



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:11 PM UTC

PDB ID : 6DHI / pdb_00006dhi
Title : Butelase 1: Auto-Catalytic Cleavage as an Evolutionary Constraint for Macro-cyclizing Endopeptidases
Authors : Bond, C.S.; Haywood, J.
Deposited on : 2018-05-20
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
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

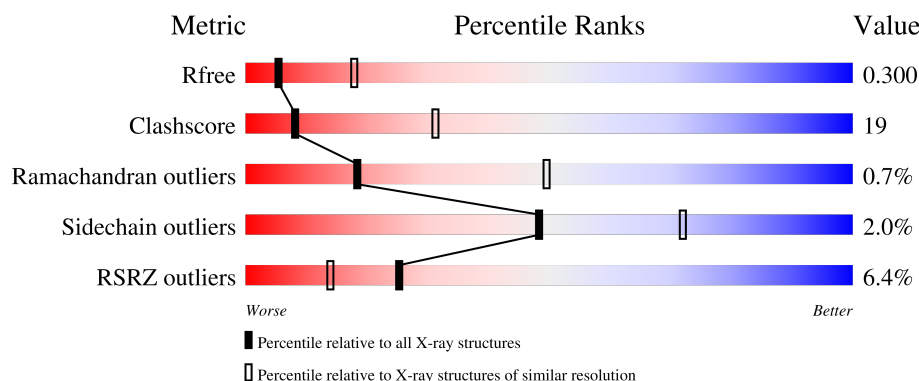
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	473	5% 65% 21% • 12%
1	B	473	7% 64% 24% • 9%
1	C	473	5% 63% 26% • 9%
1	D	473	5% 66% 18% • 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SNN	B	164	-	-	X	-
1	SNN	C	164	-	-	X	-
1	SNN	D	164	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13184 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 Asparaginyl endopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3258	2061	559	618	20			
1	B	431	Total	C	N	O	S	0	0	0
			3366	2130	577	639	20			
1	C	429	Total	C	N	O	S	0	0	0
			3355	2124	575	636	20			
1	D	406	Total	C	N	O	S	0	0	0
			3179	2016	545	598	20			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	expression tag	UNP A0A060D9Z7
A	10	ARG	-	expression tag	UNP A0A060D9Z7
A	11	GLY	-	expression tag	UNP A0A060D9Z7
A	12	SER	-	expression tag	UNP A0A060D9Z7
A	13	HIS	-	expression tag	UNP A0A060D9Z7
A	14	HIS	-	expression tag	UNP A0A060D9Z7
A	15	HIS	-	expression tag	UNP A0A060D9Z7
A	16	HIS	-	expression tag	UNP A0A060D9Z7
A	17	HIS	-	expression tag	UNP A0A060D9Z7
A	18	HIS	-	expression tag	UNP A0A060D9Z7
A	19	GLY	-	expression tag	UNP A0A060D9Z7
A	20	SER	-	expression tag	UNP A0A060D9Z7
A	164	SNN	ASP	conflict	UNP A0A060D9Z7
A	447	LEU	-	expression tag	UNP A0A060D9Z7
A	448	CYS	-	expression tag	UNP A0A060D9Z7
A	449	ASN	-	expression tag	UNP A0A060D9Z7
A	450	ALA	-	expression tag	UNP A0A060D9Z7
A	451	GLY	-	expression tag	UNP A0A060D9Z7
A	452	ILE	-	expression tag	UNP A0A060D9Z7
A	453	ARG	-	expression tag	UNP A0A060D9Z7
A	454	LYS	-	expression tag	UNP A0A060D9Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	455	GLU	-	expression tag	UNP A0A060D9Z7
A	456	GLN	-	expression tag	UNP A0A060D9Z7
A	457	MET	-	expression tag	UNP A0A060D9Z7
A	458	ALA	-	expression tag	UNP A0A060D9Z7
A	459	GLU	-	expression tag	UNP A0A060D9Z7
A	460	ALA	-	expression tag	UNP A0A060D9Z7
A	461	SER	-	expression tag	UNP A0A060D9Z7
A	462	ALA	-	expression tag	UNP A0A060D9Z7
A	463	GLN	-	expression tag	UNP A0A060D9Z7
A	464	ALA	-	expression tag	UNP A0A060D9Z7
A	465	CYS	-	expression tag	UNP A0A060D9Z7
A	466	VAL	-	expression tag	UNP A0A060D9Z7
A	467	SER	-	expression tag	UNP A0A060D9Z7
A	468	ILE	-	expression tag	UNP A0A060D9Z7
A	469	PRO	-	expression tag	UNP A0A060D9Z7
A	470	ASP	-	expression tag	UNP A0A060D9Z7
A	471	ASN	-	expression tag	UNP A0A060D9Z7
A	472	PRO	-	expression tag	UNP A0A060D9Z7
A	473	TRP	-	expression tag	UNP A0A060D9Z7
A	474	SER	-	expression tag	UNP A0A060D9Z7
A	475	SER	-	expression tag	UNP A0A060D9Z7
A	476	LEU	-	expression tag	UNP A0A060D9Z7
A	477	HIS	-	expression tag	UNP A0A060D9Z7
A	478	ALA	-	expression tag	UNP A0A060D9Z7
A	479	GLY	-	expression tag	UNP A0A060D9Z7
A	480	PHE	-	expression tag	UNP A0A060D9Z7
A	481	SER	-	expression tag	UNP A0A060D9Z7
B	9	MET	-	expression tag	UNP A0A060D9Z7
B	10	ARG	-	expression tag	UNP A0A060D9Z7
B	11	GLY	-	expression tag	UNP A0A060D9Z7
B	12	SER	-	expression tag	UNP A0A060D9Z7
B	13	HIS	-	expression tag	UNP A0A060D9Z7
B	14	HIS	-	expression tag	UNP A0A060D9Z7
B	15	HIS	-	expression tag	UNP A0A060D9Z7
B	16	HIS	-	expression tag	UNP A0A060D9Z7
B	17	HIS	-	expression tag	UNP A0A060D9Z7
B	18	HIS	-	expression tag	UNP A0A060D9Z7
B	19	GLY	-	expression tag	UNP A0A060D9Z7
B	20	SER	-	expression tag	UNP A0A060D9Z7
B	164	SNN	ASP	conflict	UNP A0A060D9Z7
B	447	LEU	-	expression tag	UNP A0A060D9Z7
B	448	CYS	-	expression tag	UNP A0A060D9Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	449	ASN	-	expression tag	UNP A0A060D9Z7
B	450	ALA	-	expression tag	UNP A0A060D9Z7
B	451	GLY	-	expression tag	UNP A0A060D9Z7
B	452	ILE	-	expression tag	UNP A0A060D9Z7
B	453	ARG	-	expression tag	UNP A0A060D9Z7
B	454	LYS	-	expression tag	UNP A0A060D9Z7
B	455	GLU	-	expression tag	UNP A0A060D9Z7
B	456	GLN	-	expression tag	UNP A0A060D9Z7
B	457	MET	-	expression tag	UNP A0A060D9Z7
B	458	ALA	-	expression tag	UNP A0A060D9Z7
B	459	GLU	-	expression tag	UNP A0A060D9Z7
B	460	ALA	-	expression tag	UNP A0A060D9Z7
B	461	SER	-	expression tag	UNP A0A060D9Z7
B	462	ALA	-	expression tag	UNP A0A060D9Z7
B	463	GLN	-	expression tag	UNP A0A060D9Z7
B	464	ALA	-	expression tag	UNP A0A060D9Z7
B	465	CYS	-	expression tag	UNP A0A060D9Z7
B	466	VAL	-	expression tag	UNP A0A060D9Z7
B	467	SER	-	expression tag	UNP A0A060D9Z7
B	468	ILE	-	expression tag	UNP A0A060D9Z7
B	469	PRO	-	expression tag	UNP A0A060D9Z7
B	470	ASP	-	expression tag	UNP A0A060D9Z7
B	471	ASN	-	expression tag	UNP A0A060D9Z7
B	472	PRO	-	expression tag	UNP A0A060D9Z7
B	473	TRP	-	expression tag	UNP A0A060D9Z7
B	474	SER	-	expression tag	UNP A0A060D9Z7
B	475	SER	-	expression tag	UNP A0A060D9Z7
B	476	LEU	-	expression tag	UNP A0A060D9Z7
B	477	HIS	-	expression tag	UNP A0A060D9Z7
B	478	ALA	-	expression tag	UNP A0A060D9Z7
B	479	GLY	-	expression tag	UNP A0A060D9Z7
B	480	PHE	-	expression tag	UNP A0A060D9Z7
B	481	SER	-	expression tag	UNP A0A060D9Z7
C	9	MET	-	expression tag	UNP A0A060D9Z7
C	10	ARG	-	expression tag	UNP A0A060D9Z7
C	11	GLY	-	expression tag	UNP A0A060D9Z7
C	12	SER	-	expression tag	UNP A0A060D9Z7
C	13	HIS	-	expression tag	UNP A0A060D9Z7
C	14	HIS	-	expression tag	UNP A0A060D9Z7
C	15	HIS	-	expression tag	UNP A0A060D9Z7
C	16	HIS	-	expression tag	UNP A0A060D9Z7
C	17	HIS	-	expression tag	UNP A0A060D9Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	HIS	-	expression tag	UNP A0A060D9Z7
C	19	GLY	-	expression tag	UNP A0A060D9Z7
C	20	SER	-	expression tag	UNP A0A060D9Z7
C	164	SNN	ASP	conflict	UNP A0A060D9Z7
C	447	LEU	-	expression tag	UNP A0A060D9Z7
C	448	CYS	-	expression tag	UNP A0A060D9Z7
C	449	ASN	-	expression tag	UNP A0A060D9Z7
C	450	ALA	-	expression tag	UNP A0A060D9Z7
C	451	GLY	-	expression tag	UNP A0A060D9Z7
C	452	ILE	-	expression tag	UNP A0A060D9Z7
C	453	ARG	-	expression tag	UNP A0A060D9Z7
C	454	LYS	-	expression tag	UNP A0A060D9Z7
C	455	GLU	-	expression tag	UNP A0A060D9Z7
C	456	GLN	-	expression tag	UNP A0A060D9Z7
C	457	MET	-	expression tag	UNP A0A060D9Z7
C	458	ALA	-	expression tag	UNP A0A060D9Z7
C	459	GLU	-	expression tag	UNP A0A060D9Z7
C	460	ALA	-	expression tag	UNP A0A060D9Z7
C	461	SER	-	expression tag	UNP A0A060D9Z7
C	462	ALA	-	expression tag	UNP A0A060D9Z7
C	463	GLN	-	expression tag	UNP A0A060D9Z7
C	464	ALA	-	expression tag	UNP A0A060D9Z7
C	465	CYS	-	expression tag	UNP A0A060D9Z7
C	466	VAL	-	expression tag	UNP A0A060D9Z7
C	467	SER	-	expression tag	UNP A0A060D9Z7
C	468	ILE	-	expression tag	UNP A0A060D9Z7
C	469	PRO	-	expression tag	UNP A0A060D9Z7
C	470	ASP	-	expression tag	UNP A0A060D9Z7
C	471	ASN	-	expression tag	UNP A0A060D9Z7
C	472	PRO	-	expression tag	UNP A0A060D9Z7
C	473	TRP	-	expression tag	UNP A0A060D9Z7
C	474	SER	-	expression tag	UNP A0A060D9Z7
C	475	SER	-	expression tag	UNP A0A060D9Z7
C	476	LEU	-	expression tag	UNP A0A060D9Z7
C	477	HIS	-	expression tag	UNP A0A060D9Z7
C	478	ALA	-	expression tag	UNP A0A060D9Z7
C	479	GLY	-	expression tag	UNP A0A060D9Z7
C	480	PHE	-	expression tag	UNP A0A060D9Z7
C	481	SER	-	expression tag	UNP A0A060D9Z7
D	9	MET	-	expression tag	UNP A0A060D9Z7
D	10	ARG	-	expression tag	UNP A0A060D9Z7
D	11	GLY	-	expression tag	UNP A0A060D9Z7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	12	SER	-	expression tag	UNP A0A060D9Z7
D	13	HIS	-	expression tag	UNP A0A060D9Z7
D	14	HIS	-	expression tag	UNP A0A060D9Z7
D	15	HIS	-	expression tag	UNP A0A060D9Z7
D	16	HIS	-	expression tag	UNP A0A060D9Z7
D	17	HIS	-	expression tag	UNP A0A060D9Z7
D	18	HIS	-	expression tag	UNP A0A060D9Z7
D	19	GLY	-	expression tag	UNP A0A060D9Z7
D	20	SER	-	expression tag	UNP A0A060D9Z7
D	164	SNN	ASP	conflict	UNP A0A060D9Z7
D	447	LEU	-	expression tag	UNP A0A060D9Z7
D	448	CYS	-	expression tag	UNP A0A060D9Z7
D	449	ASN	-	expression tag	UNP A0A060D9Z7
D	450	ALA	-	expression tag	UNP A0A060D9Z7
D	451	GLY	-	expression tag	UNP A0A060D9Z7
D	452	ILE	-	expression tag	UNP A0A060D9Z7
D	453	ARG	-	expression tag	UNP A0A060D9Z7
D	454	LYS	-	expression tag	UNP A0A060D9Z7
D	455	GLU	-	expression tag	UNP A0A060D9Z7
D	456	GLN	-	expression tag	UNP A0A060D9Z7
D	457	MET	-	expression tag	UNP A0A060D9Z7
D	458	ALA	-	expression tag	UNP A0A060D9Z7
D	459	GLU	-	expression tag	UNP A0A060D9Z7
D	460	ALA	-	expression tag	UNP A0A060D9Z7
D	461	SER	-	expression tag	UNP A0A060D9Z7
D	462	ALA	-	expression tag	UNP A0A060D9Z7
D	463	GLN	-	expression tag	UNP A0A060D9Z7
D	464	ALA	-	expression tag	UNP A0A060D9Z7
D	465	CYS	-	expression tag	UNP A0A060D9Z7
D	466	VAL	-	expression tag	UNP A0A060D9Z7
D	467	SER	-	expression tag	UNP A0A060D9Z7
D	468	ILE	-	expression tag	UNP A0A060D9Z7
D	469	PRO	-	expression tag	UNP A0A060D9Z7
D	470	ASP	-	expression tag	UNP A0A060D9Z7
D	471	ASN	-	expression tag	UNP A0A060D9Z7
D	472	PRO	-	expression tag	UNP A0A060D9Z7
D	473	TRP	-	expression tag	UNP A0A060D9Z7
D	474	SER	-	expression tag	UNP A0A060D9Z7
D	475	SER	-	expression tag	UNP A0A060D9Z7
D	476	LEU	-	expression tag	UNP A0A060D9Z7
D	477	HIS	-	expression tag	UNP A0A060D9Z7
D	478	ALA	-	expression tag	UNP A0A060D9Z7

