-8.70	99.55	110.95
2	L	95	PRO	N-CA-C	-8.65	100.15	110.70
5	B	106	GLY	CA-C-O	-8.63	116.61	122.22
1	H	97	ARG	CB-CG-CD	-8.61	91.50	111.30
5	B	146	PRO	CA-N-CD	-8.61	99.45	111.50
3	R	507	PRO	CA-N-CD	-8.50	100.10	112.00
3	R	501	ASN	CB-CA-C	-8.44	94.57	110.51
1	H	53	SER	O-C-N	8.43	130.86	122.09
1	H	154	PRO	N-CA-CB	-8.41	93.34	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	141	PRO	N-CD-CG	-8.16	94.00	103.80
2	L	204	PRO	CB-CA-C	-8.15	98.12	111.56
4	A	19	ARG	CG-CD-NE	-8.12	94.14	112.00
4	A	126	ALA	N-CA-C	8.10	120.37	110.41
2	L	79	GLN	O-C-N	-8.05	113.95	121.20
4	A	172	THR	CB-CA-C	-8.04	97.99	110.37
3	R	426	PRO	CA-N-CD	-7.97	100.84	112.00
5	B	75	ASP	CA-CB-CG	7.81	120.41	112.60
1	H	53	SER	CA-C-N	7.80	129.88	120.14
1	H	53	SER	C-N-CA	7.80	129.88	120.14
4	A	3	GLN	CB-CA-C	-7.78	96.57	109.80
1	H	67	PHE	CB-CA-C	-7.77	93.97	109.35
2	L	91	LEU	CB-CA-C	7.67	128.66	111.78
2	L	93	SER	N-CA-CB	7.64	123.65	110.81
2	L	101	GLY	CA-C-O	-7.57	115.26	121.77
4	A	161	PRO	N-CA-CB	-7.48	94.37	102.60
5	B	177	THR	CB-CA-C	-7.37	97.24	110.36
2	L	94	TYR	N-CA-CB	7.36	120.72	110.11
5	B	211	THR	CB-CA-C	-7.30	96.87	109.65
2	L	113	PRO	N-CA-CB	-7.29	95.60	103.25
5	B	5	THR	CB-CA-C	-7.27	96.93	109.65
5	B	11	LEU	CA-C-O	-7.22	112.83	119.62
4	A	13	GLN	O-C-N	-7.19	113.37	121.43
1	H	13	GLN	CB-CA-C	-7.09	97.93	109.56
1	H	170	THR	CB-CA-C	7.08	122.15	110.74
2	L	92	ASN	CB-CA-C	-7.00	99.81	111.23
5	B	30	LEU	O-C-N	7.00	131.20	123.22
4	A	161	PRO	CA-N-CD	-6.91	101.82	111.50
4	A	179	PRO	CB-CA-C	-6.91	101.10	110.85
3	R	391	CYS	CA-CB-SG	6.88	130.22	114.40
2	L	183	LYS	N-CA-C	-6.85	103.60	112.23
1	H	151	PHE	CB-CA-C	6.84	119.37	109.45
2	L	178	THR	CA-CB-OG1	-6.84	99.34	109.60
3	R	334	ASN	CA-C-N	6.83	130.54	120.90
3	R	334	ASN	C-N-CA	6.83	130.54	120.90
4	A	95	TYR	CA-C-O	-6.83	112.98	120.36
5	B	131	LYS	N-CA-C	-6.83	103.43	112.72
1	H	207	PRO	CA-N-CD	-6.80	102.48	112.00
1	H	112	THR	CA-CB-OG1	-6.79	99.42	109.60
5	B	64	PRO	N-CA-CB	-6.78	97.63	103.32
4	A	106	ASP	N-CA-C	-6.77	98.99	108.54
1	H	124	PRO	CB-CA-C	-6.77	102.08	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	92	ASN	CA-CB-CG	6.73	119.33	112.60
2	L	22	THR	CA-CB-OG1	-6.69	99.56	109.60
5	B	145	TYR	CA-C-O	6.68	125.80	119.72
4	A	39	GLN	CA-C-N	6.64	129.93	120.49
4	A	39	GLN	C-N-CA	6.64	129.93	120.49
1	H	154	PRO	N-CA-C	6.63	129.34	112.10
2	L	45	LYS	CB-CA-C	-6.63	97.70	109.70
4	A	226	LYS	CB-CA-C	6.60	122.41	109.35
2	L	48	ILE	N-CA-CB	-6.59	102.29	111.19
1	H	149	ASP	N-CA-C	6.52	118.54	110.91
3	R	368	LEU	N-CA-C	-6.51	102.84	111.24
3	R	350	VAL	CA-C-O	-6.46	113.88	121.05
2	L	116	PHE	CB-CA-C	-6.44	96.94	109.68
2	L	137	ASN	CB-CA-C	-6.41	97.97	109.71
1	H	170	THR	CA-CB-OG1	-6.41	99.99	109.60
2	L	91	LEU	CA-C-O	-6.40	114.08	121.82
3	R	415	THR	CB-CA-C	-6.37	96.46	109.38
5	B	169	THR	CB-CA-C	-6.35	97.81	111.78
4	A	105	TYR	N-CA-C	-6.34	104.09	113.72
3	R	342	PHE	CB-CA-C	-6.33	98.14	110.11
4	A	214	PRO	CB-CA-C	-6.32	101.13	111.56
2	L	199	GLN	CB-CA-C	-6.30	98.24	110.46
4	A	102	ARG	CG-CD-NE	-6.28	98.18	112.00
4	A	133	VAL	N-CA-CB	-6.28	104.55	112.15
1	H	77	THR	N-CA-CB	6.26	120.48	110.46
3	R	371	SER	O-C-N	6.26	128.79	122.03
4	A	195	THR	CA-CB-OG1	-6.26	100.21	109.60
3	R	365	TYR	N-CA-C	-6.25	106.34	112.97
4	A	183	GLN	CA-C-O	-6.22	114.62	121.89
5	B	49	PRO	N-CA-C	6.21	120.21	111.33
