



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:14 AM UTC

PDB ID : 2ID0 / pdb_00002id0
Title : Escherichia coli RNase II
Authors : Zuo, Y.; Zhang, J.; Wang, Y.; Malhotra, A.
Deposited on : 2006-09-13
Resolution : 2.35 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

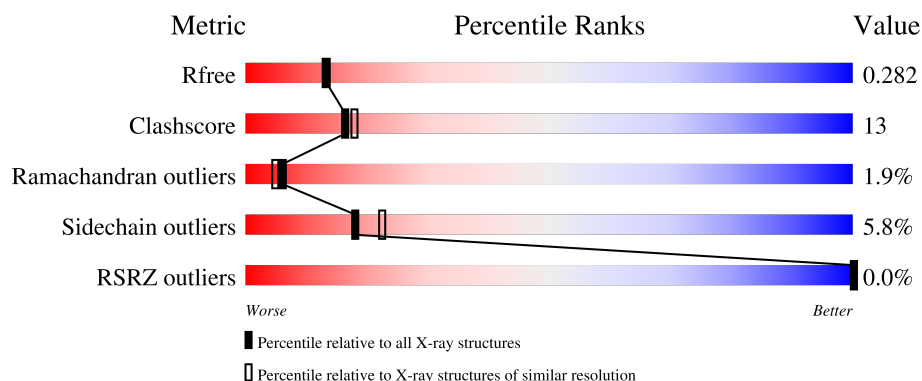
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

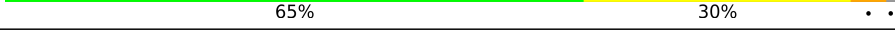
The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	644	
1	B	644	
1	C	644	
1	D	644	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19820 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 Exoribonuclease 2.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	Se		0	0	0
			4838	3078	860	879	7	14				
1	B	636	Total	C	N	O	S	Se		0	0	0
			4937	3128	879	909	7	14				
1	C	636	Total	C	N	O	S	Se		0	0	0
			4930	3129	876	904	7	14				
1	D	636	Total	C	N	O	S	Se		0	0	0
			4824	3072	853	878	7	14				

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P30850
A	51	MSE	MET	modified residue	UNP P30850
A	55	MSE	MET	modified residue	UNP P30850
A	132	MSE	MET	modified residue	UNP P30850
A	182	MSE	MET	modified residue	UNP P30850
A	208	MSE	MET	modified residue	UNP P30850
A	261	MSE	MET	modified residue	UNP P30850
A	286	MSE	MET	modified residue	UNP P30850
A	393	MSE	MET	modified residue	UNP P30850
A	417	MSE	MET	modified residue	UNP P30850
A	505	MSE	MET	modified residue	UNP P30850
A	531	MSE	MET	modified residue	UNP P30850
A	540	MSE	MET	modified residue	UNP P30850
A	576	MSE	MET	modified residue	UNP P30850
A	633	MSE	MET	modified residue	UNP P30850
B	1	MSE	MET	modified residue	UNP P30850
B	51	MSE	MET	modified residue	UNP P30850
B	55	MSE	MET	modified residue	UNP P30850
B	132	MSE	MET	modified residue	UNP P30850
B	182	MSE	MET	modified residue	UNP P30850
B	208	MSE	MET	modified residue	UNP P30850

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Chain	Residue	Modelled	Actual	Comment	Reference
B	261	MSE	MET	modified residue	UNP P30850
B	286	MSE	MET	modified residue	UNP P30850
B	393	MSE	MET	modified residue	UNP P30850
B	417	MSE	MET	modified residue	UNP P30850
B	505	MSE	MET	modified residue	UNP P30850
B	531	MSE	MET	modified residue	UNP P30850
B	540	MSE	MET	modified residue	UNP P30850
B	576	MSE	MET	modified residue	UNP P30850
B	633	MSE	MET	modified residue	UNP P30850
C	1	MSE	MET	modified residue	UNP P30850
C	51	MSE	MET	modified residue	UNP P30850
C	55	MSE	MET	modified residue	UNP P30850
C	132	MSE	MET	modified residue	UNP P30850
C	182	MSE	MET	modified residue	UNP P30850
C	208	MSE	MET	modified residue	UNP P30850
C	261	MSE	MET	modified residue	UNP P30850
C	286	MSE	MET	modified residue	UNP P30850
C	393	MSE	MET	modified residue	UNP P30850
C	417	MSE	MET	modified residue	UNP P30850
C	505	MSE	MET	modified residue	UNP P30850
C	531	MSE	MET	modified residue	UNP P30850
C	540	MSE	MET	modified residue	UNP P30850
C	576	MSE	MET	modified residue	UNP P30850
C	633	MSE	MET	modified residue	UNP P30850
D	1	MSE	MET	modified residue	UNP P30850
D	51	MSE	MET	modified residue	UNP P30850
D	55	MSE	MET	modified residue	UNP P30850
D	132	MSE	MET	modified residue	UNP P30850
D	182	MSE	MET	modified residue	UNP P30850
D	208	MSE	MET	modified residue	UNP P30850
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D	417	MSE	MET	modified residue	UNP P30850
D	505	MSE	MET	modified residue	UNP P30850
D	531	MSE	MET	modified residue	UNP P30850
D	540	MSE	MET	modified residue	UNP P30850
D	576	MSE	MET	modified residue	UNP P30850
D	633	MSE	MET	modified residue	UNP P30850

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0

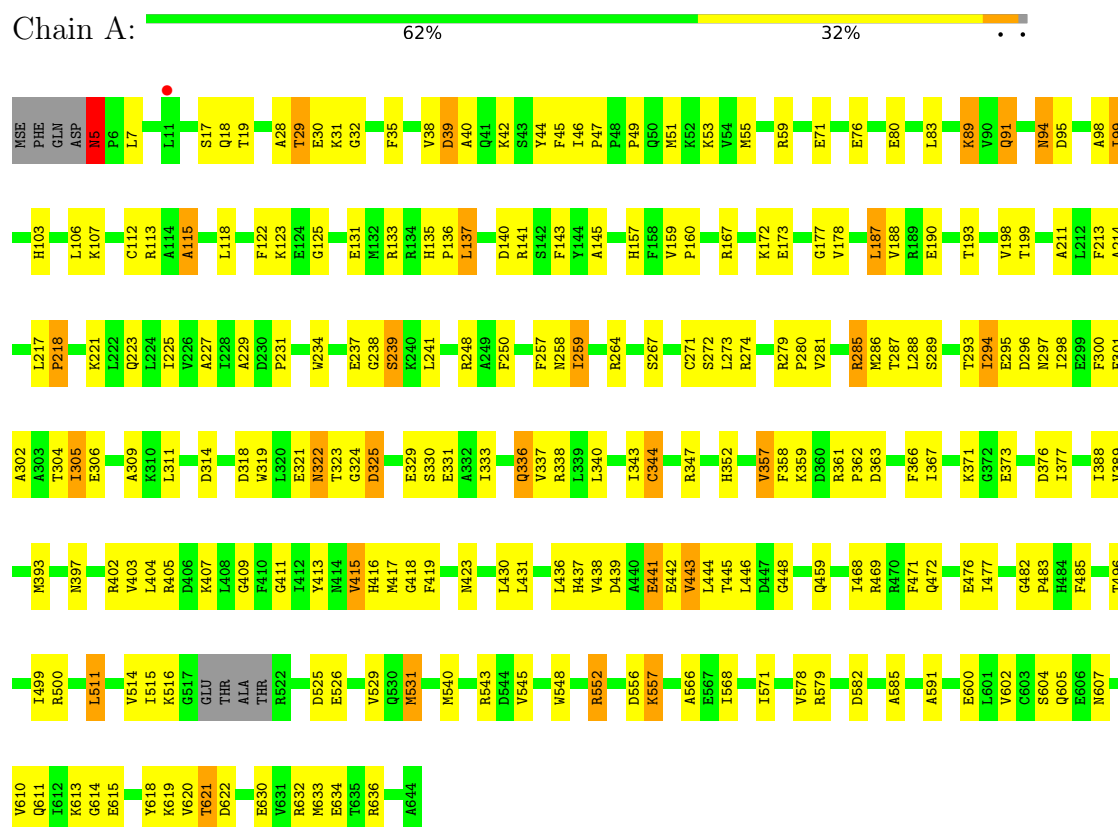
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	96	Total 96	O 96	0	0
3	C	82	Total 82	O 82	0	0
3	D	59	Total 59	O 59	0	0