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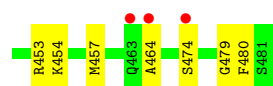
Chain	Residue	Modelled	Actual	Comment	Reference
D	479	GLY	-	expression tag	UNP A0A060D9Z7
D	480	PHE	-	expression tag	UNP A0A060D9Z7
D	481	SER	-	expression tag	UNP A0A060D9Z7

- Molecule 2 is water.

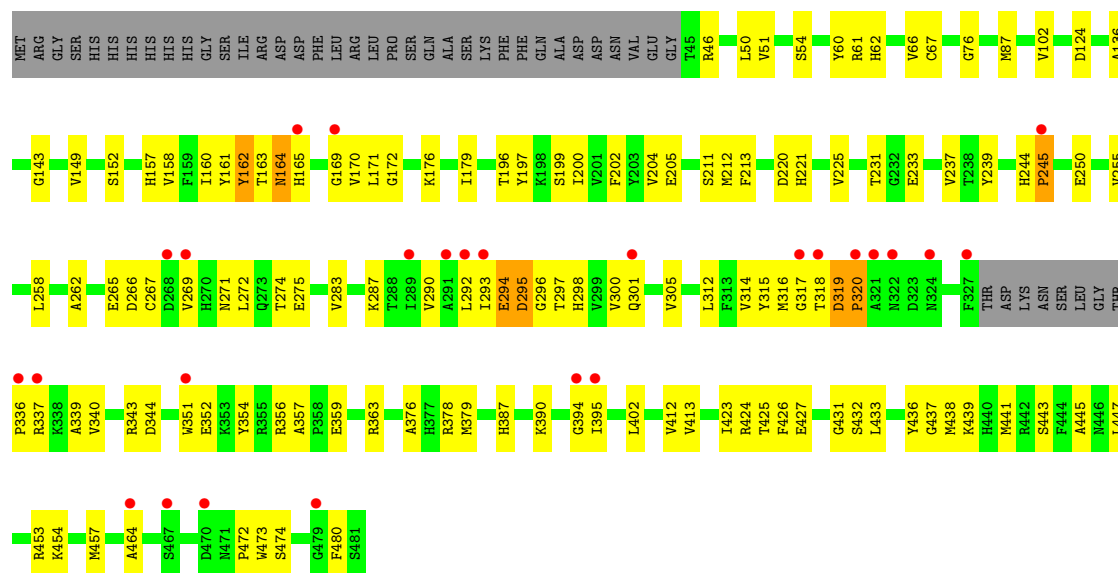
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	6	Total O 6 6	0	0
2	C	7	Total O 7 7	0	0
2	D	3	Total O 3 3	0	0

