Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 01:38 PM EST

PDB ID	:	6DHI
Title	:	Butelase 1: Auto-Catalytic Cleavage as an Evolutionary Constraint for Macrocyclizing 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:

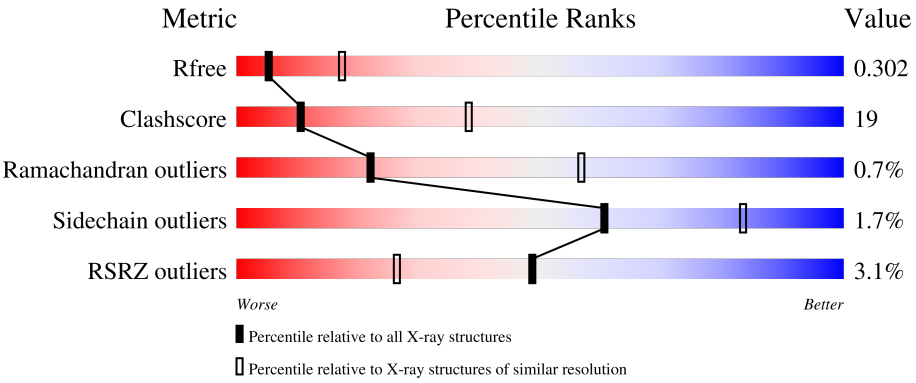
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=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	3% 67% 20% • 12%
1	B	473	2% 66% 23% • 9%
1	C	473	3% 66% 23% • 9%
1	D	473	3% 67% 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 (i)

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.

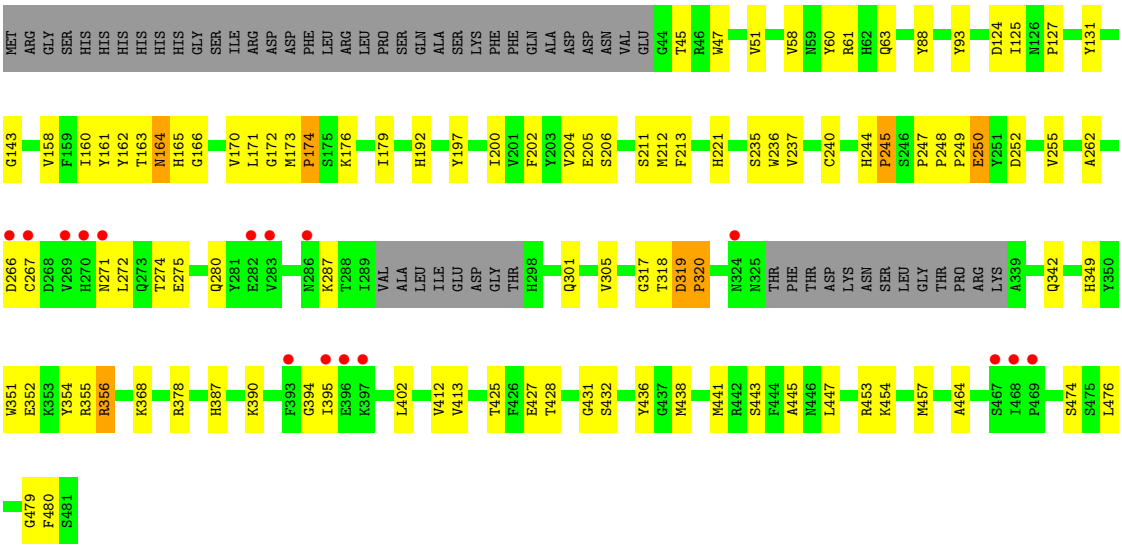
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	6	Total O 6 6	0	0
2	C	7	Total O 7 7	0	0
2	D	3	Total O 3 3	0	0

3 Residue-property plots (i)

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.

