



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:01 PM UTC

PDB ID : 6R1R / pdb_00006r1r
Title : RIBONUCLEOTIDE REDUCTASE E441D 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

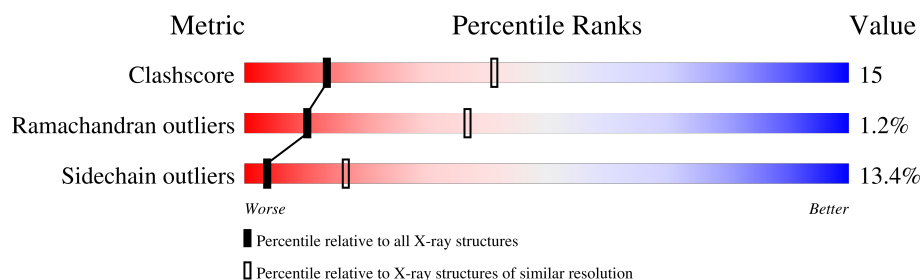
1 Overall quality at a glance

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	52% 35% 9% ..
1	B	761	54% 32% 10% ..
1	C	761	54% 32% 10% ..
2	D	20	65% 15% 10% 10%
2	E	20	60% 20% 10% 10%
2	F	20	55% 25% 10% 10%
2	P	20	5% 5% 10% 80%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18163 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
			5874	3728	1010	1111	25			
1	B	738	Total	C	N	O	S	0	0	0
			5874	3728	1010	1111	25			
1	C	738	Total	C	N	O	S	0	0	0
			5874	3728	1010	1111	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	441	ASP	GLU	engineered mutation	UNP P00452
B	441	ASP	GLU	engineered mutation	UNP P00452
C	441	ASP	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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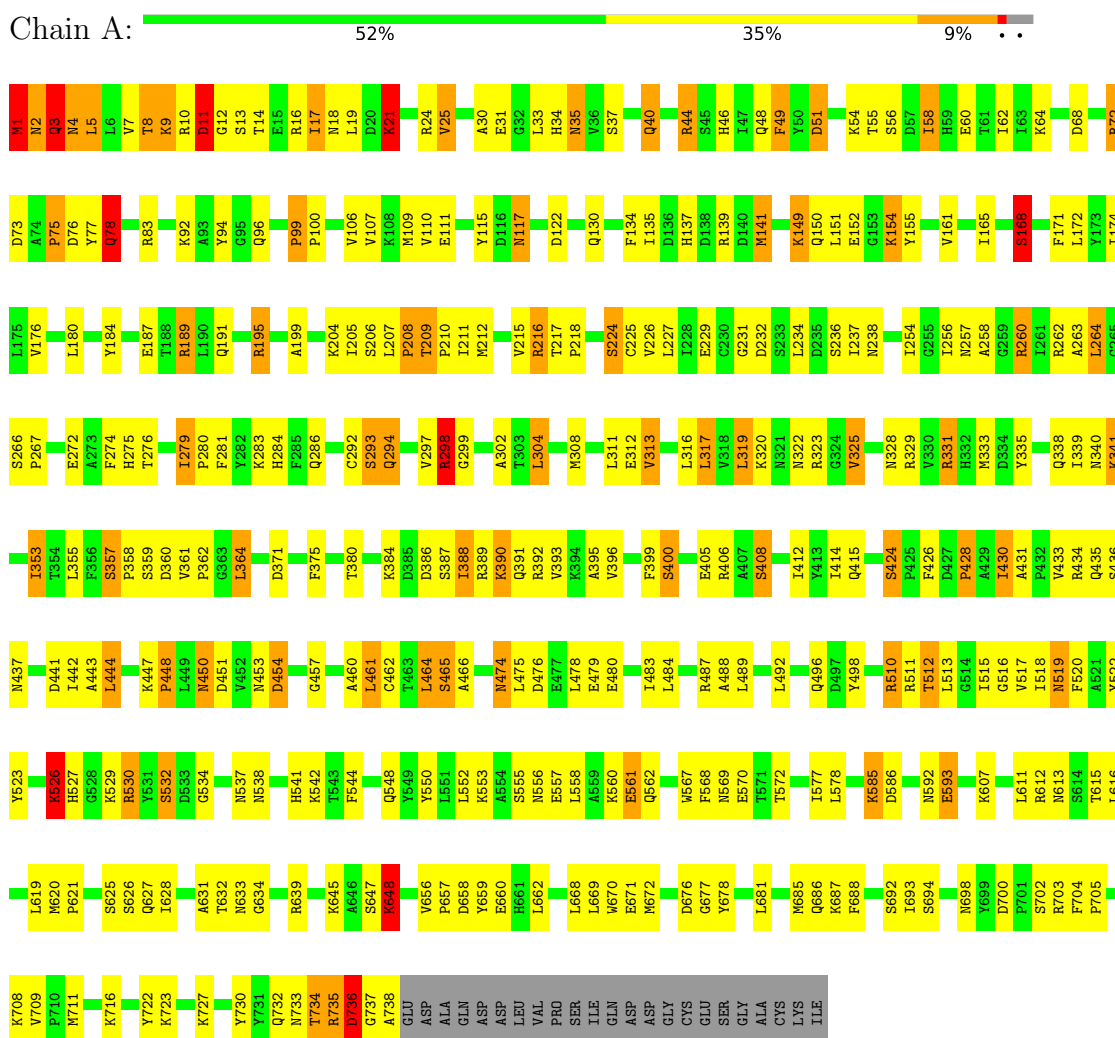
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	30	Total	O	0	0
			30	30		
3	C	32	Total	O	0	0
			32	32		

3 Residue-property plots

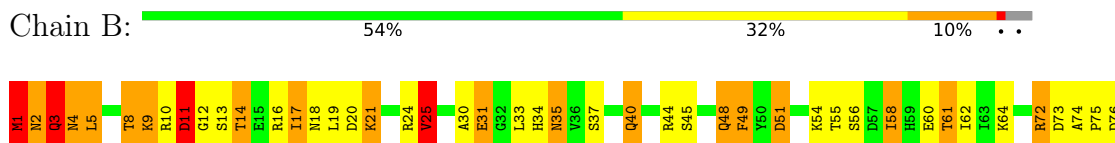
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

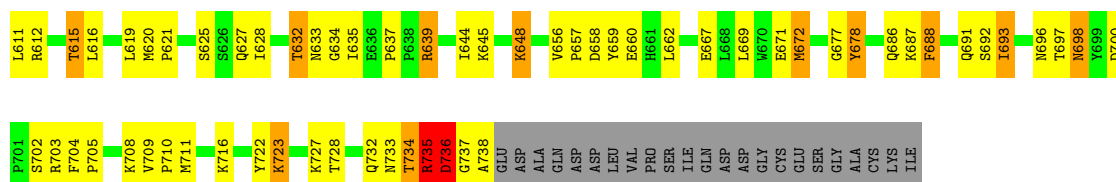


• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN





P499	H419	V325	V248	I165	S71	N1
I500	C420	N328	R251	S168	R72	N2
R510	M421	R329	G253	A74	D73	Q3
R511	S424	V330	G252	I171	A74	N4
T512	P425	R331	I254	L172	P75	L5
L513	F426	H332	G255	T173	D76	L6
G514	D427	M333	L256	I174	T77	V7
G515	P428	D334	N257	L175	Q78	T8
G516	A429	R335	A258	V176	K9	K9
V517	I430	V335	A258	R83	R10	R10
I518	A431	Q338	G259	L180	R83	R11
N519	F432	Q338	R260	I186	G12	D11
F520	V433	K341	I261	L184	S13	G12
A521	R434	E435	A263	R185	R89	T14
Y522	Q435	L348	L264	I186	R90	E15
				K92	K91	R16
				K92	K92	I17
				K93	K93	N18
				K94	K94	L19
				K95	K95	L20
				K96	K96	I22
				K97	K97	K21
				K98	K98	K22
				K99	K99	H23
				K100	K100	R24
				K101	K101	V25
				K102	K102	
				K103	K103	A30
				K104	K104	E31
				K105	K105	G32
				K106	K106	L33
				K107	K107	H34
				K108	K108	N35
				K109	K109	V36
				K110	K110	S37
				K111	K111	
				K112	K112	Q40
				K113	K113	
				K114	K114	R44
				K115	K115	S45
				K116	K116	H46
				K117	K117	I47
				K118	K118	Q48
				K119	K119	F49
				K120	K120	Y50
				K121	K121	D51
				K122	K122	
				K123	K123	K54
				K124	K124	T55
				K125	K125	S56
				K126	K126	D57
				K127	K127	I58
				K128	K128	H59
				K129	K129	E60
				K130	K130	T61
				K131	K131	
				K132	K132	K64
				K133	K133	
				K134	K134	D68
				K135	K135	L69
				K136	K136	L70



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain D: 65% 15% 10% 10%



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain E: 60% 20% 10% 10%



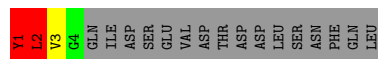
● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain F: 55% 25% 10% 10%



● Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain P: 5% 5% 10% 80%



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	224.49Å 224.49Å 336.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	89.7 (20.00-3.10)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
Refinement program	TNT, REFMAC	Depositor
R, R_{free}	0.194 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18163	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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	0.60	0/6002	1.76	128/8129 (1.6%)
1	B	0.60	0/6002	1.79	128/8129 (1.6%)
1	C	0.64	0/6002	1.81	137/8129 (1.7%)
2	D	0.44	0/140	1.44	1/188 (0.5%)
2	E	0.47	0/140	1.41	1/188 (0.5%)
2	F	0.47	0/140	1.44	0/188
2	P	0.91	0/31	2.62	3/41 (7.3%)
All	All	0.61	0/18457	1.78	398/24992 (1.6%)

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	2
1	B	0	2
1	C	0	2
All	All	0	6

There are no bond length outliers.