- Molecule 1: Asparaginyl endopeptidase

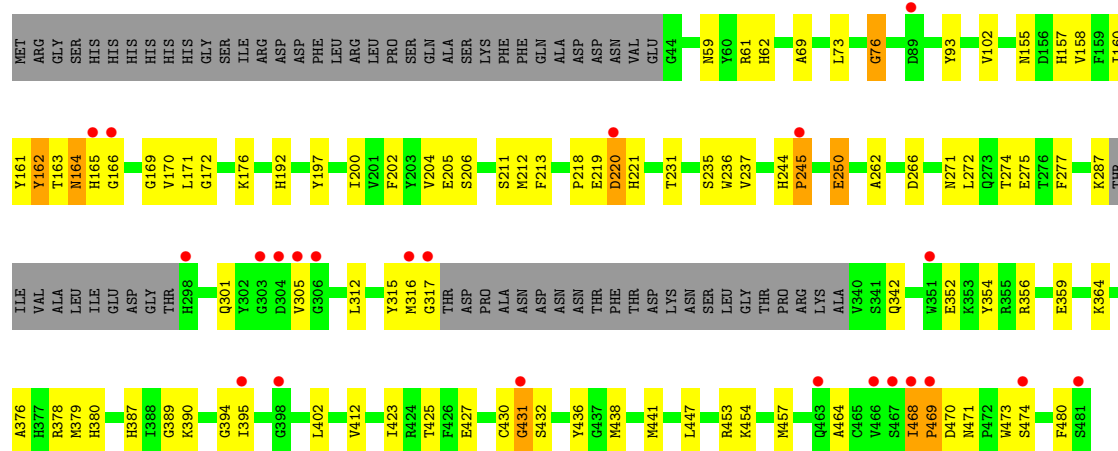




• Molecule 1: Asparaginyl endopeptidase



• Molecule 1: Asparaginyl endopeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.36Å 147.69Å 183.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 3.10 49.42 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.42-3.10) 99.9 (49.42-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.274 , 0.309 0.270 , 0.300	Depositor DCC
R_{free} test set	1844 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13184	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.73	2/3334 (0.1%)	0.93	6/4519 (0.1%)
1	B	0.73	1/3445 (0.0%)	0.90	2/4672 (0.0%)
1	C	0.68	0/3434	0.90	1/4656 (0.0%)
1	D	0.76	3/3254 (0.1%)	0.94	1/4407 (0.0%)
All	All	0.72	6/13467 (0.0%)	0.92	10/18254 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	431	GLY	C-O	-6.52	1.20	1.24
1	A	287	LYS	CA-C	6.43	1.61	1.52
1	D	469	PRO	N-CA	-5.44	1.40	1.47
1	D	431	GLY	C-O	-5.34	1.20	1.23
1	B	244	HIS	CA-CB	5.07	1.61	1.53
1	D	220	ASP	CG-OD1	-5.07	1.15	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	MET	CA-C-N	-7.91	111.32	120.89
1	A	173	MET	C-N-CA	-7.91	111.32	120.89
1	C	339	ALA	N-CA-C	6.61	118.90	108.79
1	D	76	GLY	N-CA-C	6.19	121.48	114.67
1	B	173	MET	CA-C-N	-6.08	113.71	120.45
1	B	173	MET	C-N-CA	-6.08	113.71	120.45
1	A	288	THR	CA-C-O	-5.94	114.97	121.87
1	A	287	LYS	CA-C-O	5.57	126.38	119.97
1	A	58	VAL	CB-CA-C	-5.52	104.81	112.04
1	A	288	THR	N-CA-C	5.16	117.34	110.53

There are no chirality outliers.

There are no planarity outliers.

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	3258	0	3114	103	0
1	B	3366	0	3227	159	0
1	C	3355	0	3218	149	0
1	D	3179	0	3046	105	0
2	A	10	0	0	0	0
2	B	6	0	0	0	0
2	C	7	0	0	0	0
2	D	3	0	0	0	0
All	All	13184	0	12605	499	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 19.

