



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:59 PM GMT

PDB ID : 6R1R
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

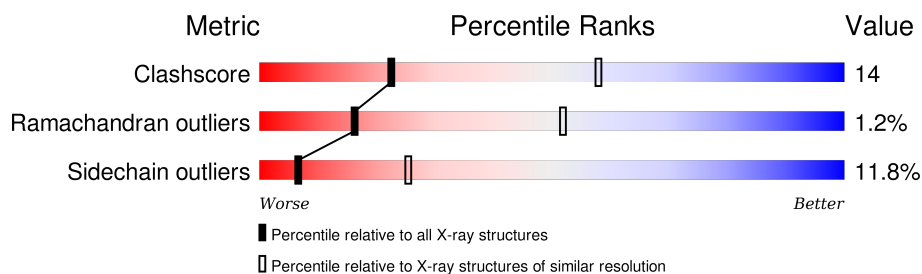
1 Overall quality at a glance

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	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	761	
1	B	761	
1	C	761	
2	D	20	
2	E	20	
2	F	20	
2	P	20	

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	UNP P00452
B	441	ASP	GLU	ENGINEERED	UNP P00452
C	441	ASP	GLU	ENGINEERED	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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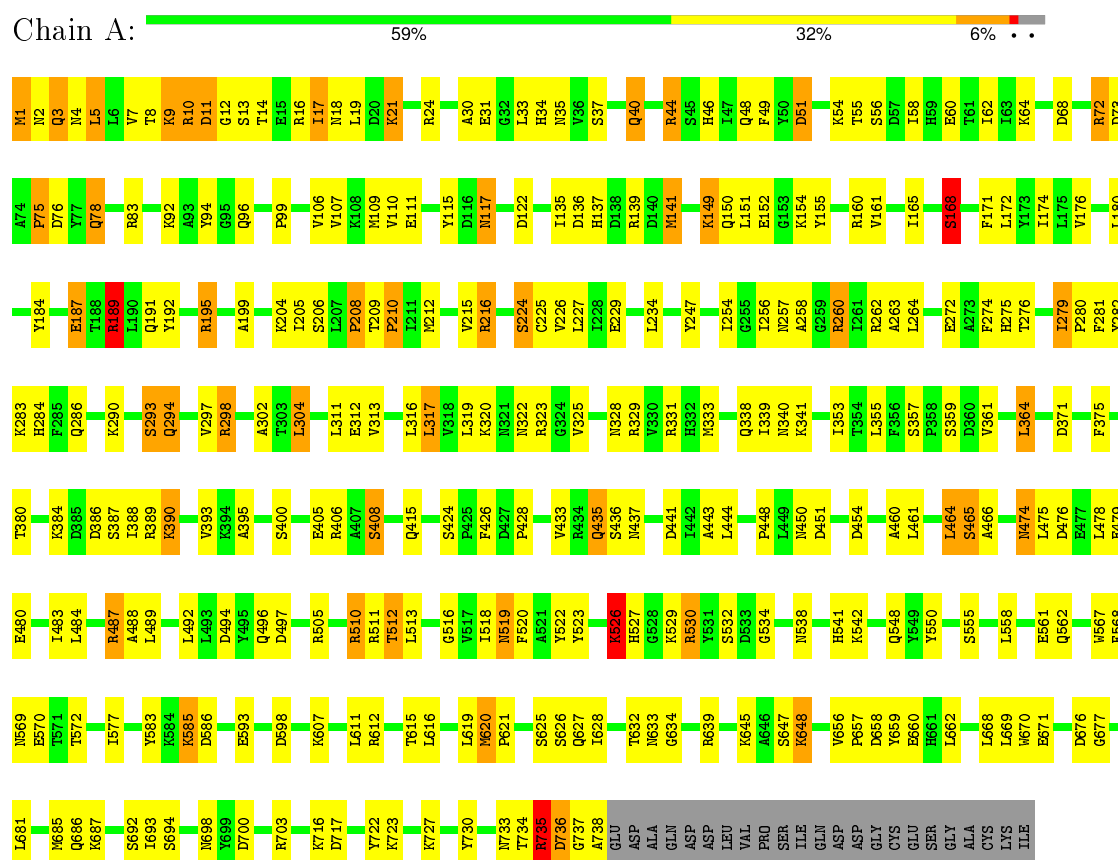
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	30	Total	O	0	0
			30	30		
3	C	32	Total	O	0	0
			32	32		

3 Residue-property plots

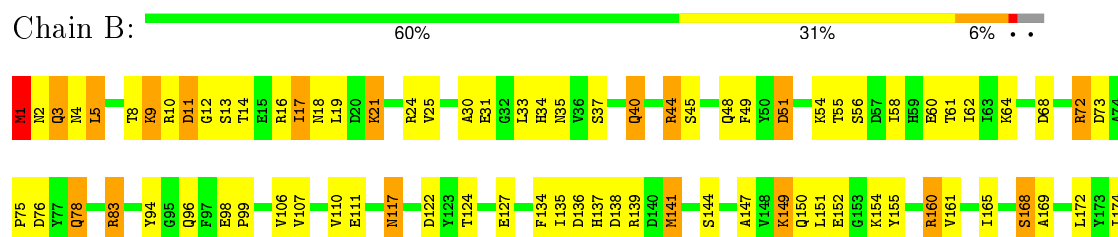
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

