Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 03:34 am GMT

PDB ID	:	7R1R
Title	:	RIBONUCLEOTIDE REDUCTASE E441Q 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949
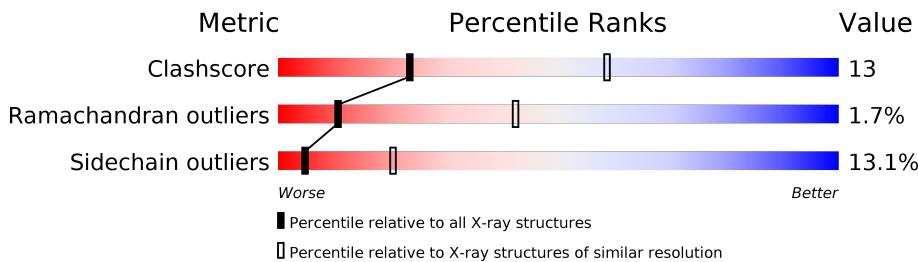
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.
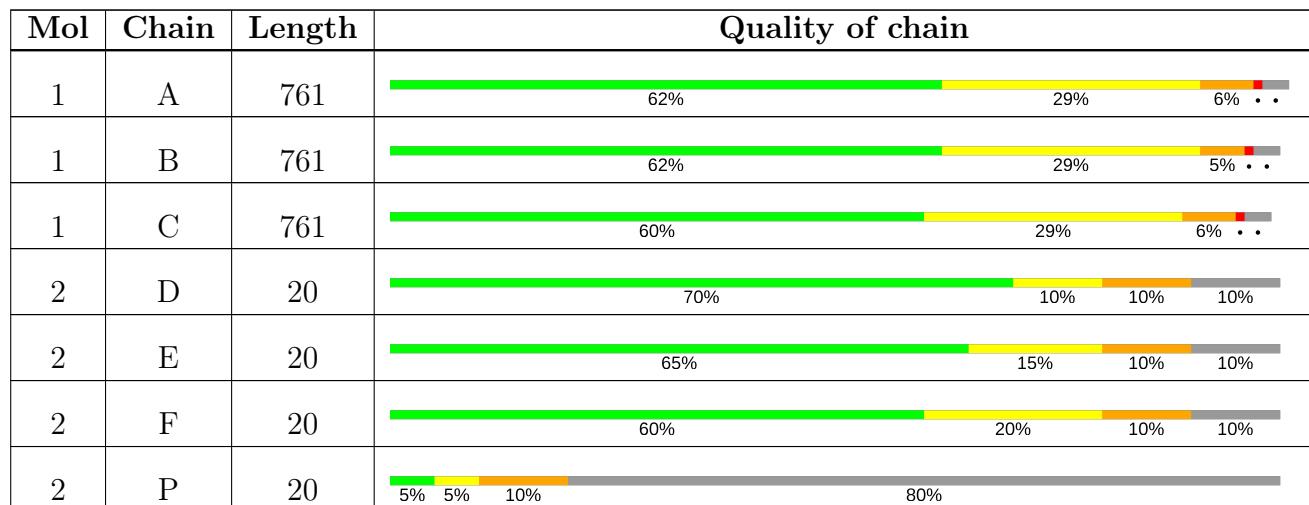
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)

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 <=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	62% 29% 6% • •
1	B	761	62% 29% 5% • •
1	C	761	60% 29% 6% • •
2	D	20	70% 10% 10% 10%
2	E	20	65% 15% 10% 10%
2	F	20	60% 20% 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 18166 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
			5875	3729	1011	1110	25			
1	B	738	Total	C	N	O	S	0	0	0
			5875	3729	1011	1110	25			
1	C	738	Total	C	N	O	S	0	0	0
			5875	3729	1011	1110	25			

There are 3 discrepancies between the modelled and reference sequences:

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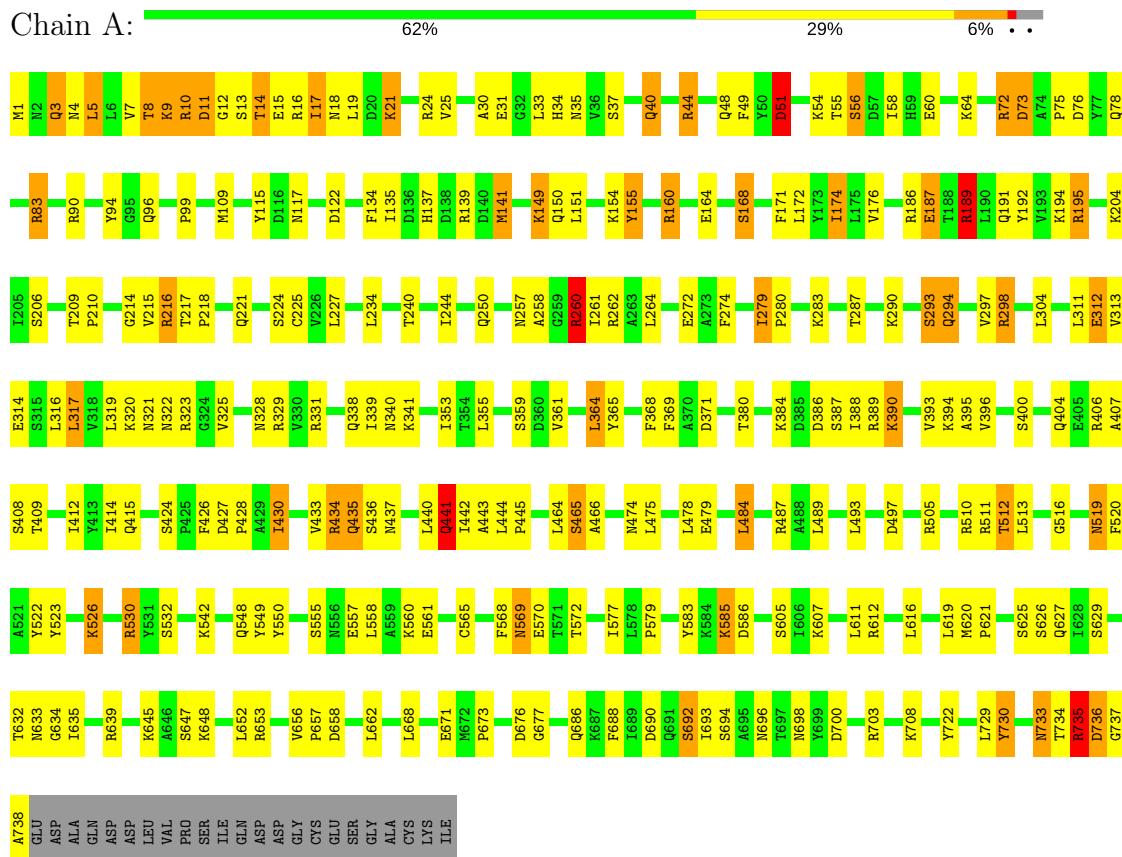
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	30	Total O 30 30		0	0
3	C	32	Total O 32 32		0	0