All (499) 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:C:163:THR:CG2	1:C:205:GLU:HB3	1.58	1.33
1:A:163:THR:HG22	1:A:205:GLU:CB	1.59	1.30
1:A:163:THR:CG2	1:A:205:GLU:HB3	1.68	1.23
1:D:162:TYR:CE1	1:D:171:LEU:HD22	1.78	1.16
1:D:163:THR:HG22	1:D:205:GLU:HB3	1.14	1.14
1:C:163:THR:HG22	1:C:205:GLU:CB	1.79	1.11
1:B:192:HIS:CE1	1:B:221:HIS:CD2	2.39	1.11
1:D:430:CYS:O	1:D:468:ILE:HG21	1.53	1.09
1:B:163:THR:HG22	1:B:205:GLU:HB3	1.36	1.05
1:D:163:THR:HG22	1:D:205:GLU:CB	1.90	1.01
1:B:283:VAL:HG12	1:B:287:LYS:HE2	1.41	1.00
1:B:335:THR:OG1	1:B:336:PRO:HD2	1.61	0.99
1:D:163:THR:CG2	1:D:205:GLU:HB3	1.91	0.99
1:C:319:ASP:HB2	1:C:320:PRO:CD	1.93	0.98
1:C:262:ALA:HB1	1:C:287:LYS:HD2	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HD12	1:A:317:GLY:C	1.92	0.94
1:C:163:THR:HG22	1:C:205:GLU:HB3	0.95	0.94
1:B:253:VAL:HG13	1:B:349:HIS:CD2	2.03	0.91
1:B:160:ILE:HB	1:B:202:PHE:HD1	1.36	0.90
1:C:283:VAL:HG12	1:C:287:LYS:HE2	1.53	0.90
1:B:192:HIS:CE1	1:B:221:HIS:HD2	1.89	0.89
1:C:319:ASP:HB2	1:C:320:PRO:HD2	1.54	0.89
1:B:233:GLU:CD	1:B:297:THR:H	1.82	0.87
1:B:271:ASN:HD22	1:B:274:THR:HG23	1.38	0.87
1:C:294:GLU:OE2	1:C:295:ASP:N	2.08	0.87
1:C:199:SER:HB3	1:C:315:TYR:OH	1.75	0.87
1:B:340:VAL:HG12	1:B:341:SER:N	1.89	0.86
1:D:387:HIS:ND1	1:D:464:ALA:HB2	1.91	0.86
1:B:340:VAL:HG12	1:B:341:SER:H	1.39	0.85
1:D:430:CYS:O	1:D:468:ILE:CG2	2.23	0.85
1:C:163:THR:CG2	1:C:205:GLU:CB	2.49	0.85
1:B:192:HIS:NE2	1:B:221:HIS:CD2	2.45	0.84
1:B:233:GLU:HB3	1:B:297:THR:HG22	1.59	0.84
1:A:262:ALA:HB1	1:A:287:LYS:HD2	1.59	0.84
1:A:271:ASN:HD22	1:A:274:THR:HG23	1.43	0.84
1:D:162:TYR:HE1	1:D:171:LEU:HD22	1.40	0.83
1:C:294:GLU:CD	1:C:295:ASP:H	1.85	0.83
1:D:164:SNN:C5	1:D:165:HIS:O	2.20	0.83
1:B:236:TRP:CE2	1:B:290:VAL:HG21	2.14	0.82
1:B:262:ALA:HB1	1:B:287:LYS:HD2	1.61	0.82
1:B:390:LYS:HA	1:B:394:GLY:O	1.78	0.81
1:C:244:HIS:CE1	1:D:250:GLU:HG3	2.14	0.81
1:D:453:ARG:NH2	1:D:454:LYS:CB	2.44	0.81
1:D:76:GLY:CA	1:D:317:GLY:HA3	2.10	0.81
1:C:162:TYR:OH	1:C:171:LEU:HB3	1.82	0.80
1:B:283:VAL:CG1	1:B:287:LYS:HE2	2.10	0.79
1:C:390:LYS:HA	1:C:394:GLY:O	1.82	0.79
1:C:162:TYR:CZ	1:C:171:LEU:HB3	2.17	0.78
1:B:164:SNN:C5	1:B:165:HIS:O	2.31	0.78
1:D:390:LYS:HA	1:D:394:GLY:O	1.84	0.78
1:B:163:THR:HG22	1:B:205:GLU:CB	2.11	0.78
1:B:236:TRP:CD2	1:B:290:VAL:HG21	2.20	0.77
1:D:271:ASN:HD22	1:D:274:THR:HG23	1.48	0.77
1:C:283:VAL:CG1	1:C:287:LYS:HE2	2.14	0.77
1:D:453:ARG:NH2	1:D:454:LYS:HB2	1.99	0.77
1:B:160:ILE:HB	1:B:202:PHE:CD1	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:CB	1:B:202:PHE:HD1	1.98	0.76
1:B:453:ARG:NH1	1:B:454:LYS:HB2	2.01	0.76
1:B:453:ARG:NH1	1:B:454:LYS:CB	2.49	0.75
1:C:164:SNN:O5	1:C:172:GLY:HA3	1.85	0.75
1:C:319:ASP:CB	1:C:320:PRO:CD	2.64	0.75
1:C:352:GLU:O	1:C:356:ARG:HG2	1.85	0.75
1:B:335:THR:OG1	1:B:336:PRO:CD	2.33	0.75
1:C:312:LEU:HB3	1:C:316:MET:HE3	1.67	0.75
1:C:61:ARG:HD3	1:C:237:VAL:HG11	1.69	0.73
1:A:67:CYS:SG	1:A:87:MET:HE1	2.29	0.73
1:D:202:PHE:CE2	1:D:204:VAL:CG2	2.72	0.72
1:B:125:ILE:O	1:B:173:MET:HE3	1.89	0.72
1:C:169:GLY:N	1:C:211:SER:OG	2.22	0.72
1:C:233:GLU:HG2	1:C:296:GLY:HA3	1.70	0.72
1:B:161:TYR:OH	1:B:163:THR:HG21	1.90	0.72
1:A:447:LEU:HD12	1:A:457:MET:HE1	1.69	0.71
1:B:271:ASN:ND2	1:B:274:THR:HG23	2.04	0.71
1:D:157:HIS:HB3	1:D:315:TYR:CE1	2.25	0.71
1:C:272:LEU:HD12	1:C:317:GLY:C	2.15	0.71
1:B:160:ILE:CG2	1:B:202:PHE:CD1	2.73	0.71
1:C:301:GLN:NE2	1:C:305:VAL:HG11	2.06	0.71
1:B:164:SNN:O5	1:B:165:HIS:O	2.07	0.71
1:B:340:VAL:CG1	1:B:341:SER:H	2.04	0.71
1:C:295:ASP:OD1	1:C:296:GLY:N	2.23	0.71
1:C:162:TYR:HE1	1:C:171:LEU:HD22	1.56	0.70
1:D:161:TYR:HH	1:D:163:THR:HG21	1.56	0.70
1:D:453:ARG:NH2	1:D:454:LYS:HB3	2.06	0.70
1:D:387:HIS:CG	1:D:464:ALA:HB1	2.27	0.70
1:D:272:LEU:HD22	1:D:312:LEU:HD12	1.72	0.70
1:D:76:GLY:HA3	1:D:317:GLY:HA3	1.74	0.69
1:D:202:PHE:CE2	1:D:204:VAL:HG22	2.27	0.69
1:A:164:SNN:C5	1:A:165:HIS:O	2.31	0.69
1:A:271:ASN:ND2	1:A:274:THR:HG23	2.06	0.69
1:C:163:THR:CB	1:C:205:GLU:HB3	2.23	0.69
1:C:262:ALA:HB1	1:C:287:LYS:CD	2.20	0.69
1:C:453:ARG:NH2	1:C:454:LYS:HB2	2.08	0.68
1:D:271:ASN:ND2	1:D:274:THR:HG23	2.09	0.68
1:D:387:HIS:CE1	1:D:464:ALA:HB2	2.28	0.68
1:A:252:ASP:OD1	1:A:356:ARG:HD2	1.93	0.68
1:B:57:TYR:CE2	1:B:253:VAL:HG21	2.29	0.68
1:C:295:ASP:O	1:C:297:THR:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:GLU:OE2	1:C:295:ASP:HB3	1.93	0.67
1:C:199:SER:CB	1:C:315:TYR:OH	2.41	0.67
1:B:88:TYR:CE2	1:B:122:GLY:O	2.48	0.67
1:C:319:ASP:CB	1:C:320:PRO:HD2	2.25	0.67
1:B:221:HIS:O	1:B:222:ASN:HB2	1.94	0.67
1:B:272:LEU:HD12	1:B:317:GLY:C	2.20	0.67
1:C:447:LEU:HD12	1:C:457:MET:HE1	1.74	0.67
1:C:272:LEU:HD12	1:C:317:GLY:O	1.96	0.66
1:C:319:ASP:HB2	1:C:320:PRO:HD3	1.76	0.66
1:D:218:PRO:HG2	1:D:221:HIS:CE1	2.31	0.66
1:A:160:ILE:HB	1:A:202:PHE:HD1	1.61	0.65
1:D:427:GLU:OE1	1:D:480:PHE:HA	1.96	0.65
1:C:164:SNN:O5	1:C:165:HIS:HB2	1.96	0.65
1:A:379:MET:HE1	1:C:376:ALA:HB2	1.77	0.65
1:C:160:ILE:HB	1:C:202:PHE:HD1	1.61	0.65
1:B:88:TYR:CD2	1:B:122:GLY:O	2.49	0.65
1:D:453:ARG:HH22	1:D:454:LYS:HB2	1.61	0.65
1:D:202:PHE:CE2	1:D:213:PHE:HZ	2.14	0.65
1:B:447:LEU:HD12	1:B:457:MET:HE1	1.78	0.64
1:B:160:ILE:HG21	1:B:202:PHE:CE1	2.32	0.64
1:A:162:TYR:CE1	1:A:171:LEU:HD22	2.32	0.64
1:C:54:SER:OG	1:C:62:HIS:HD2	1.80	0.64
1:A:427:GLU:HA	1:A:431:GLY:O	1.97	0.63
1:C:162:TYR:CE1	1:C:171:LEU:HD22	2.32	0.63
1:D:427:GLU:HG2	1:D:431:GLY:O	1.98	0.63
1:D:387:HIS:CG	1:D:464:ALA:CB	2.80	0.63
1:D:447:LEU:HD12	1:D:457:MET:HE1	1.80	0.63
1:D:166:GLY:HA3	1:D:206:SER:HB2	1.80	0.63
1:A:176:LYS:HD2	1:A:479:GLY:HA2	1.81	0.62