All (398) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	736	ASP	CA-CB-CG	12.37	124.97	112.60
1	C	195	ARG	CD-NE-CZ	11.91	141.07	124.40
1	B	195	ARG	CD-NE-CZ	11.30	140.22	124.40
1	B	736	ASP	CA-CB-CG	10.24	122.84	112.60
1	A	24	ARG	CD-NE-CZ	10.01	138.41	124.40
1	A	464	LEU	N-CA-C	9.75	125.26	110.14
1	B	24	ARG	CD-NE-CZ	9.70	137.99	124.40
1	C	691	GLN	CA-C-O	9.61	123.51	117.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	444	LEU	CA-C-O	9.43	129.17	120.50
1	C	450	ASN	CA-CB-CG	-9.28	103.32	112.60
1	A	444	LEU	CA-C-O	9.28	129.04	120.50
1	C	331	ARG	N-CA-C	9.04	122.30	111.82
1	A	736	ASP	CA-CB-CG	8.95	121.55	112.60
1	A	530	ARG	NE-CZ-NH1	8.89	130.39	121.50
1	A	195	ARG	CD-NE-CZ	8.77	136.68	124.40
1	B	293	SER	CA-C-N	8.74	138.24	121.54
1	B	293	SER	C-N-CA	8.74	138.24	121.54
1	C	464	LEU	N-CA-C	8.72	123.66	110.14
1	A	224	SER	N-CA-CB	8.71	123.74	110.42
1	A	293	SER	CA-C-N	8.55	137.87	121.54
1	A	293	SER	C-N-CA	8.55	137.87	121.54
1	B	474	ASN	OD1-CG-ND2	8.52	131.12	122.60
1	C	530	ARG	NE-CZ-NH1	8.52	130.02	121.50
1	C	24	ARG	CD-NE-CZ	8.51	136.31	124.40
1	B	450	ASN	CA-CB-CG	-8.49	104.11	112.60
1	A	4	ASN	N-CA-C	8.46	124.15	111.04
1	B	51	ASP	CA-C-O	-8.42	108.47	120.51
1	B	703	ARG	NE-CZ-NH2	-8.35	111.69	119.20
1	C	293	SER	CA-C-N	8.33	137.46	121.54
1	C	293	SER	C-N-CA	8.33	137.46	121.54
1	B	293	SER	CA-C-O	8.24	130.49	120.60
1	A	51	ASP	CA-C-O	-8.22	108.76	120.51
1	A	293	SER	CA-C-O	8.20	130.44	120.60
1	C	224	SER	N-CA-CB	8.18	122.94	110.42
1	C	14	THR	N-CA-C	8.09	120.75	110.24
1	B	444	LEU	CA-C-O	8.04	127.89	120.50
1	C	293	SER	CA-C-O	8.04	130.24	120.60
1	C	444	LEU	O-C-N	-7.99	116.60	121.71
1	A	450	ASN	CA-CB-CG	-7.99	104.61	112.60
1	B	224	SER	N-CA-CB	7.98	122.62	110.42
1	B	464	LEU	N-CA-C	7.96	122.42	109.85
1	B	338	GLN	OE1-CD-NE2	7.94	130.54	122.60
1	B	532	SER	N-CA-C	7.87	122.92	113.16
1	C	532	SER	N-CA-C	7.79	122.79	113.28
1	A	72	ARG	NE-CZ-NH2	7.52	125.97	119.20
1	B	14	THR	N-CA-C	7.51	120.01	110.24
1	C	51	ASP	CA-C-O	-7.51	109.77	120.51
1	B	421	ASN	CA-CB-CG	-7.45	105.15	112.60
1	B	217	THR	CA-C-N	7.43	127.10	119.82
1	B	217	THR	C-N-CA	7.43	127.10	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	544	PHE	CA-CB-CG	-7.42	106.38	113.80
1	B	72	ARG	NE-CZ-NH2	7.42	125.88	119.20
1	A	211	ILE	CA-C-O	-7.38	113.39	121.29
1	C	4	ASN	N-CA-C	7.35	122.43	111.04
1	C	134	PHE	CA-CB-CG	7.35	121.15	113.80
1	C	530	ARG	CD-NE-CZ	7.33	134.67	124.40
1	A	35	ASN	OD1-CG-ND2	7.32	129.92	122.60
1	C	678	TYR	CA-C-O	-7.30	113.34	121.00
1	B	211	ILE	CA-C-O	-7.29	113.45	121.17
1	C	154	LYS	N-CA-C	7.18	121.44	112.03
1	C	11	ASP	CA-C-O	7.17	130.77	120.51
1	A	408	SER	CB-CA-C	-7.14	99.96	110.96
1	A	517	VAL	N-CA-CB	-7.12	104.22	112.34
1	B	134	PHE	CA-CB-CG	7.04	120.84	113.80
1	C	72	ARG	NE-CZ-NH2	7.03	125.53	119.20
1	C	515	ILE	CA-C-O	-7.01	113.06	120.57
1	C	530	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	A	544	PHE	CA-CB-CG	-6.98	106.82	113.80
1	C	703	ARG	NE-CZ-NH1	6.97	128.47	121.50
1	B	319	LEU	CA-C-O	-6.96	112.23	120.10
1	C	68	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	703	ARG	NE-CZ-NH1	6.92	128.42	121.50
1	B	4	ASN	N-CA-C	6.92	121.76	111.04
2	P	3	VAL	N-CA-C	6.90	123.68	109.34
1	C	46	HIS	O-C-N	-6.88	114.82	122.12
1	B	1	MET	CA-C-N	6.87	134.67	121.54
1	B	1	MET	C-N-CA	6.87	134.67	121.54
1	B	697	THR	CA-C-O	-6.83	112.98	120.36
1	A	232	ASP	CA-CB-CG	6.83	119.43	112.60
1	C	154	LYS	N-CA-CB	-6.82	99.49	111.42
1	B	208	PRO	N-CA-CB	6.81	109.79	103.39
1	B	656	VAL	CA-C-N	6.79	127.19	119.93
1	B	656	VAL	C-N-CA	6.79	127.19	119.93
1	A	68	ASP	CA-CB-CG	6.78	119.38	112.60
1	B	530	ARG	CD-NE-CZ	6.77	133.88	124.40
1	C	639	ARG	CD-NE-CZ	6.77	133.88	124.40
1	A	532	SER	N-CA-C	6.76	121.53	113.28
1	C	370	ALA	N-CA-C	6.76	121.61	113.23
1	C	61	THR	CA-C-O	-6.75	113.75	120.70
1	B	11	ASP	CA-C-O	6.74	130.15	120.51
1	B	544	PHE	CA-CB-CG	-6.71	107.09	113.80
1	B	526	LYS	N-CA-CB	6.69	121.49	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ILE	N-CA-C	6.69	117.67	108.84
1	B	448	PRO	N-CA-CB	6.66	109.15	103.35
1	A	448	PRO	CA-C-O	-6.65	113.85	121.56
1	C	25	VAL	CB-CA-C	-6.64	103.18	112.14
1	A	134	PHE	CA-CB-CG	6.62	120.42	113.80
1	C	1	MET	CA-C-N	6.61	134.17	121.54
1	C	1	MET	C-N-CA	6.61	134.17	121.54
1	B	408	SER	CB-CA-C	-6.57	100.84	110.96
1	A	224	SER	N-CA-C	-6.57	104.91	113.12
1	A	217	THR	CA-C-N	6.56	126.69	119.87
1	A	217	THR	C-N-CA	6.56	126.69	119.87
1	C	399	PHE	CA-CB-CG	-6.55	107.25	113.80
1	B	253	GLY	CA-C-O	-6.54	115.62	121.64
1	B	526	LYS	CA-CB-CG	6.54	127.18	114.10
1	A	732	GLN	OE1-CD-NE2	6.52	129.12	122.60
1	B	447	LYS	CA-C-N	6.52	126.49	119.78
1	B	447	LYS	C-N-CA	6.52	126.49	119.78
1	C	421	ASN	CA-CB-CG	-6.51	106.09	112.60
1	A	430	ILE	CB-CA-C	-6.46	105.37	111.06
1	A	526	LYS	CA-CB-CG	6.46	127.01	114.10
1	A	11	ASP	CA-C-O	6.44	129.72	120.51
1	A	448	PRO	N-CA-CB	6.44	108.95	103.35
1	A	209	THR	CA-C-O	6.41	125.01	118.73
1	A	1	MET	CA-C-N	6.41	133.77	121.54
1	A	1	MET	C-N-CA	6.41	133.77	121.54
1	C	253	GLY	CA-C-O	-6.40	115.75	121.64
1	B	25	VAL	CB-CA-C	-6.39	103.52	112.14
1	A	299	GLY	CA-C-O	-6.38	118.07	122.22
1	A	399	PHE	CA-CB-CG	-6.37	107.43	113.80
1	C	319	LEU	CA-C-O	-6.34	112.94	120.10
1	C	526	LYS	N-CA-CB	6.34	120.91	110.39
1	C	648	LYS	N-CA-C	-6.34	105.37	113.23
1	A	444	LEU	O-C-N	-6.33	117.66	121.71
1	B	74	ALA	CA-C-N	6.29	125.91	119.56
1	B	74	ALA	C-N-CA	6.29	125.91	119.56
1	A	25	VAL	CB-CA-C	-6.26	103.84	112.04
1	B	72	ARG	NE-CZ-NH1	-6.26	115.24	121.50
1	A	319	LEU	CA-C-O	-6.24	113.04	120.10
1	C	430	ILE	CB-CA-C	-6.24	105.57	111.06
1	A	462	CYS	CA-C-O	-6.23	114.44	120.92
1	A	526	LYS	N-CA-CB	6.21	120.69	110.39
1	B	281	PHE	CA-CB-CG	-6.20	107.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	693	ILE	CA-C-O	-6.19	113.95	120.76
1	B	530	ARG	NE-CZ-NH1	6.18	127.68	121.50
1	B	357	SER	N-CA-C	-6.17	102.28	109.93
1	B	224	SER	N-CA-C	-6.16	105.42	113.12
1	A	442	ILE	O-C-N	6.16	129.46	122.93
1	B	35	ASN	OD1-CG-ND2	6.13	128.73	122.60
1	B	426	PHE	CA-CB-CG	-6.12	107.67	113.80
1	B	518	ILE	CA-C-O	-6.06	115.63	121.63
1	C	22	ILE	CB-CA-C	-6.06	104.13	111.88
1	A	168	SER	CB-CA-C	6.04	120.43	109.37
1	B	331	ARG	N-CA-C	6.04	119.84	112.23
1	A	447	LYS	CA-C-N	6.04	126.00	119.78
1	A	447	LYS	C-N-CA	6.04	126.00	119.78
1	C	656	VAL	CA-C-N	6.04	126.39	119.93
1	C	656	VAL	C-N-CA	6.04	126.39	119.93
1	A	648	LYS	N-CA-C	-6.03	105.41	112.89
1	C	526	LYS	CA-CB-CG	6.01	126.12	114.10
1	B	538	ASN	OD1-CG-ND2	-6.00	116.59	122.60
1	A	526	LYS	CA-C-O	-5.99	112.02	119.38
1	C	408	SER	CB-CA-C	-5.98	101.75	110.96
1	C	702	SER	CB-CA-C	-5.97	100.54	110.68
2	P	2	LEU	N-CA-C	5.95	117.69	109.54
1	A	2	ASN	CA-C-N	5.95	132.02	122.32
1	A	2	ASN	C-N-CA	5.95	132.02	122.32
1	C	232	ASP	CA-CB-CG	5.90	118.50	112.60
1	C	696	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	A	515	ILE	CA-C-O	-5.87	114.03	120.72
1	C	431	ALA	CA-C-N	5.87	125.84	120.21
1	C	431	ALA	C-N-CA	5.87	125.84	120.21
1	C	211	ILE	CA-C-O	-5.85	115.03	121.29
1	B	678	TYR	CA-C-O	-5.85	114.68	120.82
1	A	703	ARG	NE-CZ-NH2	-5.83	113.95	119.20
1	C	185	PRO	CA-C-O	-5.83	114.96	121.32
1	A	732	GLN	CA-C-O	-5.83	114.07	120.30
1	B	371	ASP	CA-CB-CG	5.82	118.42	112.60
1	B	185	PRO	CA-C-O	-5.81	114.99	121.32
1	B	191	GLN	N-CA-C	-5.81	104.87	111.14
1	B	648	LYS	N-CA-C	-5.81	105.69	112.89
1	C	517	VAL	CB-CA-C	-5.81	103.24	111.19
1	C	307	PRO	N-CA-CB	5.80	108.73	103.33
2	P	1	TYR	CA-CB-CG	5.80	124.34	113.90
1	B	638	PRO	N-CA-CB	5.80	108.39	103.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	490	ASP	CA-CB-CG	-5.79	106.81	112.60
1	A	218	PRO	N-CA-CB	5.78	108.84	103.41
1	A	530	ARG	NE-CZ-NH2	-5.77	114.00	119.20
1	C	428	PRO	N-CA-CB	5.77	109.63	103.39
1	A	208	PRO	N-CA-CB	5.77	109.31	103.25
1	A	424	SER	CA-C-N	5.76	125.38	119.56
1	A	424	SER	C-N-CA	5.76	125.38	119.56
1	A	702	SER	CB-CA-C	-5.75	100.90	110.68
1	B	298	ARG	N-CA-C	5.74	118.11	108.23
1	B	427	ASP	CA-C-N	5.73	125.58	119.28
1	B	427	ASP	C-N-CA	5.73	125.58	119.28
1	B	593	GLU	CA-C-N	5.73	126.21	120.14
1	B	593	GLU	C-N-CA	5.73	126.21	120.14
1	C	688	PHE	CA-CB-CG	-5.72	108.08	113.80
1	C	224	SER	N-CA-C	-5.72	105.97	113.12
1	B	89	LEU	CA-C-O	-5.71	114.46	120.63
1	A	561	GLU	N-CA-C	5.70	117.17	111.07
1	A	734	THR	CA-C-N	5.69	132.41	121.54
1	A	734	THR	C-N-CA	5.69	132.41	121.54
1	C	426	PHE	CA-CB-CG	-5.68	108.11	113.80
1	C	3	GLN	CA-C-N	5.68	129.41	120.89
1	C	3	GLN	C-N-CA	5.68	129.41	120.89