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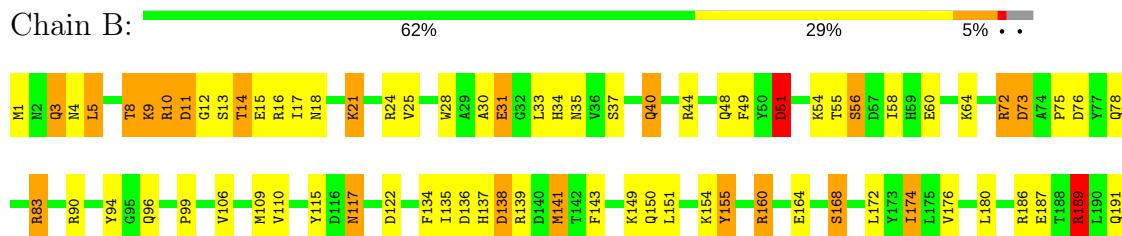
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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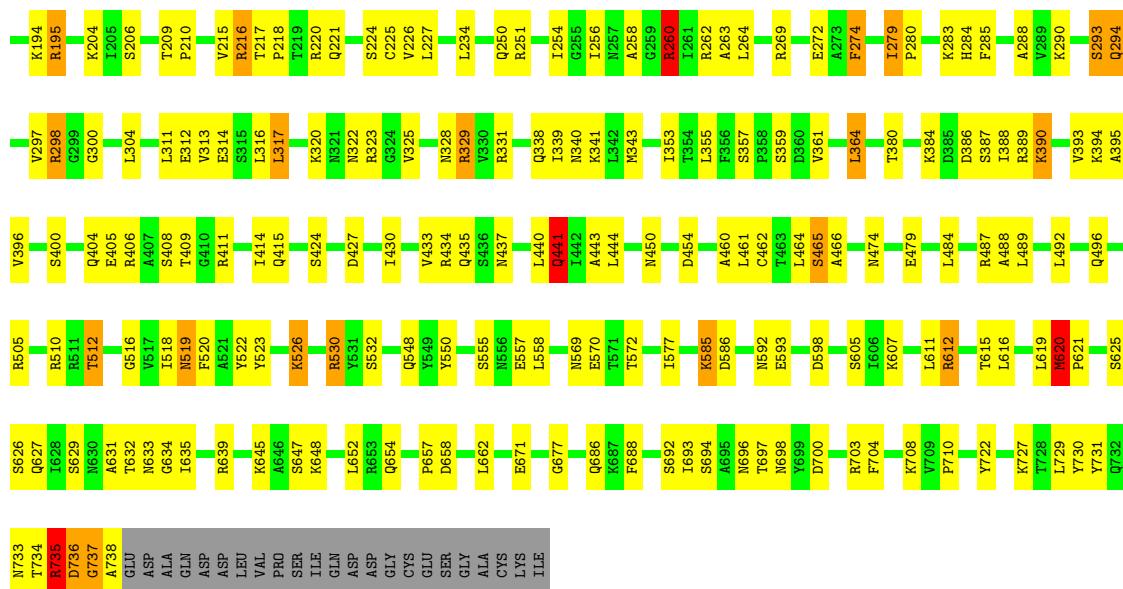
Note EDS was not executed.

• Molecule 1: RIBONUCLEOTIDE REDUCTASE R1 PROTEIN

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Chain C:

• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain D:

• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain E:

65%   15%   10%   10%

TYR LEU V358 G359 Q360 I361 D362 S371 N372 L375
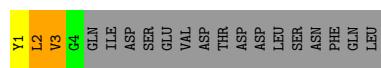
• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain F:

60%   20%   10%   10%

TYR LEU V358 G359 Q360 I361 D362 S371 N372 L375

• Molecule 2: RIBONUCLEOTIDE REDUCTASE R2 PROTEIN

Chain P: 5%   5%   10%   80%

Y1 L2 V3 G4 GLN ILE ASP SER GLU VAL ASP THR ASP ASP LEU SER ASN PHE GLN LEU

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	224.56Å 224.56Å 335.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	91.2 (20.00-3.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.200 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18166	wwPDB-VP
Average B, all atoms (Å²)	54.0	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	0.53	0/6003	1.41	47/8130 (0.6%)
1	B	0.51	0/6003	1.46	56/8130 (0.7%)
1	C	0.52	0/6003	1.47	57/8130 (0.7%)
2	D	0.47	0/140	1.12	0/188
2	E	0.46	0/140	1.03	0/188
2	F	0.49	0/140	1.16	0/188
2	P	0.96	0/31	2.59	2/41 (4.9%)
All	All	0.52	0/18460	1.45	162/24995 (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	1
1	B	0	2
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	703	ARG	NE-CZ-NH2	-21.53	109.54	120.30
1	A	703	ARG	NE-CZ-NH2	-18.65	110.97	120.30
1	B	703	ARG	NE-CZ-NH1	18.41	129.50	120.30
1	C	83	ARG	NE-CZ-NH2	-18.26	111.17	120.30
1	C	703	ARG	NE-CZ-NH1	18.14	129.37	120.30
1	A	530	ARG	NE-CZ-NH1	16.66	128.63	120.30
1	A	703	ARG	NE-CZ-NH1	15.18	127.89	120.30
1	C	703	ARG	NE-CZ-NH2	-14.95	112.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	530	ARG	NE-CZ-NH1	14.57	127.59	120.30
1	A	530	ARG	NE-CZ-NH2	-13.85	113.37	120.30
1	C	195	ARG	CD-NE-CZ	13.34	142.27	123.60
1	C	72	ARG	NE-CZ-NH2	12.81	126.71	120.30
1	C	530	ARG	NE-CZ-NH1	12.81	126.70	120.30
1	C	530	ARG	NE-CZ-NH2	-12.59	114.00	120.30
1	B	24	ARG	NE-CZ-NH1	12.58	126.59	120.30
1	A	72	ARG	NE-CZ-NH2	12.35	126.47	120.30
1	B	83	ARG	NE-CZ-NH2	-11.92	114.34	120.30
1	B	612	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	C	24	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	B	530	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	B	195	ARG	NE-CZ-NH1	11.42	126.01	120.30
1	C	44	ARG	NE-CZ-NH2	-11.29	114.65	120.30
1	B	195	ARG	CD-NE-CZ	11.11	139.15	123.60
1	A	24	ARG	CD-NE-CZ	10.64	138.50	123.60
1	A	195	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	A	83	ARG	NE-CZ-NH2	-10.43	115.09	120.30
1	B	72	ARG	NE-CZ-NH1	-10.31	115.15	120.30
1	A	195	ARG	CD-NE-CZ	10.27	137.98	123.60
1	B	72	ARG	NE-CZ-NH2	10.05	125.33	120.30
1	B	389	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	A	44	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	C	195	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	B	24	ARG	CD-NE-CZ	8.92	136.09	123.60
1	B	220	ARG	NE-CZ-NH1	8.92	124.76	120.30
1	C	72	ARG	NE-CZ-NH1	-8.91	115.85	120.30
1	A	389	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	C	487	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	C	24	ARG	CD-NE-CZ	8.60	135.64	123.60
1	B	136	ASP	CB-CG-OD1	8.49	125.94	118.30
1	C	389	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	A	224	SER	N-CA-CB	8.44	123.16	110.50
1	C	24	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	B	24	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	160	ARG	CD-NE-CZ	7.71	134.39	123.60
1	A	676	ASP	CB-CG-OD2	7.71	125.24	118.30
1	B	160	ARG	CD-NE-CZ	7.70	134.39	123.60
1	A	72	ARG	NE-CZ-NH1	-7.63	116.48	120.30
1	C	90	ARG	NE-CZ-NH2	7.49	124.04	120.30
1	B	612	ARG	NH1-CZ-NH2	7.45	127.60	119.40
1	B	138	ASP	CB-CG-OD2	-7.33	111.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	A	389	ARG	CD-NE-CZ	7.30	133.82	123.60
1	B	90	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	A	434	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	C	83	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	C	136	ASP	CB-CG-OD1	7.16	124.75	118.30
1	B	735	ARG	NE-CZ-NH2	7.15	123.88	120.30
1	B	735	ARG	NE-CZ-NH1	-7.15	116.73	120.30
1	A	441	GLN	CG-CD-OE1	7.14	135.88	121.60
1	A	10	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	B	44	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	434	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	A	653	ARG	NE-CZ-NH2	7.01	123.81	120.30
1	A	371	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	C	389	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	487	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	B	329	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	C	360	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	51	ASP	CA-C-N	6.63	129.45	116.20