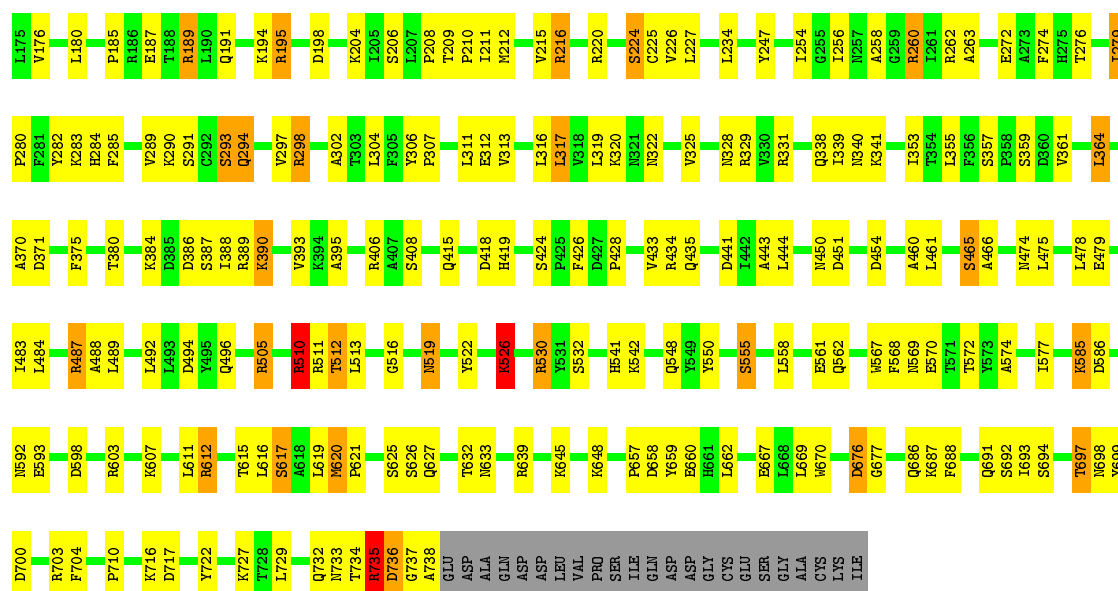
Note EDS was not executed.

• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN



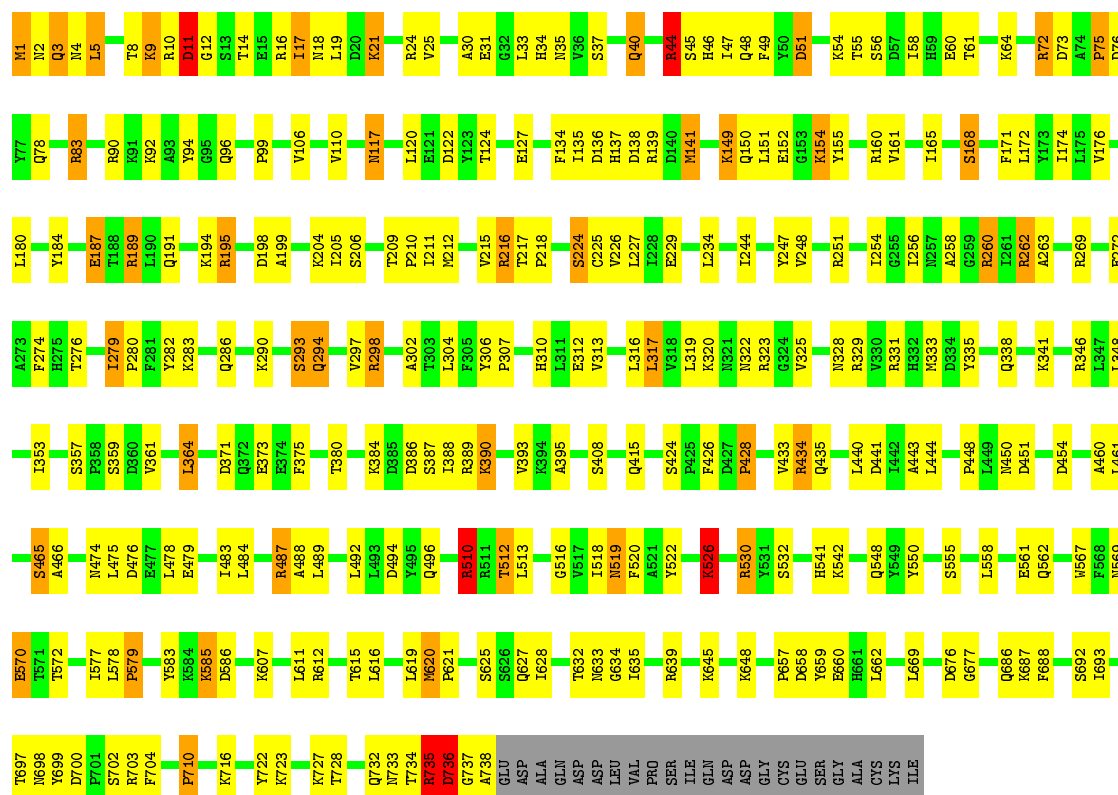
• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN





• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

Chain C: 60% 31% 6% . .



• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain D: 65% 20% 5% 10%



● 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 will therefore be 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	REFMAC, TNT	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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/6002	1.40	48/8129 (0.6%)
1	B	0.50	0/6002	1.41	53/8129 (0.7%)
1	C	0.51	0/6002	1.44	49/8129 (0.6%)
2	D	0.44	0/140	1.08	0/188
2	E	0.47	0/140	1.04	0/188
2	F	0.45	0/140	1.10	0/188
2	P	0.85	0/31	2.35	1/41 (2.4%)
All	All	0.50	0/18457	1.41	151/24992 (0.6%)