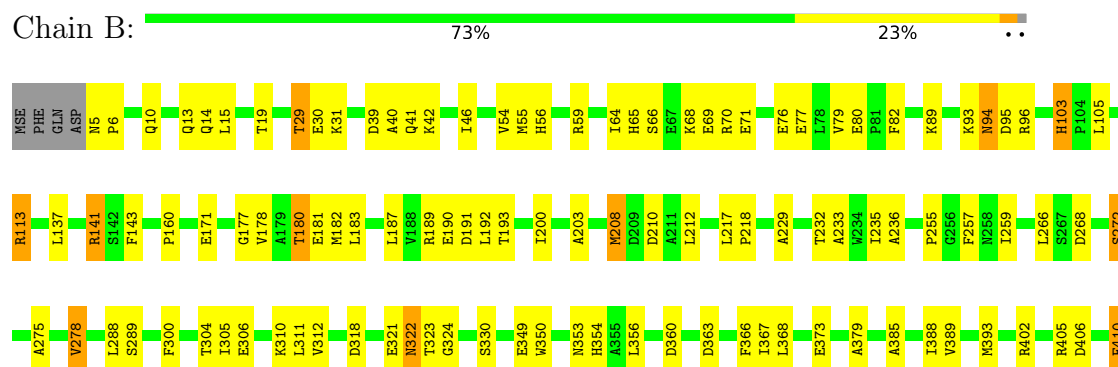
3 Residue-property plots

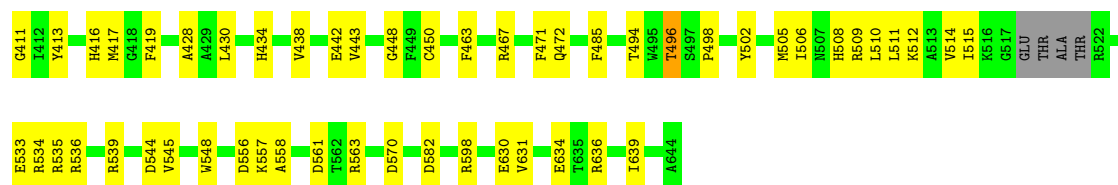
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Exoribonuclease 2



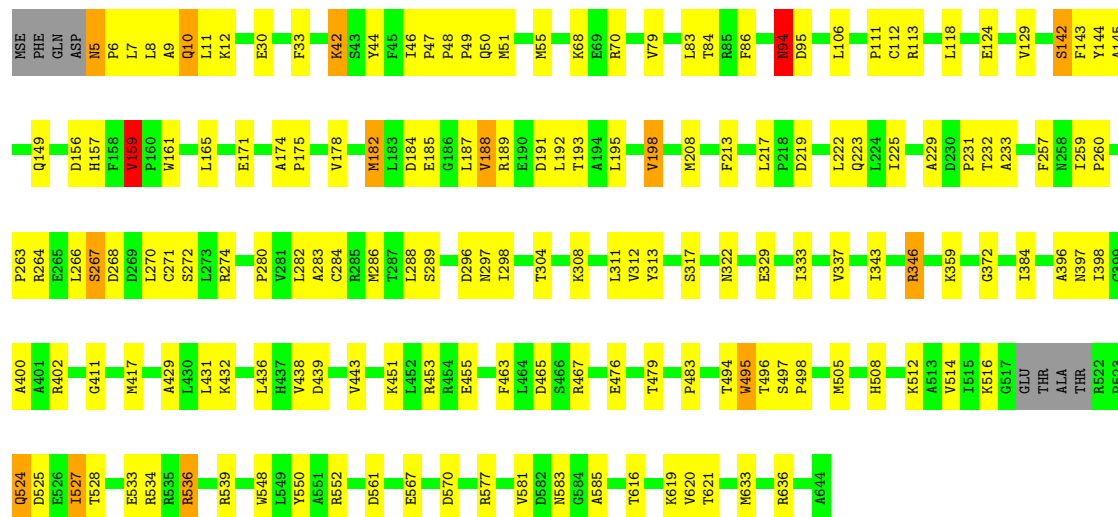
• Molecule 1: Exoribonuclease 2





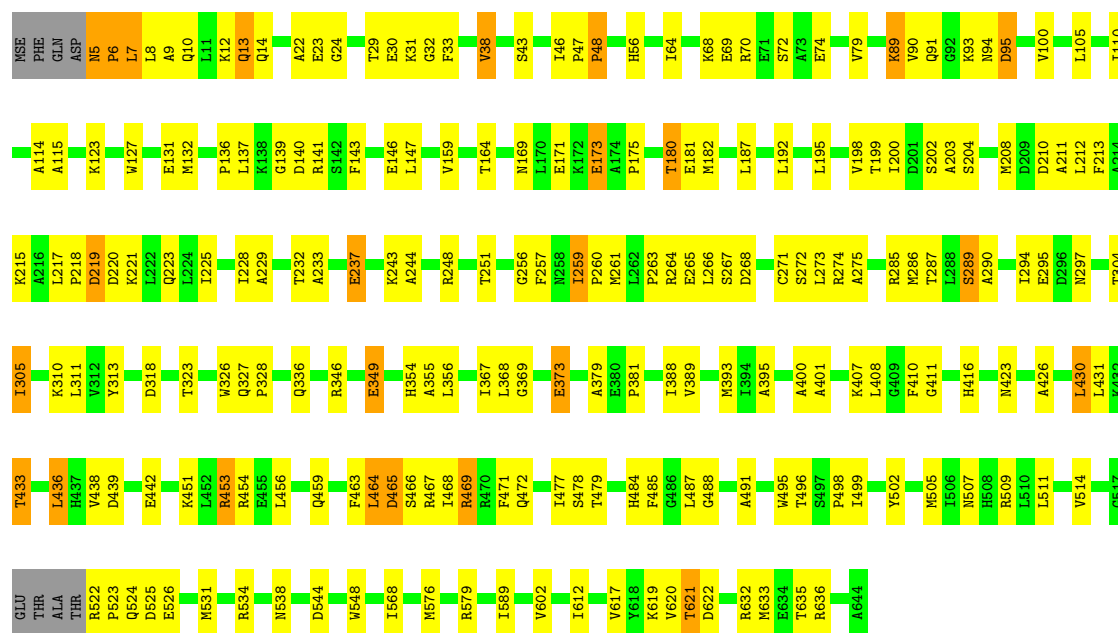
• Molecule 1: Exoribonuclease 2

Chain C: 73% 23% ..



• Molecule 1: Exoribonuclease 2

Chain D: 65% 30% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.76Å 118.43Å 122.38Å 107.80° 98.36° 91.40°	Depositor
Resolution (Å)	17.95 – 2.35 17.95 – 2.35	Depositor EDS
% Data completeness (in resolution range)	82.3 (17.95-2.35) 82.4 (17.95-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.80 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.286 0.221 , 0.282	Depositor DCC
R_{free} test set	5045 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19820	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	1.00	14/4925 (0.3%)	1.07	16/6674 (0.2%)
1	B	0.97	6/5025 (0.1%)	1.08	7/6800 (0.1%)
1	C	0.98	1/5018 (0.0%)	1.08	4/6788 (0.1%)
1	D	1.07	11/4911 (0.2%)	1.12	22/6659 (0.3%)
All	All	1.00	32/19879 (0.2%)	1.09	49/26921 (0.2%)