2	L	172	THR	CA-C-O	-6.20	114.11	121.11
2	L	202	SER	N-CA-C	-6.18	104.46	111.07
3	R	451	TYR	CA-CB-CG	-6.16	102.82	113.90
4	A	82	GLN	CB-CA-C	-6.15	100.22	110.19
2	L	197	THR	CB-CA-C	-6.15	99.15	109.48
5	B	86	GLU	CB-CG-CD	6.15	123.05	112.60
3	R	442	ASP	CB-CA-C	6.14	122.18	109.95
2	L	86	TYR	CA-C-O	-6.14	114.07	120.70
5	B	103	PHE	CB-CA-C	-6.13	98.84	111.22
4	A	159	PRO	CA-N-CD	-6.12	102.93	111.50
4	A	207	ILE	CA-C-N	-6.12	114.28	122.72
4	A	207	ILE	C-N-CA	-6.12	114.28	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	90	GLN	CB-CA-C	-6.11	99.68	109.75
1	H	77	THR	CA-CB-OG1	6.08	118.72	109.60
1	H	2	VAL	CA-C-O	-6.05	113.83	120.48
3	R	462	LYS	O-C-N	-6.03	113.98	121.64
4	A	123	VAL	N-CA-CB	-6.02	104.86	112.15
2	L	98	PHE	CB-CA-C	-6.02	97.98	109.66
4	A	135	PRO	N-CA-C	-6.01	101.72	110.80
1	H	148	LYS	CA-C-N	6.01	132.01	122.93
1	H	148	LYS	C-N-CA	6.01	132.01	122.93
4	A	61	ALA	CA-C-O	-6.01	114.20	121.05
4	A	207	ILE	CB-CA-C	-6.01	102.31	110.42
4	A	214	PRO	CA-C-N	6.00	130.25	120.23
4	A	214	PRO	C-N-CA	6.00	130.25	120.23
1	H	152	PRO	CA-N-CD	-6.00	103.10	111.50
5	B	156	ASP	CB-CA-C	5.98	120.53	111.80
3	R	515	PHE	CA-C-O	-5.95	113.71	120.32
3	R	487	ASN	CA-CB-CG	5.91	118.51	112.60
5	B	172	ASP	CB-CA-C	-5.90	97.58	109.68
1	H	210	THR	CB-CA-C	-5.90	100.37	110.16
3	R	454	ARG	CG-CD-NE	-5.89	99.05	112.00
5	B	30	LEU	CA-C-N	5.87	132.76	121.54
5	B	30	LEU	C-N-CA	5.87	132.76	121.54
4	A	135	PRO	CA-N-CD	-5.86	103.79	112.00
1	H	105	MET	N-CA-C	-5.86	100.72	109.15
5	B	102	THR	CA-C-O	-5.84	113.94	120.66
4	A	106	ASP	CA-CB-CG	5.84	118.44	112.60
5	B	25	SER	CA-C-N	5.82	128.55	120.63
5	B	25	SER	C-N-CA	5.82	128.55	120.63
4	A	136	LEU	N-CA-C	-5.79	99.30	108.73
3	R	506	GLN	O-C-N	-5.78	114.22	121.21
1	H	32	ASN	CB-CA-C	-5.76	99.01	111.11
2	L	176	SER	CA-C-O	-5.75	113.94	120.32
2	L	48	ILE	CA-C-O	-5.72	115.58	120.96
3	R	391	CYS	N-CA-CB	5.67	120.69	110.83
4	A	189	SER	CA-C-O	-5.64	113.93	120.31
1	H	172	PRO	N-CA-C	-5.64	102.33	111.19
5	B	154	LYS	CB-CA-C	-5.62	101.14	110.14
3	R	374	PHE	CB-CA-C	-5.62	98.23	109.35
4	A	79	LEU	CA-C-O	-5.60	114.58	120.80
4	A	95	TYR	CB-CA-C	-5.59	99.48	109.71
1	H	217	GLU	CB-CG-CD	5.58	122.08	112.60
4	A	125	SER	N-CA-C	-5.57	98.93	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	202	THR	CB-CA-C	-5.49	100.22	109.50
4	A	78	THR	CB-CA-C	-5.48	100.48	109.80
2	L	119	PRO	N-CD-CG	-5.47	95.00	103.20
2	L	189	HIS	N-CA-CB	-5.46	102.12	110.85
1	H	115	THR	CB-CA-C	-5.45	102.39	110.62
2	L	87	TYR	CB-CA-C	-5.45	99.84	109.70
2	L	108	ARG	CG-CD-NE	-5.44	100.02	112.00
5	B	64	PRO	CA-N-CD	-5.44	104.38	112.00
2	L	151	ASP	N-CA-C	-5.43	99.22	110.80
3	R	490	PHE	N-CA-C	-5.43	101.65	109.48
2	L	102	THR	CB-CA-C	-5.43	101.78	110.14
3	R	371	SER	N-CA-C	-5.43	105.01	111.03
4	A	91	THR	CA-CB-OG1	-5.42	101.47	109.60
4	A	135	PRO	N-CA-CB	-5.41	98.60	103.36
5	B	10	SER	CA-C-N	-5.40	114.21	122.42
5	B	10	SER	C-N-CA	-5.40	114.21	122.42
5	B	195	LYS	CA-C-N	-5.40	116.26	123.17
5	B	195	LYS	C-N-CA	-5.40	116.26	123.17
2	L	108	ARG	N-CA-CB	-5.39	102.52	111.57
5	B	105	GLN	N-CA-C	-5.38	106.67	113.18
2	L	44	PRO	N-CA-C	5.38	119.02	111.33
5	B	71	GLY	CA-C-O	-5.37	118.58	122.45
4	A	124	SER	CA-C-O	-5.37	115.49	121.23
5	B	46	GLY	CA-C-N	-5.35	114.18	122.59
5	B	46	GLY	C-N-CA	-5.35	114.18	122.59
5	B	12	PRO	N-CA-C	-5.35	101.46	112.47