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 (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	ARG	NE-CZ-NH1	20.18	130.39	120.30
1	C	530	ARG	NE-CZ-NH1	19.45	130.02	120.30
1	B	703	ARG	NE-CZ-NH2	-17.22	111.69	120.30
1	C	703	ARG	NE-CZ-NH1	16.34	128.47	120.30
1	A	703	ARG	NE-CZ-NH1	16.24	128.42	120.30
1	C	530	ARG	NE-CZ-NH2	-14.81	112.90	120.30
1	B	530	ARG	NE-CZ-NH1	14.76	127.68	120.30
1	B	703	ARG	NE-CZ-NH1	13.75	127.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	703	ARG	NE-CZ-NH2	-12.70	113.95	120.30
1	A	530	ARG	NE-CZ-NH2	-12.59	114.00	120.30
1	C	195	ARG	CD-NE-CZ	12.48	141.07	123.60
1	A	195	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	B	195	ARG	CD-NE-CZ	11.87	140.22	123.60
1	C	703	ARG	NE-CZ-NH2	-11.57	114.51	120.30
1	A	72	ARG	NE-CZ-NH2	11.34	125.97	120.30
1	C	195	ARG	NE-CZ-NH1	11.22	125.91	120.30
1	B	72	ARG	NE-CZ-NH2	11.16	125.88	120.30
1	B	195	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	C	83	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	A	24	ARG	CD-NE-CZ	10.58	138.41	123.60
1	C	72	ARG	NE-CZ-NH2	10.45	125.53	120.30
1	B	24	ARG	CD-NE-CZ	10.28	137.99	123.60
1	B	530	ARG	NE-CZ-NH2	-10.27	115.17	120.30
1	B	72	ARG	NE-CZ-NH1	-10.11	115.24	120.30
1	B	24	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	C	24	ARG	NE-CZ-NH1	9.85	125.23	120.30
1	A	195	ARG	CD-NE-CZ	9.34	136.68	123.60
1	C	24	ARG	CD-NE-CZ	9.08	136.31	123.60
1	B	44	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	A	224	SER	N-CA-CB	8.83	123.74	110.50
1	A	371	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	B	136	ASP	CB-CG-OD1	8.70	126.12	118.30
1	B	434	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	C	198	ASP	CB-CG-OD1	8.32	125.79	118.30
1	C	224	SER	N-CA-CB	8.29	122.94	110.50
1	B	224	SER	N-CA-CB	8.08	122.62	110.50
1	A	24	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	A	282	TYR	CB-CG-CD1	8.04	125.82	121.00
1	C	530	ARG	CD-NE-CZ	7.90	134.67	123.60
1	A	10	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	68	ASP	CB-CG-OD1	7.47	125.03	118.30
1	B	530	ARG	CD-NE-CZ	7.34	133.88	123.60
1	C	639	ARG	CD-NE-CZ	7.34	133.88	123.60
1	B	51	ASP	CA-C-N	7.29	130.79	116.20
1	C	510	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	A	189	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	511	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	C	282	TYR	CB-CG-CD1	7.07	125.24	121.00
1	A	497	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	C	676	ASP	CB-CG-OD1	-6.91	112.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	583	TYR	CB-CG-CD2	6.91	125.15	121.00
1	A	51	ASP	CA-C-N	6.87	129.94	116.20
1	B	276	THR	CA-CB-CG2	-6.86	102.80	112.40
1	B	220	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	487	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	A	276	THR	CA-CB-CG2	-6.68	103.05	112.40
1	C	136	ASP	CB-CG-OD1	6.66	124.30	118.30
1	B	293	SER	C-N-CA	6.61	138.24	121.70
1	A	676	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	B	136	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	C	51	ASP	CA-C-N	6.50	129.20	116.20
1	C	262	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	293	SER	C-N-CA	6.47	137.87	121.70
1	B	598	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	C	247	TYR	CB-CG-CD1	-6.42	117.14	121.00
1	B	510	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	C	293	SER	C-N-CA	6.30	137.46	121.70
1	B	526	LYS	CA-CB-CG	6.26	127.18	113.40
1	A	526	LYS	CA-CB-CG	6.19	127.01	113.40
1	C	24	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	154	LYS	N-CA-CB	-6.17	99.49	110.60
1	C	434	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	C	570	GLU	OE1-CD-OE2	-6.11	115.97	123.30
1	C	44	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	B	526	LYS	N-CA-CB	6.05	121.49	110.60
1	A	192	TYR	CB-CG-CD2	5.99	124.60	121.00
1	B	505	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	282	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	C	276	THR	CA-CB-CG2	-5.96	104.05	112.40
1	B	717	ASP	CB-CG-OD1	-5.93	112.97	118.30
1	A	530	ARG	CD-NE-CZ	5.90	131.85	123.60
1	A	195	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	494	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	83	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	511	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	B	639	ARG	CD-NE-CZ	5.85	131.78	123.60
1	B	247	TYR	CB-CG-CD2	5.84	124.51	121.00
1	B	510	ARG	NE-CZ-NH2	5.79	123.20	120.30
1	A	494	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	C	526	LYS	CA-CB-CG	5.78	126.12	113.40
1	B	371	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	373	GLU	OE1-CD-OE2	5.77	130.23	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	1	TYR	CA-CB-CG	5.76	124.34	113.40
1	C	487	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	C	699	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	136	ASP	CB-CG-OD1	5.74	123.46	118.30
1	C	526	LYS	N-CA-CB	5.73	120.91	110.60
1	A	192	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	B	699	TYR	CB-CG-CD1	5.69	124.41	121.00
1	B	612	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	B	138	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	389	ARG	CD-NE-CZ	5.67	131.54	123.60
1	C	251	ARG	CD-NE-CZ	5.66	131.53	123.60
1	B	406	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	198	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	C	136	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	C	476	ASP	CB-CG-OD1	5.64	123.37	118.30
1	B	68	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	526	LYS	N-CA-CB	5.61	120.69	110.60
1	C	247	TYR	CB-CG-CD2	5.60	124.36	121.00
1	C	51	ASP	CB-CG-OD1	5.59	123.34	118.30
1	B	51	ASP	CA-C-O	-5.54	108.47	120.10
1	A	72	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	B	389	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	639	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	639	ARG	CD-NE-CZ	5.44	131.22	123.60
1	A	168	SER	CB-CA-C	5.44	120.43	110.10
1	B	487	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	208	PRO	N-CA-CB	5.41	109.79	103.30
1	A	51	ASP	CA-C-O	-5.40	108.76	120.10
1	B	676	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	A	247	TYR	CB-CG-CD2	5.35	124.21	121.00
1	A	408	SER	CB-CA-C	-5.34	99.96	110.10
1	B	247	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	C	583	TYR	CB-CG-CD2	5.33	124.20	121.00
1	B	83	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	C	389	ARG	CD-NE-CZ	5.30	131.03	123.60
1	A	598	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	617	SER	N-CA-CB	-5.30	102.56	110.50
1	A	44	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	603	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	464	LEU	N-CA-C	5.28	125.26	111.00
1	C	428	PRO	N-CA-CB	5.27	109.63	103.30
1	A	44	ARG	NE-CZ-NH1	-5.26	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	736	ASP	CA-CB-CG	5.26	124.97	113.40
1	A	497	ASP	CB-CG-OD1	5.25	123.03	118.30
1	B	160	ARG	CD-NE-CZ	5.23	130.92	123.60
1	B	282	TYR	CB-CG-CD1	5.22	124.13	121.00
1	C	371	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	1	MET	C-N-CA	5.19	134.67	121.70
1	B	24	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	717	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	B	195	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
1	A	717	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	11	ASP	CA-C-O	5.08	130.77	120.10
1	C	335	TYR	CA-CB-CG	-5.06	103.79	113.40
1	A	494	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	702	SER	CB-CA-C	-5.03	100.54	110.10
1	C	346	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	494	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	208	PRO	N-CA-CB	5.01	109.31	103.30