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	14	GLN	C-O	19.77	1.47	1.24
1	D	5	ASN	CG-ND2	17.42	1.69	1.33
1	D	285	ARG	NE-CZ	15.44	1.50	1.33
1	A	285	ARG	CZ-NH1	15.22	1.54	1.32
1	D	14	GLN	C-N	10.84	1.48	1.33
1	B	190	GLU	CD-OE1	9.36	1.43	1.25
1	A	188	VAL	C-O	9.16	1.34	1.24
1	B	190	GLU	CD-OE2	8.89	1.42	1.25
1	A	298	ILE	C-N	8.64	1.46	1.33
1	A	302	ALA	C-N	8.36	1.41	1.33
1	D	13	GLN	CD-OE1	7.59	1.38	1.23
1	A	302	ALA	CA-C	6.96	1.61	1.52
1	A	285	ARG	CZ-NH2	6.68	1.42	1.33
1	D	5	ASN	N-CA	6.59	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ARG	CD-NE	6.23	1.54	1.46
1	D	367	ILE	CA-CB	6.04	1.60	1.53
1	A	301	PHE	C-O	5.96	1.31	1.23
1	D	12	LYS	C-O	5.92	1.31	1.24
1	A	516	LYS	C-N	5.76	1.41	1.33
1	C	159	VAL	CA-CB	5.71	1.61	1.54
1	A	188	VAL	C-N	5.57	1.41	1.33
1	D	215	LYS	C-O	5.56	1.30	1.23
1	B	82	PHE	N-CA	-5.53	1.39	1.46
1	A	99	ILE	CA-CB	5.52	1.61	1.54
1	A	301	PHE	C-N	5.51	1.40	1.33
1	D	100	VAL	CA-C	-5.49	1.48	1.53
1	B	494	THR	CA-CB	5.48	1.61	1.53
1	A	159	VAL	CA-C	5.41	1.58	1.52
1	B	639	ILE	CA-CB	5.13	1.61	1.54
1	D	159	VAL	CA-C	5.04	1.58	1.52
1	A	516	LYS	C-O	5.02	1.33	1.25
1	B	54	VAL	CA-C	-5.02	1.48	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	GLU	N-CA-C	-8.54	103.72	114.56
1	D	5	ASN	OD1-CG-ND2	8.51	131.11	122.60
1	B	46	ILE	N-CA-C	7.32	115.43	107.60
1	D	285	ARG	NE-CZ-NH2	-7.18	112.74	119.20
1	A	591	ALA	CA-C-N	-6.99	112.60	119.87
1	A	591	ALA	C-N-CA	-6.99	112.60	119.87
1	C	495	TRP	N-CA-C	-6.95	102.04	113.50
1	D	259	ILE	CA-C-N	6.71	126.62	119.85
1	D	259	ILE	C-N-CA	6.71	126.62	119.85
1	A	259	ILE	CA-C-N	6.53	126.56	119.90
1	A	259	ILE	C-N-CA	6.53	126.56	119.90
1	B	46	ILE	CA-C-N	6.49	124.40	119.66
1	B	46	ILE	C-N-CA	6.49	124.40	119.66
1	A	285	ARG	NE-CZ-NH2	-6.47	113.38	119.20
1	D	14	GLN	O-C-N	6.46	129.52	122.15
1	D	459	GLN	CA-C-N	6.25	127.65	119.84
1	D	459	GLN	C-N-CA	6.25	127.65	119.84
1	C	79	VAL	N-CA-C	-6.24	105.74	111.67
1	C	142	SER	N-CA-C	6.17	118.33	109.14
1	D	48	PRO	CA-C-N	-6.00	112.34	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	48	PRO	C-N-CA	-6.00	112.34	119.84
1	D	24	GLY	N-CA-C	5.98	118.65	110.69
1	A	459	GLN	CA-C-N	5.95	127.28	119.84
1	A	459	GLN	C-N-CA	5.95	127.28	119.84
1	D	38	VAL	N-CA-C	-5.91	105.95	111.45
1	D	46	ILE	CA-C-N	5.86	126.41	120.38
1	D	46	ILE	C-N-CA	5.86	126.41	120.38
1	D	14	GLN	CA-C-N	-5.77	112.48	120.38
1	D	14	GLN	C-N-CA	-5.77	112.48	120.38
1	A	415	VAL	N-CA-C	5.71	115.55	106.88
1	A	552	ARG	N-CA-C	5.68	117.15	111.07
1	D	5	ASN	CB-CG-ND2	-5.68	107.88	116.40
1	D	478	SER	N-CA-C	5.48	117.42	108.55
1	D	110	ILE	N-CA-C	5.37	113.18	107.76
1	B	544	ASP	N-CA-C	5.37	117.83	111.33
1	A	331	GLU	N-CA-C	-5.32	106.80	113.28
1	A	516	LYS	N-CA-C	5.26	117.16	108.48
1	A	5	ASN	CA-C-N	5.17	126.30	119.84
1	A	5	ASN	C-N-CA	5.17	126.30	119.84
1	B	496	THR	N-CA-C	5.16	117.64	111.71
1	D	48	PRO	N-CA-C	5.11	116.93	110.70
1	D	538	ASN	N-CA-C	5.11	116.84	111.28
1	A	409	GLY	N-CA-C	-5.09	107.24	115.08
1	A	516	LYS	O-C-N	5.05	126.29	120.58
1	B	103	HIS	CA-C-N	-5.03	114.43	119.56
1	B	103	HIS	C-N-CA	-5.03	114.43	119.56
1	D	173	GLU	N-CA-C	5.02	116.70	109.07
1	A	525	ASP	N-CA-C	5.01	117.12	111.11
1	C	384	ILE	N-CA-C	5.01	116.33	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	ASN	Peptide

