



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:21 AM UTC

PDB ID : 5R1R / pdb_00005r1r
Title : RIBONUCLEOTIDE REDUCTASE E441A MUTANT R1 PROTEIN FROM
ESCHERICHIA COLI
Authors : Eriksson, M.; Eklund, H.
Deposited on : 1997-09-17
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

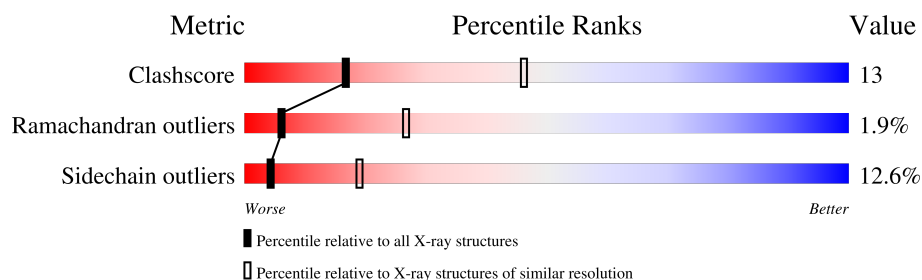
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	761	59% 30% 7% ..
1	B	761	60% 29% 6% ..
1	C	761	59% 30% 7% ..
2	D	20	70% 5% 15% 10%
2	E	20	70% 5% 15% 10%
2	F	20	70% 5% 15% 10%
2	P	20	10% 10% 80%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18154 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 RIBONUCLEOTIDE REDUCTASE R1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	738	Total	C	N	O	S	0	0	0
			5871	3727	1010	1109	25			
1	B	738	Total	C	N	O	S	0	0	0
			5871	3727	1010	1109	25			
1	C	738	Total	C	N	O	S	0	0	0
			5871	3727	1010	1109	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	ALA	GLU	engineered mutation	UNP P00452
B	441	ALA	GLU	engineered mutation	UNP P00452
C	441	ALA	GLU	engineered mutation	UNP P00452

- Molecule 2 is a protein called RIBONUCLEOTIDE REDUCTASE R2 PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	18	Total	C	N	O	0	0	0
			140	84	21	35			
2	E	18	Total	C	N	O	0	0	0
			140	84	21	35			
2	F	18	Total	C	N	O	0	0	0
			140	84	21	35			
2	P	4	Total	C	N	O	0	0	0
			31	22	4	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		

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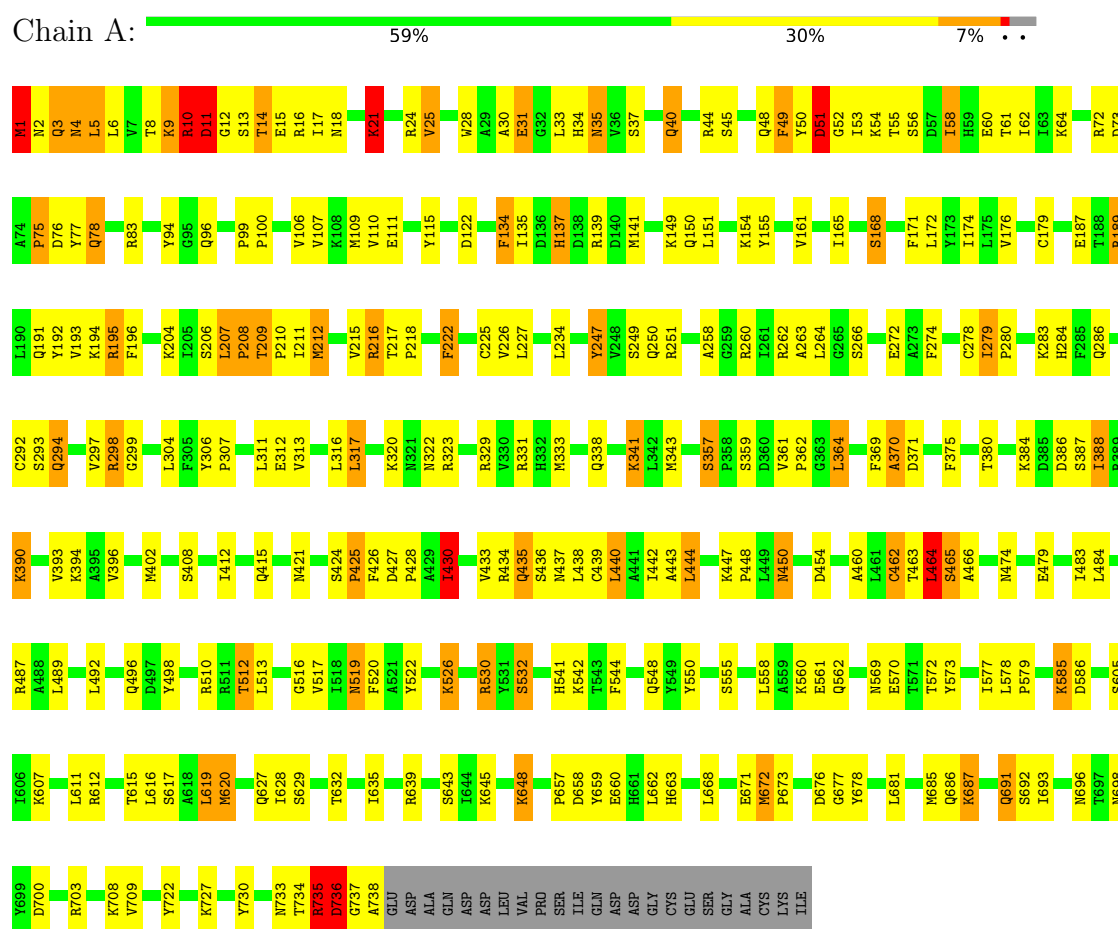
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	30	Total	O	0	0
			30	30		
3	C	32	Total	O	0	0
			32	32		

3 Residue-property plots

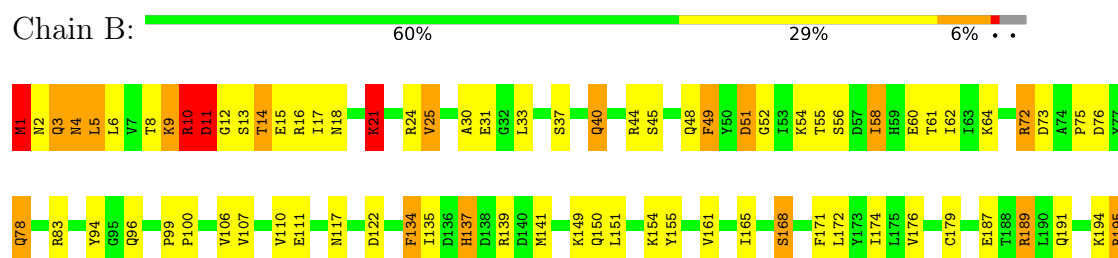
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

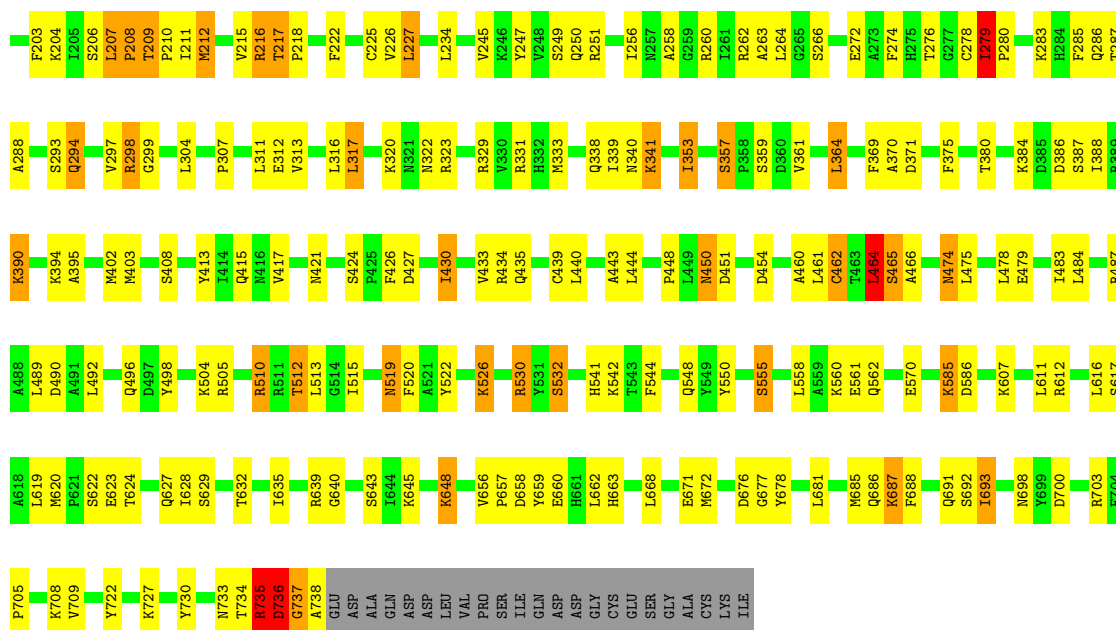
Note EDS was not executed.

• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN



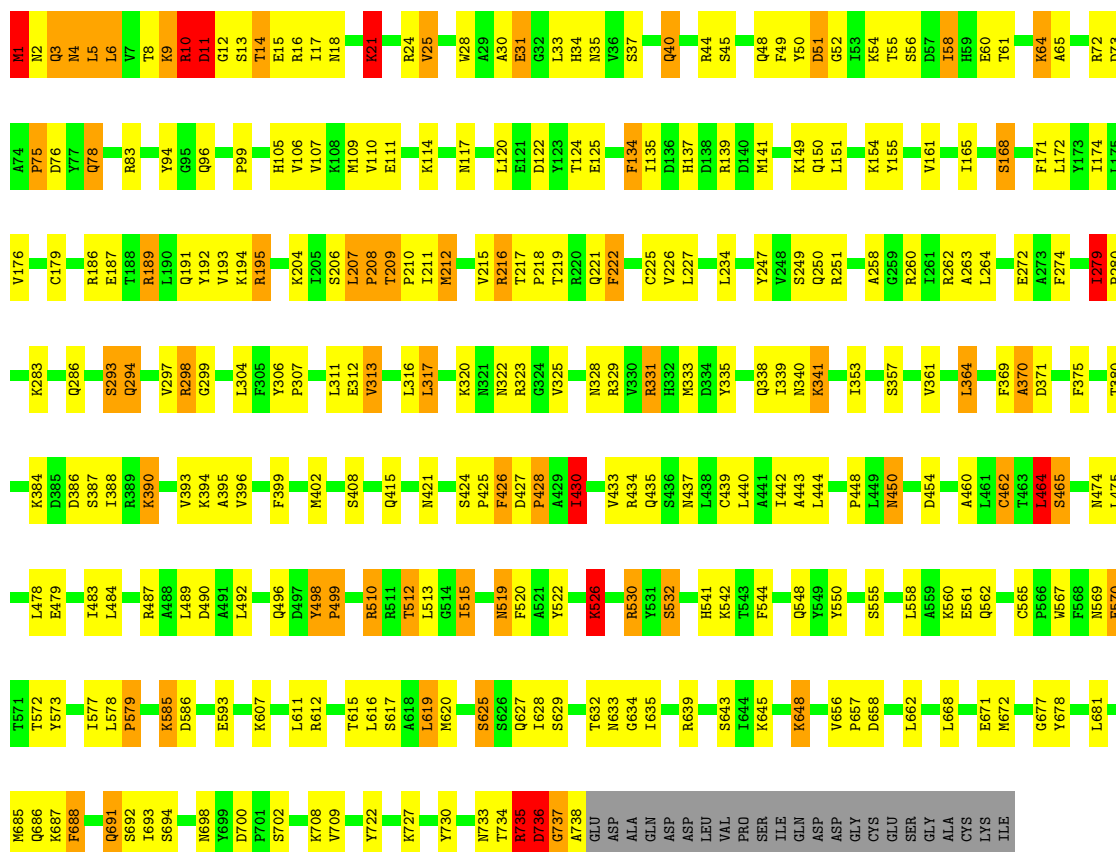
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN



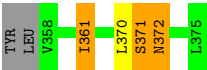


• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

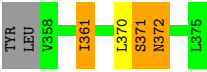
Chain C: 59% 30% 7% . .



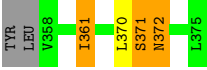
• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	223.81Å 223.81Å 334.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	90.9 (20.00-3.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	TNT, REFMAC	Depositor
R, R_{free}	0.196 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18154	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/5999	1.54	74/8125 (0.9%)
1	B	0.50	0/5999	1.55	65/8125 (0.8%)
1	C	0.54	0/5999	1.59	70/8125 (0.9%)
2	D	0.42	0/140	1.43	1/188 (0.5%)
2	E	0.43	0/140	1.44	1/188 (0.5%)
2	F	0.45	0/140	1.40	1/188 (0.5%)
2	P	0.92	0/31	2.61	2/41 (4.9%)
All	All	0.52	0/18448	1.56	214/24980 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	2
All	All	0	6

There are no bond length outliers.