1	B	703	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	C	89	LEU	CA-C-O	-5.67	113.69	120.10
1	C	313	VAL	N-CA-C	5.67	117.08	110.62
1	C	637	PRO	CA-C-N	5.67	125.62	119.78
1	C	637	PRO	C-N-CA	5.67	125.62	119.78
1	C	425	PRO	N-CA-CB	5.65	108.57	103.20
1	A	224	SER	CA-C-O	-5.65	112.94	119.78
1	C	11	ASP	CA-C-N	5.64	132.47	121.41
1	C	11	ASP	C-N-CA	5.64	132.47	121.41
1	C	209	THR	CA-C-O	5.64	124.26	118.73
1	C	593	GLU	CA-C-O	5.64	124.45	119.71
1	A	498	TYR	CA-C-N	5.64	125.31	119.05
1	A	498	TYR	C-N-CA	5.64	125.31	119.05
1	C	223	SER	CA-C-O	-5.63	114.33	120.81
1	A	688	PHE	CA-C-O	-5.63	112.68	119.27
1	A	2	ASN	CA-CB-CG	5.63	118.23	112.60
2	D	361	ILE	N-CA-C	5.62	117.90	109.20
1	C	335	TYR	CA-CB-CG	-5.62	103.79	113.90
1	B	544	PHE	CA-C-O	-5.61	113.17	119.79
1	C	90	ARG	N-CA-CB	5.61	118.12	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	593	GLU	CA-C-N	5.61	126.09	120.14
1	A	593	GLU	C-N-CA	5.61	126.09	120.14
1	A	431	ALA	CA-C-N	5.60	125.58	120.03
1	A	431	ALA	C-N-CA	5.60	125.58	120.03
1	A	35	ASN	CA-CB-CG	-5.60	107.00	112.60
1	A	3	GLN	CA-C-N	5.59	129.28	120.89
1	A	3	GLN	C-N-CA	5.59	129.28	120.89
1	B	688	PHE	CA-CB-CG	-5.59	108.21	113.80
1	A	298	ARG	N-CA-C	5.58	117.84	108.23
1	A	362	PRO	N-CA-CB	5.58	108.22	103.19
1	A	100	PRO	N-CA-CB	5.57	109.10	103.25
1	B	419	HIS	CA-C-O	-5.57	114.94	120.90
1	A	21	LYS	N-CA-C	-5.55	104.92	110.97
1	B	20	ASP	CA-CB-CG	-5.55	107.05	112.60
1	C	586	ASP	CA-C-N	5.55	127.98	120.38
1	C	586	ASP	C-N-CA	5.55	127.98	120.38
1	B	221	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	B	356	PHE	CA-CB-CG	5.53	119.33	113.80
1	B	468	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	49	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	77	TYR	CA-C-O	-5.50	114.72	120.55
1	C	70	ILE	CA-C-O	-5.50	115.31	121.36
1	C	200	VAL	CA-C-O	-5.50	115.02	120.85
1	A	331	ARG	N-CA-C	5.49	119.15	112.23
1	B	2	ASN	CA-C-N	5.48	131.25	122.32
1	B	2	ASN	C-N-CA	5.48	131.25	122.32
1	C	705	PRO	N-CA-CB	5.48	108.12	103.19
1	A	578	LEU	CA-C-N	5.47	125.56	119.32
1	A	578	LEU	C-N-CA	5.47	125.56	119.32
1	B	266	SER	CA-C-N	5.47	125.42	119.78
1	B	266	SER	C-N-CA	5.47	125.42	119.78
1	C	671	GLU	N-CA-C	-5.47	106.44	113.23
1	B	705	PRO	N-CA-CB	5.47	108.11	103.19
1	B	431	ALA	CA-C-N	5.47	125.46	120.21
1	B	431	ALA	C-N-CA	5.47	125.46	120.21
1	A	464	LEU	N-CA-CB	-5.46	102.45	110.85
1	C	368	PHE	CA-CB-CG	5.45	119.25	113.80
1	B	388	ILE	N-CA-C	5.45	116.03	108.84
1	C	2	ASN	CA-CB-CG	5.45	118.05	112.60
1	C	615	THR	CA-C-O	-5.45	114.74	121.06
1	B	231	GLY	N-CA-C	-5.45	104.29	112.89
1	C	672	MET	CA-C-N	5.44	125.05	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	672	MET	C-N-CA	5.44	125.05	119.56
1	B	462	CYS	CA-C-O	-5.42	115.28	120.92
1	A	130	GLN	OE1-CD-NE2	5.42	128.02	122.60
1	C	447	LYS	CA-C-N	5.42	125.36	119.78
1	C	447	LYS	C-N-CA	5.42	125.36	119.78
1	A	371	ASP	N-CA-CB	-5.42	102.45	110.90
1	A	154	LYS	N-CA-C	5.41	119.12	112.03
1	B	421	ASN	OD1-CG-ND2	5.41	128.01	122.60
1	C	388	ILE	N-CA-C	5.41	115.98	108.84
1	A	705	PRO	N-CA-CB	5.40	108.05	103.19
1	B	468	ASN	O-C-N	-5.40	115.83	122.68
1	B	283	LYS	CA-C-O	5.39	126.67	120.90
1	C	408	SER	N-CA-CB	5.38	117.76	109.91
1	C	456	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	613	ASN	CA-CB-CG	-5.37	107.23	112.60
1	C	2	ASN	CA-C-N	5.36	131.06	122.32
1	C	2	ASN	C-N-CA	5.36	131.06	122.32
1	C	448	PRO	N-CA-CB	5.36	108.01	103.35
1	C	217	THR	CA-C-N	5.35	125.43	119.87
1	C	217	THR	C-N-CA	5.35	125.43	119.87
1	C	593	GLU	CA-C-N	5.34	125.81	120.14
1	C	593	GLU	C-N-CA	5.34	125.81	120.14
1	C	202	THR	CA-C-O	5.34	127.04	120.15
1	C	498	TYR	CA-C-N	5.34	124.98	119.05
1	C	498	TYR	C-N-CA	5.34	124.98	119.05
1	B	49	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	530	ARG	CD-NE-CZ	5.32	131.85	124.40
1	C	207	LEU	CA-C-N	5.32	125.62	119.92
1	C	207	LEU	C-N-CA	5.32	125.62	119.92
1	A	392	ARG	CA-C-O	-5.32	114.58	120.38
1	C	279	ILE	CA-C-N	5.32	125.38	119.32
1	C	279	ILE	C-N-CA	5.32	125.38	119.32
1	B	276	THR	N-CA-C	5.31	117.81	111.71
1	B	515	ILE	CA-C-O	-5.30	114.86	120.48
1	C	735	ARG	O-C-N	-5.29	115.55	122.59
1	A	78	GLN	N-CA-CB	5.29	117.99	110.06
1	B	175	LEU	CA-C-O	-5.28	114.82	120.42
1	B	639	ARG	CD-NE-CZ	5.28	131.78	124.40
2	E	361	ILE	N-CA-C	5.27	117.21	108.99
1	C	254	ILE	CA-C-O	-5.26	114.72	120.72
1	A	276	THR	N-CA-C	5.26	118.80	112.38
1	A	408	SER	N-CA-CB	5.25	117.57	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	644	ILE	N-CA-C	5.25	116.14	108.53
1	A	360	ASP	CA-CB-CG	5.25	117.84	112.60
1	A	412	ILE	N-CA-CB	5.24	118.28	111.83
1	B	404	GLN	OE1-CD-NE2	5.24	127.84	122.60
1	B	2	ASN	CA-CB-CG	5.23	117.83	112.60
1	B	451	ASP	CA-C-O	-5.22	115.64	121.23
1	B	461	LEU	N-CA-C	5.21	118.09	109.85
1	B	498	TYR	CA-C-N	5.21	124.84	119.05
1	B	498	TYR	C-N-CA	5.21	124.84	119.05
1	C	464	LEU	CA-C-O	5.21	127.87	121.56
1	A	428	PRO	N-CA-CB	5.21	109.02	103.39
1	B	3	GLN	CA-C-N	5.21	128.71	120.89
1	B	3	GLN	C-N-CA	5.21	128.71	120.89
1	C	438	LEU	CA-C-O	-5.21	114.92	121.02
1	C	703	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	B	61	THR	CA-CB-OG1	-5.20	101.80	109.60
1	C	277	GLY	N-CA-C	5.20	120.52	112.45
1	C	734	THR	CA-C-N	5.20	131.48	121.54
1	C	734	THR	C-N-CA	5.20	131.48	121.54
1	B	357	SER	CA-C-N	5.20	125.25	119.32
1	B	357	SER	C-N-CA	5.20	125.25	119.32
1	A	453	ASN	CA-CB-CG	-5.20	107.40	112.60
1	B	200	VAL	CA-C-O	-5.20	115.34	120.85
1	A	267	PRO	N-CA-CB	5.20	107.87	103.35
1	B	48	GLN	O-C-N	5.19	128.43	122.25
1	A	231	GLY	N-CA-C	-5.18	104.70	112.89
1	B	617	SER	N-CA-CB	-5.18	102.56	110.85
1	C	253	GLY	N-CA-C	-5.18	103.50	111.64
1	B	11	ASP	CA-C-N	5.18	131.56	121.41
1	B	11	ASP	C-N-CA	5.18	131.56	121.41
1	B	31	GLU	CA-C-O	-5.18	116.01	120.88
1	A	313	VAL	N-CA-C	5.18	116.52	110.62
1	B	299	GLY	CA-C-O	-5.17	118.86	122.22
1	B	224	SER	CA-C-O	-5.17	113.52	119.78
1	C	231	GLY	N-CA-C	-5.17	104.72	112.89
1	A	99	PRO	CA-C-N	5.17	126.30	119.84
1	A	99	PRO	C-N-CA	5.17	126.30	119.84
1	A	335	TYR	CA-CB-CG	-5.17	104.60	113.90
1	B	203	PHE	N-CA-C	5.17	118.72	111.90
1	C	693	ILE	CA-C-O	-5.17	114.88	120.67
1	B	428	PRO	N-CA-CB	5.16	108.97	103.39
1	B	100	PRO	N-CA-CB	5.16	108.67	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	B	613	ASN	CA-CB-CG	-5.16	107.44	112.60
1	C	34	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	498	TYR	CA-C-O	5.15	124.47	119.62
1	B	637	PRO	CA-C-N	5.15	125.09	119.78
1	B	637	PRO	C-N-CA	5.15	125.09	119.78
1	C	202	THR	O-C-N	-5.15	115.54	122.19
1	A	44	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	A	207	LEU	CA-C-N	5.15	126.28	119.84
1	A	207	LEU	C-N-CA	5.15	126.28	119.84
1	A	704	PHE	CA-C-O	5.15	126.54	120.41
1	A	266	SER	CA-C-N	5.15	125.08	119.78
1	A	266	SER	C-N-CA	5.15	125.08	119.78
1	C	373	GLU	CB-CG-CD	-5.15	103.85	112.60
1	A	357	SER	CA-C-N	5.13	125.17	119.32
1	A	357	SER	C-N-CA	5.13	125.17	119.32
1	C	294	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	C	360	ASP	N-CA-C	5.13	119.52	113.16
1	A	358	PRO	N-CA-CB	5.12	109.10	103.26
1	C	698	ASN	OD1-CG-ND2	5.12	127.72	122.60
1	B	207	LEU	CA-C-N	5.12	125.39	119.92
1	B	207	LEU	C-N-CA	5.12	125.39	119.92
1	A	442	ILE	CA-C-O	-5.11	114.91	120.84
1	C	586	ASP	CA-CB-CG	-5.11	107.50	112.60
1	C	393	VAL	N-CA-CB	5.10	119.82	111.45
1	B	353	ILE	N-CA-CB	5.10	118.45	111.41
1	C	474	ASN	OD1-CG-ND2	5.10	127.70	122.60
1	A	389	ARG	CD-NE-CZ	5.10	131.54	124.40
1	C	557	GLU	CA-CB-CG	5.10	124.30	114.10
1	A	434	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	B	138	ASP	CA-CB-CG	-5.09	107.51	112.60
1	A	454	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	251	ARG	CD-NE-CZ	5.09	131.53	124.40
1	C	498	TYR	CA-C-O	5.08	124.39	119.62
1	A	209	THR	O-C-N	-5.07	115.97	120.48
1	C	208	PRO	N-CA-CB	5.07	108.16	103.39
1	A	457	GLY	N-CA-C	-5.06	104.90	112.89
1	C	500	ILE	CA-C-O	5.05	122.64	119.51
1	A	8	THR	N-CA-CB	5.05	118.82	110.69
1	A	353	ILE	N-CA-CB	5.03	118.35	111.41
1	A	461	LEU	N-CA-C	5.03	117.79	109.85
1	C	7	VAL	CA-C-O	-5.03	115.41	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	499	PRO	N-CA-CB	5.03	108.86	103.33
1	B	702	SER	CB-CA-C	-5.03	102.14	110.68
1	C	632	THR	CA-C-O	-5.02	116.08	121.56
1	B	274	PHE	N-CA-CB	5.02	117.89	110.56
1	A	537	ASN	CA-C-O	-5.02	115.55	121.07
1	C	464	LEU	N-CA-CB	-5.02	103.12	110.85
1	A	238	ASN	OD1-CG-ND2	-5.02	117.58	122.60
1	B	568	PHE	CA-C-N	5.02	128.63	120.60
1	B	568	PHE	C-N-CA	5.02	128.63	120.60
1	B	8	THR	N-CA-CB	5.01	119.09	110.68
1	C	276	THR	N-CA-C	5.01	117.47	111.71
1	C	49	PHE	CA-CB-CG	5.00	118.80	113.80