1:D:161:TYR:OH	1:D:163:THR:HG21	1.99	0.62
1:A:163:THR:HG22	1:A:205:GLU:HB3	0.72	0.62
1:D:76:GLY:HA2	1:D:317:GLY:HA3	1.81	0.62
1:A:267:CYS:SG	1:A:280:GLN:NE2	2.64	0.62
1:C:453:ARG:NH2	1:C:454:LYS:CB	2.63	0.62
1:B:335:THR:CG2	1:B:337:ARG:HG3	2.29	0.62
1:D:301:GLN:NE2	1:D:305:VAL:HG11	2.14	0.62
1:D:387:HIS:ND1	1:D:464:ALA:CB	2.63	0.62
1:A:162:TYR:CZ	1:A:171:LEU:HB3	2.34	0.62
1:B:376:ALA:HB2	1:D:379:MET:HE1	1.81	0.62
1:C:67:CYS:SG	1:C:87:MET:HE1	2.40	0.61
1:C:267:CYS:SG	1:C:316:MET:HE1	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:NH1	1:B:454:LYS:HB3	2.15	0.61
1:B:160:ILE:CG2	1:B:202:PHE:CE1	2.83	0.61
1:B:197:TYR:CD1	1:B:200:ILE:HG12	2.36	0.61
1:D:453:ARG:HH22	1:D:454:LYS:CB	2.14	0.61
1:C:244:HIS:HB3	1:C:245:PRO:HD3	1.83	0.61
1:B:176:LYS:NZ	1:B:432:SER:HB2	2.16	0.60
1:A:162:TYR:HE1	1:A:171:LEU:HD22	1.66	0.60
1:B:202:PHE:CE2	1:B:204:VAL:CG2	2.85	0.60
1:B:202:PHE:CE2	1:B:204:VAL:HG22	2.36	0.60
1:B:427:GLU:HA	1:B:431:GLY:O	2.01	0.60
1:C:272:LEU:HB2	1:C:318:THR:HB	1.84	0.60
1:B:428:THR:CG2	1:B:480:PHE:HZ	2.14	0.60
1:A:453:ARG:NH1	1:A:454:LYS:HB2	2.17	0.60
1:B:233:GLU:CG	1:B:297:THR:H	2.15	0.60
1:A:376:ALA:HB2	1:C:379:MET:HE1	1.84	0.60
1:B:295:ASP:O	1:B:297:THR:HG23	2.02	0.60
1:A:162:TYR:OH	1:A:171:LEU:HB3	2.01	0.59
1:B:253:VAL:CG1	1:B:349:HIS:CD2	2.81	0.59
1:A:160:ILE:HB	1:A:202:PHE:CD1	2.38	0.59
1:B:288:THR:HB	1:B:290:VAL:HG12	1.85	0.59
1:A:202:PHE:CE2	1:A:204:VAL:HG22	2.38	0.59
1:C:51:VAL:HB	1:C:162:TYR:HB2	1.83	0.59
1:A:453:ARG:NH1	1:A:454:LYS:CB	2.66	0.59
1:D:352:GLU:O	1:D:356:ARG:HG2	2.03	0.59
1:D:262:ALA:HB1	1:D:287:LYS:HD2	1.83	0.59
1:A:319:ASP:HB2	1:A:320:PRO:HD2	1.85	0.58
1:C:202:PHE:CE2	1:C:204:VAL:CG2	2.87	0.58
1:B:283:VAL:O	1:B:287:LYS:HG3	2.04	0.58
1:B:319:ASP:HB2	1:B:320:PRO:HD2	1.85	0.58
1:A:163:THR:CG2	1:A:205:GLU:CB	2.52	0.58
1:C:61:ARG:CD	1:C:237:VAL:HG11	2.33	0.58
1:D:425:THR:HG21	1:D:454:LYS:HG3	1.84	0.58
1:C:76:GLY:O	1:C:317:GLY:HA3	2.03	0.58
1:C:390:LYS:HG2	1:C:395:ILE:HA	1.85	0.58
1:B:160:ILE:HG21	1:B:202:PHE:CD1	2.39	0.58
1:A:202:PHE:CE2	1:A:204:VAL:CG2	2.86	0.58
1:D:76:GLY:O	1:D:317:GLY:HA2	2.03	0.58
1:B:453:ARG:HH12	1:B:454:LYS:HB2	1.68	0.57
1:B:253:VAL:CG1	1:B:349:HIS:CG	2.87	0.57
1:A:453:ARG:HG3	1:A:454:LYS:N	2.18	0.57
1:B:221:HIS:O	1:B:222:ASN:CB	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:PHE:CE2	1:C:204:VAL:HG22	2.40	0.57
1:C:312:LEU:HD13	1:C:316:MET:HE1	1.87	0.57
1:D:427:GLU:CB	1:D:431:GLY:O	2.52	0.57
1:B:161:TYR:CE1	1:B:163:THR:HG23	2.39	0.57
1:B:202:PHE:CE2	1:B:213:PHE:HZ	2.23	0.57
1:B:262:ALA:HB1	1:B:287:LYS:CD	2.34	0.57
1:B:378:ARG:HG2	1:B:436:TYR:CG	2.40	0.57
1:B:296:GLY:O	1:B:297:THR:OG1	2.13	0.56
1:B:335:THR:HG22	1:B:337:ARG:HG3	1.86	0.56
1:B:294:GLU:HG3	1:D:359:GLU:HG3	1.86	0.56
1:C:426:PHE:CE2	1:C:433:LEU:HD21	2.40	0.56
1:C:438:MET:HA	1:C:441:MET:HG2	1.87	0.56
1:B:160:ILE:CG2	1:B:202:PHE:HD1	2.14	0.56
1:B:253:VAL:HG13	1:B:349:HIS:CG	2.39	0.56
1:B:67:CYS:SG	1:B:87:MET:HE1	2.44	0.56
1:D:163:THR:CB	1:D:205:GLU:HB3	2.35	0.56
1:A:272:LEU:H	1:A:318:THR:HB	1.71	0.56
1:B:176:LYS:HD2	1:B:479:GLY:HA2	1.88	0.56
1:A:202:PHE:CE2	1:A:213:PHE:HZ	2.25	0.55
1:A:428:THR:CG2	1:A:480:PHE:HZ	2.19	0.55
1:C:202:PHE:CE2	1:C:213:PHE:HZ	2.24	0.55
1:A:301:GLN:NE2	1:A:305:VAL:HG11	2.22	0.55
1:D:161:TYR:CZ	1:D:163:THR:HG21	2.41	0.55
1:B:351:TRP:NE1	1:B:355:ARG:HD3	2.20	0.55
1:D:469:PRO:O	1:D:471:ASN:N	2.40	0.55
1:D:202:PHE:CE2	1:D:213:PHE:CZ	2.95	0.55
1:C:170:VAL:HG23	1:C:179:ILE:O	2.06	0.55
1:C:271:ASN:HA	1:C:318:THR:OG1	2.07	0.55
1:B:236:TRP:CE3	1:B:340:VAL:C	2.85	0.55
1:B:289:ILE:O	1:B:289:ILE:HG23	2.07	0.55
1:C:170:VAL:N	1:C:212:MET:SD	2.80	0.54
1:C:233:GLU:CG	1:C:296:GLY:HA3	2.35	0.54
1:B:312:LEU:HB3	1:B:316:MET:HE3	1.88	0.54
1:A:378:ARG:HG2	1:A:436:TYR:CG	2.43	0.53
1:B:340:VAL:CG1	1:B:341:SER:N	2.58	0.53
1:D:162:TYR:CZ	1:D:171:LEU:HB3	2.43	0.53
1:D:169:GLY:N	1:D:211:SER:OG	2.36	0.53
1:A:125:ILE:O	1:A:174:PRO:HD2	2.08	0.53
1:B:387:HIS:ND1	1:B:464:ALA:HB2	2.23	0.53
1:C:357:ALA:HA	1:C:363:ARG:HH22	1.74	0.53
1:A:428:THR:HG23	1:A:480:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:HH12	1:B:454:LYS:CB	2.22	0.53
1:A:387:HIS:ND1	1:A:464:ALA:HB2	2.24	0.53
1:A:51:VAL:CG1	1:A:162:TYR:HD2	2.21	0.53
1:A:170:VAL:N	1:A:212:MET:SD	2.82	0.53
1:C:233:GLU:CD	1:C:296:GLY:HA3	2.34	0.52
1:C:162:TYR:CE1	1:C:171:LEU:HB3	2.45	0.52
1:B:342:GLN:O	1:B:345:ALA:N	2.40	0.52
1:C:162:TYR:CD1	1:C:162:TYR:C	2.87	0.52
1:C:258:LEU:HD11	1:C:337:ARG:HG2	1.92	0.52
1:D:161:TYR:CE1	1:D:163:THR:CG2	2.92	0.52
1:B:236:TRP:CE2	1:B:290:VAL:CG2	2.90	0.52
1:A:272:LEU:HB2	1:A:318:THR:HB	1.91	0.52
1:B:433:LEU:HB3	1:B:437:GLY:HA3	1.91	0.52
1:C:164:SNN:C5	1:C:165:HIS:O	2.58	0.52
1:C:427:GLU:HA	1:C:431:GLY:O	2.10	0.52
1:B:244:HIS:HB3	1:B:245:PRO:HD3	1.90	0.52
1:B:272:LEU:HD22	1:B:312:LEU:HB2	1.91	0.52
1:C:225:VAL:O	1:C:301:GLN:HA	2.10	0.52
1:B:192:HIS:CD2	1:B:221:HIS:CD2	2.97	0.52
1:B:271:ASN:HD22	1:B:274:THR:CG2	2.15	0.52
1:B:379:MET:HE1	1:D:376:ALA:HB2	1.92	0.52
1:C:197:TYR:CD1	1:C:200:ILE:HG12	2.45	0.52
1:B:266:ASP:OD2	1:B:275:GLU:OE2	2.28	0.52
1:B:233:GLU:HB3	1:B:297:THR:CG2	2.36	0.51
1:A:244:HIS:HB3	1:A:245:PRO:HD3	1.92	0.51
1:B:197:TYR:CE1	1:B:200:ILE:HG12	2.44	0.51
1:C:266:ASP:OD2	1:C:275:GLU:OE2	2.28	0.51
1:D:427:GLU:CG	1:D:431:GLY:O	2.58	0.51
1:C:425:THR:HG21	1:C:454:LYS:HG3	1.92	0.51
1:A:271:ASN:HD22	1:A:274:THR:CG2	2.18	0.51
1:C:312:LEU:HB3	1:C:316:MET:CE	2.36	0.51
1:A:166:GLY:HA3	1:A:206:SER:HB2	1.93	0.51
1:B:253:VAL:HG12	1:B:349:HIS:HB2	1.93	0.51
1:C:76:GLY:CA	1:C:317:GLY:HA3	2.41	0.51