All (214) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	736	ASP	CA-CB-CG	10.27	122.86	112.60
1	C	736	ASP	CA-CB-CG	9.59	122.19	112.60
1	C	691	GLN	CA-C-O	9.54	123.47	117.94
1	C	195	ARG	CD-NE-CZ	9.44	137.62	124.40
1	B	195	ARG	CD-NE-CZ	8.93	136.91	124.40
1	A	464	LEU	N-CA-C	8.43	123.21	110.14
1	B	293	SER	CA-C-O	8.43	130.65	120.28
1	C	450	ASN	CA-CB-CG	-8.04	104.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	464	LEU	N-CA-C	8.03	122.59	110.14
1	A	293	SER	CA-C-O	8.02	130.14	120.28
1	C	293	SER	CA-C-O	7.93	130.03	120.28
1	C	421	ASN	CA-CB-CG	-7.91	104.69	112.60
1	A	736	ASP	CA-CB-CG	7.90	120.50	112.60
1	C	4	ASN	N-CA-C	7.81	123.14	111.04
1	B	464	LEU	N-CA-C	7.69	122.06	110.14
1	A	208	PRO	N-CA-CB	7.65	109.75	103.32
1	B	293	SER	CA-C-N	7.65	136.15	121.54
1	B	293	SER	C-N-CA	7.65	136.15	121.54
1	C	530	ARG	CD-NE-CZ	7.62	135.07	124.40
1	A	293	SER	CA-C-N	7.57	135.99	121.54
1	A	293	SER	C-N-CA	7.57	135.99	121.54
1	C	293	SER	CA-C-N	7.44	135.75	121.54
1	C	293	SER	C-N-CA	7.44	135.75	121.54
1	B	208	PRO	N-CA-CB	7.38	109.77	103.35
1	B	450	ASN	CA-CB-CG	-7.32	105.28	112.60
2	P	3	VAL	N-CA-C	7.28	124.47	109.34
1	A	299	GLY	CA-C-O	-7.26	117.50	122.22
1	C	620	MET	CB-CA-C	-7.16	97.99	109.37
1	C	530	ARG	NE-CZ-NH1	7.07	128.57	121.50
1	A	544	PHE	CA-CB-CG	-7.03	106.78	113.80
1	C	544	PHE	CA-CB-CG	-7.02	106.78	113.80
1	B	421	ASN	CA-CB-CG	-6.95	105.65	112.60
1	A	4	ASN	N-CA-C	6.92	123.99	110.56
1	A	278	CYS	N-CA-C	6.91	118.90	111.36
2	D	361	ILE	N-CA-C	6.86	119.02	109.29
1	C	25	VAL	CB-CA-C	-6.83	103.13	111.88
2	P	1	TYR	CA-CB-CG	6.82	126.17	113.90
1	A	24	ARG	CD-NE-CZ	6.79	133.91	124.40
1	A	195	ARG	CD-NE-CZ	6.77	133.88	124.40
1	A	462	CYS	CA-C-N	-6.75	113.47	122.85
1	A	462	CYS	C-N-CA	-6.75	113.47	122.85
1	C	430	ILE	CB-CA-C	-6.56	105.29	111.06
1	C	209	THR	CA-C-O	6.54	124.64	118.63
1	B	703	ARG	NE-CZ-NH2	-6.51	113.34	119.20
1	B	462	CYS	CA-C-N	-6.47	113.85	122.85
1	B	462	CYS	C-N-CA	-6.47	113.85	122.85
1	A	450	ASN	CA-CB-CG	-6.46	106.14	112.60
1	C	464	LEU	CA-C-O	6.45	129.36	121.56
1	B	1	MET	CA-C-N	6.44	133.85	121.54
1	B	1	MET	C-N-CA	6.44	133.85	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	PRO	N-CA-CB	6.42	108.94	103.35
1	B	357	SER	N-CA-C	-6.38	102.02	109.93
2	E	361	ILE	N-CA-C	6.37	118.01	108.96
1	A	11	ASP	CA-C-O	6.37	129.62	120.51
1	A	530	ARG	NE-CZ-NH1	6.35	127.85	121.50
1	B	278	CYS	N-CA-C	6.34	118.27	111.36
1	B	530	ARG	CD-NE-CZ	6.33	133.26	124.40
1	A	388	ILE	N-CA-C	6.32	117.19	108.84
1	A	134	PHE	CA-CB-CG	6.32	120.12	113.80
1	A	1	MET	CA-C-N	6.29	133.56	121.54
1	A	1	MET	C-N-CA	6.29	133.56	121.54
1	C	134	PHE	CA-CB-CG	6.29	120.09	113.80
1	B	530	ARG	NE-CZ-NH1	6.29	127.79	121.50
1	C	212	MET	N-CA-C	6.27	118.92	111.33
1	B	451	ASP	CA-C-O	-6.26	114.53	121.23
1	C	11	ASP	CA-C-O	6.25	129.45	120.51
1	A	35	ASN	CA-CB-CG	-6.22	106.38	112.60
1	B	298	ARG	N-CA-C	6.19	118.88	107.99
1	A	517	VAL	N-CA-CB	-6.18	105.29	112.34
1	B	544	PHE	CA-CB-CG	-6.18	107.62	113.80
1	A	298	ARG	N-CA-C	6.17	118.84	107.99
1	C	532	SER	N-CA-C	6.13	120.60	113.18
1	C	1	MET	CA-C-N	6.13	133.25	121.54
1	C	1	MET	C-N-CA	6.13	133.25	121.54
1	B	209	THR	CA-C-O	6.09	124.23	118.63
1	B	4	ASN	N-CA-C	6.08	122.35	110.56
1	C	371	ASP	CA-CB-CG	6.07	118.67	112.60
1	C	370	ALA	N-CA-C	6.07	120.85	112.90
1	A	217	THR	CA-C-N	6.06	125.75	119.82
1	A	217	THR	C-N-CA	6.06	125.75	119.82
1	A	21	LYS	CA-CB-CG	6.05	126.21	114.10
1	B	24	ARG	CD-NE-CZ	6.03	132.83	124.40
1	B	21	LYS	CA-CB-CG	6.00	126.10	114.10
1	C	694	SER	CA-C-O	-6.00	115.10	122.36
1	B	656	VAL	CA-C-N	5.98	126.33	119.93
1	B	656	VAL	C-N-CA	5.98	126.33	119.93
1	B	11	ASP	CA-C-O	5.94	129.01	120.51
1	A	620	MET	CB-CA-C	-5.93	99.94	109.37
1	B	134	PHE	CA-CB-CG	5.92	119.72	113.80
1	B	25	VAL	CB-CA-C	-5.92	104.30	111.88
1	B	490	ASP	CA-CB-CG	-5.92	106.68	112.60
1	A	247	TYR	N-CA-C	5.91	117.80	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	353	ILE	N-CA-CB	5.87	119.51	111.41
1	A	25	VAL	CB-CA-C	-5.85	104.39	111.88
1	A	532	SER	N-CA-C	5.84	120.25	113.18
1	B	217	THR	CA-C-N	5.84	125.94	119.87
1	B	217	THR	C-N-CA	5.84	125.94	119.87
1	C	688	PHE	CA-CB-CG	-5.84	107.96	113.80
1	C	393	VAL	N-CA-CB	5.83	121.00	111.45
1	C	656	VAL	CA-C-N	5.82	126.15	119.93
1	C	656	VAL	C-N-CA	5.82	126.15	119.93
1	C	21	LYS	CA-CB-CG	5.76	125.62	114.10
1	C	279	ILE	CA-C-N	5.71	125.83	119.32
1	C	279	ILE	C-N-CA	5.71	125.83	119.32
1	C	498	TYR	CA-C-N	5.68	125.53	119.28
1	C	498	TYR	C-N-CA	5.68	125.53	119.28
1	C	490	ASP	CA-CB-CG	-5.68	106.92	112.60
1	B	532	SER	N-CA-C	5.67	120.20	113.28
1	A	357	SER	N-CA-C	-5.67	102.90	109.93
1	B	51	ASP	CA-C-O	-5.67	112.41	120.51
1	B	245	VAL	CA-C-O	-5.67	115.16	121.17
1	B	417	VAL	CA-C-O	-5.66	114.36	120.47
1	C	593	GLU	CA-C-O	5.63	124.44	119.71
1	A	77	TYR	CA-C-O	-5.61	114.57	120.63
1	A	218	PRO	N-CA-CB	5.61	108.84	103.52
1	A	530	ARG	CD-NE-CZ	5.60	132.24	124.40
1	A	448	PRO	N-CA-CB	5.59	108.21	103.35
1	A	51	ASP	CA-C-O	-5.57	112.54	120.51
1	C	399	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	703	ARG	NE-CZ-NH2	-5.54	114.21	119.20
1	C	311	LEU	CA-C-O	-5.53	114.66	120.63
1	A	209	THR	CA-C-O	5.52	123.71	118.63
1	A	498	TYR	CA-C-N	5.51	125.34	119.28
1	A	498	TYR	C-N-CA	5.51	125.34	119.28
1	B	624	THR	N-CA-C	5.50	117.13	111.03
1	A	444	LEU	CA-C-O	5.49	125.55	120.50
1	A	447	LYS	CA-C-N	5.48	125.43	119.78
1	A	447	LYS	C-N-CA	5.48	125.43	119.78
1	A	100	PRO	N-CA-CB	5.48	109.00	103.25
1	C	530	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	A	425	PRO	N-CA-CB	5.47	108.39	103.20
1	A	207	LEU	CA-C-N	5.46	125.46	119.89
1	A	207	LEU	C-N-CA	5.46	125.46	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	331	ARG	N-CA-C	5.45	119.64	112.89
1	A	615	THR	CA-C-O	-5.43	114.76	121.06
1	C	207	LEU	CA-C-N	5.41	125.35	119.78
1	C	207	LEU	C-N-CA	5.41	125.35	119.78
1	A	311	LEU	CA-C-O	-5.41	114.79	120.63
1	A	619	LEU	CA-C-O	5.40	126.67	120.84
1	B	498	TYR	CA-C-N	5.40	125.22	119.28
1	B	498	TYR	C-N-CA	5.40	125.22	119.28
1	C	462	CYS	CA-C-N	-5.39	115.17	123.14
1	C	462	CYS	C-N-CA	-5.39	115.17	123.14
1	B	426	PHE	CA-CB-CG	-5.38	108.42	113.80
1	B	207	LEU	CA-C-N	5.38	125.32	119.78
1	B	207	LEU	C-N-CA	5.38	125.32	119.78
1	B	299	GLY	CA-C-O	-5.36	118.74	122.22
1	A	371	ASP	CA-CB-CG	5.35	117.95	112.60
1	C	448	PRO	N-CA-CB	5.34	108.00	103.35
1	A	578	LEU	CA-C-N	5.33	124.78	119.24
1	A	578	LEU	C-N-CA	5.33	124.78	119.24
1	C	498	TYR	CA-C-O	5.33	124.63	119.62
1	A	393	VAL	N-CA-CB	5.31	120.15	111.45
1	B	227	LEU	CA-C-O	-5.30	114.62	120.24
1	B	466	ALA	N-CA-C	5.29	117.30	108.99
1	A	362	PRO	N-CA-CB	5.29	107.95	103.19
1	C	11	ASP	CA-C-N	5.29	131.78	121.41
1	C	11	ASP	C-N-CA	5.29	131.78	121.41
1	A	266	SER	CA-C-N	5.28	125.20	119.76
1	A	266	SER	C-N-CA	5.28	125.20	119.76
1	B	705	PRO	N-CA-CB	5.27	108.02	103.27
1	A	53	ILE	CA-C-O	-5.27	114.84	121.11
1	B	448	PRO	N-CA-CB	5.27	107.93	103.35
1	A	438	LEU	CA-C-O	-5.26	114.86	121.02
1	B	72	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	C	313	VAL	N-CA-C	5.25	116.60	110.62
1	C	648	LYS	N-CA-C	-5.23	106.74	113.23
1	B	49	PHE	CA-CB-CG	5.23	119.03	113.80
1	B	203	PHE	N-CA-C	5.23	118.81	111.90
1	B	266	SER	CA-C-N	5.23	125.14	119.76
1	B	266	SER	C-N-CA	5.23	125.14	119.76
1	B	212	MET	N-CA-C	5.22	117.64	111.33
1	C	299	GLY	CA-C-O	-5.21	118.63	122.23
1	C	565	CYS	CA-C-N	5.21	126.36	119.84
1	C	565	CYS	C-N-CA	5.21	126.36	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	691	GLN	CA-C-O	5.21	120.96	117.94
1	C	702	SER	CB-CA-C	-5.21	101.83	110.68
1	A	357	SER	CA-C-N	5.19	125.24	119.32
1	A	357	SER	C-N-CA	5.19	125.24	119.32