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	4838	0	4707	146	0
1	B	4937	0	4850	100	0
1	C	4930	0	4860	105	0
1	D	4824	0	4698	151	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	50	0	0	5	0
3	B	96	0	0	3	0
3	C	82	0	0	2	0
3	D	59	0	0	3	0
All	All	19820	0	19115	502	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 (502) 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:D:5:ASN:ND2	1:D:5:ASN:CG	1.69	1.49
1:A:431:LEU:HD13	1:A:438:VAL:HG21	1.30	1.12
1:D:217:LEU:HB3	1:D:218:PRO:HD2	1.30	1.07
1:D:5:ASN:HB2	1:D:6:PRO:HD3	1.44	0.99
1:D:393:MSE:SE	1:D:496:THR:HG21	2.16	0.95
1:A:439:ASP:O	1:A:443:VAL:HG23	1.69	0.93
1:D:275:ALA:H	1:D:310:LYS:HE3	1.34	0.90
1:B:103:HIS:HE1	1:B:105:LEU:HD12	1.38	0.88
1:A:59:ARG:HH21	1:A:80:GLU:HG2	1.38	0.88
1:D:5:ASN:HB2	1:D:6:PRO:CD	2.06	0.86
1:D:217:LEU:HB3	1:D:218:PRO:CD	2.05	0.84
1:C:68:LYS:HB3	1:C:70:ARG:O	1.76	0.84
1:B:582:ASP:OD2	3:B:1044:HOH:O	1.96	0.83
1:D:407:LYS:HG3	1:D:514:VAL:HG13	1.61	0.82
1:B:217:LEU:HB3	1:B:218:PRO:HD2	1.61	0.81
1:B:416:HIS:HB3	1:B:485:PHE:H	1.45	0.81
1:A:115:ALA:O	3:A:1051:HOH:O	1.99	0.80
1:A:318:ASP:HB3	1:A:323:THR:HG21	1.64	0.79
1:D:182:MSE:HE2	1:D:233:ALA:HB1	1.64	0.78
1:A:264:ARG:HA	1:A:267:SER:OG	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:GLU:CD	1:A:632:ARG:HE	1.93	0.76
1:C:182:MSE:HE3	1:C:233:ALA:HB1	1.68	0.76
1:C:451:LYS:O	1:C:455:GLU:HG3	1.85	0.76
1:A:430:LEU:HD22	1:A:471:PHE:HE1	1.51	0.76
1:A:403:VAL:HG13	1:A:407:LYS:HE3	1.68	0.75
1:D:208:MSE:HE3	1:D:310:LYS:HE2	1.69	0.75
1:B:180:THR:HG22	1:B:181:GLU:H	1.52	0.74
1:D:318:ASP:HB3	1:D:323:THR:HB	1.67	0.74
1:D:275:ALA:H	1:D:310:LYS:CE	2.00	0.74
1:D:379:ALA:O	1:D:381:PRO:HD3	1.88	0.74
1:D:416:HIS:HB3	1:D:485:PHE:H	1.51	0.74
1:B:498:PRO:HG3	1:B:508:HIS:NE2	2.01	0.74
1:B:182:MSE:HE3	1:B:233:ALA:HB1	1.70	0.74
1:D:393:MSE:SE	1:D:496:THR:CG2	2.85	0.74
1:C:182:MSE:CE	1:C:233:ALA:HB1	2.18	0.73
1:D:469:ARG:HA	1:D:472:GLN:HE21	1.51	0.73
1:A:620:VAL:O	1:A:621:THR:HB	1.88	0.73
1:B:39:ASP:HB3	1:B:42:LYS:HB3	1.70	0.72
1:B:39:ASP:OD1	1:B:40:ALA:N	2.23	0.71
1:A:55:MSE:SE	1:A:83:LEU:HD12	2.40	0.71
1:B:217:LEU:HB3	1:B:218:PRO:CD	2.21	0.70
1:D:198:VAL:HG22	1:D:199:THR:N	2.06	0.70
1:C:182:MSE:HE3	1:C:233:ALA:CB	2.22	0.70
1:D:93:LYS:HG2	1:D:94:ASN:H	1.55	0.70
1:A:468:ILE:O	1:A:471:PHE:HB2	1.92	0.70
1:D:439:ASP:HB3	1:D:442:GLU:HB2	1.72	0.70
1:B:305:ILE:HG22	1:B:306:GLU:N	2.07	0.69
1:B:76:GLU:HG2	1:B:77:GLU:HG3	1.74	0.68
1:A:29:THR:HG22	1:A:30:GLU:H	1.57	0.68
1:A:214:ALA:HA	1:A:223:GLN:O	1.94	0.68
1:B:318:ASP:HB3	1:B:323:THR:HB	1.75	0.68
1:A:611:GLN:HA	1:A:615:GLU:O	1.93	0.68
1:B:417:MSE:HA	1:B:417:MSE:HE2	1.76	0.68
1:D:484:HIS:CE1	1:D:487:LEU:HG	2.28	0.68
1:B:598:ARG:NH1	3:B:1073:HOH:O	2.27	0.67
1:C:525:ASP:O	1:C:528:THR:HG22	1.94	0.67
1:D:132:MSE:CE	1:D:143:PHE:HD2	2.08	0.67
1:A:411:GLY:HA3	1:A:413:TYR:HE1	1.58	0.67
1:D:463:PHE:CE2	1:D:467:ARG:HD2	2.29	0.67
1:D:453:ARG:HD3	1:D:456:LEU:HD12	1.76	0.67
1:A:397:ASN:HD21	1:A:496:THR:HB	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:VAL:HG21	1:D:311:LEU:CD1	2.25	0.66
1:B:511:LEU:O	1:B:514:VAL:HG12	1.96	0.66
1:A:39:ASP:OD1	1:A:42:LYS:HB2	1.96	0.66
1:B:13:GLN:HG3	1:B:14:GLN:HG2	1.77	0.66
1:C:55:MSE:HE3	1:C:143:PHE:CE2	2.31	0.65
1:D:290:ALA:O	1:D:346:ARG:HD2	1.96	0.65
1:D:431:LEU:HD22	1:D:436:LEU:HD22	1.77	0.65
1:D:355:ALA:HA	1:D:488:GLY:O	1.96	0.65
1:A:319:TRP:HH2	1:A:338:ARG:HG3	1.62	0.64
1:A:411:GLY:HA3	1:A:413:TYR:CE1	2.32	0.64
1:A:53:LYS:HG2	1:A:137:LEU:HD23	1.80	0.64
1:D:423:ASN:HB3	1:D:471:PHE:HD2	1.64	0.63
1:A:38:VAL:HB	1:A:42:LYS:HB3	1.79	0.63
1:D:132:MSE:HE1	1:D:143:PHE:HD2	1.63	0.63
1:B:416:HIS:HB3	1:B:485:PHE:N	2.14	0.63
1:A:604:SER:OG	1:A:607:ASN:HB2	1.99	0.63
1:C:161:TRP:O	1:C:165:LEU:HD12	1.99	0.63
1:D:430:LEU:O	1:D:433:THR:HB	1.99	0.62
1:D:182:MSE:HE2	1:D:233:ALA:CB	2.29	0.61
1:A:571:ILE:HD13	1:A:610:VAL:HG23	1.82	0.61
1:A:499:ILE:HG23	1:A:500:ARG:NE	2.16	0.61
1:C:47:PRO:C	1:C:49:PRO:HD2	2.25	0.61
1:A:340:LEU:HA	1:A:343:ILE:HD12	1.83	0.61
1:D:5:ASN:CB	1:D:6:PRO:CD	2.78	0.61
1:B:512:LYS:HA	1:B:515:ILE:HD12	1.80	0.61
1:C:498:PRO:HG3	1:C:508:HIS:CE1	2.36	0.61
1:A:431:LEU:HD22	1:A:436:LEU:HD23	1.83	0.61
1:A:199:THR:O	1:A:311:LEU:HB2	2.01	0.61
1:C:175:PRO:HG2	1:C:263:PRO:HD3	1.84	0.60
1:C:561:ASP:OD1	3:C:1048:HOH:O	2.15	0.60
1:D:620:VAL:O	1:D:621:THR:HB	2.01	0.60
1:A:371:LYS:HE2	1:A:373:GLU:HB2	1.82	0.60
1:D:524:GLN:C	1:D:526:GLU:H	2.08	0.60
1:B:356:LEU:HD21	1:B:450:CYS:HA	1.84	0.60
1:C:5:ASN:HB2	1:C:6:PRO:CD	2.32	0.60
1:C:174:ALA:HB2	1:C:260:PRO:HG2	1.83	0.59
1:B:208:MSE:HE3	1:B:310:LYS:HG2	1.84	0.59
1:A:294:ILE:H	1:A:294:ILE:HD12	1.67	0.59
1:D:198:VAL:CG2	1:D:199:THR:N	2.65	0.59
1:A:213:PHE:HD2	1:A:225:ILE:HD12	1.66	0.59
1:A:630:GLU:OE2	1:A:632:ARG:NE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ILE:CG2	1:B:306:GLU:N	2.65	0.59
1:C:229:ALA:HB1	1:C:271:CYS:HB3	1.85	0.59
1:B:535:ARG:O	1:B:539:ARG:HG3	2.03	0.59
1:A:568:ILE:HD12	1:A:622:ASP:HB2	1.85	0.59
1:C:439:ASP:O	1:C:443:VAL:HG23	2.03	0.58
1:D:633:MSE:HG2	3:D:1015:HOH:O	2.03	0.58
1:B:389:VAL:O	1:B:393:MSE:HG2	2.03	0.58
1:A:619:LYS:HE2	1:A:622:ASP:OD1	2.03	0.58
1:C:189:ARG:HH21	1:C:280:PRO:HB2	1.69	0.58
1:A:267:SER:O	1:A:272:SER:HB2	2.04	0.58
1:D:257:PHE:CE2	1:D:259:ILE:HD11	2.39	0.58
1:D:507:ASN:O	1:D:511:LEU:HB2	2.04	0.57
1:C:195:LEU:HD22	1:C:213:PHE:CZ	2.38	0.57
1:D:213:PHE:CD2	1:D:225:ILE:HD12	2.40	0.57
1:A:177:GLY:HA2	1:A:241:LEU:HD21	1.85	0.57
1:A:198:VAL:HG12	1:A:309:ALA:HB3	1.87	0.57
1:D:5:ASN:ND2	1:D:5:ASN:CB	2.65	0.57
1:C:329:GLU:O	1:C:329:GLU:HG3	2.03	0.57
1:C:616:THR:HG21	1:C:619:LYS:HE3	1.86	0.57
1:A:367:ILE:HD12	1:A:376:ASP:HB3	1.87	0.56
1:A:403:VAL:O	1:A:407:LYS:HG2	2.05	0.56
1:C:229:ALA:O	1:C:231:PRO:HD3	2.06	0.56
1:C:189:ARG:NH2	1:C:280:PRO:HB2	2.21	0.56
1:A:415:VAL:HG12	1:A:482:GLY:HA3	1.88	0.56
1:B:556:ASP:OD1	1:B:557:LYS:NZ	2.37	0.56
1:B:305:ILE:CG2	1:B:306:GLU:H	2.19	0.56
1:B:113:ARG:CZ	1:B:113:ARG:HB2	2.35	0.55
1:A:439:ASP:OD1	1:A:441:GLU:HB3	2.06	0.55
1:C:296:ASP:O	1:C:298:ILE:N	2.35	0.55
1:C:5:ASN:HB2	1:C:6:PRO:HD3	1.88	0.55
1:D:304:THR:C	1:D:305:ILE:HG12	2.32	0.55
1:D:568:ILE:HD12	1:D:622:ASP:HB2	1.88	0.55
1:B:278:VAL:HG13	1:B:304:THR:HG22	1.89	0.55
1:A:39:ASP:CG	1:A:40:ALA:N	2.64	0.54
1:A:419:PHE:HA	1:A:472:GLN:HA	1.87	0.54
1:D:400:ALA:HB2	1:D:495:TRP:CD1	2.41	0.54
1:D:416:HIS:HB3	1:D:485:PHE:N	2.19	0.54
1:D:408:LEU:HB2	1:D:410:PHE:H	1.72	0.54
1:C:68:LYS:HG3	1:C:70:ARG:H	1.71	0.54
1:D:93:LYS:HG2	1:D:94:ASN:N	2.21	0.54
1:C:174:ALA:CB	1:C:260:PRO:HG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:HIS:HB3	1:A:106:LEU:HD12	1.90	0.54
1:D:23:GLU:O	1:D:38:VAL:HG13	2.07	0.54
1:B:442:GLU:O	1:B:448:GLY:HA3	2.07	0.54
1:B:141:ARG:O	1:B:141:ARG:HG2	2.07	0.54
1:C:431:LEU:HD13	1:C:438:VAL:HG21	1.89	0.54
1:D:171:GLU:CD	1:D:171:GLU:H	2.16	0.54
1:A:294:ILE:HD11	1:A:347:ARG:HH12	1.72	0.53
1:D:198:VAL:HG21	1:D:311:LEU:HD12	1.89	0.53
1:D:208:MSE:HB3	1:D:273:LEU:HB2	1.91	0.53
1:A:477:ILE:HD13	1:A:531:MSE:HE2	1.90	0.53
1:D:173:GLU:O	1:D:248:ARG:NH2	2.36	0.53
1:D:423:ASN:HB3	1:D:471:PHE:CD2	2.44	0.53
1:D:620:VAL:O	1:D:621:THR:CB	2.57	0.53
1:B:463:PHE:CZ	1:B:467:ARG:HD3	2.44	0.53
1:D:89:LYS:HD3	1:D:127:TRP:CZ2	2.43	0.53
1:D:175:PRO:O	1:D:263:PRO:HG3	2.09	0.53
1:A:257:PHE:CE2	1:A:259:ILE:HD11	2.43	0.53
1:A:272:SER:O	1:A:279:ARG:HD2	2.09	0.53
1:A:47:PRO:HB2	1:A:49:PRO:HD2	1.91	0.53
1:C:431:LEU:HD22	1:C:436:LEU:HD23	1.91	0.53