1	A	511	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	C	557	GLU	CA-CB-CG	6.57	127.86	113.40
1	B	51	ASP	CA-C-N	6.51	129.23	116.20
1	C	160	ARG	CD-NE-CZ	6.45	132.63	123.60
1	A	73	ASP	CB-CG-OD1	6.43	124.08	118.30
1	C	251	ARG	CD-NE-CZ	6.42	132.58	123.60
1	C	293	SER	C-N-CA	6.40	137.70	121.70
1	B	389	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	730	TYR	CB-CG-CD1	6.32	124.79	121.00
1	C	10	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	C	620	MET	CB-CA-C	-6.26	97.89	110.40
1	A	189	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	612	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	C	510	ARG	NE-CZ-NH1	-6.21	117.20	120.30
1	A	293	SER	C-N-CA	6.20	137.19	121.70
1	B	293	SER	C-N-CA	6.17	137.14	121.70
1	C	154	LYS	N-CA-CB	-6.06	99.69	110.60
1	B	598	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	192	TYR	CB-CG-CD2	6.02	124.61	121.00
1	C	224	SER	N-CA-CB	6.01	119.52	110.50
1	A	523	TYR	CA-CB-CG	6.00	124.81	113.40
1	B	186	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	C	690	ASP	CB-CG-OD2	-5.95	112.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	530	ARG	CD-NE-CZ	5.94	131.91	123.60
1	C	51	ASP	CA-C-N	5.89	127.97	116.20
1	B	251	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	690	ASP	CB-CG-OD1	-5.79	113.09	118.30
2	P	3	VAL	N-CA-C	5.74	126.49	111.00
1	B	224	SER	N-CA-CB	5.73	119.10	110.50
1	C	434	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	C	441	GLN	CG-CD-OE1	5.73	133.06	121.60
1	B	441	GLN	CG-CD-OE1	5.73	133.06	121.60
1	C	730	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	C	389	ARG	CD-NE-CZ	5.70	131.57	123.60
1	B	427	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	B	189	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	260	ARG	CD-NE-CZ	5.64	131.50	123.60
1	B	434	ARG	NH1-CZ-NH2	5.62	125.58	119.40
1	C	393	VAL	N-CA-CB	5.61	123.85	111.50
1	B	73	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	373	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	A	484	LEU	CA-CB-CG	5.57	128.10	115.30
1	C	676	ASP	CB-CG-OD1	-5.56	113.30	118.30
1	B	260	ARG	CD-NE-CZ	5.54	131.36	123.60
1	B	523	TYR	CA-CB-CG	5.54	123.92	113.40
1	A	44	ARG	NH1-CZ-NH2	5.52	125.47	119.40
1	C	428	PRO	N-CA-CB	5.51	109.91	103.30
1	A	464	LEU	N-CA-C	5.49	125.83	111.00
1	B	557	GLU	CA-CB-CG	5.49	125.48	113.40
1	A	583	TYR	CB-CG-CD2	5.47	124.28	121.00
1	C	736	ASP	CA-CB-CG	5.47	125.44	113.40
1	C	451	ASP	CB-CG-OD2	5.46	123.22	118.30
2	P	2	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	214	GLY	N-CA-C	5.40	126.61	113.10
1	A	155	TYR	CB-CG-CD1	5.39	124.23	121.00
1	C	155	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	C	68	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	497	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	389	ARG	CD-NE-CZ	5.36	131.10	123.60
1	B	671	GLU	OE1-CD-OE2	-5.35	116.88	123.30
1	A	164	GLU	CA-CB-CG	5.34	125.14	113.40
1	A	312	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	A	186	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	83	ARG	NH1-CZ-NH2	5.32	125.25	119.40
1	B	434	ARG	NE-CZ-NH1	-5.30	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	487	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
1	B	155	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	A	557	GLU	CA-CB-CG	5.29	125.04	113.40
1	B	155	TYR	CA-CB-CG	5.26	123.39	113.40
1	A	733	ASN	N-CA-CB	5.24	120.03	110.60
1	C	329	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	389	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	549	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	B	195	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
1	B	269	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	C	136	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	220	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	425	PRO	N-CA-CB	5.19	109.53	103.30
1	B	51	ASP	CA-C-O	-5.19	109.20	120.10
1	B	155	TYR	CB-CG-CD1	5.14	124.09	121.00
1	B	405	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	C	699	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	C	260	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	B	164	GLU	CA-CB-CG	5.10	124.61	113.40
1	C	155	TYR	CB-CG-CD1	5.09	124.06	121.00
1	B	136	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	260	ARG	CG-CD-NE	5.07	122.44	111.80
1	C	186	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	83	ARG	NH1-CZ-NH2	5.04	124.94	119.40
1	A	293	SER	CA-C-O	5.04	130.68	120.10
1	C	717	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	C	499	PRO	N-CA-CB	5.03	109.33	103.30
1	B	10	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	579	PRO	Mainchain
1	B	620	MET	Mainchain
1	B	697	THR	Mainchain
1	C	579	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	5875	0	5801	152	0
1	B	5875	0	5801	145	0
1	C	5875	0	5801	155	0
2	D	140	0	123	2	0
2	E	140	0	123	2	0
2	F	140	0	123	3	0
2	P	31	0	34	4	0
3	A	28	0	0	2	0
3	B	30	0	0	3	0
3	C	32	0	0	3	0
All	All	18166	0	17806	454	0