1	A	222	PHE	CA-C-N	5.19	128.47	121.05
1	A	222	PHE	C-N-CA	5.19	128.47	121.05
1	B	413	TYR	CA-C-O	5.17	127.82	121.72
1	B	464	LEU	CA-C-O	5.17	127.81	121.56
1	B	693	ILE	CA-C-O	-5.15	114.82	120.43
1	B	279	ILE	CA-C-N	5.15	125.19	119.32
1	B	279	ILE	C-N-CA	5.15	125.19	119.32
1	C	335	TYR	CA-CB-CG	-5.14	104.65	113.90
1	C	515	ILE	CA-C-O	-5.14	115.07	120.57
1	C	526	LYS	N-CA-CB	5.12	118.11	110.22
1	A	435	GLN	OE1-CD-NE2	5.10	127.70	122.60
1	C	625	SER	CA-C-O	-5.09	115.16	120.55
1	C	615	THR	CA-C-O	-5.09	114.50	120.60
1	A	430	ILE	CB-CA-C	-5.08	106.59	111.06
1	C	24	ARG	CD-NE-CZ	5.08	131.51	124.40
1	C	428	PRO	N-CA-CB	5.08	108.88	103.39
1	C	499	PRO	N-CA-CB	5.07	108.87	103.39
1	B	311	LEU	CA-C-O	-5.07	115.15	120.63
1	B	688	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	370	ALA	N-CA-C	5.07	119.49	112.45
1	C	426	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	72	ARG	NE-CZ-NH1	-5.06	116.44	121.50
2	F	361	ILE	N-CA-C	5.06	117.04	109.20
1	C	619	LEU	CA-C-O	5.03	126.28	120.84
1	A	212	MET	N-CA-C	5.03	117.42	111.33
1	A	412	ILE	N-CA-CB	5.03	118.01	111.83
1	A	421	ASN	CA-CB-CG	-5.03	107.57	112.60
1	C	298	ARG	N-CA-C	5.02	116.83	107.99
1	A	672	MET	CA-C-N	5.02	124.63	119.56
1	A	672	MET	C-N-CA	5.02	124.63	119.56
1	C	222	PHE	CA-C-N	5.02	127.89	120.82
1	C	222	PHE	C-N-CA	5.02	127.89	120.82
1	B	100	PRO	N-CA-CB	5.01	108.51	103.25
1	A	49	PHE	CA-CB-CG	5.00	118.81	113.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	HIS	Mainchain
1	A	579	PRO	Mainchain
1	A	75	PRO	Mainchain
1	B	137	HIS	Mainchain
1	C	579	PRO	Mainchain
1	C	75	PRO	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	A	5871	0	5798	153	0
1	B	5871	0	5798	147	0
1	C	5871	0	5798	157	0
2	D	140	0	123	2	0
2	E	140	0	123	2	0
2	F	140	0	123	2	0
2	P	31	0	34	5	0
3	A	28	0	0	3	0
3	B	30	0	0	4	0
3	C	32	0	0	6	0
All	All	18154	0	17797	460	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (460) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:SER:HB3	1:B:40:GLN:HB2	1.47	0.96
1:A:37:SER:HB3	1:A:40:GLN:HB2	1.51	0.93
1:C:37:SER:HB3	1:C:40:GLN:HB2	1.51	0.93
1:A:83:ARG:HG2	1:A:141:MET:HG3	1.56	0.87
1:A:698:ASN:ND2	1:A:733:ASN:HD22	1.72	0.86
1:C:191:GLN:HE21	1:C:195:ARG:HH21	1.21	0.86
1:B:83:ARG:HG2	1:B:141:MET:HG3	1.58	0.85
1:B:698:ASN:ND2	1:B:733:ASN:HD22	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLN:HE21	1:A:195:ARG:HH21	1.26	0.82
1:B:191:GLN:HE21	1:B:195:ARG:HH21	1.27	0.80
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.64	0.80
1:A:4:ASN:O	1:A:5:LEU:HB2	1.80	0.80
1:B:658:ASP:HB3	1:B:662:LEU:HD12	1.65	0.79
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.63	0.79
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.65	0.78
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.65	0.78
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.65	0.77
1:C:698:ASN:ND2	1:C:733:ASN:HD22	1.83	0.76
1:C:83:ARG:HG2	1:C:141:MET:HG3	1.67	0.76
1:B:9:LYS:HE2	1:B:55:THR:HG21	1.68	0.76
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.69	0.75
1:C:9:LYS:HE2	1:C:55:THR:HG21	1.68	0.75
1:A:150:GLN:HE21	1:A:627:GLN:NE2	1.85	0.75
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.68	0.75
1:B:4:ASN:O	1:B:5:LEU:HB2	1.84	0.75
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.68	0.74
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.66	0.74
1:A:1:MET:H2	1:A:3:GLN:HG3	1.53	0.74
1:C:4:ASN:O	1:C:5:LEU:HB2	1.87	0.73
1:C:150:GLN:HE21	1:C:627:GLN:NE2	1.87	0.72
1:B:294:GLN:HB2	1:B:298:ARG:HB3	1.71	0.70
1:B:1:MET:H2	1:B:3:GLN:HG3	1.57	0.70
1:B:215:VAL:O	1:B:216:ARG:HB3	1.90	0.70
1:A:9:LYS:HE2	1:A:55:THR:HG21	1.72	0.70
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.74	0.69
1:A:294:GLN:HB2	1:A:298:ARG:HB3	1.73	0.69
1:B:150:GLN:HE21	1:B:627:GLN:NE2	1.91	0.68
1:A:215:VAL:O	1:A:216:ARG:HB3	1.94	0.67
1:C:294:GLN:HB2	1:C:298:ARG:HB3	1.75	0.67
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.76	0.67
1:C:322:ASN:HA	1:C:331:ARG:NH1	2.10	0.66
1:B:734:THR:O	1:B:735:ARG:HB2	1.96	0.66
1:B:207:LEU:CB	1:B:212:MET:HE3	2.26	0.66
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.77	0.65
1:B:698:ASN:HD21	1:B:733:ASN:HD22	1.44	0.65
1:B:519:ASN:ND2	1:B:632:THR:H	1.94	0.65
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.77	0.65
1:B:234:LEU:HG	1:B:272:GLU:HG2	1.78	0.65
1:B:465:SER:HB2	1:B:489:LEU:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.77	0.64
1:A:489:LEU:HB3	1:A:513:LEU:HD22	1.79	0.64
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.78	0.64
1:C:1:MET:H2	1:C:3:GLN:HG3	1.63	0.64
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.78	0.64
1:C:734:THR:O	1:C:735:ARG:HB2	1.97	0.64
1:A:234:LEU:HG	1:A:272:GLU:HG2	1.80	0.64
1:A:522:TYR:CE2	1:A:526:LYS:HD3	2.33	0.64
1:C:361:VAL:HG21	1:C:364:LEU:HD12	1.78	0.64
1:B:361:VAL:HG21	1:B:364:LEU:HD12	1.79	0.63
1:B:686:GLN:NE2	1:B:727:LYS:HD2	2.14	0.63
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.82	0.62
1:B:322:ASN:HA	1:B:331:ARG:NH1	2.14	0.62
1:C:215:VAL:O	1:C:216:ARG:HB3	2.00	0.62
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.80	0.62
1:C:234:LEU:HG	1:C:272:GLU:HG2	1.81	0.62
1:A:207:LEU:CB	1:A:212:MET:HE3	2.30	0.62
1:A:361:VAL:HG21	1:A:364:LEU:HD12	1.80	0.62
1:C:465:SER:HB2	1:C:489:LEU:HD11	1.81	0.62
1:A:322:ASN:HA	1:A:331:ARG:NH1	2.15	0.61
1:C:522:TYR:CE2	1:C:526:LYS:HD3	2.35	0.61
1:A:555:SER:HB3	1:A:611:LEU:HD22	1.83	0.61
1:C:94:TYR:OH	1:C:168:SER:HB3	2.01	0.61
1:C:120:LEU:HD13	2:P:1:TYR:HB3	1.83	0.61
1:B:370:ALA:HB1	3:B:786:HOH:O	2.00	0.61
1:B:700:ASP:OD2	1:B:736:ASP:HB3	2.01	0.60
1:B:94:TYR:OH	1:B:168:SER:HB3	2.02	0.60
1:B:106:VAL:O	1:B:110:VAL:HG23	2.01	0.60
1:A:734:THR:O	1:A:735:ARG:HB2	2.01	0.60
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.83	0.60
1:C:172:LEU:O	1:C:176:VAL:HG23	2.02	0.60
1:C:207:LEU:CB	1:C:212:MET:HE3	2.31	0.60
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.82	0.60
1:B:561:GLU:HG2	1:B:562:GLN:HG2	1.83	0.59
1:B:489:LEU:HB3	1:B:513:LEU:HD22	1.85	0.59
1:A:94:TYR:OH	1:A:168:SER:HB3	2.00	0.59
1:A:585:LYS:HD3	1:A:586:ASP:OD1	2.02	0.59
1:C:187:GLU:HB2	3:C:782:HOH:O	2.02	0.59
1:A:272:GLU:HB3	1:A:274:PHE:HE1	1.67	0.59
1:A:698:ASN:HD21	1:A:733:ASN:HD22	1.47	0.59
1:B:555:SER:HB3	1:B:611:LEU:HD22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:GLU:HB3	1:C:274:PHE:HE1	1.68	0.59
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.85	0.58
1:A:18:ASN:ND2	1:A:21:LYS:HE3	2.18	0.58
1:C:700:ASP:OD2	1:C:736:ASP:HB3	2.03	0.58
1:A:585:LYS:HD2	1:A:585:LYS:N	2.19	0.58
1:A:519:ASN:ND2	1:A:522:TYR:HB3	2.19	0.58
1:B:585:LYS:HD2	1:B:585:LYS:N	2.17	0.58
1:C:286:GLN:HG3	1:C:333:MET:HG3	1.84	0.58
1:C:585:LYS:HD3	1:C:586:ASP:OD1	2.03	0.58
1:C:120:LEU:HD13	2:P:1:TYR:CG	2.38	0.58
1:A:369:PHE:CG	1:A:434:ARG:HG2	2.39	0.58
1:C:56:SER:O	1:C:60:GLU:HG2	2.03	0.57
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.85	0.57
1:C:698:ASN:HD21	1:C:733:ASN:HD22	1.52	0.57
1:B:215:VAL:O	1:B:216:ARG:CB	2.52	0.57
1:B:56:SER:O	1:B:60:GLU:HG2	2.04	0.57
1:B:585:LYS:HD3	1:B:586:ASP:OD1	2.05	0.57
1:C:106:VAL:O	1:C:110:VAL:HG23	2.05	0.57
1:B:479:GLU:HB2	1:B:550:TYR:CE1	2.40	0.57
1:A:176:VAL:HG22	3:A:787:HOH:O	2.05	0.57
1:B:207:LEU:HB2	1:B:212:MET:HE3	1.85	0.57
1:B:522:TYR:CE2	1:B:526:LYS:HD3	2.39	0.57
1:B:541:HIS:NE2	1:B:687:LYS:HE2	2.20	0.56
1:B:272:GLU:HB3	1:B:274:PHE:HE1	1.69	0.56
1:C:489:LEU:HB3	1:C:513:LEU:HD22	1.87	0.56
1:C:548:GLN:HA	1:C:548:GLN:NE2	2.20	0.56
1:A:427:ASP:HB3	1:A:430:ILE:HD12	1.87	0.56
1:A:33:LEU:HB3	1:A:76:ASP:HB3	1.87	0.56