1:A:211:ALA:HB3	1:A:227:ALA:HB3	1.90	0.53
1:C:400:ALA:HB2	1:C:495:TRP:CD1	2.44	0.53
1:A:279:ARG:HH11	1:A:280:PRO:HD2	1.74	0.53
1:C:217:LEU:HD11	1:C:223:GLN:HB2	1.91	0.53
1:B:208:MSE:CE	1:B:310:LYS:HG2	2.39	0.53
1:C:533:GLU:OE1	1:C:536:ARG:NH2	2.42	0.53
1:D:463:PHE:CZ	1:D:467:ARG:HD2	2.43	0.52
1:B:6:PRO:O	1:B:10:GLN:HG3	2.09	0.52
1:C:453:ARG:HH22	1:C:465:ASP:CG	2.17	0.52
1:D:136:PRO:HA	1:D:141:ARG:O	2.09	0.52
1:A:118:LEU:HD21	1:A:122:PHE:CE1	2.45	0.52
1:A:446:LEU:HG	1:A:485:PHE:CZ	2.45	0.52
1:C:548:TRP:HA	1:C:636:ARG:HG2	1.90	0.52
1:C:620:VAL:O	1:C:621:THR:HB	2.09	0.52
1:B:366:PHE:HB3	1:B:368:LEU:HD21	1.92	0.52
1:A:352:HIS:HA	1:A:357:VAL:HG22	1.90	0.52
1:A:611:GLN:NE2	1:A:614:GLY:O	2.42	0.52
1:A:29:THR:HG22	1:A:30:GLU:HG3	1.92	0.52
1:C:5:ASN:HD21	1:C:8:LEU:H	1.57	0.52
1:A:431:LEU:HB3	1:A:436:LEU:HB3	1.92	0.52
1:D:612:ILE:HD12	1:D:617:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLU:O	1:B:322:ASN:CB	2.58	0.52
1:C:208:MSE:HE1	1:C:274:ARG:HA	1.91	0.52
1:C:5:ASN:ND2	1:C:8:LEU:H	2.08	0.51
1:D:251:THR:HG23	1:D:260:PRO:HA	1.91	0.51
1:D:401:ALA:HB1	1:D:491:ALA:HB1	1.92	0.51
1:A:579:ARG:HA	1:A:585:ALA:O	2.11	0.51
1:B:203:ALA:HB2	1:B:312:VAL:HG22	1.91	0.51
1:C:286:MSE:HE1	1:C:396:ALA:HA	1.92	0.51
1:D:438:VAL:HG22	1:D:439:ASP:N	2.26	0.51
1:D:465:ASP:O	1:D:468:ILE:HG12	2.09	0.51
1:A:39:ASP:CG	1:A:40:ALA:H	2.17	0.51
1:A:227:ALA:HB1	1:A:281:VAL:HG11	1.93	0.51
1:A:89:LYS:HB3	1:A:89:LYS:HZ2	1.76	0.51
1:A:366:PHE:CE2	1:A:377:ILE:HD13	2.45	0.51
1:D:115:ALA:HA	1:D:146:GLU:OE2	2.11	0.51
1:C:174:ALA:HB2	1:C:260:PRO:CG	2.41	0.51
1:D:389:VAL:O	1:D:393:MSE:HG2	2.11	0.51
1:B:305:ILE:HG22	1:B:306:GLU:H	1.76	0.51
1:C:188:VAL:HG12	1:C:188:VAL:O	2.11	0.51
1:D:208:MSE:HB2	1:D:273:LEU:H	1.76	0.51
1:B:59:ARG:HG2	1:B:79:VAL:HB	1.92	0.50
1:D:579:ARG:NH2	3:D:1041:HOH:O	2.32	0.50
1:C:438:VAL:CG1	1:C:443:VAL:CG2	2.89	0.50
1:D:632:ARG:HB2	1:D:635:THR:CG2	2.41	0.50
1:A:393:MSE:SE	1:A:496:THR:OG1	2.79	0.50
1:C:417:MSE:HE1	1:C:483:PRO:HD2	1.94	0.50
1:D:408:LEU:HB3	1:D:410:PHE:CD1	2.47	0.50
1:B:275:ALA:HB2	1:B:310:LYS:HG3	1.93	0.50
1:A:330:SER:HB2	1:A:333:ILE:HG12	1.94	0.50
1:B:428:ALA:HA	1:B:438:VAL:HG12	1.94	0.50
1:C:550:TYR:OH	1:C:583:ASN:O	2.24	0.50
1:D:217:LEU:CD1	1:D:287:THR:HG23	2.42	0.50
1:D:286:MSE:SE	1:D:395:ALA:HB1	2.62	0.49
1:A:571:ILE:O	1:A:605:GLN:HA	2.12	0.49
1:D:180:THR:HG22	1:D:181:GLU:H	1.77	0.49
1:A:407:LYS:HG3	1:A:514:VAL:HG22	1.94	0.49
1:C:112:CYS:HA	1:C:145:ALA:O	2.12	0.49
1:D:451:LYS:HA	1:D:454:ARG:HE	1.78	0.49
1:D:477:ILE:HD13	1:D:531:MSE:HE2	1.95	0.49
1:D:524:GLN:C	1:D:526:GLU:N	2.70	0.49
1:A:213:PHE:CD2	1:A:225:ILE:HD12	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ILE:HD11	1:B:266:LEU:CD2	2.43	0.49
1:C:46:ILE:HG22	1:C:50:GLN:HB2	1.94	0.49
1:C:397:ASN:OD1	1:C:494:THR:HA	2.12	0.49
1:A:238:GLY:O	1:A:239:SER:C	2.55	0.49
1:B:419:PHE:HD2	1:B:471:PHE:O	1.94	0.49
1:D:198:VAL:CG2	1:D:199:THR:H	2.26	0.49
1:D:275:ALA:N	1:D:310:LYS:HE3	2.16	0.49
1:B:561:ASP:HB2	1:B:563:ARG:NH2	2.27	0.49
1:C:570:ASP:OD2	1:C:577:ARG:HD3	2.13	0.49
1:D:200:ILE:HG22	1:D:313:TYR:CE2	2.47	0.49
1:A:112:CYS:HA	1:A:145:ALA:O	2.13	0.49
1:A:431:LEU:HD13	1:A:438:VAL:CG2	2.21	0.49
1:B:55:MSE:HE3	1:B:143:PHE:CE2	2.48	0.49
1:B:10:GLN:O	1:B:13:GLN:HG2	2.13	0.48
1:D:213:PHE:HA	1:D:336:GLN:OE1	2.13	0.48
1:A:295:GLU:C	1:A:297:ASN:H	2.21	0.48
1:B:29:THR:C	1:B:31:LYS:H	2.21	0.48
1:A:229:ALA:O	1:A:231:PRO:HD3	2.13	0.48
1:D:274:ARG:HA	1:D:310:LYS:HE2	1.96	0.48
1:B:300:PHE:CD2	1:B:511:LEU:HD22	2.48	0.48
1:A:300:PHE:O	1:A:515:ILE:HG12	2.13	0.48
1:B:323:THR:OG1	1:B:324:GLY:N	2.47	0.48
1:C:55:MSE:HG3	1:C:106:LEU:HD22	1.94	0.48
1:D:22:ALA:HB3	1:D:64:ILE:HD11	1.95	0.48
1:D:182:MSE:CE	1:D:233:ALA:CB	2.92	0.48
1:A:59:ARG:NH2	1:A:80:GLU:HG2	2.17	0.48
1:A:91:GLN:NE2	1:A:98:ALA:HB3	2.29	0.48
1:C:33:PHE:HB3	1:C:48:PRO:HD3	1.95	0.48
1:C:142:SER:HB3	3:C:1055:HOH:O	2.13	0.48
1:D:632:ARG:HB2	1:D:635:THR:HG22	1.96	0.48
1:B:191:ASP:O	1:B:193:THR:N	2.43	0.48
1:D:139:GLY:O	1:D:140:ASP:HB2	2.14	0.48
1:A:135:HIS:CE1	1:A:137:LEU:HB2	2.49	0.47
1:A:389:VAL:O	1:A:393:MSE:HG2	2.14	0.47
1:A:468:ILE:HG13	1:A:469:ARG:N	2.29	0.47
1:C:156:ASP:HB3	1:C:159:VAL:HG23	1.96	0.47
1:A:113:ARG:HD2	3:A:1037:HOH:O	2.14	0.47
1:A:333:ILE:O	1:A:337:VAL:HG23	2.14	0.47
1:A:526:GLU:O	1:A:529:VAL:HB	2.14	0.47
1:B:171:GLU:H	1:B:171:GLU:CD	2.22	0.47
1:B:278:VAL:HA	1:B:305:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:VAL:HB	1:C:149:GLN:HB3	1.96	0.47
1:D:7:LEU:O	1:D:10:GLN:HB2	2.14	0.47
1:D:576:MSE:HE2	1:D:589:ILE:HD12	1.96	0.47
1:A:402:ARG:O	1:A:405:ARG:HB3	2.14	0.47
1:A:442:GLU:HG2	1:A:448:GLY:HA3	1.96	0.47
1:B:177:GLY:O	1:B:178:VAL:C	2.57	0.47
1:A:600:GLU:HG2	1:A:613:LYS:HG3	1.96	0.47
1:B:548:TRP:HA	1:B:636:ARG:HG2	1.96	0.47
1:C:266:LEU:HD23	1:C:270:LEU:HD12	1.96	0.47
1:C:463:PHE:CZ	1:C:467:ARG:HD3	2.50	0.47
1:A:32:GLY:O	1:A:51:MSE:HG3	2.14	0.47
1:B:257:PHE:CE2	1:B:259:ILE:HD11	2.48	0.47
1:A:28:ALA:HB2	1:A:51:MSE:CE	2.45	0.47
1:A:118:LEU:HD21	1:A:122:PHE:HE1	1.79	0.47
1:A:234:TRP:HH2	1:A:280:PRO:CG	2.27	0.47
1:B:438:VAL:HG22	1:B:443:VAL:HG13	1.97	0.47
1:A:250:PHE:HE1	1:A:531:MSE:O	1.97	0.47
1:B:65:HIS:O	1:B:71:GLU:HA	2.15	0.47
1:B:182:MSE:HE2	1:B:182:MSE:HB3	1.84	0.47
1:D:327:GLN:HG2	1:D:328:PRO:HD2	1.95	0.47
1:A:566:ALA:HB1	1:A:578:VAL:HB	1.96	0.47
1:B:93:LYS:O	1:B:94:ASN:C	2.57	0.47
1:D:318:ASP:HB3	1:D:323:THR:CB	2.40	0.47
1:A:404:LEU:HD21	1:A:511:LEU:HD13	1.97	0.47
1:A:416:HIS:CE1	1:A:418:GLY:HA2	2.49	0.47
1:A:620:VAL:O	1:A:621:THR:CB	2.60	0.46
1:D:263:PRO:HB2	1:D:266:LEU:HG	1.96	0.46
1:A:499:ILE:HG23	1:A:500:ARG:HE	1.79	0.46
1:A:556:ASP:OD1	1:A:557:LYS:HE2	2.15	0.46
1:A:540:MSE:HE3	1:A:543:ARG:HH22	1.80	0.46
1:B:66:SER:HB3	1:B:71:GLU:HG2	1.96	0.46
1:C:157:HIS:HE1	1:C:372:GLY:HA3	1.80	0.46
1:D:164:THR:HG21	1:D:544:ASP:HB2	1.98	0.46
1:A:107:LYS:HE3	3:A:1030:HOH:O	2.14	0.46
1:A:416:HIS:O	1:A:485:PHE:HB2	2.16	0.46
1:D:132:MSE:HE2	1:D:143:PHE:HD2	1.79	0.46
1:D:164:THR:CG2	1:D:544:ASP:HB2	2.45	0.46
1:C:232:THR:OG1	1:C:512:LYS:NZ	2.34	0.46
1:D:264:ARG:O	1:D:268:ASP:N	2.40	0.46
1:A:404:LEU:HB2	1:A:413:TYR:OH	2.16	0.46
1:B:19:THR:HG22	1:B:64:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:PHE:CE2	1:C:259:ILE:HD11	2.51	0.46
1:B:94:ASN:O	1:B:95:ASP:C	2.58	0.46
1:D:23:GLU:OE2	1:D:79:VAL:HG21	2.15	0.46
1:D:132:MSE:HE1	1:D:143:PHE:CD2	2.48	0.46
1:D:217:LEU:HD11	1:D:223:GLN:HB2	1.98	0.46
1:D:349:GLU:OE1	1:D:349:GLU:HA	2.16	0.46
1:D:484:HIS:HE1	1:D:487:LEU:HG	1.80	0.46
1:D:524:GLN:O	1:D:526:GLU:N	2.49	0.46
1:B:558:ALA:HB2	1:B:631:VAL:HG23	1.97	0.46
1:D:171:GLU:CD	1:D:534:ARG:HH12	2.23	0.46
1:D:548:TRP:HA	1:D:636:ARG:HG2	1.97	0.46
1:A:28:ALA:HB2	1:A:51:MSE:HE1	1.98	0.46
1:A:286:MSE:HE3	1:A:294:ILE:HG12	1.98	0.46
1:C:184:ASP:HA	1:C:187:LEU:HD11	1.97	0.46
1:D:323:THR:HG21	1:D:326:TRP:O	2.16	0.46
1:A:55:MSE:SE	1:A:83:LEU:CD1	3.14	0.45
1:B:29:THR:C	1:B:31:LYS:N	2.71	0.45
1:C:94:ASN:HB2	1:C:95:ASP:H	1.60	0.45
1:D:636:ARG:N	1:D:636:ARG:HD3	2.31	0.45
1:A:376:ASP:OD1	1:A:377:ILE:N	2.48	0.45
1:A:430:LEU:HD22	1:A:471:PHE:CE1	2.42	0.45
1:A:446:LEU:HD21	1:A:483:PRO:HB2	1.97	0.45
1:C:5:ASN:ND2	1:C:8:LEU:HB3	2.30	0.45
1:C:225:ILE:HA	1:C:284:CYS:O	2.16	0.45
1:C:333:ILE:O	1:C:337:VAL:HG23	2.15	0.45
1:B:416:HIS:ND1	1:B:485:PHE:HB2	2.31	0.45
1:C:5:ASN:HD22	1:C:8:LEU:HB3	1.81	0.45
1:A:231:PRO:HA	1:A:271:CYS:SG	2.56	0.45
1:B:68:LYS:HB2	1:B:69:GLU:H	1.50	0.45