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	46	HIS	Mainchain
1	A	75	PRO	Mainchain
1	B	667	GLU	Mainchain
1	B	697	THR	Mainchain
1	C	46	HIS	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	5874	0	5797	181	0
1	B	5874	0	5797	167	0
1	C	5874	0	5797	170	0
2	D	140	0	123	4	0
2	E	140	0	123	3	0
2	F	140	0	123	5	0
2	P	31	0	34	3	0
3	A	28	0	0	3	0
3	B	30	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	32	0	0	3	0
All	All	18163	0	17794	525	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 15.

All (525) 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:A:191:GLN:HE21	1:A:195:ARG:HH21	1.04	0.98
1:B:191:GLN:HE21	1:B:195:ARG:HH21	1.03	0.94
1:C:191:GLN:HE21	1:C:195:ARG:HH21	0.95	0.91
1:A:1:MET:H2	1:A:3:GLN:HG3	1.40	0.87
1:C:1:MET:H2	1:C:3:GLN:HG3	1.40	0.87
1:B:698:ASN:ND2	1:B:733:ASN:HD22	1.77	0.83
1:C:191:GLN:NE2	1:C:195:ARG:HH21	1.75	0.83
1:A:4:ASN:O	1:A:5:LEU:HB2	1.77	0.83
1:B:1:MET:H2	1:B:3:GLN:HG3	1.43	0.82
1:C:37:SER:HB3	1:C:40:GLN:HB2	1.61	0.82
1:B:37:SER:HB3	1:B:40:GLN:HB2	1.62	0.81
1:B:658:ASP:HB3	1:B:662:LEU:HD12	1.62	0.81
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.62	0.80
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.64	0.80
1:A:698:ASN:ND2	1:A:733:ASN:HD22	1.81	0.78
1:B:234:LEU:HG	1:B:272:GLU:HG2	1.65	0.78
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.66	0.78
1:C:191:GLN:HE21	1:C:195:ARG:NH2	1.78	0.77
1:B:215:VAL:O	1:B:216:ARG:HB3	1.83	0.77
1:A:94:TYR:OH	1:A:168:SER:HB3	1.84	0.77
1:C:698:ASN:ND2	1:C:733:ASN:HD22	1.83	0.77
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.66	0.76
1:B:191:GLN:NE2	1:B:195:ARG:HH21	1.81	0.76
1:A:191:GLN:NE2	1:A:195:ARG:HH21	1.84	0.76
1:A:37:SER:HB3	1:A:40:GLN:HB2	1.69	0.75
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.67	0.75
1:C:489:LEU:HB3	1:C:513:LEU:HD22	1.69	0.75
1:A:234:LEU:HG	1:A:272:GLU:HG2	1.67	0.75
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.68	0.74
1:A:279:ILE:HD13	1:A:319:LEU:HD21	1.69	0.74
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.69	0.74
1:B:489:LEU:HB3	1:B:513:LEU:HD22	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:GLN:HB2	1:B:298:ARG:HB3	1.70	0.74
1:C:279:ILE:HD13	1:C:319:LEU:HD21	1.68	0.74
1:B:4:ASN:O	1:B:5:LEU:HB2	1.86	0.74
1:A:294:GLN:HB2	1:A:298:ARG:HB3	1.70	0.72
1:A:489:LEU:HB3	1:A:513:LEU:HD22	1.72	0.72
1:C:215:VAL:O	1:C:216:ARG:HB3	1.90	0.71
1:C:465:SER:HB2	1:C:489:LEU:HD11	1.70	0.71
1:C:9:LYS:HE2	1:C:55:THR:HG21	1.71	0.71
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.71	0.70
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.73	0.70
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.73	0.70
1:A:215:VAL:O	1:A:216:ARG:HB3	1.90	0.70
1:B:9:LYS:HE2	1:B:55:THR:HG21	1.72	0.70
1:A:191:GLN:HE21	1:A:195:ARG:NH2	1.87	0.70
1:A:672:MET:HE1	1:A:678:TYR:HB2	1.72	0.70
1:C:294:GLN:HB2	1:C:298:ARG:HB3	1.75	0.69
1:B:400:SER:HB3	1:B:711:MET:HE3	1.75	0.69
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.74	0.69
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.74	0.69
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.75	0.69
1:B:465:SER:HB2	1:B:489:LEU:HD11	1.75	0.68
1:C:234:LEU:HG	1:C:272:GLU:HG2	1.75	0.68
1:C:4:ASN:O	1:C:5:LEU:HB2	1.93	0.68
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.75	0.68
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.75	0.68
1:C:94:TYR:OH	1:C:168:SER:HB3	1.95	0.67
1:B:75:PRO:O	1:B:78:GLN:HG2	1.93	0.67
1:B:279:ILE:HD13	1:B:319:LEU:HD21	1.75	0.67
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.76	0.66
1:B:361:VAL:HG21	1:B:364:LEU:HD12	1.77	0.66
1:C:522:TYR:CE2	1:C:526:LYS:HD3	2.32	0.64
1:B:176:VAL:HG11	1:B:212:MET:HE1	1.80	0.64
1:B:734:THR:O	1:B:735:ARG:HB2	1.99	0.63
1:B:479:GLU:HB2	1:B:550:TYR:CE1	2.33	0.63
1:C:700:ASP:OD2	1:C:736:ASP:HB3	1.98	0.63
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.79	0.63
1:A:519:ASN:ND2	1:A:522:TYR:HB3	2.14	0.63
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.80	0.62
1:A:83:ARG:HG2	1:A:141:MET:HG3	1.81	0.62
1:B:191:GLN:HE21	1:B:195:ARG:NH2	1.88	0.62
1:B:698:ASN:ND2	1:B:733:ASN:ND2	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:VAL:O	1:B:216:ARG:CB	2.47	0.62
1:A:522:TYR:CE2	1:A:526:LYS:HD3	2.35	0.62
1:A:361:VAL:HG21	1:A:364:LEU:HD12	1.81	0.62
1:B:700:ASP:OD2	1:B:736:ASP:HB3	2.00	0.62
1:B:94:TYR:OH	1:B:168:SER:HB3	2.00	0.62
1:A:400:SER:HB3	1:A:711:MET:HE3	1.82	0.62
1:B:313:VAL:HG22	1:B:317:LEU:HD22	1.82	0.61
1:B:686:GLN:NE2	1:B:727:LYS:HD2	2.16	0.61
1:B:322:ASN:HA	1:B:331:ARG:NH1	2.16	0.61
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.81	0.61
1:A:176:VAL:HG22	3:A:787:HOH:O	2.01	0.61
1:C:322:ASN:HA	1:C:331:ARG:NH1	2.16	0.61
1:B:172:LEU:O	1:B:176:VAL:HG23	2.00	0.61
1:A:176:VAL:HG11	1:A:212:MET:HE1	1.84	0.59
1:A:187:GLU:HB2	3:C:762:HOH:O	2.01	0.59
1:A:322:ASN:HA	1:A:331:ARG:NH1	2.16	0.59
1:A:9:LYS:HE2	1:A:55:THR:HG21	1.84	0.59
1:B:519:ASN:ND2	1:B:632:THR:H	2.01	0.59
1:C:120:LEU:HD13	2:P:1:TYR:HB3	1.85	0.59
1:C:75:PRO:O	1:C:78:GLN:HG2	2.03	0.59
1:C:215:VAL:O	1:C:216:ARG:CB	2.51	0.59
1:B:215:VAL:HB	3:B:789:HOH:O	2.03	0.58
1:B:329:ARG:HG3	1:B:331:ARG:NH1	2.18	0.58
1:B:522:TYR:CE2	1:B:526:LYS:HD3	2.38	0.58
1:C:56:SER:O	1:C:60:GLU:HG2	2.03	0.58
1:C:122:ASP:O	1:C:189:ARG:NH2	2.37	0.58
1:C:444:LEU:HD12	1:C:460:ALA:HB1	1.84	0.58
1:A:686:GLN:HE22	1:A:692:SER:HA	1.68	0.58
1:B:83:ARG:HG2	1:B:141:MET:HG3	1.84	0.58
1:C:10:ARG:O	1:C:11:ASP:C	2.47	0.58
1:C:483:ILE:HG23	1:C:487:ARG:HD2	1.85	0.58
1:B:444:LEU:HD12	1:B:460:ALA:HB1	1.86	0.57
1:C:361:VAL:HG21	1:C:364:LEU:HD12	1.85	0.57
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.85	0.57
1:C:5:LEU:HD23	1:C:51:ASP:HA	1.86	0.57
1:C:176:VAL:HG22	3:C:791:HOH:O	2.04	0.57
1:A:75:PRO:O	1:A:78:GLN:HG2	2.04	0.57
1:A:698:ASN:ND2	1:A:733:ASN:ND2	2.51	0.57
1:C:329:ARG:HG3	1:C:331:ARG:NH1	2.20	0.57
1:C:672:MET:HE1	1:C:678:TYR:HB2	1.86	0.57
1:A:479:GLU:HB2	1:A:550:TYR:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:SER:HB3	1:C:611:LEU:HD22	1.87	0.57
1:B:338:GLN:HE21	1:B:415:GLN:NE2	2.03	0.57
1:B:672:MET:HE1	1:B:678:TYR:HB2	1.86	0.57
1:A:33:LEU:HB3	1:A:76:ASP:HB3	1.86	0.56
1:C:172:LEU:O	1:C:176:VAL:HG23	2.05	0.56
1:C:176:VAL:HG11	1:C:212:MET:HE1	1.86	0.56
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.87	0.56
1:A:532:SER:HA	1:A:677:GLY:HA3	1.86	0.56
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.86	0.56
1:C:686:GLN:CD	1:C:727:LYS:HD2	2.31	0.56
1:B:620:MET:HB2	1:B:621:PRO:HD2	1.87	0.56
1:C:272:GLU:HB3	1:C:274:PHE:HE1	1.70	0.56
1:C:353:ILE:HG13	1:C:395:ALA:HB2	1.87	0.56
1:A:10:ARG:O	1:A:11:ASP:C	2.49	0.55
1:B:353:ILE:HG13	1:B:395:ALA:HB2	1.89	0.55
1:C:187:GLU:HB2	3:C:782:HOH:O	2.05	0.55
1:C:519:ASN:ND2	1:C:522:TYR:HB3	2.21	0.55
1:A:106:VAL:O	1:A:110:VAL:HG23	2.05	0.55
1:A:215:VAL:O	1:A:216:ARG:CB	2.54	0.55
1:B:621:PRO:HD3	1:B:694:SER:OG	2.06	0.55
1:C:572:THR:HB	1:C:577:ILE:HB	1.88	0.55
1:C:83:ARG:HG2	1:C:141:MET:HG3	1.87	0.55
1:A:329:ARG:HG3	1:A:331:ARG:NH1	2.22	0.55
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.87	0.55
1:C:561:GLU:HG2	1:C:562:GLN:HG2	1.87	0.55
1:A:548:GLN:HA	1:A:548:GLN:NE2	2.20	0.55
1:A:272:GLU:HB3	1:A:274:PHE:HE1	1.72	0.55
1:B:99:PRO:HG2	1:B:137:HIS:CG	2.42	0.54
1:C:21:LYS:O	1:C:25:VAL:HG23	2.07	0.54
1:B:10:ARG:O	1:B:11:ASP:C	2.50	0.54
1:B:532:SER:HA	1:B:677:GLY:HA3	1.89	0.54
1:A:585:LYS:HD2	1:A:585:LYS:N	2.23	0.54
1:C:548:GLN:HA	1:C:548:GLN:NE2	2.21	0.54
1:A:444:LEU:HD12	1:A:460:ALA:HB1	1.89	0.54
1:A:555:SER:HB3	1:A:611:LEU:HD22	1.88	0.54
1:B:272:GLU:HB3	1:B:274:PHE:HE1	1.71	0.54
1:B:149:LYS:HE3	1:B:152:GLU:OE1	2.08	0.54
1:B:479:GLU:HB2	1:B:550:TYR:CD1	2.42	0.54
1:B:117:ASN:H	1:B:117:ASN:ND2	2.04	0.54
1:A:56:SER:O	1:A:60:GLU:HG2	2.08	0.54
1:A:561:GLU:HG2	1:A:562:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:ASN:HD22	1:A:733:ASN:HD22	1.56	0.54
1:C:263:ALA:HB3	1:C:357:SER:HB2	1.90	0.54
1:A:150:GLN:OE1	1:A:154:LYS:HE3	2.08	0.53
1:C:260:ARG:HG2	1:C:260:ARG:HH11	1.73	0.53
1:A:686:GLN:CD	1:A:727:LYS:HD2	2.33	0.53
1:B:124:THR:HG23	1:B:127:GLU:OE1	2.08	0.53
1:B:686:GLN:CD	1:B:727:LYS:HD2	2.32	0.53
1:B:548:GLN:HA	1:B:548:GLN:NE2	2.24	0.53