1:B:548:GLN:HA	1:B:548:GLN:NE2	2.21	0.56
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.88	0.55
1:B:585:LYS:HD2	1:B:585:LYS:H	1.70	0.55
1:B:176:VAL:HG22	3:B:789:HOH:O	2.06	0.55
1:B:215:VAL:HB	3:B:789:HOH:O	2.06	0.55
1:C:686:GLN:NE2	1:C:727:LYS:HD2	2.22	0.55
1:A:56:SER:O	1:A:60:GLU:HG2	2.07	0.55
1:C:150:GLN:NE2	1:C:627:GLN:NE2	2.54	0.55
1:C:176:VAL:HG22	3:C:791:HOH:O	2.05	0.55
1:A:99:PRO:HG2	1:A:137:HIS:CD2	2.42	0.55
1:A:106:VAL:O	1:A:110:VAL:HG23	2.06	0.55
1:A:686:GLN:HE22	1:A:692:SER:HA	1.71	0.55
1:A:187:GLU:HB2	3:C:762:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:THR:N	1:B:210:PRO:HD2	2.21	0.54
1:C:541:HIS:NE2	1:C:687:LYS:HE2	2.21	0.54
1:A:99:PRO:HG2	1:A:137:HIS:CG	2.43	0.54
1:A:150:GLN:NE2	1:A:627:GLN:NE2	2.54	0.54
1:A:561:GLU:HG2	1:A:562:GLN:HG2	1.88	0.54
1:A:272:GLU:HB3	1:A:274:PHE:CE1	2.43	0.54
1:A:479:GLU:HB2	1:A:550:TYR:CE1	2.43	0.54
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.36	0.54
1:A:585:LYS:HD2	1:A:585:LYS:H	1.72	0.54
2:D:372:ASN:H	2:D:372:ASN:ND2	2.04	0.54
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.90	0.54
1:B:462:CYS:HB3	1:B:464:LEU:HD21	1.89	0.54
1:B:122:ASP:O	1:B:189:ARG:NH2	2.41	0.54
1:C:49:PHE:CZ	1:C:58:ILE:HG23	2.42	0.54
1:A:522:TYR:CZ	1:A:526:LYS:HD3	2.42	0.54
1:C:10:ARG:O	1:C:11:ASP:C	2.50	0.54
1:C:99:PRO:HG2	1:C:137:HIS:CG	2.42	0.54
1:B:427:ASP:HB3	1:B:430:ILE:HD12	1.89	0.54
1:A:464:LEU:HD11	1:A:620:MET:HE2	1.90	0.53
1:A:672:MET:HE1	1:A:678:TYR:HB2	1.90	0.53
1:B:294:GLN:HG2	1:B:298:ARG:HD3	1.90	0.53
1:A:172:LEU:O	1:A:176:VAL:HG23	2.09	0.53
1:B:286:GLN:HG3	1:B:333:MET:HG3	1.89	0.53
1:C:561:GLU:HG2	1:C:562:GLN:HG2	1.89	0.53
1:C:686:GLN:CD	1:C:727:LYS:HD2	2.34	0.53
1:C:548:GLN:HA	1:C:548:GLN:HE21	1.72	0.53
1:C:555:SER:HB3	1:C:611:LEU:HD22	1.90	0.53
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.91	0.53
1:A:548:GLN:HA	1:A:548:GLN:NE2	2.24	0.53
1:A:700:ASP:OD2	1:A:736:ASP:HB3	2.08	0.53
1:B:99:PRO:HG2	1:B:137:HIS:CD2	2.44	0.53
1:B:99:PRO:HG2	1:B:137:HIS:CG	2.43	0.53
1:B:686:GLN:CD	1:B:727:LYS:HD2	2.33	0.53
1:C:700:ASP:CG	1:C:736:ASP:HB3	2.34	0.53
1:B:18:ASN:ND2	1:B:21:LYS:HE3	2.24	0.53
1:C:122:ASP:O	1:C:189:ARG:NH2	2.41	0.53
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.91	0.53
1:A:698:ASN:ND2	1:A:733:ASN:ND2	2.51	0.53
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.91	0.53
1:C:99:PRO:HG2	1:C:137:HIS:CD2	2.44	0.53
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ASN:ND2	1:C:522:TYR:HB3	2.24	0.52
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.91	0.52
1:A:541:HIS:NE2	1:A:687:LYS:HE2	2.23	0.52
1:B:172:LEU:O	1:B:176:VAL:HG23	2.10	0.52
1:C:120:LEU:HD13	2:P:1:TYR:CB	2.40	0.52
1:C:427:ASP:HB3	1:C:430:ILE:HD12	1.90	0.52
1:B:83:ARG:CG	1:B:141:MET:HG3	2.36	0.52
1:A:215:VAL:O	1:A:216:ARG:CB	2.58	0.52
1:C:483:ILE:HG23	1:C:487:ARG:HD2	1.91	0.52
1:C:519:ASN:ND2	1:C:632:THR:H	2.08	0.52
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.92	0.52
1:A:548:GLN:HA	1:A:548:GLN:HE21	1.75	0.52
1:B:272:GLU:HB3	1:B:274:PHE:CE1	2.44	0.52
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.92	0.52
1:C:215:VAL:O	1:C:216:ARG:CB	2.58	0.52
1:A:294:GLN:HG2	1:A:298:ARG:HD3	1.91	0.52
1:A:208:PRO:HG2	1:A:211:ILE:HD12	1.91	0.52
1:B:10:ARG:O	1:B:11:ASP:C	2.53	0.52
1:B:250:GLN:O	1:B:251:ARG:HB2	2.10	0.52
1:C:272:GLU:HB3	1:C:274:PHE:CE1	2.43	0.52
1:C:522:TYR:CZ	1:C:526:LYS:HD3	2.45	0.51
1:A:49:PHE:CZ	1:A:58:ILE:HG23	2.45	0.51
1:A:522:TYR:CD1	1:A:657:PRO:HB2	2.44	0.51
1:B:698:ASN:ND2	1:B:733:ASN:ND2	2.52	0.51
1:B:700:ASP:CG	1:B:736:ASP:HB3	2.35	0.51
1:C:585:LYS:HD2	1:C:585:LYS:N	2.24	0.51
1:A:286:GLN:HG3	1:A:333:MET:HG3	1.91	0.51
1:C:444:LEU:HD12	1:C:460:ALA:HB1	1.91	0.51
2:F:372:ASN:ND2	2:F:372:ASN:H	2.08	0.51
1:A:250:GLN:O	1:A:251:ARG:HB2	2.10	0.51
1:C:33:LEU:HB3	1:C:76:ASP:HB3	1.91	0.51
1:B:33:LEU:HB3	1:B:76:ASP:HB3	1.92	0.51
1:A:122:ASP:O	1:A:189:ARG:NH2	2.43	0.51
1:A:209:THR:N	1:A:210:PRO:HD2	2.26	0.51
1:B:672:MET:HE1	1:B:678:TYR:HB2	1.93	0.51
1:C:522:TYR:CD1	1:C:657:PRO:HB2	2.46	0.51
1:A:464:LEU:CD1	1:A:620:MET:HE2	2.41	0.51
1:B:49:PHE:CZ	1:B:58:ILE:HG23	2.46	0.51
1:C:209:THR:N	1:C:210:PRO:HD2	2.26	0.51
1:B:263:ALA:HB3	1:B:357:SER:HB2	1.92	0.51
1:B:548:GLN:HA	1:B:548:GLN:HE21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:O	1:A:111:GLU:HG3	2.11	0.50
1:C:18:ASN:ND2	1:C:21:LYS:HE3	2.26	0.50
1:B:388:ILE:O	1:B:390:LYS:HE3	2.12	0.50
2:E:372:ASN:H	2:E:372:ASN:ND2	2.08	0.50
1:A:686:GLN:CD	1:A:727:LYS:HD2	2.36	0.50
1:A:415:GLN:HE22	1:A:435:GLN:HA	1.76	0.50
1:A:10:ARG:O	1:A:11:ASP:C	2.55	0.50
1:A:150:GLN:HE21	1:A:627:GLN:HE22	1.56	0.49
1:B:171:PHE:HA	1:B:174:ILE:HG22	1.94	0.49
1:B:313:VAL:HG22	1:B:317:LEU:HD22	1.93	0.49
1:B:450:ASN:HB2	1:B:454:ASP:OD2	2.12	0.49
1:B:150:GLN:NE2	1:B:627:GLN:NE2	2.60	0.49
1:B:522:TYR:CZ	1:B:526:LYS:HD3	2.47	0.49
1:C:633:ASN:O	1:C:634:GLY:C	2.55	0.49
1:A:171:PHE:HA	1:A:174:ILE:HG22	1.93	0.49
1:B:312:GLU:O	1:B:316:LEU:HG	2.13	0.49
1:C:479:GLU:HB2	1:C:550:TYR:CE1	2.48	0.49
1:C:369:PHE:CG	1:C:434:ARG:HG2	2.47	0.49
1:A:444:LEU:HD12	1:A:460:ALA:HB1	1.94	0.49
1:C:191:GLN:HE21	1:C:195:ARG:NH2	2.00	0.49
1:A:207:LEU:HB3	1:A:212:MET:HE3	1.95	0.49
1:A:329:ARG:HG3	1:A:331:ARG:NH1	2.27	0.49
1:B:208:PRO:HG2	1:B:211:ILE:HD12	1.94	0.49
1:B:444:LEU:HD12	1:B:460:ALA:HB1	1.94	0.49
1:B:681:LEU:O	1:B:685:MET:HG3	2.12	0.49
1:B:21:LYS:O	1:B:25:VAL:HG23	2.13	0.49
1:C:75:PRO:O	1:C:78:GLN:HG3	2.13	0.49
1:C:263:ALA:HB3	1:C:357:SER:HB2	1.95	0.49
1:C:151:LEU:HA	1:C:155:TYR:HB2	1.94	0.49
1:C:475:LEU:O	1:C:478:LEU:HB2	2.12	0.49
1:C:207:LEU:HB2	1:C:212:MET:HE3	1.94	0.48
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.95	0.48
1:B:341:LYS:HG2	1:B:722:TYR:OH	2.13	0.48
1:C:21:LYS:O	1:C:25:VAL:HG23	2.13	0.48
1:B:329:ARG:HG3	1:B:331:ARG:NH1	2.27	0.48
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.94	0.48
1:B:134:PHE:CE2	1:B:194:LYS:HB2	2.47	0.48
1:C:569:ASN:H	1:C:569:ASN:ND2	2.11	0.48
1:C:28:TRP:O	1:C:31:GLU:HB2	2.14	0.48
1:C:492:LEU:O	1:C:496:GLN:HG2	2.13	0.48
1:A:6:LEU:O	1:A:52:GLY:HA2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:HIS:O	1:A:35:ASN:HB2	2.12	0.48
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.95	0.48
1:A:686:GLN:NE2	1:A:727:LYS:HD2	2.28	0.48
1:A:698:ASN:HD22	1:A:733:ASN:HD22	1.60	0.48
1:A:45:SER:CB	1:A:61:THR:HG22	2.43	0.48
1:A:207:LEU:HB2	1:A:212:MET:HE3	1.95	0.48
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.95	0.47
1:A:263:ALA:HB3	1:A:357:SER:HB2	1.95	0.47
1:B:369:PHE:CG	1:B:434:ARG:HG2	2.49	0.47
1:C:45:SER:CB	1:C:61:THR:HG22	2.45	0.47
1:C:307:PRO:HA	1:C:338:GLN:HB2	1.96	0.47
1:B:187:GLU:HB2	3:B:780:HOH:O	2.14	0.47
1:B:492:LEU:O	1:B:496:GLN:HG2	2.14	0.47
1:A:434:ARG:O	1:A:435:GLN:HB3	2.14	0.47
1:A:532:SER:HA	1:A:677:GLY:HA3	1.95	0.47
1:B:439:CYS:HA	1:B:730:TYR:CE1	2.49	0.47
1:C:462:CYS:HB3	1:C:464:LEU:HD21	1.95	0.47
1:B:222:PHE:HD2	1:B:496:GLN:HB3	1.79	0.47
1:C:171:PHE:HA	1:C:174:ILE:HG22	1.95	0.47
1:C:569:ASN:H	1:C:569:ASN:HD22	1.62	0.47
1:B:617:SER:O	1:B:691:GLN:HG3	2.15	0.47
1:C:341:LYS:HG2	1:C:722:TYR:OH	2.13	0.47
1:C:572:THR:HB	1:C:577:ILE:HB	1.95	0.47
1:A:483:ILE:HG23	1:A:487:ARG:HD2	1.97	0.47
1:B:522:TYR:CD1	1:B:657:PRO:HB2	2.49	0.47
1:B:668:LEU:HB2	1:B:671:GLU:HG3	1.97	0.47
1:C:120:LEU:HB3	2:P:1:TYR:CE1	2.50	0.47
1:C:686:GLN:HE22	1:C:692:SER:HA	1.80	0.47
1:A:75:PRO:O	1:A:78:GLN:HG3	2.15	0.47
1:A:519:ASN:ND2	1:A:632:THR:H	2.12	0.47
1:A:700:ASP:CG	1:A:736:ASP:HB3	2.40	0.47
1:B:686:GLN:HE22	1:B:692:SER:HA	1.80	0.47