1:C:229:ALA:C	1:C:231:PRO:HD3	2.41	0.45
1:B:506:ILE:O	1:B:510:LEU:HG	2.17	0.45
1:A:305:ILE:HG22	1:A:306:GLU:H	1.81	0.45
1:C:198:VAL:HG21	1:C:311:LEU:HD11	1.99	0.45
1:C:185:GLU:H	1:C:187:LEU:HG	1.80	0.45
1:C:222:LEU:HD12	1:C:346:ARG:HD2	1.99	0.45
1:C:398:ILE:O	1:C:402:ARG:HG3	2.17	0.45
1:C:438:VAL:CG1	1:C:443:VAL:HG21	2.47	0.45
1:C:533:GLU:OE1	1:C:533:GLU:HA	2.17	0.45
1:A:319:TRP:CH2	1:A:338:ARG:HG3	2.47	0.45
1:B:430:LEU:O	1:B:434:HIS:HD2	2.00	0.45
1:B:235:ILE:O	1:B:509:ARG:NH2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:ALA:HB1	1:B:630:GLU:HA	1.99	0.44
1:C:5:ASN:O	1:C:9:ALA:HB2	2.17	0.44
1:D:237:GLU:HB2	1:D:509:ARG:CZ	2.46	0.44
1:D:289:SER:HB3	1:D:290:ALA:H	1.56	0.44
1:D:633:MSE:C	1:D:635:THR:H	2.24	0.44
1:A:548:TRP:HA	1:A:636:ARG:HG2	2.00	0.44
1:A:633:MSE:HG2	3:A:1012:HOH:O	2.16	0.44
1:C:30:GLU:HA	1:C:30:GLU:OE1	2.17	0.44
1:D:137:LEU:HD23	1:D:137:LEU:HA	1.70	0.44
1:C:192:LEU:HB3	1:C:195:LEU:HD12	2.00	0.44
1:C:552:ARG:HA	1:C:633:MSE:HE1	2.00	0.44
1:A:135:HIS:ND1	1:A:137:LEU:HB2	2.31	0.44
1:A:344:CYS:HB2	1:A:388:ILE:HA	1.98	0.44
1:A:221:LYS:HD3	1:A:289:SER:HB3	1.99	0.44
1:D:263:PRO:HB3	1:D:265:GLU:OE1	2.16	0.44
1:D:33:PHE:HB3	1:D:48:PRO:HG3	1.98	0.44
1:D:369:GLY:HA3	1:D:373:GLU:OE1	2.18	0.44
1:A:321:GLU:O	1:A:322:ASN:CB	2.65	0.44
1:D:522:ARG:HA	1:D:523:PRO:HD3	1.90	0.44
1:C:182:MSE:HE3	1:C:233:ALA:HB3	2.00	0.44
1:D:208:MSE:HB2	1:D:273:LEU:N	2.33	0.44
1:D:579:ARG:NE	3:D:1041:HOH:O	2.48	0.44
1:A:423:ASN:HB3	1:A:471:PHE:CD2	2.53	0.43
1:B:373:GLU:HG3	3:B:1055:HOH:O	2.18	0.43
1:C:42:LYS:HE2	1:C:44:TYR:CE1	2.52	0.43
1:C:312:VAL:O	1:C:313:TYR:C	2.61	0.43
1:D:32:GLY:O	1:D:48:PRO:HA	2.18	0.43
1:A:157:HIS:CE1	1:A:552:ARG:NH1	2.87	0.43
1:C:308:LYS:HA	1:C:308:LYS:HD3	1.86	0.43
1:D:295:GLU:C	1:D:297:ASN:N	2.75	0.43
1:D:426:ALA:HB3	1:D:471:PHE:HE2	1.83	0.43
1:A:279:ARG:O	1:A:281:VAL:HG23	2.18	0.43
1:B:113:ARG:NH1	1:B:113:ARG:CB	2.81	0.43
1:C:550:TYR:CD2	1:C:585:ALA:HB2	2.54	0.43
1:D:47:PRO:HA	1:D:48:PRO:HD3	1.87	0.43
1:D:114:ALA:HA	1:D:147:LEU:HB2	2.01	0.43
1:B:10:GLN:HA	1:B:13:GLN:HG2	2.01	0.43
1:B:502:TYR:O	1:B:505:MSE:HB2	2.19	0.43
1:C:411:GLY:O	1:C:479:THR:HA	2.18	0.43
1:B:385:ALA:HA	1:B:388:ILE:HD12	2.01	0.43
1:D:95:ASP:OD1	1:D:95:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ALA:HB3	1:D:499:ILE:HD11	2.00	0.43
1:B:275:ALA:H	1:B:310:LYS:HE3	1.83	0.43
1:B:349:GLU:O	1:B:353:ASN:ND2	2.51	0.43
1:C:111:PRO:HD2	1:C:143:PHE:O	2.19	0.43
1:C:191:ASP:OD1	1:C:193:THR:HB	2.19	0.43
1:D:453:ARG:HD3	1:D:453:ARG:HA	1.72	0.43
1:A:35:PHE:HA	1:A:44:TYR:O	2.18	0.43
1:B:570:ASP:OD1	1:B:570:ASP:N	2.50	0.43
1:C:467:ARG:HA	1:C:467:ARG:NE	2.34	0.43
1:A:157:HIS:HD2	1:A:371:LYS:O	2.02	0.43
1:B:56:HIS:NE2	1:B:105:LEU:HD13	2.34	0.43
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.81	0.43
1:B:182:MSE:HE1	1:B:189:ARG:HH12	1.84	0.43
1:B:502:TYR:CE2	1:B:506:ILE:HD11	2.54	0.42
1:D:619:LYS:N	1:D:622:ASP:OD2	2.50	0.42
1:C:524:GLN:OE1	1:C:527:ILE:HG13	2.19	0.42
1:D:9:ALA:O	1:D:13:GLN:HB2	2.19	0.42
1:A:99:ILE:HG23	1:A:99:ILE:O	2.18	0.42
1:B:363:ASP:O	1:B:379:ALA:HA	2.20	0.42
1:A:217:LEU:HB3	1:A:218:PRO:CD	2.49	0.42
1:C:429:ALA:HA	1:C:432:LYS:HG2	2.02	0.42
1:B:533:GLU:CD	1:B:536:ARG:HH21	2.27	0.42
1:C:359:LYS:HE2	1:C:359:LYS:HB3	1.73	0.42
1:D:356:LEU:HB2	1:D:487:LEU:C	2.45	0.42
1:D:411:GLY:O	1:D:479:THR:HA	2.19	0.42
1:A:160:PRO:O	1:A:545:VAL:HG22	2.20	0.42
1:B:103:HIS:CE1	1:B:105:LEU:HD12	2.30	0.42
1:B:402:ARG:O	1:B:406:ASP:OD2	2.37	0.42
1:C:48:PRO:O	1:C:51:MSE:HB2	2.19	0.42
1:C:171:GLU:CD	1:C:534:ARG:HH12	2.27	0.42
1:C:514:VAL:C	1:C:516:LYS:H	2.27	0.42
1:D:295:GLU:C	1:D:297:ASN:H	2.26	0.42
1:A:324:GLY:O	1:A:325:ASP:HB2	2.19	0.42
1:C:5:ASN:CB	1:C:6:PRO:CD	2.97	0.42
1:D:466:SER:OG	1:D:620:VAL:HG21	2.20	0.42
1:A:600:GLU:CD	1:A:613:LYS:HD2	2.45	0.42
1:B:561:ASP:HB2	1:B:563:ARG:HH21	1.85	0.42
1:D:275:ALA:HB2	1:D:310:LYS:HG3	2.02	0.42
1:B:5:ASN:HB2	1:B:6:PRO:HD2	2.01	0.41
1:C:55:MSE:CE	1:C:143:PHE:CE2	3.01	0.41
1:D:192:LEU:HB3	1:D:195:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:MSE:HE3	1:A:143:PHE:CE2	2.54	0.41
1:A:136:PRO:HA	1:A:140:ASP:O	2.20	0.41
1:A:173:GLU:O	1:A:248:ARG:NH2	2.49	0.41
1:A:280:PRO:HA	1:A:304:THR:HG22	2.01	0.41
1:B:59:ARG:HB3	1:B:80:GLU:HB2	2.01	0.41
1:D:29:THR:O	1:D:30:GLU:C	2.63	0.41
1:D:408:LEU:HB3	1:D:410:PHE:HD1	1.85	0.41
1:A:257:PHE:HE2	1:A:259:ILE:HD11	1.83	0.41
1:A:362:PRO:O	1:A:363:ASP:C	2.62	0.41
1:B:212:LEU:HD21	1:B:393:MSE:CE	2.51	0.41
1:D:243:LYS:HG3	1:D:244:ALA:N	2.35	0.41
1:A:336:GLN:NE2	1:A:336:GLN:HA	2.34	0.41
1:D:416:HIS:ND1	1:D:485:PHE:HB2	2.35	0.41
1:A:221:LYS:NZ	1:A:289:SER:HB3	2.35	0.41
1:C:111:PRO:HB2	1:C:144:TYR:CD1	2.55	0.41
1:C:288:LEU:HD11	1:C:343:ILE:HG23	2.02	0.41
1:D:228:ILE:HG13	1:D:496:THR:HA	2.01	0.41
1:D:318:ASP:C	1:D:323:THR:HB	2.46	0.41
1:D:453:ARG:HG2	1:D:453:ARG:HH11	1.85	0.41
1:A:288:LEU:HD23	1:A:294:ILE:HG13	2.03	0.41
1:B:350:TRP:CD1	1:B:354:HIS:HD2	2.38	0.41
1:A:59:ARG:HB3	1:A:80:GLU:HB3	2.03	0.41
1:B:200:ILE:HG12	1:B:311:LEU:HD12	2.03	0.41
1:D:169:ASN:HD22	1:D:169:ASN:HA	1.68	0.41
1:D:407:LYS:HG3	1:D:514:VAL:CG1	2.39	0.41
1:D:633:MSE:C	1:D:635:THR:N	2.79	0.41
1:A:287:THR:H	1:A:294:ILE:HG23	1.85	0.41
1:C:10:GLN:O	1:C:11:LEU:C	2.64	0.41
1:C:83:LEU:HD13	1:C:86:PHE:CD2	2.56	0.41
1:A:89:LYS:NZ	1:A:125:GLY:O	2.54	0.41
1:B:41:GLN:OE1	1:B:41:GLN:HA	2.19	0.41
1:B:268:ASP:O	1:B:272:SER:HB3	2.21	0.41
1:B:410:PHE:CD1	1:B:410:PHE:C	2.98	0.41
1:C:271:CYS:O	1:C:272:SER:C	2.64	0.41
1:D:90:VAL:CG1	1:D:91:GLN:N	2.84	0.41
1:D:211:ALA:O	1:D:212:LEU:HD23	2.21	0.41
1:D:256:GLY:HA3	1:D:368:LEU:HD12	2.03	0.41
1:D:464:LEU:HD23	1:D:464:LEU:N	2.35	0.41
1:C:5:ASN:HD22	1:C:5:ASN:N	2.19	0.41
1:C:118:LEU:HD12	1:C:118:LEU:HA	1.97	0.41
1:D:56:HIS:CE1	1:D:105:LEU:HD13	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:HIS:CD2	1:A:371:LYS:O	2.74	0.40
1:A:442:GLU:O	1:A:443:VAL:C	2.63	0.40
1:D:198:VAL:HG22	1:D:199:THR:H	1.84	0.40
1:D:218:PRO:O	1:D:219:ASP:C	2.63	0.40
1:A:29:THR:C	1:A:31:LYS:H	2.29	0.40
1:A:46:ILE:HA	1:A:47:PRO:HD3	1.78	0.40
1:A:95:ASP:HB2	3:A:1039:HOH:O	2.21	0.40
1:A:288:LEU:CD2	1:A:294:ILE:HG13	2.52	0.40
1:A:602:VAL:O	1:A:610:VAL:HA	2.21	0.40
1:B:534:ARG:HD3	1:B:534:ARG:HA	1.88	0.40
1:C:264:ARG:HA	1:C:267:SER:OG	2.21	0.40
1:D:203:ALA:O	1:D:204:SER:C	2.64	0.40
1:D:271:CYS:O	1:D:272:SER:C	2.64	0.40
1:D:502:TYR:CD1	1:D:505:MSE:HE2	2.55	0.40
1:A:135:HIS:HA	1:A:136:PRO:HD2	1.91	0.40
1:B:498:PRO:HG3	1:B:508:HIS:CE1	2.55	0.40
1:C:7:LEU:O	1:C:8:LEU:C	2.64	0.40
1:C:282:LEU:HD12	1:C:283:ALA:H	1.87	0.40
1:D:199:THR:HG22	1:D:210:ASP:O	2.21	0.40
1:D:498:PRO:HB2	1:D:505:MSE:HG2	2.03	0.40
1:B:160:PRO:O	1:B:545:VAL:HG22	2.21	0.40
1:D:304:THR:O	1:D:305:ILE:HG12	2.22	0.40
1:A:273:LEU:HD22	1:A:281:VAL:HG22	2.02	0.40
1:A:568:ILE:HD13	1:A:618:TYR:HB3	2.03	0.40
1:B:183:LEU:HD11	1:B:236:ALA:HB2	2.02	0.40
1:B:187:LEU:HD22	1:B:189:ARG:HH21	1.87	0.40
1:B:411:GLY:O	1:B:413:TYR:HD1	2.04	0.40
1:C:55:MSE:HE3	1:C:55:MSE:HB2	1.92	0.40
1:C:55:MSE:CG	1:C:106:LEU:HD22	2.52	0.40
1:C:400:ALA:CB	1:C:495:TRP:CD1	3.05	0.40
1:C:539:ARG:HG3	1:C:539:ARG:HH11	1.86	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	632/644 (98%)	546 (86%)	68 (11%)	18 (3%)	4	2
1	B	632/644 (98%)	577 (91%)	47 (7%)	8 (1%)	9	8
1	C	632/644 (98%)	580 (92%)	45 (7%)	7 (1%)	11	11
1	D	632/644 (98%)	557 (88%)	61 (10%)	14 (2%)	5	3
All	All	2528/2576 (98%)	2260 (89%)	221 (9%)	47 (2%)	6	5