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	167	0
1	B	5874	0	5797	156	0
1	C	5874	0	5797	161	0
2	D	140	0	123	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	140	0	123	2	0
2	F	140	0	123	4	0
2	P	31	0	34	3	0
3	A	28	0	0	3	0
3	B	30	0	0	4	0
3	C	32	0	0	3	0
All	All	18163	0	17794	490	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 14.

All (490) 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:C:1:MET:H2	1:C:3:GLN:HG3	1.40	0.87
1:A:1:MET:H2	1:A:3:GLN:HG3	1.40	0.86
1:C:191:GLN:NE2	1:C:195:ARG:HH21	1.75	0.83
1:B:698:ASN:ND2	1:B:733:ASN:HD22	1.77	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	1.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:HG	1:A:272:GLU:HG2	1.67	0.75
1:A:279:ILE:HD13	1:A:319:LEU:HD21	1.69	0.74
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.68	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
1:C:279:ILE:HD13	1:C:319:LEU:HD21	1.68	0.74
1:B:294:GLN:HB2	1:B:298:ARG:HB3	1.70	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:C:135:ILE:HD11	1:C:174:ILE:HG21	1.73	0.70
1:B:558:LEU:HD23	1:B:612:ARG:HG2	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:C:294:GLN:HB2	1:C:298:ARG:HB3	1.75	0.69
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.74	0.69
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.75	0.69
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.74	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:734:THR:O	1:B:735:ARG:HB2	1.99	0.63
1:C:700:ASP:OD2	1:C:736:ASP:HB3	1.98	0.63
1:B:479:GLU:HB2	1:B:550:TYR:CE1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:B:519:ASN:ND2	1:B:632:THR:H	2.01	0.59
1:A:9:LYS:HE2	1:A:55:THR:HG21	1.84	0.59
1:C:120:LEU:HD13	2:P:1:TYR:HB3	1.85	0.59
1:C:215:VAL:O	1:C:216:ARG:CB	2.51	0.59
1:C:75:PRO:O	1:C:78:GLN:HG2	2.03	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:444:LEU:HD12	1:C:460:ALA:HB1	1.84	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: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: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: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:A:75:PRO:O	1:A:78:GLN:HG2	2.04	0.57
1:C:555:SER:HB3	1:C:611:LEU:HD22	1.87	0.57
1:A:479:GLU:HB2	1:A:550:TYR:CE1	2.40	0.57
1:B:338:GLN:HE21	1:B:415:GLN:NE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:O	1:C:176:VAL:HG23	2.05	0.56
1:A:548:GLN:HA	1:A:548:GLN:NE2	2.20	0.56
1:A:33:LEU:HB3	1:A:76:ASP:HB3	1.86	0.56
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.86	0.56
1:A:532:SER:HA	1:A:677:GLY:HA3	1.86	0.56
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.87	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:C:519:ASN:ND2	1:C:522:TYR:HB3	2.21	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:A:176:VAL:HG11	1:A:212:MET:HE1	1.89	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:A:106:VAL:O	1:A:110:VAL:HG23	2.05	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:B:176:VAL:HG11	1:B:212:MET:HE1	1.89	0.55
1:A:272:GLU:HB3	1:A:274:PHE:HE1	1.72	0.55
1:C:548:GLN:HA	1:C:548:GLN:NE2	2.21	0.55
1:C:21:LYS:O	1:C:25:VAL:HG23	2.07	0.54
1:B:99:PRO:HG2	1:B:137:HIS:CG	2.42	0.54
1:B:532:SER:HA	1:B:677:GLY:HA3	1.89	0.54
1:A:585:LYS:N	1:A:585:LYS:HD2	2.23	0.54
1:B:272:GLU:HB3	1:B:274:PHE:HE1	1.71	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: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:ND2	1:B:117:ASN:H	2.04	0.54
1:A:698:ASN:HD22	1:A:733:ASN:HD22	1.56	0.54
1:A:561:GLU:HG2	1:A:562:GLN:HG2	1.90	0.54
1:C:263:ALA:HB3	1:C:357:SER:HB2	1.90	0.54
1:A:56:SER:O	1:A:60:GLU:HG2	2.08	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:B:124:THR:HG23	1:B:127:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:GLN:NE2	1:B:548:GLN:HA	2.24	0.53
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.89	0.53
1:A:620:MET:HB2	1:A:621:PRO:HD2	1.89	0.53
1:C:10:ARG:O	1:C:11:ASP:C	2.47	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:353:ILE:HG13	1:A:395:ALA:HB2	1.91	0.53
1:B:226:VAL:HG12	1:B:461:LEU:CD2	2.39	0.53
1:B:122:ASP:O	1:B:189:ARG:NH2	2.42	0.53
1:A:149:LYS:HE3	1:A:152:GLU:OE1	2.08	0.53