2	L	129	THR	CA-CB-OG1	-5.34	101.58	109.60
1	H	101	GLU	CB-CG-CD	5.34	121.68	112.60
2	L	144	ALA	CA-C-O	-5.34	115.02	120.89
5	B	145	TYR	CA-C-N	5.33	139.80	127.00
5	B	145	TYR	C-N-CA	5.33	139.80	127.00
1	H	81	GLN	CB-CA-C	-5.33	101.15	109.84
3	R	523	THR	CA-C-N	-5.33	113.72	122.67
3	R	523	THR	C-N-CA	-5.33	113.72	122.67
1	H	15	GLY	N-CA-C	-5.32	108.58	115.59
2	L	146	VAL	CA-C-O	-5.31	115.49	120.22
3	R	515	PHE	O-C-N	5.30	129.51	123.31
4	A	98	LYS	CA-C-O	-5.30	114.61	120.38
4	A	105	TYR	CB-CA-C	5.30	120.98	110.65
1	H	19	ARG	CB-CA-C	-5.29	101.67	110.14
4	A	119	THR	CA-CB-OG1	-5.29	101.67	109.60
4	A	135	PRO	O-C-N	5.26	128.99	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	33	ASN	CB-CA-C	-5.24	100.00	110.42
5	B	77	THR	CA-CB-OG1	-5.22	101.77	109.60
4	A	206	TYR	CB-CA-C	5.21	118.34	109.80
4	A	90	ASP	CA-C-N	-5.20	115.28	122.30
4	A	90	ASP	C-N-CA	-5.20	115.28	122.30
2	L	113	PRO	N-CD-CG	5.19	110.98	103.20
4	A	32	TYR	CB-CA-C	-5.19	100.77	109.48
4	A	107	TYR	CA-C-O	-5.17	115.46	121.15
1	H	153	GLU	N-CA-C	-5.16	102.64	110.39
4	A	195	THR	CA-C-O	-5.15	115.25	120.71
3	R	451	TYR	CA-C-O	-5.14	115.29	120.84
2	L	35	TRP	CA-C-O	-5.13	114.79	120.38
1	H	11	LEU	CA-C-N	-5.12	114.86	122.70
1	H	11	LEU	C-N-CA	-5.12	114.86	122.70
1	H	66	ARG	CG-CD-NE	-5.12	100.74	112.00
4	A	123	VAL	CA-CB-CG1	5.12	119.09	110.40
5	B	196	VAL	O-C-N	5.12	127.67	122.71
4	A	127	SER	N-CA-C	-5.11	99.92	110.80
2	L	153	ALA	CA-C-O	-5.07	114.90	120.43
5	B	59	ARG	CA-C-O	-5.07	115.61	121.19
1	H	217	GLU	CB-CA-C	-5.06	101.44	109.09
3	R	468	ILE	CB-CA-C	-5.05	105.74	112.46
5	B	45	PRO	N-CA-CB	-5.05	98.92	103.36
4	A	35	ASN	CA-CB-CG	5.03	117.63	112.60
2	L	168	SER	CA-C-O	-5.03	112.54	119.12
5	B	87	ASP	CB-CA-C	-5.03	102.23	110.72
2	L	18	ARG	CA-C-O	-5.02	114.99	120.36
2	L	172	THR	CB-CA-C	-5.02	99.44	109.33
1	H	33	TYR	CA-C-O	-5.01	115.22	120.58
4	A	99	THR	CA-CB-OG1	-5.01	102.09	109.60
1	H	140	THR	CA-CB-OG1	-5.01	102.09	109.60

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	159	0
2	L	1604	0	1569	125	1
3	R	1498	0	1408	138	0
4	A	1636	0	1597	173	1
5	B	1659	0	1616	163	0
All	All	7956	0	7724	709	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 (709) 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:CD	1.86	1.33
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:222:LYS:HZ2	4:A:224:GLU:CD	1.43	1.20
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: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
1:H:82:MET:HE1	1:H:93:TYR:CZ	1.88	1.09
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
2:L:150:VAL:CG1	2:L:189:HIS:HD2	1.68	1.06
1:H:139:GLY:C	1:H:191:SER:HG	1.64	1.05
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
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
4:A:112:LYS:NZ	5:B:94:MET:HE1	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:R:388:ASN:O	3:R:526:GLY:C	2.13	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
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
4:A:112:LYS:HZ3	5:B:94:MET:HE1	1.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:86:ARG:CD	1:H:88:GLU:CD	2.52	0.83
1:H:139:GLY:C	1:H:191:SER:OG	2.17	0.83
4:A:161:PRO:HD2	4:A:161:PRO:O	1.79	0.83
1:H:82:MET:HE1	1:H:93:TYR:CE2	2.15	0.82
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