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	218	PRO
1	A	274	ARG
1	A	322	ASN
1	A	325	ASP
1	A	437	HIS
1	A	443	VAL
1	B	322	ASN
1	C	297	ASN
1	D	31	LYS
1	D	221	LYS
1	D	289	SER
1	D	433	THR
1	A	115	ALA
1	A	123	LYS
1	A	187	LEU
1	A	621	THR
1	C	42	LYS
1	C	289	SER
1	C	322	ASN
1	D	68	LYS
1	D	219	ASP
1	D	469	ARG
1	D	525	ASP
1	D	621	THR
1	A	190	GLU
1	A	239	SER
1	A	441	GLU
1	B	15	LEU
1	B	192	LEU

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Mol	Chain	Res	Type
1	B	272	SER
1	C	94	ASN
1	C	182	MSE
1	D	237	GLU
1	D	465	ASP
1	A	39	ASP
1	A	193	THR
1	A	296	ASP
1	B	30	GLU
1	D	220	ASP
1	B	94	ASN
1	B	229	ALA
1	C	188	VAL
1	D	6	PRO
1	A	361	ARG
1	B	255	PRO
1	D	388	ILE

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	480/522 (92%)	438 (91%)	42 (9%)	9	10
1	B	505/522 (97%)	484 (96%)	21 (4%)	26	35
1	C	504/522 (97%)	479 (95%)	25 (5%)	22	27
1	D	479/522 (92%)	453 (95%)	26 (5%)	20	24
All	All	1968/2088 (94%)	1854 (94%)	114 (6%)	18	22