1:B:176:VAL:HG22	3:B:789:HOH:O	2.07	0.53
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.91	0.53
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.90	0.52
1:B:441:ASP:OD2	1:B:620:MET:HB3	2.10	0.52
1:B:56:SER:O	1:B:60:GLU:HG2	2.09	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:C:734:THR:O	1:C:735:ARG:HB2	2.09	0.52
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.37	0.52
1:A:107:VAL:O	1:A:111:GLU:HG3	2.10	0.52
1:C:176:VAL:HG11	1:C:212:MET:HE1	1.91	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:C:686:GLN:CD	1:C:727:LYS:HD2	2.31	0.51
1:C:199:ALA:HB1	1:C:205:ILE:HD12	1.92	0.51
1:B:263:ALA:HB3	1:B:357:SER:HB2	1.92	0.51
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:A:17:ILE:HD12	1:A:19:LEU:HD23	1.93	0.51
1:C:519:ASN:ND2	1:C:632:THR:H	2.09	0.51
1:C:149:LYS:HE3	1:C:152:GLU:OE1	2.10	0.51
1:C:99:PRO:HG2	1:C:137:HIS:CG	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:HD12	1:A:19:LEU:CD2	2.40	0.51
1:A:172:LEU:O	1:A:176:VAL:HG23	2.11	0.51
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.93	0.51
1:A:483:ILE:HG23	1:A:487:ARG:HD2	1.93	0.51
1:A:99:PRO:HG2	1:A:137:HIS:CD2	2.45	0.51
1:A:10:ARG:O	1:A:11:ASP:C	2.49	0.51
1:A:99:PRO:HG2	1:A:137:HIS:CG	2.46	0.51
2:D:372:ASN:ND2	2:D:372:ASN:H	2.07	0.51
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.38	0.51
1:B:49:PHE:CZ	1:B:58:ILE:HG23	2.46	0.51
1:C:49:PHE:CZ	1:C:58:ILE:HG23	2.45	0.51
1:B:697:THR:O	1:B:732:GLN:HA	2.11	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:C:698:ASN:ND2	1:C:733:ASN:ND2	2.58	0.50
1:C:569:ASN:ND2	1:C:569:ASN:H	2.08	0.50
1:B:106:VAL:O	1:B:110:VAL:HG23	2.12	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:686:GLN:NE2	1:A:727:LYS:HD2	2.26	0.50
1:B:10:ARG:O	1:B:11:ASP:C	2.50	0.50
1:A:209:THR:N	1:A:210:PRO:HD2	2.27	0.50
1:A:325:VAL:HG13	1:A:328:ASN:HB2	1.94	0.49
1:B:698:ASN:HD21	1:B:733:ASN:HD22	1.54	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: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: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:C:226:VAL:HG12	1:C:461:LEU:CD2	2.42	0.49
1:C:686:GLN:NE2	1:C:727:LYS:HD2	2.27	0.49
1:A:415:GLN:HE22	1:A:435:GLN:HA	1.77	0.49
1:C:341:LYS:HG2	1:C:722:TYR:OH	2.13	0.49
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.93	0.49
1:A:199:ALA:HB1	1:A:205:ILE:HD12	1.93	0.49
1:A:585:LYS:H	1:A:585:LYS:HD2	1.77	0.49
1:B:341:LYS:HG2	1:B:722:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:PRO:HA	1:C:338:GLN:HB2	1.95	0.49
1:A:569:ASN:H	1:A:569:ASN:ND2	2.10	0.49
1:A:426:PHE:O	1:A:428:PRO:HD3	2.13	0.49
1:B:555:SER:HB3	1:B:611:LEU:HD22	1.93	0.49
1:A:260:ARG:HG2	1:A:260:ARG:HH11	1.78	0.49
1:C:585:LYS:HD2	1:C:585:LYS:N	2.27	0.49
1:C:1:MET:HA	1:C:3:GLN:HE21	1.77	0.49
1:A:34:HIS:O	1:A:35:ASN:HB2	2.13	0.49
1:B:585:LYS:H	1:B:585:LYS:HD2	1.77	0.49
1:C:532:SER:HA	1:C:677:GLY:HA3	1.95	0.49
1:B:686:GLN:CD	1:B:727:LYS:HD2	2.32	0.48
1:A:686:GLN:CD	1:A:727:LYS:HD2	2.33	0.48
1:A:475:LEU:O	1:A:478:LEU:HB2	2.13	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: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:A:737:GLY:O	1:A:738:ALA:HB3	2.14	0.48
1:B:572:THR:HB	1:B:577:ILE:HB	1.95	0.48
1:B:483:ILE:HG23	1:B:487:ARG:HD2	1.94	0.48
1:B:700:ASP:CG	1:B:736:ASP:HB3	2.34	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: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:C:120:LEU:HD13	2:P:1:TYR:CG	2.49	0.47
1:B:512:THR:HG22	1:B:615:THR:HG23	1.96	0.47
1:A:621:PRO:HD3	1:A:694:SER:OG	2.14	0.47
1:A:263:ALA:HB3	1:A:357:SER:HB2	1.95	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:B:272:GLU:HB3	1:B:274:PHE:CE1	2.49	0.47
1:A:441:ASP:OD2	1:A:620:MET:HB3	2.13	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:518:ILE:HA	1:C:634:GLY:HA2	1.96	0.47
1:C:479:GLU:HB2	1:C:550:TYR:CE1	2.50	0.47
1:A:569:ASN:H	1:A:569:ASN:HD22	1.63	0.47
1:A:229:GLU:O	1:A:448:PRO:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:O	1:A:189:ARG:NH2	2.48	0.47
1:C:138:ASP:O	1:C:141:MET:HB2	2.15	0.47
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.97	0.47
1:B:262:ARG:HB3	1:B:359:SER:HB3	1.96	0.47