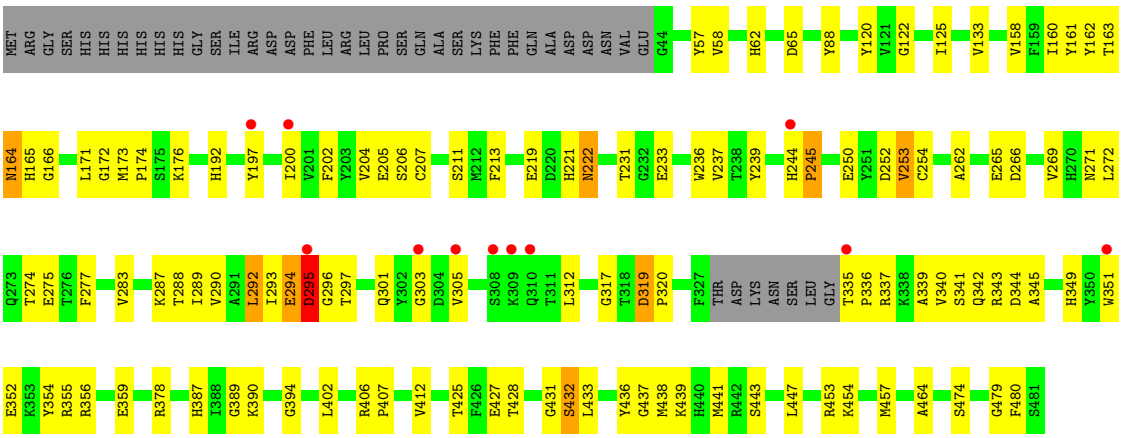
• Molecule 1: Asparaginyl endopeptidase

Chain A:

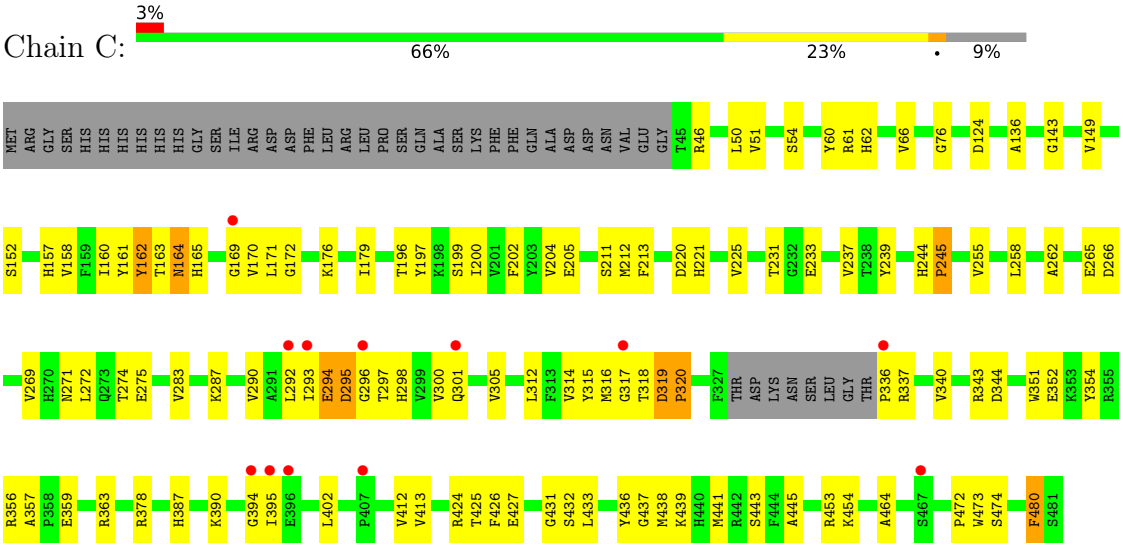


• Molecule 1: Asparaginyl endopeptidase

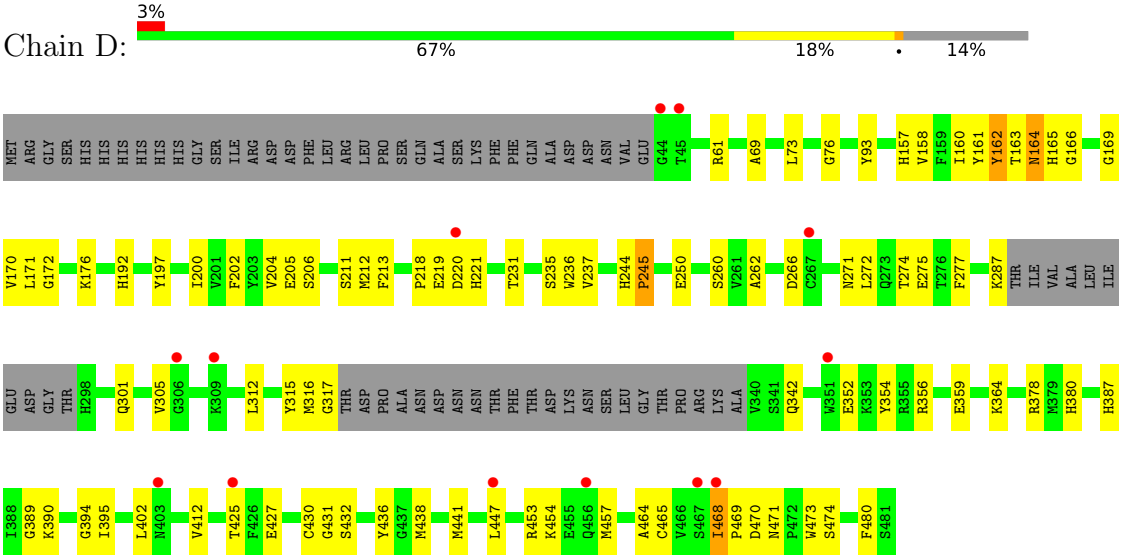
Chain B:



• Molecule 1: Asparaginyl endopeptidase



- Molecule 1: Asparaginyl endopeptidase



4 Data and refinement statistics (i)

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) 100.0 (49.42-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.274 , 0.309 0.272 , 0.302	Depositor DCC
R_{free} test set	1844 reflections (5.13%)	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)	0.30 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.55	0/3334	0.70	0/4519
1	B	0.56	0/3445	0.67	0/4672
1	C	0.54	0/3434	0.68	0/4656
1	D	0.59	0/3254	0.70	0/4407
All	All	0.56	0/13467	0.69	0/18254

There are no bond length outliers.

There are no bond angle outliers.

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	98	0
1	B	3366	0	3227	150	0
1	C	3355	0	3218	141	0
1	D	3179	0	3046	101	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	477	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 (477) 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
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:A:272:LEU:HD12	1:A:317:GLY:C	1.92	0.89
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: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:D:164:SNN:C5	1:D:165:HIS:O	2.20	0.83
1:B:233:GLU:CD	1:B:297:THR:H	1.82	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:294:GLU:CD	1:C:295:ASP:H	1.85	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
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:61:ARG:HD3	1:C:237:VAL:HG11	1.69	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: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: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:453:ARG:NH2	1:D:454:LYS:HB3	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:272:LEU:HD12	1:C:317:GLY:C	2.15	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:272:LEU:HD12	1:B:317:GLY:C	2.20	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: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:D:161:TYR:HH	1:D:163:THR:HG21	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:202:PHE:CE2	1:C:204:VAL:HG22	2.40	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: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:C:312:LEU:HB3	1:C:316:MET:CE	2.36	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:318:THR:HG23	1:C:318:THR:O	2.09	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
1:B:296:GLY:O	1:B:297:THR:OG1	2.13	0.53
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: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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:SNN:O5	1:A:172:GLY:HA3	2.11	0.51
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: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: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:236:TRP:CE3	1:B:340:VAL:C	2.85	0.50
1:B:378:ARG:HG2	1:B:436:TYR:CD2	2.46	0.50
1:C:170:VAL:HG11	1:C:441:MET:HE2	1.93	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:A:447:LEU:HD12	1:A:457:MET:HE1	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG22	1:B:349:HIS:ND1	2.29	0.48
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:C:60:TYR:CE1	1:C:255:VAL:HG12	2.49	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:C:233:GLU:CD	1:C:296:GLY:HA3	2.34	0.47
1:C:162:TYR:CD1	1:C:162:TYR:C	2.87	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:C:312:LEU:HB3	1:C:316:MET:HE2	1.96	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:162:TYR:CD1	1:D:162:TYR:C	2.89	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:B:164:SNN:O5	1:B:165:HIS:C	2.54	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:272:LEU:HD12	1:D:317:GLY:C	2.38	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:312:LEU:HD13	1:C:316:MET:CE	2.48	0.44
1:C:472:PRO:HG2	1:C:473:TRP:CD1	2.52	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: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: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: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:C:169:GLY:C	1:C:212:MET:SD	2.96	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: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
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:C:258:LEU:CD1	1:C:337:ARG:CG	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:76:GLY:C	1:C:317:GLY:HA3	2.40	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:A:45:THR:HG1	1:A:47:TRP:HE1	1.66	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:C:295:ASP:O	1:C:296:GLY:C	2.58	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:D:447:LEU:HD12	1:D:457:MET:HE1	2.01	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:C:312:LEU:HB3	1:C:316:MET:HE3	2.02	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
1:B:253:VAL:O	1:B:254:CYS:C	2.58	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:161:TYR:HH	1:D:260:SER:CB	2.33	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:B:447:LEU:HD12	1:B:457:MET:HE1	2.02	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:B:342:GLN:O	1:B:343:ARG:C	2.59	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