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

All (454) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.46	0.96
1:B:191:GLN:HE21	1:B:195:ARG:HH21	1.11	0.94
1:A:191:GLN:HE21	1:A:195:ARG:HH21	1.12	0.93
1:C:441:GLN:NE2	1:C:620:MET:HB3	1.85	0.92
1:C:441:GLN:HE21	1:C:620:MET:HB3	1.34	0.92
1:C:191:GLN:HE21	1:C:195:ARG:HH21	1.08	0.91
1:B:441:GLN:HE21	1:B:620:MET:HB3	1.31	0.91
1:B:441:GLN:NE2	1:B:620:MET:HB3	1.88	0.89
1:B:37:SER:HB3	1:B:40:GLN:HB2	1.56	0.88
1:A:465:SER:HB2	1:A:489:LEU:HD11	1.56	0.88
1:C:465:SER:HB2	1:C:489:LEU:HD11	1.57	0.86
1:C:37:SER:HB3	1:C:40:GLN:HB2	1.58	0.86
1:C:260:ARG:HG2	1:C:260:ARG:HH11	1.40	0.84
1:B:465:SER:HB2	1:B:489:LEU:HD11	1.59	0.83
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.61	0.82
1:B:294:GLN:HB2	1:B:298:ARG:HB3	1.62	0.82
1:A:294:GLN:HB2	1:A:298:ARG:HB3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ARG:HG2	1:B:260:ARG:HH11	1.45	0.81
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.63	0.80
1:B:75:PRO:O	1:B:78:GLN:HG3	1.80	0.80
1:A:4:ASN:O	1:A:5:LEU:HB2	1.82	0.79
1:C:75:PRO:O	1:C:78:GLN:HG3	1.83	0.78
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.64	0.78
1:A:37:SER:HB3	1:A:40:GLN:HB2	1.66	0.78
1:B:4:ASN:O	1:B:5:LEU:HB2	1.83	0.78
1:C:294:GLN:HB2	1:C:298:ARG:HB3	1.67	0.77
1:C:658:ASP:HB3	1:C:662:LEU:HD12	1.67	0.77
1:C:4:ASN:O	1:C:5:LEU:HB2	1.86	0.75
1:B:215:VAL:O	1:B:216:ARG:HB3	1.85	0.75
1:C:325:VAL:HG13	1:C:328:ASN:HB2	1.69	0.75
1:A:260:ARG:HG2	1:A:260:ARG:HH11	1.50	0.74
1:A:83:ARG:HG2	1:A:141:MET:HG3	1.71	0.73
1:B:658:ASP:HB3	1:B:662:LEU:HD12	1.70	0.72
1:A:75:PRO:O	1:A:78:GLN:HG3	1.88	0.72
1:A:150:GLN:OE1	1:A:154:LYS:HE3	1.92	0.70
1:A:325:VAL:HG13	1:A:328:ASN:HB2	1.74	0.70
1:A:686:GLN:HE22	1:A:692:SER:HA	1.56	0.70
1:A:734:THR:O	1:A:735:ARG:HB2	1.91	0.70
1:B:325:VAL:HG13	1:B:328:ASN:HB2	1.73	0.70
1:A:215:VAL:O	1:A:216:ARG:HB3	1.90	0.70
1:A:94:TYR:OH	1:A:168:SER:HB3	1.90	0.70
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.74	0.70
1:C:734:THR:O	1:C:735:ARG:HB2	1.93	0.69
1:B:734:THR:O	1:B:735:ARG:HB2	1.91	0.68
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.76	0.68
1:A:522:TYR:CE2	1:A:526:LYS:HD3	2.29	0.67
1:C:215:VAL:O	1:C:216:ARG:HB3	1.94	0.67
1:A:548:GLN:HE21	1:A:548:GLN:HA	1.59	0.67
1:C:548:GLN:HA	1:C:548:GLN:HE21	1.59	0.67
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.76	0.67
1:A:548:GLN:NE2	1:A:548:GLN:HA	2.11	0.66
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.78	0.65
1:B:519:ASN:ND2	1:B:632:THR:H	1.95	0.65
1:B:548:GLN:HE21	1:B:548:GLN:HA	1.62	0.65
1:B:548:GLN:NE2	1:B:548:GLN:HA	2.12	0.65
1:B:700:ASP:OD2	1:B:736:ASP:HB3	1.97	0.65
1:C:150:GLN:OE1	1:C:154:LYS:HE3	1.95	0.65
1:C:700:ASP:OD2	1:C:736:ASP:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.78	0.64
1:B:361:VAL:HG21	1:B:364:LEU:HD12	1.79	0.63
1:B:94:TYR:OH	1:B:168:SER:HB3	1.98	0.63
1:C:548:GLN:HA	1:C:548:GLN:NE2	2.14	0.63
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.80	0.63
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.81	0.63
1:B:234:LEU:HG	1:B:272:GLU:HG2	1.79	0.63
1:A:532:SER:HA	1:A:677:GLY:HA3	1.81	0.63
1:C:322:ASN:HA	1:C:331:ARG:NH1	2.14	0.63
1:A:620:MET:HB2	1:A:621:PRO:HD2	1.81	0.62
1:C:209:THR:N	1:C:210:PRO:HD2	2.14	0.62
1:A:441:GLN:HE21	1:A:620:MET:HA	1.64	0.62
1:A:441:GLN:NE2	1:A:620:MET:HB3	2.15	0.62
1:C:620:MET:HB2	1:C:621:PRO:HD2	1.82	0.62
1:B:83:ARG:HG2	1:B:141:MET:HG3	1.81	0.62
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.82	0.62
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.81	0.62
1:B:620:MET:HB2	1:B:621:PRO:HD2	1.82	0.62
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.79	0.61
1:C:94:TYR:OH	1:C:168:SER:HB3	2.00	0.61
1:A:234:LEU:HG	1:A:272:GLU:HG2	1.83	0.61
1:C:522:TYR:CE2	1:C:526:LYS:HD3	2.34	0.61
1:C:519:ASN:ND2	1:C:632:THR:H	1.98	0.61
1:C:441:GLN:NE2	1:C:620:MET:CB	2.62	0.61
1:A:569:ASN:H	1:A:569:ASN:HD22	1.48	0.61
1:B:215:VAL:HB	3:B:789:HOH:O	2.00	0.61
1:B:322:ASN:HA	1:B:331:ARG:NH1	2.16	0.61
1:A:176:VAL:HG22	3:A:787:HOH:O	2.01	0.61
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.82	0.60
1:A:522:TYR:CZ	1:A:526:LYS:HD3	2.37	0.60
1:C:83:ARG:HG2	1:C:141:MET:HG3	1.83	0.60
1:B:215:VAL:O	1:B:216:ARG:CB	2.50	0.60
1:B:33:LEU:HB3	1:B:76:ASP:HB3	1.83	0.60
1:A:441:GLN:NE2	1:A:620:MET:CB	2.65	0.60
1:A:361:VAL:HG21	1:A:364:LEU:HD12	1.82	0.59
1:B:532:SER:HA	1:B:677:GLY:HA3	1.84	0.59
1:C:532:SER:HA	1:C:677:GLY:HA3	1.84	0.59
1:C:272:GLU:HB3	1:C:274:PHE:HE1	1.66	0.59
1:C:260:ARG:NH1	1:C:260:ARG:HG2	2.15	0.59
1:C:34:HIS:O	1:C:35:ASN:HB2	2.02	0.59
1:B:522:TYR:CE2	1:B:526:LYS:HD3	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HB3	1:A:76:ASP:HB3	1.83	0.59
1:A:519:ASN:ND2	1:A:632:THR:H	2.00	0.59
1:B:176:VAL:HG22	3:B:789:HOH:O	2.01	0.59
1:B:686:GLN:HE22	1:B:692:SER:HA	1.67	0.59
1:C:191:GLN:NE2	1:C:195:ARG:HH21	1.90	0.59
1:B:698:ASN:ND2	1:B:733:ASN:ND2	2.51	0.58
1:C:361:VAL:HG21	1:C:364:LEU:HD12	1.84	0.58
1:A:700:ASP:OD2	1:A:736:ASP:HB3	2.03	0.58
1:C:122:ASP:O	1:C:189:ARG:NH2	2.36	0.58
1:B:272:GLU:HB3	1:B:274:PHE:HE1	1.68	0.58