1:C:161:TYR:OH	1:C:163:THR:HG21	2.11	0.51
1:A:428:THR:HG23	1:A:480:PHE:HZ	1.76	0.51
1:C:318:THR:HG23	1:C:318:THR:O	2.09	0.51
1:B:164:SNN:O5	1:B:172:GLY:HA3	2.11	0.51
1:B:425:THR:HG21	1:B:454:LYS:HG3	1.93	0.51
1:C:157:HIS:HB3	1:C:315:TYR:CE1	2.46	0.51
1:A:164:SNN:O5	1:A:172:GLY:HA3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:MET:HA	1:A:441:MET:HG2	1.93	0.50
1:D:161:TYR:CE1	1:D:163:THR:HG23	2.45	0.50
1:D:197:TYR:CD1	1:D:200:ILE:HG12	2.46	0.50
1:D:162:TYR:CD1	1:D:162:TYR:C	2.89	0.50
1:C:161:TYR:HH	1:C:163:THR:HG21	1.76	0.50
1:C:378:ARG:HG2	1:C:436:TYR:CG	2.47	0.50
1:D:164:SNN:O5	1:D:165:HIS:O	2.29	0.50
1:C:164:SNN:O5	1:C:172:GLY:CA	2.58	0.50
1:D:272:LEU:HB2	1:D:317:GLY:O	2.12	0.50
1:B:164:SNN:O5	1:B:165:HIS:C	2.54	0.50
1:B:272:LEU:HD22	1:B:312:LEU:CB	2.42	0.50
1:B:428:THR:CG2	1:B:480:PHE:CZ	2.94	0.50
1:D:161:TYR:CZ	1:D:163:THR:CG2	2.94	0.50
1:B:57:TYR:CE2	1:B:253:VAL:CG2	2.95	0.50
1:B:341:SER:HB3	1:B:344:ASP:HB2	1.92	0.50
1:C:343:ARG:HH21	1:C:439:LYS:N	2.10	0.50
1:A:262:ALA:CB	1:A:287:LYS:HD2	2.37	0.50
1:B:378:ARG:HG2	1:B:436:TYR:CD2	2.46	0.50
1:D:69:ALA:O	1:D:73:LEU:HG	2.12	0.49
1:D:170:VAL:N	1:D:212:MET:SD	2.85	0.49
1:C:272:LEU:HD13	1:C:316:MET:HB2	1.93	0.49
1:D:427:GLU:HA	1:D:431:GLY:O	2.13	0.49
1:C:272:LEU:HD22	1:C:312:LEU:HB2	1.94	0.49
1:C:298:HIS:O	1:C:300:VAL:HG13	2.13	0.49
1:A:378:ARG:HG2	1:A:436:TYR:CD2	2.48	0.49
1:C:424:ARG:HG2	1:C:480:PHE:CD2	2.47	0.49
1:B:161:TYR:CZ	1:B:163:THR:CG2	2.94	0.49
1:B:453:ARG:HG3	1:B:454:LYS:N	2.28	0.49
1:A:164:SNN:O5	1:A:165:HIS:O	2.30	0.49
1:A:351:TRP:O	1:A:355:ARG:N	2.46	0.49
1:D:271:ASN:HD22	1:D:274:THR:CG2	2.22	0.49
1:A:197:TYR:CD1	1:A:200:ILE:HG12	2.48	0.49
1:A:447:LEU:CD1	1:A:457:MET:HE1	2.41	0.49
1:B:219:GLU:HG2	1:B:303:GLY:CA	2.43	0.49
1:C:233:GLU:CG	1:C:297:THR:H	2.26	0.49
1:A:427:GLU:CA	1:A:431:GLY:O	2.61	0.48
1:A:236:TRP:CH2	1:C:359:GLU:HG2	2.48	0.48
1:C:54:SER:OG	1:C:62:HIS:CD2	2.65	0.48
1:B:160:ILE:HG21	1:B:202:PHE:HE1	1.78	0.48
1:A:176:LYS:NZ	1:A:432:SER:HB2	2.29	0.48
1:B:58:VAL:HG22	1:B:349:HIS:ND1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:TYR:CE1	1:B:163:THR:CG2	2.96	0.48
1:C:233:GLU:HB3	1:C:297:THR:H	1.78	0.48
1:D:272:LEU:HD12	1:D:317:GLY:C	2.38	0.48
1:B:447:LEU:CD1	1:B:457:MET:HE1	2.44	0.48
1:C:60:TYR:CE1	1:C:255:VAL:HG12	2.49	0.48
1:C:169:GLY:C	1:C:212:MET:SD	2.96	0.48
1:A:124:ASP:OD1	1:A:143:GLY:HA3	2.14	0.48
1:C:46:ARG:HD3	1:C:314:VAL:O	2.14	0.48
1:D:438:MET:HA	1:D:441:MET:HG2	1.95	0.48
1:B:62:HIS:NE2	1:B:164:SNN:O	2.47	0.48
1:B:161:TYR:CZ	1:B:163:THR:HG21	2.48	0.48
1:B:406:ARG:HG2	1:B:407:PRO:HD2	1.96	0.48
1:D:423:ILE:HD13	1:D:441:MET:HE1	1.96	0.47
1:A:93:TYR:CE1	1:B:269:VAL:HB	2.49	0.47
1:A:425:THR:HG21	1:A:454:LYS:HG3	1.96	0.47
1:B:120:TYR:CE2	1:B:133:VAL:HG21	2.49	0.47
1:B:125:ILE:HB	1:B:174:PRO:HG2	1.96	0.47
1:B:160:ILE:O	1:B:202:PHE:HA	2.14	0.47
1:B:378:ARG:HG2	1:B:436:TYR:CD1	2.48	0.47
1:B:443:SER:O	1:B:447:LEU:HG	2.15	0.47
1:A:390:LYS:HA	1:A:394:GLY:O	2.15	0.47
1:B:164:SNN:O5	1:B:165:HIS:HB2	2.12	0.47
1:D:164:SNN:O5	1:D:172:GLY:HA3	2.14	0.47
1:D:170:VAL:O	1:D:170:VAL:HG13	2.12	0.47
1:A:158:VAL:HB	1:A:200:ILE:CD1	2.44	0.47
1:A:163:THR:HG22	1:A:205:GLU:CG	2.37	0.47
1:C:50:LEU:HB3	1:C:66:VAL:HG13	1.97	0.47
1:A:51:VAL:HB	1:A:162:TYR:HB2	1.96	0.47
1:A:158:VAL:HB	1:A:200:ILE:HD12	1.96	0.47
1:A:272:LEU:H	1:A:318:THR:CB	2.28	0.47
1:A:453:ARG:NH1	1:A:454:LYS:HB3	2.30	0.47
1:C:271:ASN:HD22	1:C:274:THR:HG23	1.79	0.47
1:D:244:HIS:HB3	1:D:245:PRO:HD3	1.97	0.47
1:A:423:ILE:HD13	1:A:441:MET:HE1	1.96	0.47
1:D:192:HIS:CD2	1:D:221:HIS:CD2	3.03	0.47
1:B:351:TRP:HE1	1:B:355:ARG:HD3	1.80	0.47
1:C:76:GLY:C	1:C:317:GLY:HA3	2.40	0.47
1:A:428:THR:CG2	1:A:480:PHE:CZ	2.98	0.47
1:B:343:ARG:NH1	1:B:439:LYS:N	2.62	0.47
1:C:262:ALA:O	1:C:287:LYS:HE3	2.15	0.47
1:D:380:HIS:NE2	1:D:468:ILE:HG23	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:LEU:HD22	1:C:312:LEU:CB	2.45	0.46
1:A:51:VAL:O	1:A:162:TYR:HA	2.14	0.46
1:C:295:ASP:O	1:C:296:GLY:C	2.58	0.46
1:B:427:GLU:CA	1:B:431:GLY:O	2.63	0.46
1:D:158:VAL:HB	1:D:200:ILE:CD1	2.46	0.46
1:B:65:ASP:HB3	1:B:161:TYR:OH	2.16	0.46
1:B:294:GLU:HG3	1:D:359:GLU:CG	2.46	0.46
1:B:438:MET:HA	1:B:441:MET:HG2	1.97	0.46
1:C:290:VAL:O	1:C:290:VAL:HG22	2.16	0.46
1:C:378:ARG:HG2	1:C:436:TYR:CD1	2.51	0.46
1:C:340:VAL:CG1	1:C:344:ASP:HB3	2.46	0.46
1:B:158:VAL:HB	1:B:200:ILE:HD12	1.97	0.46
1:B:253:VAL:O	1:B:254:CYS:C	2.58	0.46
1:D:160:ILE:HB	1:D:202:PHE:HD1	1.81	0.46
1:A:240:CYS:O	1:A:247:PRO:HD2	2.15	0.46
1:A:351:TRP:CD1	1:C:351:TRP:CD1	3.04	0.46
1:B:292:LEU:O	1:B:292:LEU:HD22	2.16	0.46
1:D:378:ARG:HG2	1:D:436:TYR:CG	2.51	0.46
1:D:389:GLY:HA3	1:D:402:LEU:HD11	1.97	0.46
1:B:342:GLN:O	1:B:344:ASP:N	2.48	0.46
1:C:423:ILE:HD13	1:C:441:MET:HE1	1.98	0.46
1:D:61:ARG:HD2	1:D:237:VAL:HG13	1.97	0.46
1:D:432:SER:OG	1:D:473:TRP:O	2.30	0.46
1:B:340:VAL:HG11	1:B:344:ASP:OD2	2.15	0.45
1:D:390:LYS:HG2	1:D:395:ILE:HA	1.99	0.45
1:A:351:TRP:CD1	1:C:351:TRP:NE1	2.84	0.45
1:D:73:LEU:HD22	1:D:316:MET:HG2	1.99	0.45
1:A:127:PRO:HB3	1:A:179:ILE:HG12	1.97	0.45
1:A:351:TRP:CZ2	1:A:355:ARG:HG3	2.50	0.45
1:C:220:ASP:O	1:C:221:HIS:HD2	1.99	0.45
1:C:239:TYR:OH	1:C:265:GLU:OE2	2.34	0.45
1:D:76:GLY:O	1:D:317:GLY:CA	2.64	0.45
1:B:301:GLN:NE2	1:B:305:VAL:HG11	2.32	0.45
1:C:244:HIS:CE1	1:D:250:GLU:CG	2.94	0.45
1:C:244:HIS:CD2	1:C:336:PRO:HB2	2.52	0.45
1:A:413:VAL:CG2	1:A:445:ALA:HB1	2.47	0.45
1:B:342:GLN:O	1:B:343:ARG:C	2.59	0.45
1:C:387:HIS:ND1	1:C:464:ALA:HB2	2.31	0.45
1:C:453:ARG:NH2	1:C:454:LYS:HB3	2.32	0.45