1:A:620:MET:HB2	1:A:621:PRO:HD2	1.89	0.53
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.89	0.53
1:B:585:LYS:HD2	1:B:585:LYS:N	2.23	0.53
1:A:700:ASP:OD2	1:A:736:ASP:HB3	2.09	0.53
1:B:33:LEU:HB3	1:B:76:ASP:HB3	1.91	0.53
1:A:149:LYS:HE3	1:A:152:GLU:OE1	2.08	0.53
1:A:353:ILE:HG13	1:A:395:ALA:HB2	1.91	0.53
1:B:122:ASP:O	1:B:189:ARG:NH2	2.42	0.53
1:B:226:VAL:HG12	1:B:461:LEU:CD2	2.39	0.53
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.91	0.53
1:B:176:VAL:HG22	3:B:789:HOH:O	2.07	0.53
1:B:700:ASP:CG	1:B:736:ASP:HB3	2.34	0.53
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.90	0.52
1:B:56:SER:O	1:B:60:GLU:HG2	2.09	0.52
1:B:441:ASP:OD2	1:B:620:MET:HB3	2.10	0.52
1:A:534:GLY:HA2	3:A:776:HOH:O	2.09	0.52
1:B:209:THR:N	1:B:210:PRO:HD2	2.24	0.52
1:B:212:MET:HE2	1:B:212:MET:HA	1.91	0.52
1:C:734:THR:O	1:C:735:ARG:HB2	2.09	0.52
1:A:107:VAL:O	1:A:111:GLU:HG3	2.10	0.52
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.37	0.52
1:C:325:VAL:HG13	1:C:328:ASN:HB2	1.92	0.52
1:B:541:HIS:NE2	1:B:687:LYS:HE2	2.24	0.52
1:C:180:LEU:HD12	1:C:488:ALA:HB1	1.91	0.52
1:C:492:LEU:O	1:C:496:GLN:HG2	2.10	0.52
1:B:312:GLU:O	1:B:316:LEU:HG	2.10	0.52
1:C:686:GLN:HE22	1:C:692:SER:HA	1.75	0.52
1:A:734:THR:O	1:A:735:ARG:HB2	2.09	0.52
1:B:686:GLN:HE22	1:B:692:SER:HA	1.75	0.52
1:C:33:LEU:HB3	1:C:76:ASP:HB3	1.92	0.52
2:E:372:ASN:H	2:E:372:ASN:ND2	2.08	0.51
1:A:17:ILE:HD12	1:A:19:LEU:HD23	1.93	0.51
1:B:263:ALA:HB3	1:B:357:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:TRP:HB3	1:B:570:GLU:HG3	1.92	0.51
1:C:124:THR:HG23	1:C:127:GLU:OE1	2.10	0.51
1:C:199:ALA:HB1	1:C:205:ILE:HD12	1.92	0.51
1:C:149:LYS:HE3	1:C:152:GLU:OE1	2.10	0.51
1:C:519:ASN:ND2	1:C:632:THR:H	2.09	0.51
1:C:99:PRO:HG2	1:C:137:HIS:CG	2.46	0.51
1:C:700:ASP:CG	1:C:736:ASP:HB3	2.36	0.51
1:A:17:ILE:HD12	1:A:19:LEU:CD2	2.40	0.51
1:C:633:ASN:O	1:C:634:GLY:C	2.53	0.51
1:A:99:PRO:HG2	1:A:137:HIS:CD2	2.45	0.51
1:A:172:LEU:O	1:A:176:VAL:HG23	2.11	0.51
1:A:308:MET:HE3	1:A:339:ILE:HG12	1.92	0.51
1:A:483:ILE:HG23	1:A:487:ARG:HD2	1.93	0.51
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.93	0.51
1:A:99:PRO:HG2	1:A:137:HIS:CG	2.46	0.51
2:D:372:ASN:H	2:D:372:ASN:ND2	2.07	0.51
1:B:49:PHE:CZ	1:B:58:ILE:HG23	2.46	0.51
1:B:697:THR:O	1:B:732:GLN:HA	2.11	0.51
1:C:49:PHE:CZ	1:C:58:ILE:HG23	2.45	0.51
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.38	0.51
1:B:99:PRO:HG2	1:B:137:HIS:CD2	2.46	0.50
1:C:441:ASP:OD2	1:C:620:MET:HB3	2.11	0.50
1:B:180:LEU:HD12	1:B:488:ALA:HB1	1.94	0.50
1:B:475:LEU:O	1:B:478:LEU:HB2	2.11	0.50
1:C:106:VAL:O	1:C:110:VAL:HG23	2.11	0.50
1:B:106:VAL:O	1:B:110:VAL:HG23	2.12	0.50
1:C:569:ASN:H	1:C:569:ASN:ND2	2.08	0.50
1:C:698:ASN:ND2	1:C:733:ASN:ND2	2.58	0.50
1:A:669:LEU:HD11	1:A:698:ASN:ND2	2.27	0.50
1:C:522:TYR:CD1	1:C:657:PRO:HB2	2.47	0.50
1:A:209:THR:N	1:A:210:PRO:HD2	2.27	0.50
1:A:212:MET:HE2	1:A:212:MET:HA	1.93	0.50
1:A:686:GLN:NE2	1:A:727:LYS:HD2	2.26	0.50
1:C:723:LYS:NZ	2:F:374:GLN:O	2.44	0.50
1:A:325:VAL:HG13	1:A:328:ASN:HB2	1.94	0.49
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.93	0.49
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.93	0.49
1:B:698:ASN:HD21	1:B:733:ASN:HD22	1.54	0.49
1:B:519:ASN:ND2	1:B:522:TYR:HB3	2.27	0.49
1:C:99:PRO:HG2	1:C:137:HIS:CD2	2.48	0.49
1:C:226:VAL:HG12	1:C:461:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:620:MET:HB2	1:C:621:PRO:HD2	1.94	0.49
1:C:704:PHE:CD2	1:C:710:PRO:HD3	2.47	0.49
1:A:304:LEU:HD13	1:A:333:MET:HE1	1.94	0.49
1:A:415:GLN:HE22	1:A:435:GLN:HA	1.77	0.49
1:C:686:GLN:NE2	1:C:727:LYS:HD2	2.27	0.49
1:C:341:LYS:HG2	1:C:722:TYR:OH	2.13	0.49
1:A:199:ALA:HB1	1:A:205:ILE:HD12	1.93	0.49
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.93	0.49
1:C:304:LEU:HD13	1:C:333:MET:HE1	1.94	0.49
1:C:400:SER:HB3	1:C:711:MET:HE3	1.95	0.49
1:A:426:PHE:O	1:A:428:PRO:HD3	2.13	0.49
1:A:569:ASN:ND2	1:A:569:ASN:H	2.10	0.49
1:A:585:LYS:HD2	1:A:585:LYS:H	1.77	0.49
1:B:341:LYS:HG2	1:B:722:TYR:OH	2.12	0.49
1:C:307:PRO:HA	1:C:338:GLN:HB2	1.95	0.49
1:A:260:ARG:HH11	1:A:260:ARG:HG2	1.78	0.49
1:B:555:SER:HB3	1:B:611:LEU:HD22	1.93	0.49
1:C:585:LYS:HD2	1:C:585:LYS:N	2.27	0.49
1:A:34:HIS:O	1:A:35:ASN:HB2	2.13	0.49
1:C:1:MET:HA	1:C:3:GLN:HE21	1.77	0.49
1:B:585:LYS:HD2	1:B:585:LYS:H	1.77	0.49
1:C:532:SER:HA	1:C:677:GLY:HA3	1.95	0.49
1:A:475:LEU:O	1:A:478:LEU:HB2	2.13	0.48
1:B:304:LEU:CD1	1:B:333:MET:HE1	2.43	0.48
1:A:572:THR:HB	1:A:577:ILE:HB	1.94	0.48
1:C:272:GLU:HB3	1:C:274:PHE:CE1	2.48	0.48
1:A:737:GLY:O	1:A:738:ALA:HB3	2.14	0.48
1:B:1:MET:HA	1:B:3:GLN:HE21	1.78	0.48
1:B:522:TYR:CD1	1:B:657:PRO:HB2	2.49	0.48
1:B:483:ILE:HG23	1:B:487:ARG:HD2	1.94	0.48
1:B:572:THR:HB	1:B:577:ILE:HB	1.95	0.48
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.95	0.48
1:B:415:GLN:HE22	1:B:435:GLN:HA	1.79	0.48
1:B:659:TYR:O	1:B:660:GLU:C	2.56	0.48
1:C:450:ASN:HB2	1:C:454:ASP:OD2	2.13	0.48
1:B:698:ASN:HD22	1:B:733:ASN:HD22	1.59	0.48
1:C:313:VAL:HG22	1:C:317:LEU:HD22	1.94	0.48
1:B:512:THR:HG22	1:B:615:THR:HG23	1.96	0.47
1:C:120:LEU:HD13	2:P:1:TYR:CG	2.49	0.47
1:A:263:ALA:HB3	1:A:357:SER:HB2	1.95	0.47
1:A:621:PRO:HD3	1:A:694:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:TYR:O	1:A:660:GLU:C	2.57	0.47
1:C:18:ASN:HB3	1:C:21:LYS:HB2	1.96	0.47
1:C:426:PHE:O	1:C:428:PRO:HD3	2.15	0.47
1:A:441:ASP:OD2	1:A:620:MET:HB3	2.13	0.47
1:B:272:GLU:HB3	1:B:274:PHE:CE1	2.49	0.47
1:B:388:ILE:O	1:B:390:LYS:HE3	2.14	0.47
1:A:567:TRP:HB3	1:A:570:GLU:HG3	1.96	0.47
1:B:561:GLU:HG2	1:B:562:GLN:HG2	1.97	0.47
1:C:479:GLU:HB2	1:C:550:TYR:CE1	2.50	0.47
1:C:518:ILE:HA	1:C:634:GLY:HA2	1.96	0.47
1:A:122:ASP:O	1:A:189:ARG:NH2	2.48	0.47
1:A:229:GLU:O	1:A:448:PRO:HA	2.14	0.47
1:A:569:ASN:H	1:A:569:ASN:HD22	1.63	0.47
1:C:487:ARG:HH22	1:C:561:GLU:CD	2.22	0.47
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.97	0.47
1:C:138:ASP:O	1:C:141:MET:HB2	2.15	0.47
1:C:659:TYR:O	1:C:660:GLU:C	2.58	0.47
1:A:317:LEU:O	1:A:405:GLU:HG3	2.14	0.47
1:B:256:ILE:O	1:B:304:LEU:HA	2.14	0.47
1:B:262:ARG:HB3	1:B:359:SER:HB3	1.96	0.47
1:A:487:ARG:HH22	1:A:561:GLU:CD	2.23	0.47
1:C:209:THR:N	1:C:210:PRO:HD2	2.29	0.47
1:C:260:ARG:HG2	1:C:260:ARG:NH1	2.30	0.47
1:C:150:GLN:OE1	1:C:154:LYS:HE3	2.15	0.46
1:A:388:ILE:O	1:A:390:LYS:HE3	2.16	0.46
1:C:475:LEU:O	1:C:478:LEU:HB2	2.14	0.46
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.97	0.46
1:C:134:PHE:CE2	1:C:194:LYS:HB2	2.50	0.46
1:C:548:GLN:HB2	1:C:688:PHE:HB3	1.97	0.46
1:B:729:LEU:HD23	1:B:729:LEU:HA	1.79	0.46
1:C:34:HIS:O	1:C:35:ASN:HB2	2.15	0.46
1:A:341:LYS:HG2	1:A:722:TYR:OH	2.14	0.46
1:A:492:LEU:O	1:A:496:GLN:HG2	2.16	0.46
1:A:312:GLU:O	1:A:316:LEU:HG	2.15	0.46
1:B:585:LYS:HD3	1:B:586:ASP:OD1	2.15	0.46
1:C:117:ASN:ND2	1:C:117:ASN:H	2.13	0.46
1:C:388:ILE:O	1:C:390:LYS:HE3	2.15	0.46
1:A:49:PHE:CZ	1:A:58:ILE:HG23	2.50	0.46
1:A:272:GLU:HB3	1:A:274:PHE:CE1	2.50	0.46
1:A:518:ILE:HA	1:A:634:GLY:HA2	1.97	0.46
1:B:364:LEU:HD22	1:B:375:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:SER:CB	1:C:61:THR:HG22	2.46	0.46
1:C:415:GLN:HE22	1:C:435:GLN:HA	1.80	0.46
2:F:372:ASN:ND2	2:F:372:ASN:H	2.14	0.46
1:B:172:LEU:C	1:B:172:LEU:HD23	2.41	0.46
1:C:567:TRP:HB3	1:C:570:GLU:HG3	1.98	0.46
1:C:585:LYS:HD3	1:C:586:ASP:OD1	2.16	0.46
1:B:370:ALA:HB1	3:B:786:HOH:O	2.16	0.46
1:C:37:SER:CB	1:C:40:GLN:HB2	2.41	0.46
1:B:5:LEU:HD23	1:B:51:ASP:HA	1.97	0.45
1:C:440:LEU:HD12	1:C:728:THR:HB	1.98	0.45
1:A:541:HIS:NE2	1:A:687:LYS:HE2	2.30	0.45
1:C:262:ARG:HD2	1:C:274:PHE:HB2	1.97	0.45
1:C:669:LEU:HD11	1:C:698:ASN:ND2	2.31	0.45
1:A:700:ASP:CG	1:A:736:ASP:HB3	2.41	0.45
1:B:426:PHE:O	1:B:428:PRO:HD3	2.17	0.45
1:B:450:ASN:HB2	1:B:454:ASP:OD2	2.16	0.45
1:A:5:LEU:HD23	1:A:51:ASP:HA	1.98	0.45
1:A:262:ARG:HB3	1:A:359:SER:HB3	1.98	0.45
1:B:510:ARG:HB2	1:B:512:THR:HG23	1.97	0.45
1:C:737:GLY:O	1:C:738:ALA:HB3	2.16	0.45
2:D:370:LEU:O	2:D:371:SER:C	2.59	0.45
1:B:592:ASN:O	1:B:593:GLU:C	2.60	0.45
1:A:522:TYR:CD1	1:A:657:PRO:HB2	2.51	0.45
1:A:585:LYS:HD3	1:A:586:ASP:OD1	2.16	0.45
1:B:325:VAL:HG13	1:B:328:ASN:HB2	1.99	0.45
1:B:548:GLN:HB2	1:B:688:PHE:HB3	1.99	0.45
1:C:522:TYR:CZ	1:C:526:LYS:HD3	2.51	0.45