1:A:272:GLU:HB3	1:A:274:PHE:HE1	1.68	0.58
1:C:686:GLN:HE22	1:C:692:SER:HA	1.68	0.58
1:A:262:ARG:HB3	1:A:359:SER:HB3	1.86	0.57
1:B:99:PRO:HG2	1:B:137:HIS:CD2	2.39	0.57
1:C:522:TYR:CZ	1:C:526:LYS:HD3	2.39	0.57
1:A:150:GLN:HE21	1:A:627:GLN:NE2	2.02	0.57
1:A:621:PRO:HD3	1:A:694:SER:OG	2.05	0.57
1:A:322:ASN:HA	1:A:331:ARG:NH1	2.19	0.57
1:A:34:HIS:O	1:A:35:ASN:HB2	2.05	0.57
1:C:120:LEU:HD13	2:P:1:TYR:CG	2.39	0.57
1:A:187:GLU:HB2	3:C:762:HOH:O	2.04	0.57
1:C:99:PRO:HG2	1:C:137:HIS:CD2	2.40	0.57
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.87	0.57
1:B:621:PRO:HD3	1:B:694:SER:OG	2.05	0.57
1:A:585:LYS:HD3	1:A:586:ASP:OD1	2.05	0.56
1:C:187:GLU:HB2	3:C:782:HOH:O	2.05	0.56
1:C:215:VAL:O	1:C:216:ARG:CB	2.53	0.56
1:C:262:ARG:HB3	1:C:359:SER:HB3	1.87	0.56
1:A:572:THR:HB	1:A:577:ILE:HB	1.86	0.56
1:B:313:VAL:HG22	1:B:317:LEU:HD22	1.86	0.56
1:C:33:LEU:HB3	1:C:76:ASP:HB3	1.87	0.56
1:A:257:ASN:HB2	1:A:435:GLN:OE1	2.06	0.56
1:B:441:GLN:NE2	1:B:620:MET:CB	2.65	0.56
1:A:569:ASN:H	1:A:569:ASN:ND2	2.04	0.56
1:B:522:TYR:CZ	1:B:526:LYS:HD3	2.41	0.56
1:C:172:LEU:O	1:C:176:VAL:HG23	2.06	0.56
1:B:209:THR:N	1:B:210:PRO:HD2	2.20	0.56
1:B:388:ILE:O	1:B:390:LYS:HE3	2.06	0.55
1:A:585:LYS:N	1:A:585:LYS:HD2	2.22	0.55
1:B:172:LEU:O	1:B:176:VAL:HG23	2.07	0.55
1:C:5:LEU:HD23	1:C:51:ASP:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:372:ASN:ND2	2:D:372:ASN:H	2.03	0.55
1:B:191:GLN:NE2	1:B:195:ARG:HH21	1.93	0.55
1:B:441:GLN:HE21	1:B:620:MET:CB	2.12	0.55
1:C:572:THR:HB	1:C:577:ILE:HB	1.87	0.55
1:A:441:GLN:HE21	1:A:620:MET:CA	2.20	0.55
1:B:262:ARG:HB3	1:B:359:SER:HB3	1.89	0.55
1:A:209:THR:N	1:A:210:PRO:HD2	2.22	0.54
1:A:18:ASN:ND2	1:A:21:LYS:HE3	2.23	0.54
1:A:441:GLN:HE21	1:A:620:MET:CB	2.20	0.54
1:B:49:PHE:CZ	1:B:58:ILE:HG23	2.42	0.54
1:C:134:PHE:CE2	1:C:194:LYS:HB2	2.43	0.54
1:C:21:LYS:O	1:C:25:VAL:HG23	2.08	0.53
1:A:5:LEU:HD23	1:A:51:ASP:HA	1.90	0.53
1:B:312:GLU:O	1:B:316:LEU:HG	2.08	0.53
1:B:572:THR:HB	1:B:577:ILE:HB	1.89	0.53
1:C:234:LEU:HG	1:C:272:GLU:HG2	1.90	0.53
1:C:49:PHE:CZ	1:C:58:ILE:HG23	2.44	0.53
1:A:215:VAL:O	1:A:216:ARG:CB	2.57	0.53
1:A:99:PRO:HG2	1:A:137:HIS:CD2	2.44	0.53
1:B:122:ASP:O	1:B:189:ARG:NH2	2.42	0.53
2:E:372:ASN:H	2:E:372:ASN:ND2	2.05	0.53
1:A:221:GLN:NE2	1:A:250:GLN:OE1	2.42	0.53
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.90	0.53
1:B:5:LEU:HD23	1:B:51:ASP:HA	1.91	0.53
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.91	0.52
1:B:9:LYS:HE2	1:B:55:THR:HG21	1.92	0.52
1:A:18:ASN:HD22	1:A:21:LYS:HE3	1.74	0.52
1:A:388:ILE:O	1:A:390:LYS:HE3	2.10	0.52
1:C:341:LYS:HG2	1:C:722:TYR:OH	2.09	0.52
1:B:353:ILE:HG13	1:B:395:ALA:HB2	1.91	0.52
1:A:215:VAL:HB	3:A:787:HOH:O	2.10	0.52
1:A:329:ARG:HG3	1:A:331:ARG:NH1	2.25	0.52
1:B:150:GLN:OE1	1:B:154:LYS:HE3	2.09	0.52
1:B:329:ARG:HG3	1:B:331:ARG:NH1	2.24	0.52
1:C:548:GLN:HB2	1:C:688:PHE:HB3	1.92	0.52
1:C:9:LYS:HE2	1:C:55:THR:HG21	1.91	0.52
1:C:56:SER:O	1:C:60:GLU:HG2	2.09	0.52
1:C:272:GLU:HB3	1:C:274:PHE:CE1	2.45	0.51
1:C:427:ASP:HB3	1:C:430:ILE:HG13	1.93	0.51
1:C:698:ASN:ND2	1:C:733:ASN:ND2	2.58	0.51
1:A:172:LEU:O	1:A:176:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:HIS:O	1:B:35:ASN:HB2	2.08	0.51
1:B:585:LYS:HD3	1:B:586:ASP:OD1	2.10	0.51
1:C:585:LYS:HD3	1:C:586:ASP:OD1	2.10	0.51
1:A:260:ARG:HG2	1:A:260:ARG:NH1	2.23	0.51
1:A:341:LYS:HG2	1:A:722:TYR:OH	2.11	0.51
1:C:388:ILE:O	1:C:390:LYS:HE3	2.11	0.51
1:C:47:ILE:HG13	1:C:47:ILE:O	2.10	0.51
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.41	0.51
1:A:479:GLU:HB2	1:A:550:TYR:CE1	2.46	0.51
1:B:263:ALA:HB3	1:B:357:SER:HB2	1.92	0.51
1:B:272:GLU:HB3	1:B:274:PHE:CE1	2.46	0.51
1:B:479:GLU:HB2	1:B:550:TYR:CE1	2.46	0.50
1:C:176:VAL:HG22	3:C:791:HOH:O	2.10	0.50
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.94	0.50
1:B:626:SER:CB	1:B:633:ASN:HD22	2.24	0.50
1:C:260:ARG:HH11	1:C:260:ARG:CG	2.18	0.50
1:B:56:SER:O	1:B:60:GLU:HG2	2.12	0.50
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.94	0.50
1:A:272:GLU:HB3	1:A:274:PHE:CE1	2.47	0.50
1:B:585:LYS:HD2	1:B:585:LYS:N	2.26	0.50
1:C:90:ARG:HG3	1:C:90:ARG:HH11	1.77	0.50
1:A:585:LYS:H	1:A:585:LYS:HD2	1.76	0.49
1:C:585:LYS:HD2	1:C:585:LYS:N	2.26	0.49
1:B:700:ASP:CG	1:B:736:ASP:HB3	2.32	0.49
1:A:49:PHE:CZ	1:A:58:ILE:HG23	2.47	0.49
1:A:522:TYR:CD1	1:A:657:PRO:HB2	2.47	0.49
1:B:627:GLN:HG2	1:B:654:GLN:HE22	1.77	0.49
1:C:217:THR:HB	1:C:218:PRO:CD	2.41	0.49
1:A:555:SER:HB3	1:A:611:LEU:HD22	1.95	0.49
1:B:522:TYR:CD1	1:B:657:PRO:HB2	2.48	0.49
1:B:21:LYS:O	1:B:25:VAL:HG23	2.11	0.49
1:C:569:ASN:HD22	1:C:569:ASN:H	1.61	0.49
1:A:698:ASN:ND2	1:A:733:ASN:ND2	2.61	0.49
1:C:518:ILE:HA	1:C:634:GLY:HA2	1.95	0.49
1:C:180:LEU:CD1	1:C:488:ALA:HB1	2.43	0.48
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.43	0.48
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.95	0.48
2:F:372:ASN:H	2:F:372:ASN:ND2	2.10	0.48
1:B:217:THR:HB	1:B:218:PRO:HD2	1.95	0.48
1:B:341:LYS:HG2	1:B:722:TYR:OH	2.14	0.48
1:C:10:ARG:O	1:C:11:ASP:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:LEU:HD11	1:C:698:ASN:ND2	2.28	0.48
1:A:466:ALA:HA	1:A:516:GLY:O	2.13	0.48