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%)	22	57
1	B	425/473 (90%)	388 (91%)	33 (8%)	4 (1%)	17	52
1	C	423/473 (89%)	393 (93%)	27 (6%)	3 (1%)	22	57
1	D	398/473 (84%)	374 (94%)	22 (6%)	2 (0%)	29	64
All	All	1655/1892 (88%)	1541 (93%)	102 (6%)	12 (1%)	22	57

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%)	347 (99%)	4 (1%)	73	89
1	B	363/401 (90%)	355 (98%)	8 (2%)	52	78
1	C	362/401 (90%)	355 (98%)	7 (2%)	57	81
1	D	342/401 (85%)	337 (98%)	5 (2%)	65	85
All	All	1418/1604 (88%)	1394 (98%)	24 (2%)	60	83

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	PRO
1	A	250	GLU
1	A	356	ARG
1	A	474	SER
1	B	250	GLU
1	B	253	VAL
1	B	292	LEU
1	B	293	ILE
1	B	294	GLU
1	B	295	ASP
1	B	432	SER
1	B	474	SER
1	C	162	TYR
1	C	292	LEU
1	C	293	ILE
1	C	294	GLU
1	C	295	ASP
1	C	474	SER
1	C	480	PHE
1	D	162	TYR
1	D	176	LYS
1	D	465	CYS
1	D	468	ILE
1	D	474	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	B	157	HIS
1	B	192	HIS
1	B	221	HIS
1	B	271	ASN
1	B	278	GLN
1	B	279	GLN
1	B	301	GLN
1	B	325	ASN
1	C	62	HIS
1	C	221	HIS
1	C	244	HIS
1	C	301	GLN

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Mol	Chain	Res	Type
1	C	377	HIS
1	D	105	ASN
1	D	221	HIS
1	D	270	HIS
1	D	271	ASN
1	D	280	GLN
1	D	301	GLN
1	D	429	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	A	164	1	7,8,8	3.39	3 (42%)	7,11,11	1.61	2 (28%)
1	SNN	D	164	1	7,8,8	2.71	3 (42%)	7,11,11	1.54	2 (28%)
1	SNN	B	164	1	7,8,8	3.38	3 (42%)	7,11,11	1.67	2 (28%)
1	SNN	C	164	1	7,8,8	2.73	3 (42%)	7,11,11	1.75	2 (28%)