1:A:21:LYS:O	1:A:25:VAL:HG23	2.15	0.47
1:A:262:ARG:HD2	1:A:274:PHE:HB2	1.97	0.47
1:B:402:MET:HE3	1:B:403:MET:SD	2.55	0.47
1:C:134:PHE:CE2	1:C:194:LYS:HB2	2.49	0.47
1:A:737:GLY:O	1:A:738:ALA:HB3	2.15	0.46
1:B:191:GLN:HE21	1:B:195:ARG:NH2	2.03	0.46
1:C:1:MET:HA	1:C:3:GLN:NE2	2.30	0.46
1:A:83:ARG:CG	1:A:141:MET:HG3	2.36	0.46
1:C:262:ARG:HD2	1:C:274:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.41	0.46
1:B:6:LEU:O	1:B:52:GLY:HA2	2.16	0.46
1:C:450:ASN:HB2	1:C:454:ASP:OD2	2.15	0.46
1:A:572:THR:HB	1:A:577:ILE:HB	1.97	0.46
1:C:208:PRO:HG2	1:C:211:ILE:HD12	1.97	0.46
1:C:329:ARG:HG3	1:C:331:ARG:NH1	2.29	0.46
1:A:370:ALA:HB1	3:A:784:HOH:O	2.15	0.46
1:B:415:GLN:HE22	1:B:435:GLN:HA	1.81	0.46
1:A:439:CYS:HA	1:A:730:TYR:CE1	2.51	0.46
2:D:370:LEU:O	2:D:371:SER:C	2.59	0.46
1:C:222:PHE:HD2	1:C:496:GLN:HB3	1.80	0.46
1:C:737:GLY:O	1:C:738:ALA:HB3	2.15	0.46
1:B:532:SER:HA	1:B:677:GLY:HA3	1.98	0.45
1:A:191:GLN:HE21	1:A:195:ARG:NH2	2.05	0.45
1:A:341:LYS:HG2	1:A:722:TYR:OH	2.16	0.45
1:B:226:VAL:HG12	1:B:461:LEU:CD2	2.47	0.45
1:A:659:TYR:CE1	1:A:663:HIS:HB3	2.52	0.45
1:B:483:ILE:HG23	1:B:487:ARG:HD2	1.98	0.45
1:B:648:LYS:HE3	1:B:648:LYS:H	1.79	0.45
1:C:353:ILE:HG13	1:C:395:ALA:HB2	1.99	0.45
1:B:45:SER:CB	1:B:61:THR:HG22	2.47	0.45
1:B:117:ASN:H	1:B:117:ASN:ND2	2.13	0.45
1:B:464:LEU:CD1	1:B:620:MET:HE2	2.46	0.45
1:C:294:GLN:HG2	1:C:298:ARG:HD3	1.98	0.45
1:C:388:ILE:O	1:C:390:LYS:HE3	2.17	0.45
1:A:284:HIS:HA	1:B:287:THR:CB	2.47	0.45
1:A:617:SER:O	1:A:691:GLN:HG3	2.15	0.45
1:B:262:ARG:HD2	1:B:274:PHE:HB2	1.99	0.45
1:B:659:TYR:O	1:B:660:GLU:C	2.60	0.45
1:C:737:GLY:O	1:C:738:ALA:CB	2.64	0.45
1:C:6:LEU:O	1:C:52:GLY:HA2	2.17	0.45
1:C:207:LEU:HB3	1:C:212:MET:HE3	1.98	0.45
1:C:250:GLN:O	1:C:251:ARG:HB2	2.16	0.45
1:C:532:SER:HA	1:C:677:GLY:HA3	1.98	0.45
1:C:548:GLN:HB2	1:C:688:PHE:HB3	1.99	0.45
1:C:617:SER:O	1:C:691:GLN:HG3	2.17	0.45
1:A:426:PHE:O	1:A:428:PRO:HD3	2.17	0.45
1:B:58:ILE:O	1:B:62:ILE:HG23	2.16	0.45
1:B:737:GLY:O	1:B:738:ALA:HB3	2.16	0.45
1:C:50:TYR:O	1:C:51:ASP:C	2.60	0.45
1:C:520:PHE:HB3	1:C:635:ILE:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:HB	3:A:787:HOH:O	2.15	0.45
1:A:569:ASN:ND2	1:A:569:ASN:H	2.15	0.45
1:B:262:ARG:HB3	1:B:359:SER:HB3	1.99	0.44
1:C:585:LYS:HD2	1:C:585:LYS:H	1.82	0.44
1:A:58:ILE:O	1:A:62:ILE:HG23	2.18	0.44
1:B:364:LEU:HD22	1:B:375:PHE:CE1	2.52	0.44
1:C:64:LYS:O	1:C:65:ALA:C	2.59	0.44
1:C:415:GLN:HE22	1:C:435:GLN:HA	1.82	0.44
1:C:434:ARG:O	1:C:435:GLN:HB3	2.18	0.44
1:A:450:ASN:HB2	1:A:454:ASP:OD2	2.17	0.44
1:B:427:ASP:CB	1:B:430:ILE:HD12	2.48	0.44
1:A:681:LEU:O	1:A:685:MET:HG3	2.18	0.44
1:B:179:CYS:SG	1:B:216:ARG:HA	2.57	0.44
1:A:222:PHE:HD2	1:A:496:GLN:HB3	1.82	0.44
1:A:648:LYS:HE3	1:A:648:LYS:H	1.82	0.44
1:A:737:GLY:O	1:A:738:ALA:CB	2.64	0.44
1:B:1:MET:HA	1:B:3:GLN:NE2	2.33	0.44
1:B:307:PRO:HA	1:B:338:GLN:HB2	1.99	0.44
1:C:186:ARG:HG3	3:C:762:HOH:O	2.18	0.44
1:C:425:PRO:HB3	1:C:573:TYR:HE2	1.82	0.44
1:B:433:VAL:HG11	1:B:443:ALA:HB1	2.00	0.44
1:C:107:VAL:O	1:C:111:GLU:HG3	2.17	0.44
1:A:312:GLU:O	1:A:316:LEU:HG	2.18	0.44
1:A:388:ILE:O	1:A:390:LYS:HE3	2.17	0.44
1:B:207:LEU:HB3	1:B:212:MET:HE3	1.96	0.44
1:B:256:ILE:O	1:B:304:LEU:HA	2.17	0.44
1:B:353:ILE:HG13	1:B:395:ALA:HB2	2.00	0.44
1:A:150:GLN:NE2	1:A:627:GLN:HE22	2.13	0.44
1:A:462:CYS:HB3	1:A:464:LEU:HD21	2.00	0.44
1:A:659:TYR:O	1:A:660:GLU:C	2.61	0.44
1:B:465:SER:O	1:B:515:ILE:HA	2.18	0.44
1:B:339:ILE:HG22	1:B:340:ASN:N	2.31	0.43
1:B:676:ASP:O	1:B:677:GLY:C	2.58	0.43
1:A:676:ASP:O	1:A:677:GLY:C	2.60	0.43
1:C:111:GLU:O	2:P:4:GLY:HA2	2.18	0.43
1:A:262:ARG:HB3	1:A:359:SER:HB3	2.01	0.43
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.99	0.43
1:B:279:ILE:H	1:B:279:ILE:HG12	1.58	0.43
1:C:179:CYS:SG	1:C:216:ARG:HA	2.58	0.43
1:B:737:GLY:O	1:B:738:ALA:CB	2.66	0.43
1:A:134:PHE:CE2	1:A:194:LYS:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LEU:HD11	1:B:620:MET:HE2	2.00	0.43
1:C:150:GLN:NE2	1:C:627:GLN:HE22	2.15	0.43
1:C:312:GLU:O	1:C:316:LEU:HG	2.17	0.43
1:C:668:LEU:HB2	1:C:671:GLU:HG3	2.01	0.43
1:A:292:CYS:C	1:B:276:THR:HG21	2.44	0.43
1:B:504:LYS:O	1:B:505:ARG:C	2.62	0.43
1:B:510:ARG:HB2	1:B:512:THR:HG23	2.00	0.43
2:E:370:LEU:O	2:E:371:SER:C	2.62	0.43
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.54	0.42
1:B:75:PRO:O	1:B:78:GLN:HG3	2.19	0.42
1:A:179:CYS:SG	1:A:216:ARG:HA	2.59	0.42
1:A:307:PRO:HA	1:A:338:GLN:HB2	2.00	0.42
1:A:466:ALA:HA	1:A:516:GLY:O	2.19	0.42
1:A:569:ASN:H	1:A:569:ASN:HD22	1.66	0.42
1:C:510:ARG:HB2	1:C:512:THR:HG23	2.01	0.42
1:C:734:THR:O	1:C:735:ARG:CB	2.66	0.42
1:A:364:LEU:HD22	1:A:375:PHE:CE1	2.55	0.42
1:A:227:LEU:HD11	1:A:437:ASN:HB3	2.00	0.42
1:B:226:VAL:HG11	1:B:247:TYR:CD2	2.54	0.42
1:C:226:VAL:HG11	1:C:247:TYR:CD2	2.54	0.42
1:A:492:LEU:O	1:A:496:GLN:HG2	2.19	0.42
1:B:107:VAL:O	1:B:111:GLU:HG3	2.19	0.42
1:B:434:ARG:O	1:B:435:GLN:HB3	2.19	0.42
1:B:217:THR:HB	1:B:218:PRO:CD	2.50	0.42
1:C:681:LEU:O	1:C:685:MET:HG3	2.20	0.42
1:A:463:THR:HG22	1:A:489:LEU:HD22	2.02	0.42
1:C:34:HIS:O	1:C:35:ASN:HB2	2.20	0.42
1:A:50:TYR:O	1:A:51:ASP:C	2.63	0.42
1:A:284:HIS:HA	1:B:287:THR:HB	2.00	0.42
1:C:402:MET:HE2	1:C:402:MET:HB3	1.94	0.42
1:C:498:TYR:HA	1:C:499:PRO:HD2	1.94	0.42
1:C:672:MET:HE1	1:C:678:TYR:HB2	2.02	0.42
1:A:28:TRP:O	1:A:31:GLU:HB2	2.20	0.42
1:A:343:MET:HE2	1:A:343:MET:HA	2.02	0.42
1:B:285:PHE:O	1:B:288:ALA:HB3	2.20	0.42
1:C:515:ILE:O	1:C:617:SER:HA	2.19	0.42
2:F:370:LEU:O	2:F:371:SER:C	2.63	0.42
1:C:105:HIS:O	1:C:109:MET:HG2	2.20	0.41
1:C:339:ILE:HG22	1:C:340:ASN:N	2.35	0.41
1:A:18:ASN:HD22	1:A:21:LYS:HE3	1.85	0.41
1:A:306:TYR:HB2	1:A:307:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PHE:HZ	1:A:207:LEU:HD11	1.85	0.41
1:C:489:LEU:HD23	1:C:489:LEU:HA	1.88	0.41
1:A:672:MET:HA	1:A:673:PRO:HD3	1.83	0.41
1:B:474:ASN:N	1:B:474:ASN:HD22	2.18	0.41
1:B:519:ASN:HD22	1:B:519:ASN:HA	1.56	0.41
1:A:402:MET:HE2	1:A:402:MET:HB3	1.97	0.41
1:B:659:TYR:CE1	1:B:663:HIS:HB3	2.56	0.41
1:C:192:TYR:O	1:C:193:VAL:C	2.64	0.41
1:C:217:THR:OG1	1:C:219:THR:HG22	2.21	0.41
1:C:433:VAL:HG11	1:C:443:ALA:HB1	2.03	0.41
1:A:45:SER:HB3	1:A:61:THR:HG22	2.01	0.41
1:A:548:GLN:HE21	1:A:548:GLN:CA	2.32	0.41
1:A:1:MET:HA	1:A:3:GLN:NE2	2.36	0.41
1:C:227:LEU:HD11	1:C:437:ASN:HB3	2.02	0.41
1:C:442:ILE:HG13	1:C:462:CYS:SG	2.61	0.41
1:B:479:GLU:HB2	1:B:550:TYR:CD1	2.55	0.41
1:C:124:THR:O	1:C:125:GLU:C	2.63	0.41
1:C:279:ILE:H	1:C:279:ILE:HG12	1.61	0.41
1:C:221:GLN:HA	1:C:221:GLN:NE2	2.35	0.41
1:C:293:SER:HB2	1:C:298:ARG:O	2.21	0.41
1:C:313:VAL:HG22	1:C:317:LEU:HD22	2.02	0.41
1:C:370:ALA:HB1	3:C:788:HOH:O	2.20	0.41
1:C:426:PHE:O	1:C:428:PRO:HD3	2.21	0.41
1:C:567:TRP:HB3	1:C:570:GLU:HG3	2.03	0.41
1:A:226:VAL:HG11	1:A:247:TYR:CD2	2.55	0.41
1:B:338:GLN:HE21	1:B:415:GLN:NE2	2.19	0.41
1:C:117:ASN:H	1:C:117:ASN:ND2	2.19	0.41
1:A:436:SER:OG	1:A:440:LEU:HA	2.20	0.40
1:B:522:TYR:O	1:B:526:LYS:HG2	2.20	0.40
1:C:109:MET:HE3	1:C:114:LYS:HB2	2.03	0.40
1:A:442:ILE:HG13	1:A:462:CYS:SG	2.62	0.40
1:B:519:ASN:ND2	1:B:522:TYR:HB3	2.35	0.40
1:C:364:LEU:HD22	1:C:375:PHE:CE1	2.56	0.40
1:C:439:CYS:HA	1:C:730:TYR:CE1	2.56	0.40
1:A:192:TYR:O	1:A:193:VAL:C	2.62	0.40
1:B:640:GLY:HA2	1:B:668:LEU:HD13	2.03	0.40
1:C:215:VAL:HB	3:C:791:HOH:O	2.20	0.40
1:C:217:THR:HB	1:C:218:PRO:CD	2.51	0.40
1:C:306:TYR:HB2	1:C:307:PRO:HD2	2.03	0.40
1:A:425:PRO:HB3	1:A:573:TYR:HE2	1.86	0.40
1:B:475:LEU:O	1:B:478:LEU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:VAL:HG13	1:C:328:ASN:HB2	2.04	0.40