1:A:404:GLN:HG3	2:D:361:ILE:HD11	1.96	0.48
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.49	0.48
1:A:279:ILE:HD13	1:A:319:LEU:HD21	1.95	0.48
1:A:415:GLN:HE22	1:A:435:GLN:HA	1.77	0.48
1:A:737:GLY:O	1:A:738:ALA:HB3	2.14	0.48
1:A:626:SER:CB	1:A:633:ASN:HD22	2.26	0.48
1:B:117:ASN:ND2	1:B:117:ASN:H	2.12	0.48
1:B:134:PHE:CE2	1:B:194:LYS:HB2	2.49	0.48
1:B:226:VAL:HG12	1:B:461:LEU:CD2	2.44	0.48
1:C:120:LEU:HD13	2:P:1:TYR:CB	2.43	0.48
1:C:150:GLN:HE21	1:C:627:GLN:NE2	2.12	0.48
1:A:353:ILE:HG13	1:A:395:ALA:HB2	1.96	0.48
1:A:519:ASN:ND2	1:A:522:TYR:HB3	2.29	0.48
1:C:1:MET:HA	1:C:3:GLN:HE21	1.77	0.48
1:B:18:ASN:HD22	1:B:21:LYS:HE3	1.79	0.48
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.96	0.48
1:C:329:ARG:HG3	1:C:331:ARG:NH1	2.28	0.48
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.96	0.48
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.96	0.47
1:A:338:GLN:HE21	1:A:415:GLN:NE2	2.12	0.47
1:A:56:SER:O	1:A:60:GLU:HG2	2.14	0.47
1:B:338:GLN:HE21	1:B:415:GLN:NE2	2.13	0.47
1:B:569:ASN:HD22	1:B:569:ASN:H	1.61	0.47
1:C:313:VAL:HG22	1:C:317:LEU:HD22	1.96	0.47
1:A:312:GLU:O	1:A:316:LEU:HG	2.14	0.47
1:C:120:LEU:HD13	2:P:1:TYR:HB3	1.97	0.47
1:C:99:PRO:HG2	1:C:137:HIS:CG	2.49	0.47
1:C:737:GLY:O	1:C:738:ALA:HB3	2.14	0.47
1:A:548:GLN:HB2	1:A:688:PHE:HB3	1.97	0.47
1:B:414:ILE:HB	1:B:729:LEU:HB2	1.97	0.47
1:B:150:GLN:HE21	1:B:627:GLN:NE2	2.12	0.47
1:B:18:ASN:ND2	1:B:21:LYS:HE3	2.30	0.47
1:C:227:LEU:HD11	1:C:437:ASN:HB3	1.96	0.47
1:A:404:GLN:O	1:A:407:ALA:HB3	2.15	0.47
1:B:217:THR:HB	1:B:218:PRO:CD	2.44	0.47
1:B:569:ASN:ND2	1:B:569:ASN:H	2.13	0.47
1:A:414:ILE:HB	1:A:729:LEU:HB2	1.97	0.46
1:C:54:LYS:H	1:C:54:LYS:HG2	1.61	0.46
1:A:149:LYS:HA	1:A:149:LYS:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:ARG:NH2	1:C:730:TYR:O	2.47	0.46
1:A:427:ASP:HB3	1:A:430:ILE:HG13	1.97	0.46
1:B:339:ILE:HD12	1:B:414:ILE:HG23	1.97	0.46
1:C:209:THR:N	1:C:210:PRO:CD	2.79	0.46
1:C:312:GLU:O	1:C:316:LEU:HG	2.16	0.46
1:C:519:ASN:HA	1:C:519:ASN:HD22	1.59	0.46
1:A:217:THR:HB	1:A:218:PRO:CD	2.45	0.46
1:B:450:ASN:HB2	1:B:454:ASP:OD2	2.15	0.46
1:B:180:LEU:CD1	1:B:488:ALA:HB1	2.45	0.46
1:B:294:GLN:HG2	1:B:298:ARG:HD3	1.98	0.46
1:B:698:ASN:HD22	1:B:733:ASN:ND2	2.13	0.46
1:C:138:ASP:O	1:C:141:MET:HB2	2.15	0.46
1:C:257:ASN:HB2	1:C:435:GLN:OE1	2.15	0.46
1:A:489:LEU:HB3	1:A:513:LEU:HD22	1.98	0.46
1:C:254:ILE:HG22	1:C:256:ILE:HG13	1.98	0.46
1:C:700:ASP:CG	1:C:736:ASP:HB3	2.36	0.46
1:A:227:LEU:HD11	1:A:437:ASN:HB3	1.97	0.46
1:A:9:LYS:HE2	1:A:55:THR:HG21	1.97	0.46
1:B:313:VAL:HG13	1:B:314:GLU:N	2.31	0.46
1:A:668:LEU:HB2	1:A:671:GLU:HG3	1.97	0.46
1:C:1:MET:HA	1:C:3:GLN:NE2	2.31	0.46
1:C:626:SER:CB	1:C:633:ASN:HD22	2.29	0.46
1:C:414:ILE:HB	1:C:729:LEU:HB2	1.98	0.46
1:B:221:GLN:NE2	1:B:250:GLN:OE1	2.49	0.46
1:B:1:MET:HA	1:B:3:GLN:HE21	1.80	0.46
1:C:240:THR:O	1:C:244:ILE:HG13	2.16	0.45
1:B:404:GLN:HG3	2:E:361:ILE:HD11	1.98	0.45
1:A:83:ARG:CG	1:A:141:MET:HG3	2.42	0.45
1:A:7:VAL:CG1	1:A:55:THR:HG22	2.46	0.45
1:C:522:TYR:CD1	1:C:657:PRO:HB2	2.50	0.45
1:A:519:ASN:HA	1:A:519:ASN:HD22	1.59	0.45
1:C:353:ILE:HG13	1:C:395:ALA:HB2	1.98	0.45
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.99	0.45
1:C:221:GLN:NE2	1:C:250:GLN:OE1	2.49	0.45
1:A:17:ILE:HD12	1:A:19:LEU:HD23	1.97	0.45
1:A:487:ARG:NH2	1:A:561:GLU:OE1	2.42	0.45
1:B:1:MET:H2	1:B:3:GLN:HG3	1.80	0.45
1:C:633:ASN:O	1:C:634:GLY:C	2.55	0.45
1:A:21:LYS:O	1:A:25:VAL:HG23	2.17	0.45
1:C:475:LEU:O	1:C:478:LEU:HB2	2.16	0.45
1:B:411:ARG:NE	1:B:731:TYR:HE1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:ASN:HB2	1:C:454:ASP:OD2	2.17	0.45
1:A:313:VAL:HG13	1:A:314:GLU:N	2.32	0.45
1:A:8:THR:O	1:A:54:LYS:HA	2.17	0.45
1:A:565:CYS:SG	1:A:568:PHE:HB2	2.57	0.45
1:C:263:ALA:HB3	1:C:357:SER:HB2	1.99	0.45
1:C:180:LEU:HD13	1:C:488:ALA:HB1	1.98	0.45
1:B:10:ARG:O	1:B:11:ASP:C	2.55	0.44
1:B:99:PRO:HG2	1:B:137:HIS:CG	2.51	0.44
1:C:548:GLN:CA	1:C:548:GLN:HE21	2.28	0.44
1:A:10:ARG:O	1:A:11:ASP:C	2.56	0.44
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.97	0.44
1:A:406:ARG:NH2	1:A:730:TYR:O	2.46	0.44
1:B:548:GLN:HB2	1:B:688:PHE:HB3	1.99	0.44
1:A:279:ILE:HG12	1:A:279:ILE:H	1.65	0.44
1:C:620:MET:HB2	1:C:621:PRO:CD	2.45	0.44
1:B:585:LYS:H	1:B:585:LYS:HD2	1.82	0.44
1:C:117:ASN:ND2	1:C:117:ASN:H	2.16	0.44
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.99	0.44
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.98	0.44
1:C:489:LEU:HB3	1:C:513:LEU:HD22	1.98	0.44
1:C:585:LYS:HD2	1:C:585:LYS:H	1.82	0.44
1:C:348:LEU:HD11	2:F:375:LEU:HD21	2.00	0.44
1:B:698:ASN:HD22	1:B:733:ASN:HD22	1.64	0.44
1:C:203:PHE:HB3	1:C:629:SER:HB3	1.99	0.44
1:A:311:LEU:HA	1:A:355:LEU:HB3	2.00	0.44
1:B:737:GLY:O	1:B:738:ALA:HB3	2.18	0.44
1:A:240:THR:O	1:A:244:ILE:HG13	2.18	0.44
1:A:321:ASN:O	1:A:329:ARG:NE	2.50	0.44
1:A:426:PHE:O	1:A:428:PRO:HD3	2.18	0.44
1:A:698:ASN:HD22	1:A:733:ASN:ND2	2.15	0.44
1:A:122:ASP:O	1:A:189:ARG:NH2	2.51	0.44
1:C:151:LEU:HA	1:C:155:TYR:HB2	2.00	0.44
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.99	0.43
1:A:365:TYR:O	1:A:368:PHE:HB3	2.18	0.43