1:A:354:TYR:CE1	1:A:368:LYS:HB2	2.51	0.45
1:C:136:ALA:HA	1:C:149:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:LYS:NZ	1:C:432:SER:HB2	2.32	0.45
1:C:402:LEU:HD22	1:C:443:SER:HB3	1.98	0.45
1:B:359:GLU:HG2	1:D:236:TRP:HH2	1.82	0.45
1:D:219:GLU:O	1:D:220:ASP:OD1	2.35	0.45
1:B:427:GLU:OE2	1:B:432:SER:HA	2.18	0.44
1:D:266:ASP:OD2	1:D:275:GLU:OE2	2.35	0.44
1:B:211:SER:HB3	1:B:231:THR:HG23	2.00	0.44
1:C:426:PHE:HE2	1:C:433:LEU:HD21	1.80	0.44
1:C:453:ARG:HH21	1:C:454:LYS:HB2	1.78	0.44
1:B:428:THR:HG23	1:B:480:PHE:CZ	2.52	0.44
1:C:472:PRO:HG2	1:C:473:TRP:CD1	2.52	0.44
1:D:59:ASN:HB3	1:D:62:HIS:HD1	1.83	0.44
1:B:277:PHE:CE1	1:B:312:LEU:HD22	2.53	0.44
1:C:211:SER:HB2	1:C:412:VAL:CG2	2.47	0.44
1:C:295:ASP:CG	1:C:296:GLY:N	2.75	0.44
1:A:272:LEU:HD12	1:A:317:GLY:O	2.15	0.44
1:A:351:TRP:NE1	1:C:351:TRP:CD1	2.86	0.44
1:A:51:VAL:N	1:A:161:TYR:O	2.49	0.44
1:C:161:TYR:CE1	1:C:163:THR:HG23	2.53	0.44
1:C:283:VAL:O	1:C:287:LYS:HG3	2.17	0.44
1:C:312:LEU:HD13	1:C:316:MET:CE	2.48	0.44
1:D:453:ARG:HG3	1:D:454:LYS:N	2.33	0.44
1:A:211:SER:HB2	1:A:412:VAL:CG2	2.48	0.44
1:B:342:GLN:C	1:B:344:ASP:N	2.75	0.43
1:B:343:ARG:HH11	1:B:439:LYS:N	2.16	0.43
1:D:427:GLU:CA	1:D:431:GLY:O	2.66	0.43
1:C:158:VAL:HB	1:C:200:ILE:HD12	2.01	0.43
1:A:58:VAL:HG22	1:A:349:HIS:ND1	2.33	0.43
1:A:390:LYS:HG2	1:A:395:ILE:HA	2.00	0.43
1:B:166:GLY:O	1:B:207:CYS:HB2	2.18	0.43
1:D:235:SER:OG	1:D:342:GLN:HG3	2.18	0.43
1:D:272:LEU:HB3	1:D:312:LEU:HB2	2.01	0.43
1:A:170:VAL:O	1:A:170:VAL:HG13	2.18	0.43
1:C:161:TYR:CE1	1:C:163:THR:CG2	3.01	0.43
1:A:378:ARG:HG2	1:A:436:TYR:CD1	2.53	0.43
1:C:170:VAL:HG11	1:C:441:MET:HE2	2.01	0.43
1:B:239:TYR:OH	1:B:265:GLU:OE2	2.37	0.43
1:B:252:ASP:OD1	1:B:253:VAL:HG22	2.19	0.43
1:B:354:TYR:O	1:B:354:TYR:CG	2.72	0.43
1:A:61:ARG:HD2	1:A:237:VAL:HG13	2.01	0.43
1:D:158:VAL:HB	1:D:200:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:GLU:CB	1:C:297:THR:H	2.32	0.43
1:A:60:TYR:CE1	1:A:255:VAL:HG12	2.54	0.42
1:B:219:GLU:HG2	1:B:303:GLY:C	2.44	0.42
1:C:258:LEU:CD1	1:C:337:ARG:CG	2.97	0.42
1:C:267:CYS:HG	1:C:316:MET:HE1	1.83	0.42
1:B:166:GLY:HA3	1:B:206:SER:HB2	2.01	0.42
1:B:389:GLY:HA3	1:B:402:LEU:HD11	2.01	0.42
1:B:162:TYR:CE2	1:B:171:LEU:HD22	2.54	0.42
1:C:357:ALA:HA	1:C:363:ARG:NH2	2.33	0.42
1:D:202:PHE:CE2	1:D:204:VAL:HG21	2.51	0.42
1:B:423:ILE:HD13	1:B:441:MET:HE1	2.01	0.42
1:C:160:ILE:HB	1:C:202:PHE:CD1	2.49	0.42
1:C:262:ALA:CB	1:C:287:LYS:CD	2.94	0.42
1:C:354:TYR:O	1:C:354:TYR:CG	2.72	0.42
1:B:236:TRP:CD1	1:B:236:TRP:N	2.87	0.42
1:B:272:LEU:HD12	1:B:317:GLY:O	2.18	0.42
1:A:236:TRP:HH2	1:C:359:GLU:HG2	1.83	0.42
1:A:272:LEU:CB	1:A:318:THR:HB	2.49	0.42
1:A:352:GLU:O	1:A:356:ARG:HG2	2.19	0.42
1:C:433:LEU:HB3	1:C:437:GLY:HA3	2.02	0.42
1:D:354:TYR:CE1	1:D:364:LYS:HD3	2.54	0.42
1:A:427:GLU:CB	1:A:431:GLY:O	2.68	0.42
1:B:335:THR:HG23	1:B:337:ARG:HG3	1.99	0.42
1:B:352:GLU:O	1:B:356:ARG:HG2	2.19	0.42
1:C:211:SER:CB	1:C:231:THR:HG23	2.50	0.42
1:B:427:GLU:CB	1:B:431:GLY:O	2.67	0.42
1:A:250:GLU:HG2	1:B:244:HIS:CE1	2.54	0.41
1:C:244:HIS:NE2	1:C:336:PRO:HG2	2.35	0.41
1:A:162:TYR:CD1	1:A:162:TYR:C	2.98	0.41
1:A:427:GLU:OE1	1:A:480:PHE:HA	2.20	0.41
1:B:211:SER:HB2	1:B:412:VAL:CG2	2.49	0.41
1:B:237:VAL:O	1:B:339:ALA:HB1	2.21	0.41
1:C:124:ASP:OD1	1:C:143:GLY:HA3	2.20	0.41
1:C:161:TYR:CZ	1:C:163:THR:HG21	2.55	0.41
1:A:266:ASP:OD2	1:A:275:GLU:OE2	2.38	0.41
1:B:161:TYR:CZ	1:B:163:THR:HG23	2.55	0.41
1:B:160:ILE:CB	1:B:202:PHE:CD1	2.85	0.41
1:B:236:TRP:CE3	1:B:340:VAL:O	2.73	0.41
1:C:258:LEU:CD1	1:C:337:ARG:HG2	2.49	0.41
1:B:340:VAL:CG1	1:B:344:ASP:OD2	2.68	0.41
1:C:312:LEU:O	1:C:316:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ILE:HG22	1:B:202:PHE:CE1	2.55	0.41
1:B:233:GLU:HB3	1:B:297:THR:HA	2.03	0.41
1:B:236:TRP:HE3	1:B:340:VAL:C	2.28	0.41
1:C:161:TYR:CZ	1:C:163:THR:CG2	3.03	0.41
1:D:61:ARG:HD2	1:D:237:VAL:CG1	2.50	0.41
1:D:164:SNN:O5	1:D:165:HIS:HB2	2.13	0.41
1:D:277:PHE:CD1	1:D:312:LEU:HD23	2.56	0.41
1:A:63:GLN:OE1	1:A:88:TYR:O	2.39	0.41
1:A:402:LEU:HD22	1:A:443:SER:HB3	2.02	0.41
1:D:211:SER:HB2	1:D:412:VAL:CG2	2.50	0.41
1:C:152:SER:O	1:C:196:THR:HB	2.21	0.41
1:A:235:SER:OG	1:A:342:GLN:HG3	2.21	0.41
1:D:157:HIS:HB3	1:D:315:TYR:CD1	2.55	0.41
1:D:202:PHE:HE2	1:D:204:VAL:HG21	1.85	0.41
1:A:476:LEU:HD23	1:A:476:LEU:HA	1.94	0.40
1:C:162:TYR:OH	1:C:172:GLY:N	2.54	0.40
1:A:173:MET:SD	1:A:179:ILE:CD1	3.10	0.40
1:A:211:SER:HB2	1:A:412:VAL:HG21	2.03	0.40
1:A:248:PRO:HA	1:A:249:PRO:HD3	1.98	0.40
1:C:272:LEU:H	1:C:318:THR:HB	1.85	0.40
1:C:211:SER:HB2	1:C:412:VAL:HG21	2.02	0.40
1:D:163:THR:CG2	1:D:205:GLU:CB	2.73	0.40
1:D:277:PHE:CZ	1:D:315:TYR:CD2	3.09	0.40
1:A:192:HIS:CG	1:A:221:HIS:CD2	3.09	0.40
1:B:219:GLU:HG2	1:B:303:GLY:HA2	2.03	0.40
1:B:289:ILE:CG2	1:B:336:PRO:O	2.70	0.40
1:C:413:VAL:CG2	1:C:445:ALA:HB1	2.52	0.40
1:D:211:SER:HB3	1:D:231:THR:HG23	2.04	0.40
1:A:125:ILE:HB	1:A:174:PRO:HG2	2.03	0.40
1:A:131:TYR:OH	1:A:179:ILE:HG23	2.22	0.40
1:C:163:THR:HG22	1:C:205:GLU:CA	2.48	0.40
1:C:269:VAL:HB	1:D:93:TYR:CE1	2.57	0.40
1:D:169:GLY:C	1:D:212:MET:SD	3.05	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	409/473 (86%)	386 (94%)	20 (5%)	3 (1%)	18	49
1	B	425/473 (90%)	388 (91%)	33 (8%)	4 (1%)	14	44
1	C	423/473 (89%)	393 (93%)	27 (6%)	3 (1%)	18	49
1	D	398/473 (84%)	374 (94%)	22 (6%)	2 (0%)	24	57
All	All	1655/1892 (88%)	1541 (93%)	102 (6%)	12 (1%)	18	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	222	ASN
1	D	470	ASP
1	B	295	ASP
1	B	319	ASP
1	C	319	ASP
1	A	245	PRO
1	A	319	ASP
1	A	320	PRO
1	C	320	PRO
1	B	245	PRO
1	C	245	PRO
1	D	245	PRO