There are no symmetry-related clashes.

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	A	736/761 (97%)	681 (92%)	43 (6%)	12 (2%)	7	30
1	B	736/761 (97%)	679 (92%)	43 (6%)	14 (2%)	6	27
1	C	736/761 (97%)	683 (93%)	40 (5%)	13 (2%)	6	28
2	D	16/20 (80%)	14 (88%)	1 (6%)	1 (6%)	1	6
2	E	16/20 (80%)	13 (81%)	2 (12%)	1 (6%)	1	6
2	F	16/20 (80%)	14 (88%)	1 (6%)	1 (6%)	1	6
2	P	2/20 (10%)	0	1 (50%)	1 (50%)	0	0
All	All	2258/2363 (96%)	2084 (92%)	131 (6%)	43 (2%)	6	27

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	51	ASP
1	A	216	ARG
1	A	294	GLN
1	A	735	ARG
1	B	14	THR
1	B	51	ASP
1	B	294	GLN
1	B	735	ARG
1	C	14	THR

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Mol	Chain	Res	Type
1	C	51	ASP
1	C	294	GLN
1	C	735	ARG
1	A	5	LEU
1	A	11	ASP
1	B	5	LEU
1	B	11	ASP
1	B	13	SER
1	B	216	ARG
1	C	5	LEU
1	C	11	ASP
1	C	216	ARG
1	A	2	ASN
1	A	13	SER
1	B	2	ASN
1	C	2	ASN
1	C	13	SER
1	A	15	GLU
2	D	371	SER
1	B	15	GLU
1	B	622	SER
2	E	371	SER
2	F	371	SER
2	P	3	VAL
1	A	10	ARG
1	B	10	ARG
1	C	10	ARG
1	C	15	GLU
1	B	12	GLY
1	A	12	GLY
1	C	12	GLY
1	B	737	GLY
1	C	737	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	631/650 (97%)	551 (87%)	80 (13%)	4	18
1	B	631/650 (97%)	552 (88%)	79 (12%)	4	19
1	C	631/650 (97%)	552 (88%)	79 (12%)	4	19
2	D	17/19 (90%)	15 (88%)	2 (12%)	5	21
2	E	17/19 (90%)	15 (88%)	2 (12%)	5	21
2	F	17/19 (90%)	15 (88%)	2 (12%)	5	21
2	P	3/19 (16%)	2 (67%)	1 (33%)	0	0
All	All	1947/2026 (96%)	1702 (87%)	245 (13%)	4	19