1:B:260:ARG:NH1	1:B:260:ARG:HG2	2.21	0.43
1:B:256:ILE:O	1:B:304:LEU:HA	2.18	0.43
1:C:227:LEU:HB3	1:C:435:GLN:NE2	2.32	0.43
1:A:406:ARG:HG3	1:A:412:ILE:O	2.18	0.43
1:B:227:LEU:HD11	1:B:437:ASN:HB3	1.98	0.43
1:B:686:GLN:CD	1:B:727:LYS:HD2	2.38	0.43
1:A:150:GLN:NE2	1:A:627:GLN:NE2	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LYS:HA	2:P:1:TYR:N	2.34	0.43
1:A:258:ALA:HB1	1:A:261:ILE:HD12	1.99	0.43
1:B:1:MET:HA	1:B:3:GLN:NE2	2.33	0.43
1:C:520:PHE:HB3	1:C:635:ILE:HA	2.00	0.43
1:A:369:PHE:CG	1:A:434:ARG:HG2	2.54	0.43
1:B:227:LEU:HB3	1:B:435:GLN:NE2	2.34	0.43
1:B:262:ARG:HD2	1:B:274:PHE:HB2	2.00	0.43
1:C:404:GLN:HG3	2:F:361:ILE:HD11	2.00	0.43
1:C:106:VAL:O	1:C:110:VAL:HG23	2.19	0.43
1:C:18:ASN:HD22	1:C:21:LYS:HE3	1.84	0.43
1:A:294:GLN:HG2	1:A:298:ARG:HD3	2.00	0.43
1:B:548:GLN:CA	1:B:548:GLN:HE21	2.27	0.43
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.99	0.43
1:A:441:GLN:HG2	1:A:442:ILE:N	2.31	0.42
1:A:532:SER:CB	1:A:673:PRO:HD2	2.49	0.42
1:A:734:THR:O	1:A:735:ARG:CB	2.62	0.42
1:B:109:MET:HG3	1:B:115:TYR:CE2	2.54	0.42
1:C:311:LEU:HA	1:C:355:LEU:HB3	2.00	0.42
1:A:171:PHE:HA	1:A:174:ILE:HG22	2.01	0.42
1:B:519:ASN:CG	1:B:631:ALA:HB1	2.40	0.42
1:C:339:ILE:HG22	1:C:340:ASN:N	2.35	0.42
1:C:569:ASN:ND2	1:C:569:ASN:H	2.16	0.42
1:C:621:PRO:HD3	1:C:694:SER:OG	2.20	0.42
1:A:700:ASP:CG	1:A:736:ASP:HB3	2.40	0.42
1:B:406:ARG:NH2	1:B:730:TYR:O	2.50	0.42
1:A:436:SER:OG	1:A:437:ASN:N	2.52	0.42
1:B:187:GLU:HB2	3:B:780:HOH:O	2.19	0.42
1:B:492:LEU:O	1:B:496:GLN:HG2	2.19	0.42
1:C:262:ARG:HD2	1:C:274:PHE:HB2	2.00	0.42
1:C:411:ARG:NE	1:C:731:TYR:HE1	2.17	0.42
1:A:150:GLN:NE2	1:A:627:GLN:HE22	2.17	0.42
1:A:328:ASN:HA	1:A:328:ASN:HD22	1.64	0.42
1:C:217:THR:OG1	1:C:219:THR:HG22	2.19	0.42
1:C:519:ASN:HD22	1:C:632:THR:H	1.68	0.42
1:C:704:PHE:CD2	1:C:710:PRO:HD3	2.54	0.42
1:C:90:ARG:HG3	1:C:90:ARG:NH1	2.34	0.42
1:A:329:ARG:HG3	1:A:331:ARG:HH12	1.84	0.42
1:B:285:PHE:O	1:B:288:ALA:HB3	2.19	0.42
1:C:279:ILE:HD13	1:C:319:LEU:HD21	2.00	0.42
1:A:520:PHE:HB3	1:A:635:ILE:HA	2.02	0.42
1:A:548:GLN:HE21	1:A:548:GLN:CA	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:VAL:O	1:B:110:VAL:HG23	2.20	0.42
1:B:172:LEU:C	1:B:172:LEU:HD23	2.40	0.42
1:B:555:SER:HB3	1:B:611:LEU:HD22	2.01	0.42
1:A:134:PHE:CE2	1:A:194:LYS:HB2	2.54	0.42
1:B:254:ILE:HG22	1:B:256:ILE:HG13	2.02	0.42
1:C:258:ALA:HB3	1:C:304:LEU:HD21	2.01	0.42
1:A:1:MET:HA	1:A:3:GLN:HE21	1.85	0.42
1:B:227:LEU:HB2	1:B:460:ALA:HB3	2.02	0.41
1:B:8:THR:O	1:B:54:LYS:HA	2.20	0.41
1:C:176:VAL:HG11	1:C:212:MET:CE	2.49	0.41
1:C:217:THR:CB	1:C:218:PRO:CD	2.98	0.41
1:C:217:THR:HB	1:C:218:PRO:HD2	2.01	0.41
1:C:256:ILE:O	1:C:304:LEU:HA	2.20	0.41
1:C:18:ASN:ND2	1:C:21:LYS:HE3	2.35	0.41
1:A:441:GLN:HE21	1:A:620:MET:HB3	1.82	0.41
1:B:83:ARG:CG	1:B:141:MET:HG3	2.48	0.41
1:B:466:ALA:HA	1:B:516:GLY:O	2.20	0.41
1:B:519:ASN:HA	1:B:519:ASN:HD22	1.46	0.41
1:C:109:MET:HG3	1:C:115:TYR:CE2	2.56	0.41
1:C:479:GLU:HB2	1:C:550:TYR:CE1	2.56	0.41
1:A:444:LEU:HA	1:A:445:PRO:HD3	1.85	0.41
1:B:592:ASN:O	1:B:593:GLU:C	2.59	0.41
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.48	0.41
1:C:406:ARG:HG3	1:C:412:ILE:O	2.21	0.41
1:A:262:ARG:HD2	1:A:274:PHE:HB2	2.03	0.41
1:A:90:ARG:HG3	1:A:90:ARG:HH11	1.85	0.41
1:B:226:VAL:HG12	1:B:461:LEU:HD23	2.02	0.41
1:B:518:ILE:HA	1:B:634:GLY:HA2	2.01	0.41
1:C:226:VAL:HG12	1:C:461:LEU:CD2	2.50	0.41
1:A:7:VAL:HG11	1:A:55:THR:HG22	2.03	0.41
1:B:279:ILE:HG12	1:B:279:ILE:H	1.51	0.41
1:A:475:LEU:O	1:A:478:LEU:HB2	2.21	0.41
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.87	0.41
1:B:143:PHE:CZ	1:B:151:LEU:HD11	2.56	0.41
1:B:339:ILE:HG23	1:B:343:MET:HB2	2.02	0.41
1:B:704:PHE:CD2	1:B:710:PRO:HD3	2.56	0.41
1:A:339:ILE:HG22	1:A:340:ASN:N	2.36	0.41
1:A:339:ILE:HD12	1:A:414:ILE:HG23	2.03	0.41
1:A:493:LEU:HD23	1:A:493:LEU:HA	1.92	0.41
1:B:462:CYS:HB3	1:B:464:LEU:HD21	2.02	0.41
1:C:222:PHE:HD2	1:C:496:GLN:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:GLY:O	1:C:738:ALA:CB	2.69	0.41
1:A:633:ASN:O	1:A:634:GLY:C	2.59	0.41
1:B:339:ILE:HG22	1:B:340:ASN:N	2.34	0.41
1:C:1:MET:H2	1:C:3:GLN:HG3	1.85	0.41
1:C:28:TRP:O	1:C:31:GLU:HB2	2.21	0.41
1:C:8:THR:O	1:C:54:LYS:HA	2.20	0.41
1:C:669:LEU:HD11	1:C:698:ASN:CG	2.41	0.41
1:C:321:ASN:O	1:C:329:ARG:NE	2.54	0.40
1:C:441:GLN:HG2	1:C:442:ILE:N	2.32	0.40
1:C:466:ALA:HA	1:C:516:GLY:O	2.21	0.40
1:B:138:ASP:O	1:B:141:MET:HB2	2.21	0.40
1:B:734:THR:O	1:B:735:ARG:CB	2.66	0.40
1:A:99:PRO:HG2	1:A:137:HIS:CG	2.56	0.40
1:A:287:THR:OG1	1:B:284:HIS:HA	2.22	0.40
1:B:512:THR:HG22	1:B:615:THR:HG23	2.03	0.40
1:C:207:LEU:HD13	1:C:212:MET:CE	2.52	0.40
1:C:285:PHE:O	1:C:289:VAL:HG23	2.21	0.40
1:C:97:PHE:O	1:C:99:PRO:HD3	2.21	0.40
1:A:569:ASN:N	1:A:569:ASN:ND2	2.68	0.40
1:A:737:GLY:O	1:A:738:ALA:CB	2.69	0.40
1:B:28:TRP:O	1:B:31:GLU:HB2	2.21	0.40
1:B:620:MET:HB2	1:B:621:PRO:CD	2.50	0.40
1:C:492:LEU:O	1:C:496:GLN:HG2	2.22	0.40
1:A:656:VAL:HA	1:A:657:PRO:HD3	1.93	0.40
1:B:633:ASN:O	1:B:634:GLY:C	2.58	0.40
1:C:462:CYS:HB3	1:C:464:LEU:HD21	2.02	0.40
1:C:555:SER:HB3	1:C:611:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