5.3.2 Protein sidechains [i](#)

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	351/401 (88%)	346 (99%)	5 (1%)	59	76
1	B	363/401 (90%)	354 (98%)	9 (2%)	42	69
1	C	362/401 (90%)	354 (98%)	8 (2%)	45	71
1	D	342/401 (85%)	335 (98%)	7 (2%)	48	72
All	All	1418/1604 (88%)	1389 (98%)	29 (2%)	48	72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	VAL
1	A	138	LYS
1	A	250	GLU
1	A	356	ARG
1	A	474	SER
1	B	102	VAL
1	B	125	ILE
1	B	160	ILE
1	B	250	GLU
1	B	253	VAL
1	B	292	LEU
1	B	293	ILE
1	B	295	ASP
1	B	474	SER
1	C	102	VAL
1	C	162	TYR
1	C	250	GLU
1	C	292	LEU
1	C	293	ILE
1	C	294	GLU
1	C	295	ASP
1	C	474	SER
1	D	102	VAL
1	D	155	ASN
1	D	162	TYR
1	D	176	LYS
1	D	250	GLU
1	D	468	ILE
1	D	474	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	192	HIS
1	A	278	GLN
1	A	301	GLN
1	A	310	GLN
1	A	399	HIS
1	A	403	ASN
1	B	105	ASN
1	B	157	HIS
1	B	185	ASN
1	B	192	HIS
1	B	221	HIS
1	B	222	ASN
1	B	271	ASN
1	B	279	GLN
1	B	301	GLN
1	B	310	GLN
1	C	62	HIS
1	C	105	ASN
1	C	185	ASN
1	C	221	HIS
1	C	222	ASN
1	C	244	HIS
1	C	278	GLN
1	C	301	GLN
1	D	59	ASN
1	D	105	ASN
1	D	185	ASN
1	D	221	HIS
1	D	243	GLN
1	D	270	HIS
1	D	271	ASN
1	D	278	GLN
1	D	280	GLN
1	D	301	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SNN	B	164	1	7,8,8	3.27	3 (42%)	10,11,11	1.87	3 (30%)
1	SNN	C	164	1	7,8,8	2.61	3 (42%)	10,11,11	1.63	3 (30%)
1	SNN	D	164	1	7,8,8	2.58	3 (42%)	10,11,11	1.46	2 (20%)
1	SNN	A	164	1	7,8,8	3.26	3 (42%)	10,11,11	1.87	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SNN	B	164	1	-	-	0/1/1/1
1	SNN	C	164	1	-	-	0/1/1/1
1	SNN	D	164	1	-	-	0/1/1/1
1	SNN	A	164	1	-	-	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	SNN	C-N1	-6.40	1.29	1.37
1	A	164	SNN	C-N1	-6.00	1.29	1.37
1	A	164	SNN	C5-N1	-5.13	1.29	1.37
1	C	164	SNN	C-N1	-4.69	1.31	1.37
1	D	164	SNN	C-N1	-4.45	1.31	1.37
1	D	164	SNN	C5-N1	-4.36	1.30	1.37
1	C	164	SNN	C5-N1	-4.26	1.30	1.37
1	B	164	SNN	C5-N1	-4.13	1.30	1.37
1	B	164	SNN	C4-C5	-3.69	1.45	1.51
1	A	164	SNN	C4-C5	-3.33	1.46	1.51
1	D	164	SNN	C4-C5	-2.66	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	164	SNN	C4-C5	-2.50	1.47	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	SNN	C5-N1-C	3.96	117.95	113.96
1	B	164	SNN	C5-N1-C	3.71	117.69	113.96
1	C	164	SNN	O-C-CA	-3.31	123.81	126.19
1	B	164	SNN	O-C-N1	3.08	128.56	124.93
1	A	164	SNN	O-C-N1	3.00	128.46	124.93
1	B	164	SNN	O-C-CA	-2.96	124.06	126.19
1	D	164	SNN	O-C-CA	-2.88	124.12	126.19
1	A	164	SNN	O-C-CA	-2.47	124.41	126.19
1	C	164	SNN	O-C-N1	2.39	127.75	124.93
1	D	164	SNN	O-C-N1	2.39	127.75	124.93
1	C	164	SNN	C5-N1-C	2.02	116.00	113.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	164	SNN	6	0
1	C	164	SNN	4	0
1	D	164	SNN	4	0
1	A	164	SNN	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	416/473 (87%)	0.41	25 (6%)	27	15	21, 59, 92, 139	0
1	B	430/473 (90%)	0.62	33 (7%)	19	10	21, 70, 100, 134	0
1	C	428/473 (90%)	0.59	26 (6%)	27	15	21, 68, 98, 148	0
1	D	405/473 (85%)	0.56	23 (5%)	29	16	22, 69, 103, 130	0
All	All	1679/1892 (88%)	0.55	107 (6%)	25	14	21, 67, 100, 148	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169	GLY	5.8
1	C	395	ILE	5.4
1	A	395	ILE	5.3
1	B	335	THR	5.0
1	A	468	ILE	4.3
1	C	467	SER	4.2
1	B	244	HIS	4.0
1	C	293	ILE	3.7
1	D	468	ILE	3.7
1	A	467	SER	3.6
1	C	292	LEU	3.6
1	A	397	LYS	3.6
1	A	469	PRO	3.5
1	B	474	SER	3.5
1	A	351	TRP	3.5
1	B	327	PHE	3.4
1	A	289	ILE	3.4
1	B	317	GLY	3.3
1	C	317	GLY	3.3
1	D	469	PRO	3.2
1	C	321	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	351	TRP	3.2
1	D	481	SER	3.1
1	B	242	LEU	3.1
1	B	289	ILE	3.1
1	A	463	GLN	3.1
1	D	463	GLN	3.0
1	A	394	GLY	3.0
1	C	394	GLY	3.0
1	A	324	ASN	3.0
1	D	89	ASP	3.0
1	B	396	GLU	3.0
1	C	289	ILE	3.0
1	C	291	ALA	2.9
1	C	327	PHE	2.9
1	C	165	HIS	2.8
1	B	340	VAL	2.8
1	B	269	VAL	2.8
1	C	268	ASP	2.8
1	D	466	VAL	2.7
1	C	336	PRO	2.7
1	D	431	GLY	2.7
1	B	202	PHE	2.7
1	C	351	TRP	2.7
1	A	471	ASN	2.7
1	C	322	ASN	2.7
1	A	455	GLU	2.7
1	D	220	ASP	2.7
1	B	82	ASN	2.7
1	D	306	GLY	2.6
1	B	321	ALA	2.6
1	B	297	THR	2.6
1	D	395	ILE	2.6
1	D	398	GLY	2.6
1	A	435	GLU	2.5
1	B	395	ILE	2.5
1	A	165	HIS	2.5
1	B	292	LEU	2.5
1	A	477	HIS	2.5
1	A	398	GLY	2.5
1	C	301	GLN	2.5
1	C	269	VAL	2.4
1	A	288	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	298	HIS	2.4
1	C	464	ALA	2.4
1	B	337	ARG	2.3
1	D	245	PRO	2.3
1	B	243	GLN	2.3
1	B	338	LYS	2.3
1	B	463	GLN	2.3
1	B	351	TRP	2.2
1	B	322	ASN	2.2
1	A	466	VAL	2.2
1	C	324	ASN	2.2
1	A	396	GLU	2.2
1	A	464	ALA	2.2
1	C	245	PRO	2.2
1	D	316	MET	2.2
1	A	231	THR	2.2
1	D	317	GLY	2.2
1	D	467	SER	2.2
1	B	319	ASP	2.2
1	D	304	ASP	2.2
1	B	221	HIS	2.2
1	C	320	PRO	2.1
1	C	479	GLY	2.1
1	B	295	ASP	2.1
1	B	165	HIS	2.1
1	D	305	VAL	2.1
1	B	197	TYR	2.1
1	B	251	TYR	2.1
1	A	267	CYS	2.1
1	D	165	HIS	2.1
1	C	318	THR	2.1
1	B	291	ALA	2.1
1	B	431	GLY	2.1
1	D	166	GLY	2.1
1	D	303	GLY	2.1
1	A	242	LEU	2.1
1	B	293	ILE	2.1
1	C	337	ARG	2.1
1	B	464	ALA	2.1
1	A	317	GLY	2.1
1	A	393	PHE	2.1
1	B	325	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	474	SER	2.0
1	C	470	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SNN	D	164	8/8	0.77	0.14	47,48,49,50	0
1	SNN	C	164	8/8	0.82	0.14	43,43,44,44	0
1	SNN	B	164	8/8	0.83	0.13	53,54,55,56	0
1	SNN	A	164	8/8	0.85	0.12	43,44,45,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.