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLN
1	A	8	THR
1	A	9	LYS
1	A	10	ARG
1	A	14	THR
1	A	16	ARG
1	A	17	ILE
1	A	21	LYS
1	A	31	GLU
1	A	40	GLN
1	A	44	ARG
1	A	48	GLN
1	A	54	LYS
1	A	58	ILE
1	A	64	LYS
1	A	72	ARG
1	A	73	ASP
1	A	78	GLN
1	A	96	GLN
1	A	139	ARG
1	A	149	LYS
1	A	154	LYS
1	A	161	VAL
1	A	165	ILE
1	A	168	SER
1	A	189	ARG
1	A	204	LYS
1	A	206	SER

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Mol	Chain	Res	Type
1	A	225	CYS
1	A	249	SER
1	A	260	ARG
1	A	264	LEU
1	A	279	ILE
1	A	283	LYS
1	A	297	VAL
1	A	317	LEU
1	A	320	LYS
1	A	323	ARG
1	A	341	LYS
1	A	364	LEU
1	A	380	THR
1	A	384	LYS
1	A	386	ASP
1	A	387	SER
1	A	390	LYS
1	A	394	LYS
1	A	396	VAL
1	A	408	SER
1	A	424	SER
1	A	430	ILE
1	A	440	LEU
1	A	464	LEU
1	A	465	SER
1	A	474	ASN
1	A	484	LEU
1	A	510	ARG
1	A	512	THR
1	A	519	ASN
1	A	526	LYS
1	A	530	ARG
1	A	542	LYS
1	A	560	LYS
1	A	570	GLU
1	A	585	LYS
1	A	605	SER
1	A	607	LYS
1	A	616	LEU
1	A	628	ILE
1	A	629	SER
1	A	639	ARG

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Mol	Chain	Res	Type
1	A	643	SER
1	A	645	LYS
1	A	648	LYS
1	A	687	LYS
1	A	696	ASN
1	A	708	LYS
1	A	709	VAL
1	A	735	ARG
1	A	736	ASP
2	D	361	ILE
2	D	372	ASN
1	B	1	MET
1	B	3	GLN
1	B	8	THR
1	B	9	LYS
1	B	10	ARG
1	B	14	THR
1	B	16	ARG
1	B	17	ILE
1	B	21	LYS
1	B	31	GLU
1	B	40	GLN
1	B	44	ARG
1	B	48	GLN
1	B	54	LYS
1	B	58	ILE
1	B	64	LYS
1	B	72	ARG
1	B	73	ASP
1	B	78	GLN
1	B	96	GLN
1	B	139	ARG
1	B	149	LYS
1	B	154	LYS
1	B	161	VAL
1	B	165	ILE
1	B	168	SER
1	B	189	ARG
1	B	204	LYS
1	B	206	SER
1	B	225	CYS
1	B	249	SER

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Mol	Chain	Res	Type
1	B	260	ARG
1	B	264	LEU
1	B	279	ILE
1	B	283	LYS
1	B	297	VAL
1	B	317	LEU
1	B	320	LYS
1	B	323	ARG
1	B	341	LYS
1	B	364	LEU
1	B	380	THR
1	B	384	LYS
1	B	386	ASP
1	B	387	SER
1	B	390	LYS
1	B	394	LYS
1	B	408	SER
1	B	424	SER
1	B	430	ILE
1	B	440	LEU
1	B	464	LEU
1	B	465	SER
1	B	474	ASN
1	B	484	LEU
1	B	510	ARG
1	B	512	THR
1	B	519	ASN
1	B	526	LYS
1	B	530	ARG
1	B	542	LYS
1	B	555	SER
1	B	560	LYS
1	B	570	GLU
1	B	585	LYS
1	B	607	LYS
1	B	616	LEU
1	B	623	GLU
1	B	628	ILE
1	B	629	SER
1	B	639	ARG
1	B	643	SER
1	B	645	LYS

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Mol	Chain	Res	Type
1	B	648	LYS
1	B	687	LYS
1	B	708	LYS
1	B	709	VAL
1	B	735	ARG
1	B	736	ASP
2	E	361	ILE
2	E	372	ASN
1	C	1	MET
1	C	3	GLN
1	C	6	LEU
1	C	8	THR
1	C	9	LYS
1	C	10	ARG
1	C	14	THR
1	C	16	ARG
1	C	17	ILE
1	C	21	LYS
1	C	31	GLU
1	C	40	GLN
1	C	44	ARG
1	C	48	GLN
1	C	54	LYS
1	C	58	ILE
1	C	64	LYS
1	C	72	ARG
1	C	73	ASP
1	C	78	GLN
1	C	96	GLN
1	C	139	ARG
1	C	149	LYS
1	C	154	LYS
1	C	161	VAL
1	C	165	ILE
1	C	168	SER
1	C	189	ARG
1	C	204	LYS
1	C	206	SER
1	C	225	CYS
1	C	249	SER
1	C	260	ARG
1	C	264	LEU

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Mol	Chain	Res	Type
1	C	279	ILE
1	C	283	LYS
1	C	297	VAL
1	C	317	LEU
1	C	320	LYS
1	C	323	ARG
1	C	341	LYS
1	C	364	LEU
1	C	380	THR
1	C	384	LYS
1	C	386	ASP
1	C	387	SER
1	C	390	LYS
1	C	394	LYS
1	C	396	VAL
1	C	408	SER
1	C	424	SER
1	C	430	ILE
1	C	440	LEU
1	C	464	LEU
1	C	465	SER
1	C	474	ASN
1	C	484	LEU
1	C	510	ARG
1	C	512	THR
1	C	519	ASN
1	C	526	LYS
1	C	530	ARG
1	C	542	LYS
1	C	560	LYS
1	C	570	GLU
1	C	585	LYS
1	C	607	LYS
1	C	616	LEU
1	C	625	SER
1	C	628	ILE
1	C	629	SER
1	C	639	ARG
1	C	643	SER
1	C	645	LYS
1	C	648	LYS
1	C	708	LYS

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Mol	Chain	Res	Type
1	C	709	VAL
1	C	735	ARG
1	C	736	ASP
2	F	361	ILE
2	F	372	ASN
2	P	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	ASN
1	A	18	ASN
1	A	40	GLN
1	A	46	HIS
1	A	117	ASN
1	A	158	GLN
1	A	191	GLN
1	A	221	GLN
1	A	328	ASN
1	A	415	GLN
1	A	453	ASN
1	A	496	GLN
1	A	519	ASN
1	A	548	GLN
1	A	569	ASN
1	A	627	GLN
1	A	633	ASN
1	A	654	GLN
1	A	686	GLN
1	A	698	ASN
1	A	713	GLN
2	D	372	ASN
1	B	3	GLN
1	B	18	ASN
1	B	40	GLN
1	B	117	ASN
1	B	158	GLN
1	B	191	GLN
1	B	221	GLN
1	B	328	ASN
1	B	415	GLN

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Mol	Chain	Res	Type
1	B	496	GLN
1	B	519	ASN
1	B	548	GLN
1	B	569	ASN
1	B	627	GLN
1	B	633	ASN
1	B	654	GLN
1	B	686	GLN
1	B	698	ASN
1	B	713	GLN
2	E	372	ASN
1	C	3	GLN
1	C	18	ASN
1	C	40	GLN
1	C	46	HIS
1	C	117	ASN
1	C	158	GLN
1	C	191	GLN
1	C	221	GLN
1	C	328	ASN
1	C	415	GLN
1	C	496	GLN
1	C	519	ASN
1	C	548	GLN
1	C	569	ASN
1	C	627	GLN
1	C	633	ASN
1	C	654	GLN
1	C	686	GLN
1	C	698	ASN
1	C	713	GLN
1	C	732	GLN
2	F	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.