5.3　Torsion angles　ⓘ

5.3.1　Protein backbone　ⓘ

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%)	675 (92%)	51 (7%)	10 (1%)	13	47
1	B	736/761 (97%)	678 (92%)	46 (6%)	12 (2%)	11	43
1	C	736/761 (97%)	679 (92%)	47 (6%)	10 (1%)	13	47
2	D	16/20 (80%)	13 (81%)	2 (12%)	1 (6%)	1	10
2	E	16/20 (80%)	13 (81%)	1 (6%)	2 (12%)	0	1
2	F	16/20 (80%)	13 (81%)	1 (6%)	2 (12%)	0	1
2	P	2/20 (10%)	0	1 (50%)	1 (50%)	0	0
All	All	2258/2363 (96%)	2071 (92%)	149 (7%)	38 (2%)	11	42

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	735	ARG
1	B	14	THR
1	B	294	GLN
1	B	735	ARG
2	E	371	SER
1	C	294	GLN
1	C	735	ARG
2	P	3	VAL
1	A	5	LEU
1	A	11	ASP
1	A	14	THR
1	A	51	ASP
1	A	216	ARG
2	D	371	SER
1	B	5	LEU
1	B	11	ASP
1	B	216	ARG
1	C	5	LEU
1	C	11	ASP
1	C	14	THR
1	C	51	ASP
1	C	216	ARG
2	F	371	SER
1	B	13	SER
1	B	51	ASP
1	A	15	GLU
1	B	15	GLU
1	C	15	GLU

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Mol	Chain	Res	Type
1	A	13	SER
1	C	13	SER
2	E	359	GLY
1	B	12	GLY
1	A	12	GLY
1	B	300	GLY
1	B	737	GLY
1	C	12	GLY
2	F	359	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%)	548 (87%)	84 (13%)	4	20
1	B	632/651 (97%)	552 (87%)	80 (13%)	5	21
1	C	632/651 (97%)	550 (87%)	82 (13%)	5	21
2	D	17/19 (90%)	14 (82%)	3 (18%)	2	10
2	E	17/19 (90%)	14 (82%)	3 (18%)	2	10
2	F	17/19 (90%)	14 (82%)	3 (18%)	2	10
2	P	3/19 (16%)	2 (67%)	1 (33%)	0	0
All	All	1950/2029 (96%)	1694 (87%)	256 (13%)	5	20

All (256) residues with a non-rotameric sidechain are listed below:

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	31	GLU

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Mol	Chain	Res	Type
1	A	40	GLN
1	A	44	ARG
1	A	48	GLN
1	A	56	SER
1	A	64	LYS
1	A	72	ARG
1	A	73	ASP
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	168	SER
1	A	174	ILE
1	A	187	GLU
1	A	189	ARG
1	A	204	LYS
1	A	206	SER
1	A	225	CYS
1	A	260	ARG
1	A	264	LEU
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	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	394	LYS
1	A	396	VAL
1	A	400	SER
1	A	408	SER

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Mol	Chain	Res	Type
1	A	409	THR
1	A	424	SER
1	A	430	ILE
1	A	435	GLN
1	A	440	LEU
1	A	441	GLN
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	569	ASN
1	A	570	GLU
1	A	585	LYS
1	A	605	SER
1	A	607	LYS
1	A	616	LEU
1	A	625	SER
1	A	629	SER
1	A	639	ARG
1	A	645	LYS
1	A	647	SER
1	A	648	LYS
1	A	652	LEU
1	A	692	SER
1	A	696	ASN
1	A	708	LYS
1	A	735	ARG
1	A	736	ASP
2	D	361	ILE
2	D	362	ASP
2	D	372	ASN
1	B	3	GLN
1	B	8	THR
1	B	9	LYS
1	B	14	THR
1	B	16	ARG

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Mol	Chain	Res	Type
1	B	17	ILE
1	B	21	LYS
1	B	31	GLU
1	B	40	GLN
1	B	48	GLN
1	B	56	SER
1	B	64	LYS
1	B	72	ARG
1	B	73	ASP
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	168	SER
1	B	174	ILE
1	B	189	ARG
1	B	204	LYS
1	B	206	SER
1	B	225	CYS
1	B	260	ARG
1	B	264	LEU
1	B	274	PHE
1	B	279	ILE
1	B	283	LYS
1	B	290	LYS
1	B	293	SER
1	B	297	VAL
1	B	298	ARG
1	B	317	LEU
1	B	320	LYS
1	B	323	ARG
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	394	LYS
1	B	396	VAL

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Mol	Chain	Res	Type
1	B	400	SER
1	B	408	SER
1	B	409	THR
1	B	424	SER
1	B	430	ILE
1	B	440	LEU
1	B	441	GLN
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	570	GLU
1	B	585	LYS
1	B	605	SER
1	B	607	LYS
1	B	616	LEU
1	B	620	MET
1	B	625	SER
1	B	629	SER
1	B	639	ARG
1	B	645	LYS
1	B	647	SER
1	B	648	LYS
1	B	652	LEU
1	B	696	ASN
1	B	708	LYS
1	B	735	ARG
1	B	736	ASP
2	E	361	ILE
2	E	362	ASP
2	E	372	ASN
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	56	SER
1	C	64	LYS
1	C	72	ARG
1	C	73	ASP
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	168	SER
1	C	174	ILE
1	C	187	GLU
1	C	189	ARG
1	C	206	SER
1	C	225	CYS
1	C	260	ARG
1	C	264	LEU
1	C	274	PHE
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
1	C	394	LYS
1	C	396	VAL

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Mol	Chain	Res	Type
1	C	400	SER
1	C	408	SER
1	C	424	SER
1	C	430	ILE
1	C	440	LEU
1	C	441	GLN
1	C	465	SER
1	C	474	ASN
1	C	484	LEU
1	C	505	ARG
1	C	510	ARG
1	C	512	THR
1	C	519	ASN
1	C	526	LYS
1	C	530	ARG
1	C	570	GLU
1	C	585	LYS
1	C	605	SER
1	C	607	LYS
1	C	616	LEU
1	C	620	MET
1	C	625	SER
1	C	628	ILE
1	C	629	SER
1	C	639	ARG
1	C	645	LYS
1	C	647	SER
1	C	648	LYS
1	C	652	LEU
1	C	692	SER
1	C	696	ASN
1	C	708	LYS
1	C	735	ARG
1	C	736	ASP
2	F	361	ILE
2	F	362	ASP
2	F	372	ASN
2	P	2	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) 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	130	GLN
1	A	191	GLN
1	A	221	GLN
1	A	328	ASN
1	A	415	GLN
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	696	ASN
1	A	698	ASN
1	A	733	ASN
2	D	360	GLN
2	D	372	ASN
1	B	3	GLN
1	B	18	ASN
1	B	46	HIS
1	B	117	ASN
1	B	130	GLN
1	B	191	GLN
1	B	221	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	696	ASN
1	B	698	ASN
1	B	733	ASN
2	E	360	GLN

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Mol	Chain	Res	Type
2	E	372	ASN
1	C	3	GLN
1	C	18	ASN
1	C	46	HIS
1	C	117	ASN
1	C	130	GLN
1	C	191	GLN
1	C	221	GLN
1	C	328	ASN
1	C	415	GLN
1	C	496	GLN
1	C	519	ASN
1	C	548	GLN
1	C	569	ASN
1	C	627	GLN
1	C	633	ASN
1	C	654	GLN
1	C	686	GLN
1	C	696	ASN
1	C	698	ASN
1	C	733	ASN
2	F	360	GLN
2	F	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.