1:B:256:ILE:O	1:B:304:LEU:HA	2.14	0.47
1:A:317:LEU:O	1:A:405:GLU:HG3	2.14	0.47
1:C:260:ARG:NH1	1:C:260:ARG:HG2	2.30	0.47
1:C:209:THR:N	1:C:210:PRO:HD2	2.29	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:700:ASP:CG	1:C:736:ASP:HB3	2.36	0.46
1:C:548:GLN:HB2	1:C:688:PHE:HB3	1.97	0.46
1:C:134:PHE:CE2	1:C:194:LYS:HB2	2.50	0.46
1:C:633:ASN:O	1:C:634:GLY:C	2.53	0.46
1:C:34:HIS:O	1:C:35:ASN:HB2	2.15	0.46
1:B:729:LEU:HA	1:B:729:LEU:HD23	1.79	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: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:312:GLU:O	1:A:316:LEU:HG	2.15	0.46
1:A:272:GLU:HB3	1:A:274:PHE:CE1	2.50	0.46
1:B:364:LEU:HD22	1:B:375:PHE:CE2	2.50	0.46
1:C:415:GLN:HE22	1:C:435:GLN:HA	1.80	0.46
1:C:45:SER:CB	1:C:61:THR:HG22	2.46	0.46
1:A:49:PHE:CZ	1:A:58:ILE:HG23	2.50	0.46
2:F:372:ASN:H	2:F:372:ASN:ND2	2.14	0.46
1:A:518:ILE:HA	1:A:634:GLY:HA2	1.97	0.46
1:C:585:LYS:HD3	1:C:586:ASP:OD1	2.16	0.46
1:C:567:TRP:HB3	1:C:570:GLU:HG3	1.98	0.46
1:C:37:SER:CB	1:C:40:GLN:HB2	2.41	0.46
1:B:370:ALA:HB1	3:B:786:HOH:O	2.16	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:C:669:LEU:HD11	1:C:698:ASN:ND2	2.31	0.45
1:C:262:ARG:HD2	1:C:274:PHE:HB2	1.97	0.45
1:A:541:HIS:NE2	1:A:687:LYS:HE2	2.30	0.45
1:B:426:PHE:O	1:B:428:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:522:TYR:CZ	1:C:526:LYS:HD3	2.51	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:548:GLN:HB2	1:B:688:PHE:HB3	1.99	0.45
1:B:325:VAL:HG13	1:B:328:ASN:HB2	1.99	0.45
1:C:585:LYS:HD2	1:C:585:LYS:H	1.82	0.45
1:B:492:LEU:O	1:B:496:GLN:HG2	2.16	0.45
1:A:723:LYS:NZ	2:D:374:GLN:O	2.42	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:B:519:ASN:HA	1:B:519:ASN:HD22	1.53	0.45
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:117:ASN:ND2	1:A:117:ASN:H	2.15	0.44
1:A:520:PHE:O	1:A:523:TYR:HB3	2.18	0.44
1:C:569:ASN:HD22	1:C:569:ASN:H	1.66	0.44
1:A:450:ASN:HB2	1:A:454:ASP:OD2	2.16	0.44
1:C:176:VAL:HG11	1:C:212:MET:CE	2.48	0.44
1:A:479:GLU:HB2	1:A:550:TYR:CD1	2.51	0.44
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: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:C:262:ARG:HB3	1:C:359:SER:HB3	1.98	0.44
1:B:568:PHE:CE1	1:B:611:LEU:HB2	2.53	0.44
1:C:45:SER:HB2	1:C:61:THR:HG22	2.00	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:90:ARG:HG3	1:C:90:ARG:HH11	1.82	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:C:434:ARG:O	1:C:435:GLN:HB3	2.17	0.44
1:B:21:LYS:O	1:B:25:VAL:HG23	2.18	0.44
1:A:212:MET:HE2	1:A:212:MET:HA	1.99	0.44
1:A:558:LEU:HD23	1:A:612:ARG:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:O	1:A:302:ALA:HA	2.18	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:522:TYR:CZ	1:A:526:LYS:HD3	2.52	0.43
1:A:58:ILE:O	1:A:62:ILE:HG23	2.17	0.43
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.98	0.43
1:A:151:LEU:HA	1:A:155:TYR:HB2	2.00	0.43
1:A:149:LYS:HA	1:A:149:LYS:CE	2.48	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:211:ILE:HG22	1:B:212:MET:HE3	1.99	0.43
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.46	0.43
1:C:217:THR:HB	1:C:218:PRO:CD	2.48	0.43
1:B:212:MET:HE2	1:B:212:MET:HA	2.01	0.43
1:C:698:ASN:HD21	1:C:733:ASN:HD22	1.63	0.43
1:A:7:VAL:CG1	1:A:55:THR:HG22	2.49	0.43
1:B:306:TYR:HB2	1:B:307:PRO:HD2	1.99	0.43
1:A:257:ASN:HB2	1:A:435:GLN:OE1	2.18	0.43
1:C:737:GLY:O	1:C:738:ALA:CB	2.65	0.43
1:B:339:ILE:HG22	1:B:340:ASN:N	2.33	0.43
1:B:704:PHE:CD2	1:B:710:PRO:HD3	2.54	0.43
1:A:538:ASN:HB3	1:A:593:GLU:HB2	2.00	0.43
1:C:489:LEU:HA	1:C:489:LEU:HD23	1.81	0.43
1:A:519:ASN:ND2	1:A:632:THR:H	2.17	0.43
1:B:151:LEU:HD13	1:B:169:ALA:HB2	2.00	0.43
1:B:150:GLN:OE1	1:B:154:LYS:HE3	2.18	0.43
1:C:466:ALA:HA	1:C:516:GLY:O	2.18	0.43
1:A:406:ARG:NH2	1:A:730:TYR:O	2.45	0.43
1:B:187:GLU:HB2	3:B:780:HOH:O	2.17	0.43
1:B:659:TYR:O	1:B:660:GLU:C	2.56	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:B:568:PHE:CE2	1:B:574:ALA:HA	2.54	0.43
1:B:285:PHE:O	1:B:289:VAL:HG23	2.18	0.43
1:C:512:THR:HG22	1:C:615:THR:HG23	2.00	0.43
1:B:18:ASN:HB3	1:B:21:LYS:HB2	2.00	0.43
1:A:180:LEU:HD12	1:A:488:ALA:HB1	2.01	0.43