1:A:723:LYS:NZ	2:D:374:GLN:O	2.42	0.45
1:B:492:LEU:O	1:B:496:GLN:HG2	2.16	0.45
1:C:585:LYS:HD2	1:C:585:LYS:H	1.82	0.45
1:A:292:CYS:C	1:B:276:THR:HG21	2.42	0.45
1:B:519:ASN:HD22	1:B:519:ASN:HA	1.53	0.45
1:C:256:ILE:O	1:C:304:LEU:HA	2.16	0.45
1:C:262:ARG:HH12	1:C:269:ARG:HB2	1.82	0.45
1:A:117:ASN:ND2	1:A:117:ASN:H	2.15	0.44
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.76	0.44
1:C:541:HIS:NE2	1:C:687:LYS:HE2	2.32	0.44
1:A:520:PHE:O	1:A:523:TYR:HB3	2.18	0.44
1:A:450:ASN:HB2	1:A:454:ASP:OD2	2.16	0.44
1:C:569:ASN:H	1:C:569:ASN:HD22	1.66	0.44
1:A:479:GLU:HB2	1:A:550:TYR:CD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:GLY:O	1:A:738:ALA:CB	2.65	0.44
1:B:150:GLN:HE21	1:B:627:GLN:NE2	2.16	0.44
1:C:176:VAL:HG11	1:C:212:MET:CE	2.48	0.44
1:B:262:ARG:HD2	1:B:274:PHE:HB2	1.99	0.44
1:C:254:ILE:O	1:C:302:ALA:HA	2.18	0.44
1:A:215:VAL:HB	3:A:787:HOH:O	2.17	0.44
1:A:633:ASN:O	1:A:634:GLY:C	2.61	0.44
1:B:519:ASN:CG	1:B:631:ALA:HB1	2.43	0.44
1:B:568:PHE:CE1	1:B:611:LEU:HB2	2.53	0.44
1:B:626:SER:CB	1:B:633:ASN:HD22	2.31	0.44
1:B:737:GLY:O	1:B:738:ALA:HB3	2.17	0.44
1:C:45:SER:HB2	1:C:61:THR:HG22	2.00	0.44
1:C:90:ARG:HG3	1:C:90:ARG:HH11	1.82	0.44
1:C:262:ARG:HB3	1:C:359:SER:HB3	1.98	0.44
1:A:364:LEU:HD22	1:A:375:PHE:CE2	2.53	0.44
1:A:568:PHE:CE1	1:A:611:LEU:HB2	2.53	0.44
1:B:21:LYS:O	1:B:25:VAL:HG23	2.18	0.44
1:C:434:ARG:O	1:C:435:GLN:HB3	2.17	0.44
1:A:254:ILE:O	1:A:302:ALA:HA	2.18	0.44
1:A:558:LEU:HD23	1:A:612:ARG:CG	2.47	0.44
1:B:669:LEU:HD23	1:B:670:TRP:CE2	2.53	0.44
1:C:17:ILE:HG23	1:C:19:LEU:HG	1.99	0.44
1:A:58:ILE:O	1:A:62:ILE:HG23	2.17	0.43
1:A:151:LEU:HA	1:A:155:TYR:HB2	2.00	0.43
1:A:522:TYR:CZ	1:A:526:LYS:HD3	2.52	0.43
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.98	0.43
1:B:418:ASP:O	1:B:419:HIS:C	2.57	0.43
1:A:149:LYS:HA	1:A:149:LYS:CE	2.48	0.43
1:A:676:ASP:O	1:A:677:GLY:C	2.60	0.43
1:C:520:PHE:HB3	1:C:635:ILE:HA	1.99	0.43
1:A:510:ARG:HB2	1:A:512:THR:HG23	2.01	0.43
1:C:286:GLN:HG3	1:C:333:MET:HG3	1.99	0.43
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.46	0.43
1:B:492:LEU:O	1:B:493:LEU:C	2.62	0.43
2:E:370:LEU:O	2:E:371:SER:C	2.61	0.43
1:C:217:THR:HB	1:C:218:PRO:CD	2.48	0.43
1:A:7:VAL:CG1	1:A:55:THR:HG22	2.49	0.43
1:A:257:ASN:HB2	1:A:435:GLN:OE1	2.18	0.43
1:A:538:ASN:HB3	1:A:593:GLU:HB2	2.00	0.43
1:B:306:TYR:HB2	1:B:307:PRO:HD2	1.99	0.43
1:B:339:ILE:HG22	1:B:340:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ASN:O	1:B:634:GLY:C	2.60	0.43
1:B:704:PHE:CD2	1:B:710:PRO:HD3	2.54	0.43
1:C:698:ASN:HD21	1:C:733:ASN:HD22	1.63	0.43
1:C:737:GLY:O	1:C:738:ALA:CB	2.65	0.43
1:A:406:ARG:NH2	1:A:730:TYR:O	2.45	0.43
1:A:519:ASN:ND2	1:A:632:THR:H	2.17	0.43
1:B:150:GLN:OE1	1:B:154:LYS:HE3	2.18	0.43
1:B:151:LEU:HD13	1:B:169:ALA:HB2	2.00	0.43
1:B:187:GLU:HB2	3:B:780:HOH:O	2.17	0.43
1:C:466:ALA:HA	1:C:516:GLY:O	2.18	0.43
1:C:489:LEU:HD23	1:C:489:LEU:HA	1.81	0.43
1:B:175:LEU:O	1:B:176:VAL:C	2.61	0.43
1:B:285:PHE:O	1:B:289:VAL:HG23	2.18	0.43
1:B:568:PHE:CE2	1:B:574:ALA:HA	2.54	0.43
1:B:698:ASN:HD21	1:B:733:ASN:ND2	2.14	0.43
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.99	0.43
1:C:338:GLN:HE21	1:C:415:GLN:NE2	2.17	0.43
1:A:180:LEU:HD12	1:A:488:ALA:HB1	2.01	0.43
1:B:18:ASN:HB3	1:B:21:LYS:HB2	2.00	0.43
1:C:512:THR:HG22	1:C:615:THR:HG23	2.00	0.43
1:A:262:ARG:HD2	1:A:274:PHE:HB2	2.01	0.43
1:A:626:SER:CB	1:A:633:ASN:HD22	2.32	0.43
1:B:144:SER:O	1:B:147:ALA:HB3	2.18	0.43
1:B:209:THR:N	1:B:210:PRO:CD	2.82	0.43
1:B:260:ARG:HG2	1:B:260:ARG:HH11	1.84	0.43
1:B:402:MET:HE2	1:B:402:MET:HB3	1.95	0.43
1:C:47:ILE:HG13	1:C:47:ILE:O	2.18	0.43
1:A:171:PHE:HA	1:A:174:ILE:HG22	2.01	0.42
1:B:466:ALA:HA	1:B:516:GLY:O	2.19	0.42
1:A:260:ARG:HG2	1:A:260:ARG:NH1	2.35	0.42
1:A:338:GLN:HE21	1:A:415:GLN:NE2	2.17	0.42
1:B:254:ILE:O	1:B:302:ALA:HA	2.18	0.42
1:C:510:ARG:HB2	1:C:512:THR:HG23	2.01	0.42
1:A:256:ILE:O	1:A:304:LEU:HA	2.20	0.42
1:A:304:LEU:CD1	1:A:333:MET:HE1	2.49	0.42
1:A:592:ASN:O	1:A:593:GLU:C	2.61	0.42
1:C:17:ILE:HD12	1:C:19:LEU:CD2	2.49	0.42
1:C:418:ASP:O	1:C:419:HIS:C	2.60	0.42
1:B:522:TYR:CZ	1:B:526:LYS:HD3	2.54	0.42
1:A:1:MET:HA	1:A:3:GLN:HE21	1.84	0.42
1:A:18:ASN:ND2	1:A:21:LYS:HE3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ILE:O	1:B:62:ILE:HG23	2.19	0.42
1:C:212:MET:HA	1:C:212:MET:HE2	2.01	0.42
1:C:304:LEU:CD1	1:C:333:MET:HE1	2.48	0.42
1:A:18:ASN:HB3	1:A:21:LYS:HB2	2.01	0.42
1:A:548:GLN:HA	1:A:548:GLN:HE21	1.84	0.42
1:B:569:ASN:H	1:B:569:ASN:ND2	2.18	0.42
1:A:435:GLN:HG3	1:A:436:SER:O	2.20	0.42
1:C:322:ASN:HA	1:C:331:ARG:HH11	1.84	0.42
2:P:1:TYR:HB2	2:P:2:LEU:H	1.69	0.42
1:B:487:ARG:HH22	1:B:561:GLU:CD	2.27	0.42
1:C:151:LEU:HA	1:C:155:TYR:HB2	2.01	0.42
1:C:348:LEU:HD11	2:F:375:LEU:HD21	2.01	0.42
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.55	0.42
1:A:176:VAL:HG11	1:A:212:MET:CE	2.50	0.42
1:A:236:SER:O	1:A:237:ILE:C	2.62	0.42
1:A:512:THR:HG22	1:A:615:THR:HG23	2.02	0.42
1:A:700:ASP:OD1	1:A:700:ASP:C	2.61	0.42
1:B:676:ASP:O	1:B:677:GLY:C	2.60	0.42
1:B:737:GLY:O	1:B:738:ALA:CB	2.68	0.42
1:C:262:ARG:NH1	1:C:269:ARG:HB2	2.34	0.42
1:C:697:THR:O	1:C:732:GLN:HA	2.20	0.42
1:A:150:GLN:HE21	1:A:627:GLN:NE2	2.18	0.42
1:A:466:ALA:HA	1:A:516:GLY:O	2.19	0.42
1:B:294:GLN:HG2	1:B:298:ARG:HD3	2.01	0.42
1:C:171:PHE:HA	1:C:174:ILE:HG22	2.02	0.42
1:A:226:VAL:HG12	1:A:461:LEU:CD2	2.50	0.41
1:A:281:PHE:CE1	1:B:291:SER:HB2	2.55	0.41
1:A:284:HIS:CE1	1:B:284:HIS:CE1	3.08	0.41
1:A:474:ASN:OD1	1:A:476:ASP:HB2	2.20	0.41
1:A:519:ASN:CG	1:A:631:ALA:HB1	2.45	0.41
1:A:669:LEU:HD23	1:A:670:TRP:CE2	2.55	0.41
1:B:107:VAL:O	1:B:111:GLU:HG3	2.20	0.41
1:C:17:ILE:HD12	1:C:19:LEU:HD23	2.01	0.41
1:C:229:GLU:O	1:C:448:PRO:HA	2.20	0.41
1:A:339:ILE:HG22	1:A:340:ASN:N	2.34	0.41
1:B:134:PHE:CE2	1:B:194:LYS:HB2	2.56	0.41
1:B:322:ASN:HA	1:B:331:ARG:HH11	1.84	0.41
1:B:418:ASP:OD1	1:B:419:HIS:N	2.52	0.41
1:C:310:HIS:CE1	1:C:312:GLU:HG3	2.55	0.41
1:A:527:HIS:O	1:A:529:LYS:HE2	2.20	0.41
1:A:681:LEU:O	1:A:685:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:TYR:O	1:B:193:VAL:C	2.64	0.41
1:B:734:THR:O	1:B:735:ARG:CB	2.68	0.41
1:A:209:THR:N	1:A:210:PRO:CD	2.82	0.41
1:A:647:SER:OG	1:A:648:LYS:N	2.53	0.41
1:B:45:SER:HB2	1:B:61:THR:HG22	2.02	0.41
1:C:592:ASN:O	1:C:593:GLU:C	2.63	0.41
1:A:656:VAL:HA	1:A:657:PRO:HD3	1.88	0.41
1:B:307:PRO:HA	1:B:338:GLN:HB2	2.01	0.41
1:C:556:ASN:O	1:C:557:GLU:C	2.63	0.41
1:A:174:ILE:HD12	1:A:174:ILE:HA	1.94	0.41
1:A:208:PRO:HG3	1:A:464:LEU:HB2	2.02	0.41
1:B:34:HIS:O	1:B:35:ASN:HB2	2.20	0.41
1:C:150:GLN:HE21	1:C:627:GLN:NE2	2.19	0.41
1:C:217:THR:HB	1:C:218:PRO:HD2	2.02	0.41
1:C:244:ILE:O	1:C:248:VAL:HG22	2.20	0.41
1:C:364:LEU:HD22	1:C:375:PHE:CE2	2.55	0.41
1:A:7:VAL:HG11	1:A:55:THR:HG22	2.03	0.41
1:A:556:ASN:O	1:A:557:GLU:C	2.64	0.40
1:C:5:LEU:CD2	1:C:51:ASP:HA	2.50	0.40
1:A:184:TYR:O	1:A:189:ARG:HD3	2.21	0.40
1:A:311:LEU:HA	1:A:355:LEU:HB3	2.03	0.40
1:C:172:LEU:HD23	1:C:172:LEU:C	2.46	0.40
1:C:184:TYR:O	1:C:189:ARG:HD3	2.20	0.40
1:C:312:GLU:O	1:C:316:LEU:HG	2.21	0.40
1:B:17:ILE:HD12	1:B:19:LEU:CD2	2.51	0.40
1:C:144:SER:O	1:C:145:TYR:C	2.64	0.40
1:C:306:TYR:HB2	1:C:307:PRO:HD2	2.03	0.40
2:F:360:GLN:HA	2:F:360:GLN:NE2	2.36	0.40
2:F:370:LEU:O	2:F:371:SER:C	2.64	0.40
1:A:264:LEU:HD12	1:A:275:HIS:O	2.21	0.40
1:A:286:GLN:HG3	1:A:333:MET:HG3	2.03	0.40
1:A:294:GLN:HG2	1:A:298:ARG:HD3	2.03	0.40
1:A:436:SER:OG	1:A:437:ASN:N	2.53	0.40
1:A:552:LEU:O	1:A:553:LYS:C	2.63	0.40
1:C:40:GLN:NE2	1:C:44:ARG:HD2	2.37	0.40
1:A:195:ARG:NH1	1:A:480:GLU:OE2	2.42	0.40
2:D:370:LEU:O	2:D:372:ASN:N	2.54	0.40
1:B:98:GLU:HA	1:B:99:PRO:HD3	1.93	0.40
1:B:364:LEU:HD22	1:B:375:PHE:CD2	2.57	0.40
1:B:617:SER:O	1:B:691:GLN:HG3	2.21	0.40
2:E:360:GLN:NE2	2:E:360:GLN:HA	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:LEU:HD23	1:C:612:ARG:CG	2.41	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%)	680 (92%)	48 (6%)	8 (1%)	11	39
1	B	736/761 (97%)	681 (92%)	47 (6%)	8 (1%)	11	39
1	C	736/761 (97%)	685 (93%)	44 (6%)	7 (1%)	12	41
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	2 (100%)	0	100	100
All	All	2258/2363 (96%)	2087 (92%)	145 (6%)	26 (1%)	10	37