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	7	LEU
1	A	17	SER
1	A	18	GLN

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Mol	Chain	Res	Type
1	A	19	THR
1	A	29	THR
1	A	45	PHE
1	A	71	GLU
1	A	76	GLU
1	A	89	LYS
1	A	91	GLN
1	A	94	ASN
1	A	131	GLU
1	A	133	ARG
1	A	137	LEU
1	A	141	ARG
1	A	167	ARG
1	A	172	LYS
1	A	178	VAL
1	A	187	LEU
1	A	237	GLU
1	A	258	ASN
1	A	285	ARG
1	A	293	THR
1	A	294	ILE
1	A	305	ILE
1	A	314	ASP
1	A	329	GLU
1	A	336	GLN
1	A	344	CYS
1	A	357	VAL
1	A	358	PHE
1	A	359	LYS
1	A	417	MSE
1	A	444	LEU
1	A	445	THR
1	A	476	GLU
1	A	511	LEU
1	A	531	MSE
1	A	557	LYS
1	A	582	ASP
1	A	634	GLU
1	B	29	THR
1	B	70	ARG
1	B	89	LYS
1	B	96	ARG

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Mol	Chain	Res	Type
1	B	113	ARG
1	B	141	ARG
1	B	180	THR
1	B	208	MSE
1	B	210	ASP
1	B	232	THR
1	B	278	VAL
1	B	288	LEU
1	B	289	SER
1	B	330	SER
1	B	360	ASP
1	B	367	ILE
1	B	405	ARG
1	B	410	PHE
1	B	472	GLN
1	B	496	THR
1	B	634	GLU
1	C	5	ASN
1	C	10	GLN
1	C	12	LYS
1	C	84	THR
1	C	94	ASN
1	C	113	ARG
1	C	124	GLU
1	C	159	VAL
1	C	178	VAL
1	C	198	VAL
1	C	219	ASP
1	C	267	SER
1	C	268	ASP
1	C	304	THR
1	C	317	SER
1	C	346	ARG
1	C	476	GLU
1	C	496	THR
1	C	497	SER
1	C	505	MSE
1	C	524	GLN
1	C	527	ILE
1	C	536	ARG
1	C	567	GLU
1	C	581	VAL

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Mol	Chain	Res	Type
1	D	7	LEU
1	D	8	LEU
1	D	43	SER
1	D	70	ARG
1	D	72	SER
1	D	74	GLU
1	D	89	LYS
1	D	95	ASP
1	D	123	LYS
1	D	131	GLU
1	D	180	THR
1	D	187	LEU
1	D	202	SER
1	D	232	THR
1	D	261	MSE
1	D	267	SER
1	D	294	ILE
1	D	305	ILE
1	D	349	GLU
1	D	354	HIS
1	D	373	GLU
1	D	430	LEU
1	D	436	LEU
1	D	453	ARG
1	D	464	LEU
1	D	602	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	18	GLN
1	A	91	GLN
1	A	94	ASN
1	A	157	HIS
1	A	223	GLN
1	A	538	ASN
1	A	605	GLN
1	B	149	GLN
1	B	252	ASN
1	B	315	GLN
1	B	354	HIS

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Mol	Chain	Res	Type
1	B	434	HIS
1	B	472	GLN
1	B	507	ASN
1	B	607	ASN
1	C	5	ASN
1	C	157	HIS
1	C	252	ASN
1	C	315	GLN
1	C	353	ASN
1	C	354	HIS
1	C	472	GLN
1	C	611	GLN
1	D	5	ASN
1	D	13	GLN
1	D	169	ASN
1	D	297	ASN
1	D	342	GLN
1	D	437	HIS
1	D	472	GLN
1	D	607	ASN
1	D	611	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	622/644 (96%)	-1.17	1 (0%) 91 92	31, 57, 80, 89	0
1	B	622/644 (96%)	-1.29	0 100 100	33, 54, 74, 84	0
1	C	622/644 (96%)	-1.32	0 100 100	41, 53, 72, 84	0
1	D	622/644 (96%)	-1.25	0 100 100	31, 53, 74, 85	0
All	All	2488/2576 (96%)	-1.26	1 (0%) 100 100	31, 54, 76, 89	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	LEU	3.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	A	1001	1/1	0.98	0.03	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	B	1002	1/1	0.99	0.03	83,83,83,83	0
2	MN	C	1003	1/1	0.99	0.03	88,88,88,88	0
2	MN	D	1004	1/1	0.99	0.02	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.