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:86:ARG:HD2	1:H:88:GLU:CD	2.08	0.79
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:A:14:PRO:N	4:A:14:PRO:C	2.41	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:149:ASP:OD1	1:H:176:GLN:NE2	2.20	0.75
1:H:77:THR:HG22	1:H:78:LEU:N	2.01	0.74
5:B:153:TRP:CD1	5:B:184:LEU:CD1	2.69	0.74
1:H:13:GLN:CD	1:H:13:GLN:H	1.95	0.74
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:12:PRO:N	5:B:12:PRO:C	2.47	0.73
5:B:52:LEU:HA	5:B:63:VAL:HG21	1.68	0.73
1:H:22:CYS:C	1:H:77:THR:HG23	2.14	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
4:A:159:PRO:N	4:A:159:PRO:C	2.47	0.73
5:B:24:ARG:HD3	5:B:75:ASP:OD1	1.88	0.73
4:A:190:LEU:HD12	4:A:190:LEU:C	2.14	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
4:A:222:LYS:HZ1	4:A:224:GLU:CD	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:H:152:PRO:N	1:H:152:PRO:C	2.52	0.68
4:A:67:ARG:HG2	4:A:85:SER:HG	1.59	0.68
1:H:14:PRO:C	1:H:16:GLY:H	2.01	0.67
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:72:ASP:CG	1:H:75:LYS:HG3	2.20	0.66
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
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
2:L:152:ASN:HD22	2:L:152:ASN:C	2.03	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:437:ASN:CG	3:R:508:TYR:CZ	2.74	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
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
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:22:CYS:O	1:H:22:CYS:SG	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:TRP:HB3	2:L:96:PRO:HD2	1.80	0.63
3:R:371:SER:OG	3:R:373:SER:OG	2.15	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
1:H:82:MET:CE	1:H:93:TYR:CE2	2.82	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
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
5:B:160:GLN:HA	5:B:160:GLN:OE1	1.98	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:29:PHE:C	4:A:29:PHE:HD1	2.09	0.60
1:H:61:ASP:OD1	1:H:64:LYS:NZ	2.31	0.60
4:A:104:LEU:HD23	4:A:104:LEU:N	2.14	0.60
5:B:118:PRO:HG3	5:B:141:LEU:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:R:426:PRO:N	3:R:426:PRO:C	2.57	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
4:A:39:GLN:C	4:A:92:ALA:HB1	2.28	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:146:GLY:C	4:A:198:SER:HB2	2.27	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
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
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
2:L:140:TYR:CD1	2:L:140:TYR:C	2.81	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
4:A:29:PHE:C	4:A:29:PHE:CD1	2.82	0.58
5:B:4:MET:CE	5:B:23:CYS:SG	2.92	0.58
5:B:196:VAL:HG13	5:B:196:VAL:O	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:167:ASP:CG	2:L:170:ASP:OD1	2.48	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
2:L:209:PHE:CD1	2:L:209:PHE:C	2.83	0.56
4:A:219:VAL:HG12	4:A:219:VAL:O	2.06	0.56
4:A:217:THR:O	4:A:219:VAL:HG23	2.05	0.56
5:B:4:MET:HE3	5:B:23:CYS:SG	2.45	0.56
1:H:23:ALA:CA	1:H:77:THR:HG23	2.36	0.56
4:A:109:TRP:CD1	4:A:109:TRP:C	2.84	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
4:A:112:LYS:HZ1	5:B:94:MET:HE1	1.70	0.55
4:A:159:PRO:C	4:A:159:PRO:CD	2.70	0.55
5:B:129:GLN:CD	5:B:136:SER:OG	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:190:PRO:O	1:H:190:PRO:HG2	2.06	0.55