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	735	ARG
2	D	371	SER
1	B	294	GLN
1	B	735	ARG
2	E	371	SER
1	C	294	GLN
1	C	735	ARG
2	F	371	SER
1	A	5	LEU

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Mol	Chain	Res	Type
1	A	11	ASP
1	A	216	ARG
1	B	5	LEU
1	B	11	ASP
1	B	216	ARG
1	C	5	LEU
1	C	11	ASP
1	C	216	ARG
1	A	2	ASN
1	B	2	ASN
1	C	2	ASN
1	A	13	SER
1	B	13	SER
1	B	12	GLY
1	C	12	GLY
1	A	12	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	632/651 (97%)	549 (87%)	83 (13%)	4	17
1	B	632/651 (97%)	547 (87%)	85 (13%)	4	17
1	C	632/651 (97%)	546 (86%)	86 (14%)	3	16
2	D	17/19 (90%)	16 (94%)	1 (6%)	18	48
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%)	1 (33%)	2 (67%)	0	0
All	All	1950/2029 (96%)	1689 (87%)	261 (13%)	4	17

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	3	GLN
1	A	8	THR
1	A	9	LYS
1	A	14	THR
1	A	16	ARG
1	A	17	ILE
1	A	21	LYS
1	A	25	VAL
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	92	LYS
1	A	96	GLN
1	A	117	ASN
1	A	139	ARG
1	A	141	MET
1	A	149	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
1	A	224	SER
1	A	225	CYS
1	A	260	ARG
1	A	264	LEU
1	A	279	ILE
1	A	283	LYS
1	A	293	SER
1	A	297	VAL
1	A	298	ARG
1	A	304	LEU
1	A	317	LEU
1	A	320	LYS