1:A:659:TYR:O	1:A:660:GLU:C	2.57	0.43
1:A:262:ARG:HD2	1:A:274:PHE:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:THR:N	1:B:210:PRO:CD	2.82	0.43
1:A:626:SER:CB	1:A:633:ASN:HD22	2.32	0.43
1:C:47:ILE:O	1:C:47:ILE:HG13	2.18	0.43
1:B:260:ARG:HG2	1:B:260:ARG:HH11	1.84	0.43
1:B:144:SER:O	1:B:147:ALA:HB3	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:C:510:ARG:HB2	1:C:512:THR:HG23	2.01	0.42
1:A:338:GLN:HE21	1:A:415:GLN:NE2	2.17	0.42
1:A:260:ARG:HG2	1:A:260:ARG:NH1	2.35	0.42
1:B:254:ILE:O	1:B:302:ALA:HA	2.18	0.42
1:A:256:ILE:O	1:A:304:LEU:HA	2.20	0.42
1:C:17:ILE:HD12	1:C:19:LEU:CD2	2.49	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:C:487:ARG:HH22	1:C:561:GLU:CD	2.22	0.42
1:B:58:ILE:O	1:B:62:ILE:HG23	2.19	0.42
1:A:18:ASN:ND2	1:A:21:LYS:HE3	2.35	0.42
1:A:548:GLN:HE21	1:A:548:GLN:HA	1.84	0.42
1:A:18:ASN:HB3	1:A:21:LYS:HB2	2.01	0.42
1:C:659:TYR:O	1:C:660:GLU:C	2.58	0.42
1:B:569:ASN:ND2	1:B:569:ASN:H	2.18	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:A:435:GLN:HG3	1:A:436:SER:O	2.20	0.42
1:A:487:ARG:HH22	1:A:561:GLU:CD	2.23	0.42
1:C:348:LEU:HD11	2:F:375:LEU:HD21	2.01	0.42
1:C:151:LEU:HA	1:C:155:TYR:HB2	2.01	0.42
1:A:176:VAL:HG11	1:A:212:MET:CE	2.50	0.42
1:C:262:ARG:NH1	1:C:269:ARG:HB2	2.34	0.42
1:A:512:THR:HG22	1:A:615:THR:HG23	2.02	0.42
1:B:737:GLY:O	1:B:738:ALA:CB	2.68	0.42
1:C:697:THR:O	1:C:732:GLN:HA	2.20	0.42
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.55	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: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:A:669:LEU:HD23	1:A:670:TRP:CE2	2.55	0.41
1:A:226:VAL:HG12	1:A:461:LEU:CD2	2.50	0.41
1:A:284:HIS:CE1	1:B:284:HIS:CE1	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ASN:OD1	1:A:476:ASP:HB2	2.20	0.41
1:A:281:PHE:CE1	1:B:291:SER:HB2	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:B:322:ASN:HA	1:B:331:ARG:HH11	1.84	0.41
1:B:134:PHE:CE2	1:B:194:LYS:HB2	2.56	0.41
1:A:339:ILE:HG22	1:A:340:ASN:N	2.34	0.41
1:C:310:HIS:CE1	1:C:312:GLU:HG3	2.55	0.41
1:B:418:ASP:OD1	1:B:419:HIS:N	2.52	0.41
1:B:734:THR:O	1:B:735:ARG:CB	2.68	0.41
1:A:681:LEU:O	1:A:685:MET:HG3	2.20	0.41
1:A:527:HIS:O	1:A:529:LYS:HE2	2.20	0.41
1:B:172:LEU:C	1:B:172:LEU:HD23	2.41	0.41
1:A:209:THR:N	1:A:210:PRO:CD	2.82	0.41
1:C:723:LYS:NZ	2:F:374:GLN:O	2.44	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: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:B:34:HIS:O	1:B:35:ASN:HB2	2.20	0.41
1:A:174:ILE:HD12	1:A:174:ILE:HA	1.94	0.41
1:C:364:LEU:HD22	1:C:375:PHE:CE2	2.55	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:A:208:PRO:HG3	1:A:464:LEU:HB2	2.02	0.41
1:A:7:VAL:HG11	1:A:55:THR:HG22	2.03	0.41
1:A:700:ASP:CG	1:A:736:ASP:HB3	2.41	0.41
1:C:5:LEU:CD2	1:C:51:ASP:HA	2.50	0.40
1:C:211:ILE:HG22	1:C:212:MET:HE3	2.03	0.40
1:C:184:TYR:O	1:C:189:ARG:HD3	2.20	0.40
2:D:370:LEU:O	2:D:371:SER:C	2.59	0.40
1:A:184:TYR:O	1:A:189:ARG:HD3	2.21	0.40
1:C:312:GLU:O	1:C:316:LEU:HG	2.21	0.40
1:A:311:LEU:HA	1:A:355:LEU:HB3	2.03	0.40
1:B:592:ASN:O	1:B:593:GLU:C	2.60	0.40
1:C:306:TYR:HB2	1:C:307:PRO:HD2	2.03	0.40
1:B:17:ILE:HD12	1:B:19:LEU:CD2	2.51	0.40
2:F:360:GLN:NE2	2:F:360:GLN:HA	2.36	0.40
1:C:40:GLN:NE2	1:C:44:ARG:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLN:HG2	1:A:298:ARG:HD3	2.03	0.40
1:B:676:ASP:O	1:B:677:GLY:C	2.60	0.40
1:A:436:SER:OG	1:A:437:ASN:N	2.53	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:195:ARG:NH1	1:A:480:GLU:OE2	2.42	0.40
1:C:558:LEU:HD23	1:C:612:ARG:CG	2.41	0.40
1:B:364:LEU:HD22	1:B:375:PHE:CD2	2.57	0.40
1:B:98:GLU:HA	1:B:99:PRO:HD3	1.93	0.40
2:D:370:LEU:O	2:D:372:ASN:N	2.54	0.40
2:E:360:GLN:NE2	2:E:360:GLN:HA	2.37	0.40
1:B:617:SER:O	1:B:691:GLN:HG3	2.21	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%)	17	55
1	B	736/761 (97%)	681 (92%)	47 (6%)	8 (1%)	17	55
1	C	736/761 (97%)	685 (93%)	44 (6%)	7 (1%)	19	58
2	D	16/20 (80%)	14 (88%)	1 (6%)	1 (6%)	2	10
2	E	16/20 (80%)	13 (81%)	2 (12%)	1 (6%)	2	10
2	F	16/20 (80%)	14 (88%)	1 (6%)	1 (6%)	2	10
2	P	2/20 (10%)	0	2 (100%)	0	100	100
All	All	2258/2363 (96%)	2087 (92%)	145 (6%)	26 (1%)	16	52