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	A	164	1	-	-	0/1/1/1
1	SNN	D	164	1	-	-	0/1/1/1
1	SNN	B	164	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SNN	C	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	-5.99	1.29	1.37
1	A	164	SNN	C5-N1	-5.64	1.29	1.37
1	D	164	SNN	C5-N1	-4.81	1.30	1.37
1	C	164	SNN	C5-N1	-4.70	1.30	1.37
1	C	164	SNN	C-N1	-4.66	1.31	1.37
1	B	164	SNN	C5-N1	-4.56	1.30	1.37
1	D	164	SNN	C-N1	-4.42	1.31	1.37
1	B	164	SNN	C4-C5	-3.85	1.45	1.51
1	A	164	SNN	C4-C5	-3.48	1.46	1.51
1	D	164	SNN	C4-C5	-2.77	1.47	1.51
1	C	164	SNN	C4-C5	-2.61	1.47	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	164	SNN	O-C-CA	-3.28	123.81	126.18
1	B	164	SNN	O-C-N1	2.99	128.56	124.94
1	B	164	SNN	O-C-CA	-2.93	124.06	126.18
1	A	164	SNN	O-C-N1	2.90	128.46	124.94
1	D	164	SNN	O-C-CA	-2.85	124.12	126.18
1	A	164	SNN	O-C-CA	-2.45	124.41	126.18
1	C	164	SNN	O-C-N1	2.32	127.75	124.94
1	D	164	SNN	O-C-N1	2.31	127.75	124.94

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	A	164	SNN	3	0
1	D	164	SNN	4	0
1	B	164	SNN	6	0
1	C	164	SNN	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	0.10	16 (3%)	40	20	21, 59, 92, 139	0
1	B	430/473 (90%)	0.23	11 (2%)	56	33	21, 70, 100, 134	0
1	C	428/473 (90%)	0.20	12 (2%)	53	30	21, 68, 98, 148	0
1	D	405/473 (85%)	0.27	13 (3%)	47	25	22, 69, 103, 130	0
All	All	1679/1892 (88%)	0.20	52 (3%)	49	26	21, 67, 100, 148	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	SER	4.9
1	C	292	LEU	4.2
1	D	468	ILE	4.2
1	D	467	SER	3.8
1	B	303	GLY	3.8
1	A	395	ILE	3.8
1	C	467	SER	3.7
1	B	335	THR	3.5
1	A	468	ILE	3.3
1	D	403	ASN	3.3
1	C	395	ILE	3.1
1	B	308	SER	3.1
1	A	469	PRO	3.1
1	B	295	ASP	3.0
1	A	324	ASN	2.9
1	D	267	CYS	2.9
1	C	317	GLY	2.8
1	C	169	GLY	2.7
1	B	309	LYS	2.7
1	C	293	ILE	2.7
1	D	44	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	305	VAL	2.7
1	B	351	TRP	2.7
1	D	306	GLY	2.6
1	B	197	TYR	2.6
1	C	301	GLN	2.6
1	B	310	GLN	2.3
1	A	283	VAL	2.3
1	A	286	ASN	2.3
1	A	282	GLU	2.3
1	A	267	CYS	2.3
1	D	220	ASP	2.3
1	A	397	LYS	2.3
1	A	396	GLU	2.2
1	C	396	GLU	2.2
1	B	200	ILE	2.2
1	C	394	GLY	2.2
1	A	271	ASN	2.1
1	A	266	ASP	2.1
1	D	351	TRP	2.1
1	A	270	HIS	2.1
1	C	336	PRO	2.1
1	C	296	GLY	2.1
1	D	456	GLN	2.1
1	D	309	LYS	2.1
1	A	269	VAL	2.1
1	D	447	LEU	2.0
1	D	425	THR	2.0
1	A	393	PHE	2.0
1	B	244	HIS	2.0
1	D	45	THR	2.0
1	C	407	PRO	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, 95^{th} 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	0.83	0.22	47,48,49,50	0
1	SNN	C	164	8/8	0.85	0.23	43,43,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SNN	B	164	8/8	0.88	0.23	53,54,55,56	0
1	SNN	A	164	8/8	0.90	0.21	43,44,45,46	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.