3:R:338:PHE:C	3:R:340:GLU:H	2.14	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
2:L:181:LEU:HD12	2:L:181:LEU:C	2.32	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
1:H:19:ARG:CD	1:H:81:GLN:NE2	2.67	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
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
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
5:B:198:ALA:CB	5:B:213:SER:CB	2.85	0.53
1:H:39:GLN:HE22	2:L:38:GLN:CD	2.16	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
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
2:L:90:GLN:CD	2:L:93:SER:HB2	2.34	0.53
4:A:178:PHE:HD1	4:A:191:SER:O	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:B:191:TYR:C	5:B:197:TYR:HH	2.16	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
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
4:A:104:LEU:C	4:A:106:ASP:H	2.15	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:207:PRO:N	1:H:207:PRO:C	2.61	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
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
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
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
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
1:H:14:PRO:C	1:H:16:GLY:N	2.66	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:437:ASN:CG	3:R:508:TYR:CE1	2.90	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
1:H:86:ARG:HB2	1:H:88:GLU:CD	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:338:PHE:C	3:R:340:GLU:N	2.69	0.50
5:B:29:LEU:HD21	5:B:95:GLN:HB3	1.94	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
3:R:443:SER:OG	3:R:498:GLN:C	2.54	0.50
5:B:38:LEU:HD13	5:B:38:LEU:C	2.37	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:O	3:R:418:ILE:HG22	2.10	0.49
4:A:190:LEU:C	4:A:190:LEU:CD1	2.84	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
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
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
4:A:104:LEU:C	4:A:106:ASP:N	2.71	0.48
1:H:47:TRP:CG	2:L:96:PRO:HG3	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:150:VAL:CG1	2:L:192:TYR:CE1	2.91	0.48
4:A:136:LEU:HB2	4:A:151:GLY:C	2.38	0.48
4:A:159:PRO:CD	4:A:159:PRO:O	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:31:HIS:ND1	5:B:31:HIS:C	2.71	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
1:H:86:ARG:HD3	1:H:88:GLU:CD	2.19	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
1:H:150:TYR:OH	1:H:183:LEU:HD22	2.10	0.47
2:L:186:TYR:CD1	2:L:186:TYR:C	2.92	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:B:130:LEU:C	5:B:132:SER:H	2.24	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
5:B:97:LEU:HD23	5:B:97:LEU:C	2.40	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:34:MET:HB3	1:H:34:MET:HE3	1.56	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
4:A:87:ARG:O	4:A:123:VAL:HG11	2.16	0.45
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:448:ASN:N	3:R:497:PHE:O	2.46	0.45
5:B:3:VAL:O	5:B:3:VAL:CG1	2.62	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:59:TYR:HE1	4:A:108:VAL:HG21	1.82	0.44
5:B:84:GLU:C	5:B:87:ASP:OD1	2.58	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
1:H:67:PHE:CZ	1:H:82:MET:HE2	2.53	0.44