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
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%)	554 (88%)	78 (12%)	6	23
1	B	632/651 (97%)	560 (89%)	72 (11%)	7	28
1	C	632/651 (97%)	558 (88%)	74 (12%)	7	26
2	D	17/19 (90%)	16 (94%)	1 (6%)	24	60
2	E	17/19 (90%)	15 (88%)	2 (12%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	17/19 (90%)	15 (88%)	2 (12%)	6	25
2	P	3/19 (16%)	1 (33%)	2 (67%)	0	0
All	All	1950/2029 (96%)	1719 (88%)	231 (12%)	6	25

All (231) 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	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	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	160	ARG
1	A	161	VAL
1	A	165	ILE
1	A	168	SER
1	A	187	GLU
1	A	189	ARG
1	A	204	LYS
1	A	206	SER
1	A	210	PRO
1	A	224	SER
1	A	225	CYS

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Mol	Chain	Res	Type
1	A	260	ARG
1	A	279	ILE
1	A	283	LYS
1	A	290	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
1	A	323	ARG
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	393	VAL
1	A	400	SER
1	A	408	SER
1	A	424	SER
1	A	435	GLN
1	A	451	ASP
1	A	465	SER
1	A	474	ASN
1	A	484	LEU
1	A	505	ARG
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	585	LYS
1	A	607	LYS
1	A	616	LEU
1	A	620	MET
1	A	625	SER
1	A	628	ILE
1	A	645	LYS
1	A	648	LYS
1	A	716	LYS

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Mol	Chain	Res	Type
1	A	735	ARG
1	A	736	ASP
2	D	361	ILE
1	B	1	MET
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	31	GLU
1	B	40	GLN
1	B	44	ARG
1	B	48	GLN
1	B	54	LYS
1	B	64	LYS
1	B	72	ARG
1	B	73	ASP
1	B	78	GLN
1	B	96	GLN
1	B	117	ASN
1	B	139	ARG
1	B	141	MET
1	B	149	LYS
1	B	160	ARG
1	B	161	VAL
1	B	165	ILE
1	B	168	SER
1	B	185	PRO
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	279	ILE
1	B	283	LYS
1	B	290	LYS
1	B	293	SER
1	B	297	VAL
1	B	298	ARG

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Mol	Chain	Res	Type
1	B	317	LEU
1	B	320	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	393	VAL
1	B	408	SER
1	B	424	SER
1	B	451	ASP
1	B	465	SER
1	B	474	ASN
1	B	484	LEU
1	B	505	ARG
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	585	LYS
1	B	607	LYS
1	B	616	LEU
1	B	620	MET
1	B	625	SER
1	B	645	LYS
1	B	648	LYS
1	B	716	LYS
1	B	735	ARG
1	B	736	ASP
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

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Mol	Chain	Res	Type
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	64	LYS
1	C	72	ARG
1	C	73	ASP
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	160	ARG
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	279	ILE
1	C	283	LYS
1	C	290	LYS
1	C	293	SER
1	C	297	VAL
1	C	298	ARG
1	C	317	LEU
1	C	320	LYS
1	C	323	ARG
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	393	VAL

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Mol	Chain	Res	Type
1	C	408	SER
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	579	PRO
1	C	585	LYS
1	C	607	LYS
1	C	616	LEU
1	C	620	MET
1	C	625	SER
1	C	628	ILE
1	C	645	LYS
1	C	648	LYS
1	C	710	PRO
1	C	716	LYS
1	C	735	ARG
1	C	736	ASP
2	F	361	ILE
2	F	362	ASP
2	P	1	TYR
2	P	2	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	18	ASN
1	A	46	HIS
1	A	117	ASN
1	A	191	GLN
1	A	221	GLN
1	A	294	GLN
1	A	328	ASN
1	A	415	GLN

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Mol	Chain	Res	Type
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
2	D	360	GLN
2	D	372	ASN
1	B	3	GLN
1	B	18	ASN
1	B	117	ASN
1	B	150	GLN
1	B	191	GLN
1	B	221	GLN
1	B	294	GLN
1	B	328	ASN
1	B	415	GLN
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
2	E	360	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	150	GLN
1	C	191	GLN
1	C	221	GLN
1	C	294	GLN
1	C	328	ASN
1	C	415	GLN

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Mol	Chain	Res	Type
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
2	F	360	GLN
2	F	372	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.