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Mol	Chain	Res	Type
1	A	323	ARG
1	A	325	VAL
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	391	GLN
1	A	393	VAL
1	A	396	VAL
1	A	400	SER
1	A	408	SER
1	A	414	ILE
1	A	424	SER
1	A	430	ILE
1	A	451	ASP
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	585	LYS
1	A	607	LYS
1	A	616	LEU
1	A	625	SER
1	A	628	ILE
1	A	639	ARG
1	A	645	LYS
1	A	648	LYS
1	A	708	LYS
1	A	709	VAL
1	A	716	LYS
1	A	736	ASP
2	D	361	ILE
1	B	1	MET

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Mol	Chain	Res	Type
1	B	3	GLN
1	B	8	THR
1	B	9	LYS
1	B	14	THR
1	B	16	ARG
1	B	17	ILE
1	B	21	LYS
1	B	25	VAL
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	86	ILE
1	B	96	GLN
1	B	117	ASN
1	B	139	ARG
1	B	141	MET
1	B	149	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	224	SER
1	B	225	CYS
1	B	260	ARG
1	B	264	LEU
1	B	279	ILE
1	B	283	LYS
1	B	293	SER
1	B	297	VAL
1	B	298	ARG
1	B	304	LEU
1	B	317	LEU
1	B	320	LYS

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Mol	Chain	Res	Type
1	B	323	ARG
1	B	325	VAL
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	391	GLN
1	B	393	VAL
1	B	396	VAL
1	B	400	SER
1	B	408	SER
1	B	414	ILE
1	B	424	SER
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	560	LYS
1	B	570	GLU
1	B	585	LYS
1	B	607	LYS
1	B	616	LEU
1	B	625	SER
1	B	628	ILE
1	B	639	ARG
1	B	644	ILE
1	B	645	LYS
1	B	648	LYS
1	B	667	GLU
1	B	671	GLU
1	B	708	LYS
1	B	709	VAL
1	B	716	LYS
1	B	736	ASP

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Mol	Chain	Res	Type
2	E	361	ILE
2	E	362	ASP
1	C	1	MET
1	C	3	GLN
1	C	8	THR
1	C	9	LYS
1	C	14	THR
1	C	16	ARG
1	C	17	ILE
1	C	21	LYS
1	C	25	VAL
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	86	ILE
1	C	92	LYS
1	C	96	GLN
1	C	117	ASN
1	C	139	ARG
1	C	141	MET
1	C	149	LYS
1	C	161	VAL
1	C	165	ILE
1	C	168	SER
1	C	187	GLU
1	C	189	ARG
1	C	204	LYS
1	C	206	SER
1	C	224	SER
1	C	225	CYS
1	C	260	ARG
1	C	264	LEU
1	C	279	ILE
1	C	283	LYS
1	C	293	SER

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Mol	Chain	Res	Type
1	C	297	VAL
1	C	298	ARG
1	C	304	LEU
1	C	317	LEU
1	C	320	LYS
1	C	323	ARG
1	C	325	VAL
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	391	GLN
1	C	393	VAL
1	C	396	VAL
1	C	408	SER
1	C	414	ILE
1	C	424	SER
1	C	451	ASP
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	639	ARG
1	C	644	ILE
1	C	645	LYS
1	C	648	LYS
1	C	667	GLU
1	C	708	LYS

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Mol	Chain	Res	Type
1	C	709	VAL
1	C	716	LYS
1	C	723	LYS
1	C	736	ASP
2	F	361	ILE
2	F	372	ASN
2	P	1	TYR
2	P	2	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	18	ASN
1	A	40	GLN
1	A	46	HIS
1	A	96	GLN
1	A	117	ASN
1	A	150	GLN
1	A	191	GLN
1	A	221	GLN
1	A	294	GLN
1	A	328	ASN
1	A	415	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	96	GLN
1	B	117	ASN
1	B	150	GLN
1	B	158	GLN
1	B	191	GLN

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Mol	Chain	Res	Type
1	B	221	GLN
1	B	294	GLN
1	B	328	ASN
1	B	415	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	696	ASN
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	96	GLN
1	C	117	ASN
1	C	150	GLN
1	C	191	GLN
1	C	221	GLN
1	C	328	ASN
1	C	415	GLN
1	C	416	ASN
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
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 [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

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.