3:R:335:LEU:HD12	3:R:335:LEU:C	2.42	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
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
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:90:GLN:C	2:L:91:LEU:O	2.49	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
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
4:A:156:ASP:CG	4:A:183:GLN:NE2	2.74	0.43
5:B:118:PRO:HB3	5:B:144:PHE:HB3	2.00	0.43
1:H:22:CYS:C	1:H:77:THR:CG2	2.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:215:SER:OG	4:A:217:THR:OG1	2.14	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
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
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
4:A:81:LEU:HD23	4:A:81:LEU:C	2.44	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:201:LEU:HD23	4:A:201:LEU:HA	1.87	0.42
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
1:H:205:HIS:C	1:H:207:PRO:CD	2.93	0.41
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:97:LEU:C	5:B:97:LEU:CD2	2.93	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
4:A:51:ILE:O	4:A:51:ILE:CG2	2.66	0.41
4:A:64:VAL:O	4:A:64:VAL:CG1	2.68	0.41
5:B:4:MET:HE3	5:B:4:MET:HB3	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:A:34:MET:HB3	4:A:34:MET:HE3	1.68	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
2:L:175:LEU:HD23	2:L:175:LEU:C	2.46	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
1:H:60:ALA:O	1:H:63: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
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
1:H:67:PHE:CE1	1:H:82:MET:HE2	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%)	24	54
5	B	214/219 (98%)	198 (92%)	14 (6%)	2 (1%)	14	41
All	All	1031/1109 (93%)	960 (93%)	68 (7%)	3 (0%)	36	65

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	175/185 (95%)	175 (100%)	0	100	100
2	L	182/184 (99%)	182 (100%)	0	100	100
3	R	163/196 (83%)	163 (100%)	0	100	100
4	A	178/188 (95%)	178 (100%)	0	100	100
5	B	190/192 (99%)	190 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	888/945 (94%)	888 (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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	81	GLN
1	H	110	GLN
2	L	27	GLN
2	L	37	GLN
2	L	38	GLN
2	L	79	GLN
2	L	124	GLN
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	39	GLN
4	A	77	ASN
4	A	176	HIS
4	A	211	ASN
4	A	216	ASN
5	B	6	GLN
5	B	43	GLN
5	B	142	ASN
5	B	165	GLN
5	B	203	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	0.08	1 (0%) 87 78	26, 56, 80, 90	0
2	L	211/214 (98%)	0.01	1 (0%) 87 78	26, 47, 72, 81	0
3	R	189/223 (84%)	0.20	5 (2%) 57 42	20, 50, 107, 123	0
4	A	219/230 (95%)	0.49	12 (5%) 30 23	25, 56, 85, 99	0
5	B	216/219 (98%)	0.09	0 100 100	20, 52, 95, 135	0
All	All	1047/1109 (94%)	0.17	19 (1%) 67 53	20, 52, 91, 135	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	227	SER	3.9
4	A	199	SER	3.9
3	R	525	CYS	3.3
4	A	198	SER	3.1
3	R	437	ASN	2.9
3	R	382	VAL	2.8
4	A	124	SER	2.7
4	A	54	GLY	2.6
4	A	127	SER	2.5
4	A	14	PRO	2.5
3	R	391	CYS	2.3
4	A	15	GLY	2.3
2	L	92	ASN	2.3
4	A	68	PHE	2.2
4	A	138	PRO	2.2
4	A	216	ASN	2.1
3	R	387	LEU	2.1
1	H	101	GLU	2.1
4	A	104	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 oligosaccharides 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.